



Full wwPDB EM Validation Report ⓘ

Dec 5, 2022 – 03:19 pm GMT

PDB ID : 8A1S
EMDB ID : EMD-15086
Title : Structure of murine perforin-2 (Mpeg1) pore in twisted form
Authors : Yu, X.; Ni, T.; Zhang, P.; Gilbert, R.
Deposited on : 2022-06-02
Resolution : 4.00 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

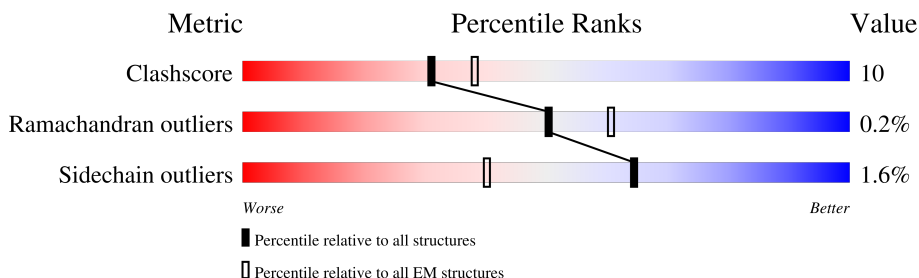
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	648	<div> <div>49%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>
1	B	648	<div> <div>54%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div>
1	C	648	<div> <div>66%</div> <div>62%</div> <div>20%</div> <div>18%</div> </div>
1	D	648	<div> <div>77%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div>
1	E	648	<div> <div>70%</div> <div>62%</div> <div>20%</div> <div>18%</div> </div>
1	F	648	<div> <div>67%</div> <div>65%</div> <div>17%</div> <div>18%</div> </div>
1	G	648	<div> <div>61%</div> <div>61%</div> <div>21%</div> <div>18%</div> </div>
1	H	648	<div> <div>55%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	648	<div> <div>53%</div> <div>64%</div> <div>17%</div> <div>18%</div> </div>
1	J	648	<div> <div>51%</div> <div>61%</div> <div>20%</div> <div>18%</div> </div>
1	K	648	<div> <div>47%</div> <div>62%</div> <div>19%</div> <div>18%</div> </div>
1	L	648	<div> <div>43%</div> <div>62%</div> <div>20%</div> <div>18%</div> </div>
1	M	648	<div> <div>44%</div> <div>62%</div> <div>19%</div> <div>18%</div> </div>
1	N	648	<div> <div>46%</div> <div>62%</div> <div>19%</div> <div>18%</div> </div>
1	O	648	<div> <div>44%</div> <div>62%</div> <div>19%</div> <div>18%</div> </div>
1	P	648	<div> <div>48%</div> <div>63%</div> <div>19%</div> <div>18%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 67152 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Macrophage-expressed gene 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	B	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	C	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	D	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	E	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	F	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	G	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	H	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	I	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	J	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	K	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	L	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	M	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	N	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	O	533	Total 4148	C 2650	N 687	O 784	S 27	0	0
1	P	533	Total 4148	C 2650	N 687	O 784	S 27	0	0

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	-	expression tag	UNP A1L314
A	18	THR	-	expression tag	UNP A1L314
A	19	GLY	-	expression tag	UNP A1L314
A	653	GLY	-	expression tag	UNP A1L314
A	654	THR	-	expression tag	UNP A1L314
A	655	LYS	-	expression tag	UNP A1L314
A	656	THR	-	expression tag	UNP A1L314
A	657	GLU	-	expression tag	UNP A1L314
A	658	THR	-	expression tag	UNP A1L314
A	659	SER	-	expression tag	UNP A1L314
A	660	GLN	-	expression tag	UNP A1L314
A	661	VAL	-	expression tag	UNP A1L314
A	662	ALA	-	expression tag	UNP A1L314
A	663	PRO	-	expression tag	UNP A1L314
A	664	ALA	-	expression tag	UNP A1L314
B	17	GLU	-	expression tag	UNP A1L314
B	18	THR	-	expression tag	UNP A1L314
B	19	GLY	-	expression tag	UNP A1L314
B	653	GLY	-	expression tag	UNP A1L314
B	654	THR	-	expression tag	UNP A1L314
B	655	LYS	-	expression tag	UNP A1L314
B	656	THR	-	expression tag	UNP A1L314
B	657	GLU	-	expression tag	UNP A1L314
B	658	THR	-	expression tag	UNP A1L314
B	659	SER	-	expression tag	UNP A1L314
B	660	GLN	-	expression tag	UNP A1L314
B	661	VAL	-	expression tag	UNP A1L314
B	662	ALA	-	expression tag	UNP A1L314
B	663	PRO	-	expression tag	UNP A1L314
B	664	ALA	-	expression tag	UNP A1L314
C	17	GLU	-	expression tag	UNP A1L314
C	18	THR	-	expression tag	UNP A1L314
C	19	GLY	-	expression tag	UNP A1L314
C	653	GLY	-	expression tag	UNP A1L314
C	654	THR	-	expression tag	UNP A1L314
C	655	LYS	-	expression tag	UNP A1L314
C	656	THR	-	expression tag	UNP A1L314
C	657	GLU	-	expression tag	UNP A1L314
C	658	THR	-	expression tag	UNP A1L314
C	659	SER	-	expression tag	UNP A1L314
C	660	GLN	-	expression tag	UNP A1L314
C	661	VAL	-	expression tag	UNP A1L314
C	662	ALA	-	expression tag	UNP A1L314

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Chain	Residue	Modelled	Actual	Comment	Reference
C	663	PRO	-	expression tag	UNP A1L314
C	664	ALA	-	expression tag	UNP A1L314
D	17	GLU	-	expression tag	UNP A1L314
D	18	THR	-	expression tag	UNP A1L314
D	19	GLY	-	expression tag	UNP A1L314
D	653	GLY	-	expression tag	UNP A1L314
D	654	THR	-	expression tag	UNP A1L314
D	655	LYS	-	expression tag	UNP A1L314
D	656	THR	-	expression tag	UNP A1L314
D	657	GLU	-	expression tag	UNP A1L314
D	658	THR	-	expression tag	UNP A1L314
D	659	SER	-	expression tag	UNP A1L314
D	660	GLN	-	expression tag	UNP A1L314
D	661	VAL	-	expression tag	UNP A1L314
D	662	ALA	-	expression tag	UNP A1L314
D	663	PRO	-	expression tag	UNP A1L314
D	664	ALA	-	expression tag	UNP A1L314
E	17	GLU	-	expression tag	UNP A1L314
E	18	THR	-	expression tag	UNP A1L314
E	19	GLY	-	expression tag	UNP A1L314
E	653	GLY	-	expression tag	UNP A1L314
E	654	THR	-	expression tag	UNP A1L314
E	655	LYS	-	expression tag	UNP A1L314
E	656	THR	-	expression tag	UNP A1L314
E	657	GLU	-	expression tag	UNP A1L314
E	658	THR	-	expression tag	UNP A1L314
E	659	SER	-	expression tag	UNP A1L314
E	660	GLN	-	expression tag	UNP A1L314
E	661	VAL	-	expression tag	UNP A1L314
E	662	ALA	-	expression tag	UNP A1L314
E	663	PRO	-	expression tag	UNP A1L314
E	664	ALA	-	expression tag	UNP A1L314
F	17	GLU	-	expression tag	UNP A1L314
F	18	THR	-	expression tag	UNP A1L314
F	19	GLY	-	expression tag	UNP A1L314
F	653	GLY	-	expression tag	UNP A1L314
F	654	THR	-	expression tag	UNP A1L314
F	655	LYS	-	expression tag	UNP A1L314
F	656	THR	-	expression tag	UNP A1L314
F	657	GLU	-	expression tag	UNP A1L314
F	658	THR	-	expression tag	UNP A1L314
F	659	SER	-	expression tag	UNP A1L314

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Chain	Residue	Modelled	Actual	Comment	Reference
F	660	GLN	-	expression tag	UNP A1L314
F	661	VAL	-	expression tag	UNP A1L314
F	662	ALA	-	expression tag	UNP A1L314
F	663	PRO	-	expression tag	UNP A1L314
F	664	ALA	-	expression tag	UNP A1L314
G	17	GLU	-	expression tag	UNP A1L314
G	18	THR	-	expression tag	UNP A1L314
G	19	GLY	-	expression tag	UNP A1L314
G	653	GLY	-	expression tag	UNP A1L314
G	654	THR	-	expression tag	UNP A1L314
G	655	LYS	-	expression tag	UNP A1L314
G	656	THR	-	expression tag	UNP A1L314
G	657	GLU	-	expression tag	UNP A1L314
G	658	THR	-	expression tag	UNP A1L314
G	659	SER	-	expression tag	UNP A1L314
G	660	GLN	-	expression tag	UNP A1L314
G	661	VAL	-	expression tag	UNP A1L314
G	662	ALA	-	expression tag	UNP A1L314
G	663	PRO	-	expression tag	UNP A1L314
G	664	ALA	-	expression tag	UNP A1L314
H	17	GLU	-	expression tag	UNP A1L314
H	18	THR	-	expression tag	UNP A1L314
H	19	GLY	-	expression tag	UNP A1L314
H	653	GLY	-	expression tag	UNP A1L314
H	654	THR	-	expression tag	UNP A1L314
H	655	LYS	-	expression tag	UNP A1L314
H	656	THR	-	expression tag	UNP A1L314
H	657	GLU	-	expression tag	UNP A1L314
H	658	THR	-	expression tag	UNP A1L314
H	659	SER	-	expression tag	UNP A1L314
H	660	GLN	-	expression tag	UNP A1L314
H	661	VAL	-	expression tag	UNP A1L314
H	662	ALA	-	expression tag	UNP A1L314
H	663	PRO	-	expression tag	UNP A1L314
H	664	ALA	-	expression tag	UNP A1L314
I	17	GLU	-	expression tag	UNP A1L314
I	18	THR	-	expression tag	UNP A1L314
I	19	GLY	-	expression tag	UNP A1L314
I	653	GLY	-	expression tag	UNP A1L314
I	654	THR	-	expression tag	UNP A1L314
I	655	LYS	-	expression tag	UNP A1L314
I	656	THR	-	expression tag	UNP A1L314

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Chain	Residue	Modelled	Actual	Comment	Reference
I	657	GLU	-	expression tag	UNP A1L314
I	658	THR	-	expression tag	UNP A1L314
I	659	SER	-	expression tag	UNP A1L314
I	660	GLN	-	expression tag	UNP A1L314
I	661	VAL	-	expression tag	UNP A1L314
I	662	ALA	-	expression tag	UNP A1L314
I	663	PRO	-	expression tag	UNP A1L314
I	664	ALA	-	expression tag	UNP A1L314
J	17	GLU	-	expression tag	UNP A1L314
J	18	THR	-	expression tag	UNP A1L314
J	19	GLY	-	expression tag	UNP A1L314
J	653	GLY	-	expression tag	UNP A1L314
J	654	THR	-	expression tag	UNP A1L314
J	655	LYS	-	expression tag	UNP A1L314
J	656	THR	-	expression tag	UNP A1L314
J	657	GLU	-	expression tag	UNP A1L314
J	658	THR	-	expression tag	UNP A1L314
J	659	SER	-	expression tag	UNP A1L314
J	660	GLN	-	expression tag	UNP A1L314
J	661	VAL	-	expression tag	UNP A1L314
J	662	ALA	-	expression tag	UNP A1L314
J	663	PRO	-	expression tag	UNP A1L314
J	664	ALA	-	expression tag	UNP A1L314
K	17	GLU	-	expression tag	UNP A1L314
K	18	THR	-	expression tag	UNP A1L314
K	19	GLY	-	expression tag	UNP A1L314
K	653	GLY	-	expression tag	UNP A1L314
K	654	THR	-	expression tag	UNP A1L314
K	655	LYS	-	expression tag	UNP A1L314
K	656	THR	-	expression tag	UNP A1L314
K	657	GLU	-	expression tag	UNP A1L314
K	658	THR	-	expression tag	UNP A1L314
K	659	SER	-	expression tag	UNP A1L314
K	660	GLN	-	expression tag	UNP A1L314
K	661	VAL	-	expression tag	UNP A1L314
K	662	ALA	-	expression tag	UNP A1L314
K	663	PRO	-	expression tag	UNP A1L314
K	664	ALA	-	expression tag	UNP A1L314
L	17	GLU	-	expression tag	UNP A1L314
L	18	THR	-	expression tag	UNP A1L314
L	19	GLY	-	expression tag	UNP A1L314
L	653	GLY	-	expression tag	UNP A1L314

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Chain	Residue	Modelled	Actual	Comment	Reference
L	654	THR	-	expression tag	UNP A1L314
L	655	LYS	-	expression tag	UNP A1L314
L	656	THR	-	expression tag	UNP A1L314
L	657	GLU	-	expression tag	UNP A1L314
L	658	THR	-	expression tag	UNP A1L314
L	659	SER	-	expression tag	UNP A1L314
L	660	GLN	-	expression tag	UNP A1L314
L	661	VAL	-	expression tag	UNP A1L314
L	662	ALA	-	expression tag	UNP A1L314
L	663	PRO	-	expression tag	UNP A1L314
L	664	ALA	-	expression tag	UNP A1L314
M	17	GLU	-	expression tag	UNP A1L314
M	18	THR	-	expression tag	UNP A1L314
M	19	GLY	-	expression tag	UNP A1L314
M	653	GLY	-	expression tag	UNP A1L314
M	654	THR	-	expression tag	UNP A1L314
M	655	LYS	-	expression tag	UNP A1L314
M	656	THR	-	expression tag	UNP A1L314
M	657	GLU	-	expression tag	UNP A1L314
M	658	THR	-	expression tag	UNP A1L314
M	659	SER	-	expression tag	UNP A1L314
M	660	GLN	-	expression tag	UNP A1L314
M	661	VAL	-	expression tag	UNP A1L314
M	662	ALA	-	expression tag	UNP A1L314
M	663	PRO	-	expression tag	UNP A1L314
M	664	ALA	-	expression tag	UNP A1L314
N	17	GLU	-	expression tag	UNP A1L314
N	18	THR	-	expression tag	UNP A1L314
N	19	GLY	-	expression tag	UNP A1L314
N	653	GLY	-	expression tag	UNP A1L314
N	654	THR	-	expression tag	UNP A1L314
N	655	LYS	-	expression tag	UNP A1L314
N	656	THR	-	expression tag	UNP A1L314
N	657	GLU	-	expression tag	UNP A1L314
N	658	THR	-	expression tag	UNP A1L314
N	659	SER	-	expression tag	UNP A1L314
N	660	GLN	-	expression tag	UNP A1L314
N	661	VAL	-	expression tag	UNP A1L314
N	662	ALA	-	expression tag	UNP A1L314
N	663	PRO	-	expression tag	UNP A1L314
N	664	ALA	-	expression tag	UNP A1L314
O	17	GLU	-	expression tag	UNP A1L314

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Chain	Residue	Modelled	Actual	Comment	Reference
O	18	THR	-	expression tag	UNP A1L314
O	19	GLY	-	expression tag	UNP A1L314
O	653	GLY	-	expression tag	UNP A1L314
O	654	THR	-	expression tag	UNP A1L314
O	655	LYS	-	expression tag	UNP A1L314
O	656	THR	-	expression tag	UNP A1L314
O	657	GLU	-	expression tag	UNP A1L314
O	658	THR	-	expression tag	UNP A1L314
O	659	SER	-	expression tag	UNP A1L314
O	660	GLN	-	expression tag	UNP A1L314
O	661	VAL	-	expression tag	UNP A1L314
O	662	ALA	-	expression tag	UNP A1L314
O	663	PRO	-	expression tag	UNP A1L314
O	664	ALA	-	expression tag	UNP A1L314
P	17	GLU	-	expression tag	UNP A1L314
P	18	THR	-	expression tag	UNP A1L314
P	19	GLY	-	expression tag	UNP A1L314
P	653	GLY	-	expression tag	UNP A1L314
P	654	THR	-	expression tag	UNP A1L314
P	655	LYS	-	expression tag	UNP A1L314
P	656	THR	-	expression tag	UNP A1L314
P	657	GLU	-	expression tag	UNP A1L314
P	658	THR	-	expression tag	UNP A1L314
P	659	SER	-	expression tag	UNP A1L314
P	660	GLN	-	expression tag	UNP A1L314
P	661	VAL	-	expression tag	UNP A1L314
P	662	ALA	-	expression tag	UNP A1L314
P	663	PRO	-	expression tag	UNP A1L314
P	664	ALA	-	expression tag	UNP A1L314

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



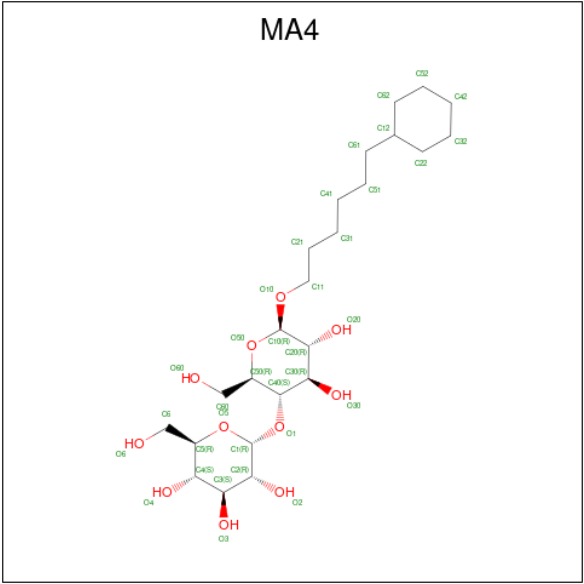
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	
2	E	1	Total	C	N	O	0
			14	8	1	5	
2	F	1	Total	C	N	O	0
			14	8	1	5	
2	G	1	Total	C	N	O	0
			14	8	1	5	
2	H	1	Total	C	N	O	0
			14	8	1	5	
2	I	1	Total	C	N	O	0
			14	8	1	5	
2	J	1	Total	C	N	O	0
			14	8	1	5	
2	K	1	Total	C	N	O	0
			14	8	1	5	
2	L	1	Total	C	N	O	0
			14	8	1	5	
2	M	1	Total	C	N	O	0
			14	8	1	5	
2	N	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
2	O	1	Total	C	N	O	0
			14	8	1	5	
2	P	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CYCLOHEXYL-HEXYL-BETA-D-MALTOSIDE (three-letter code: MA4) (formula: C₂₄H₄₄O₁₁) (labeled as "Ligand of Interest" by depositor).



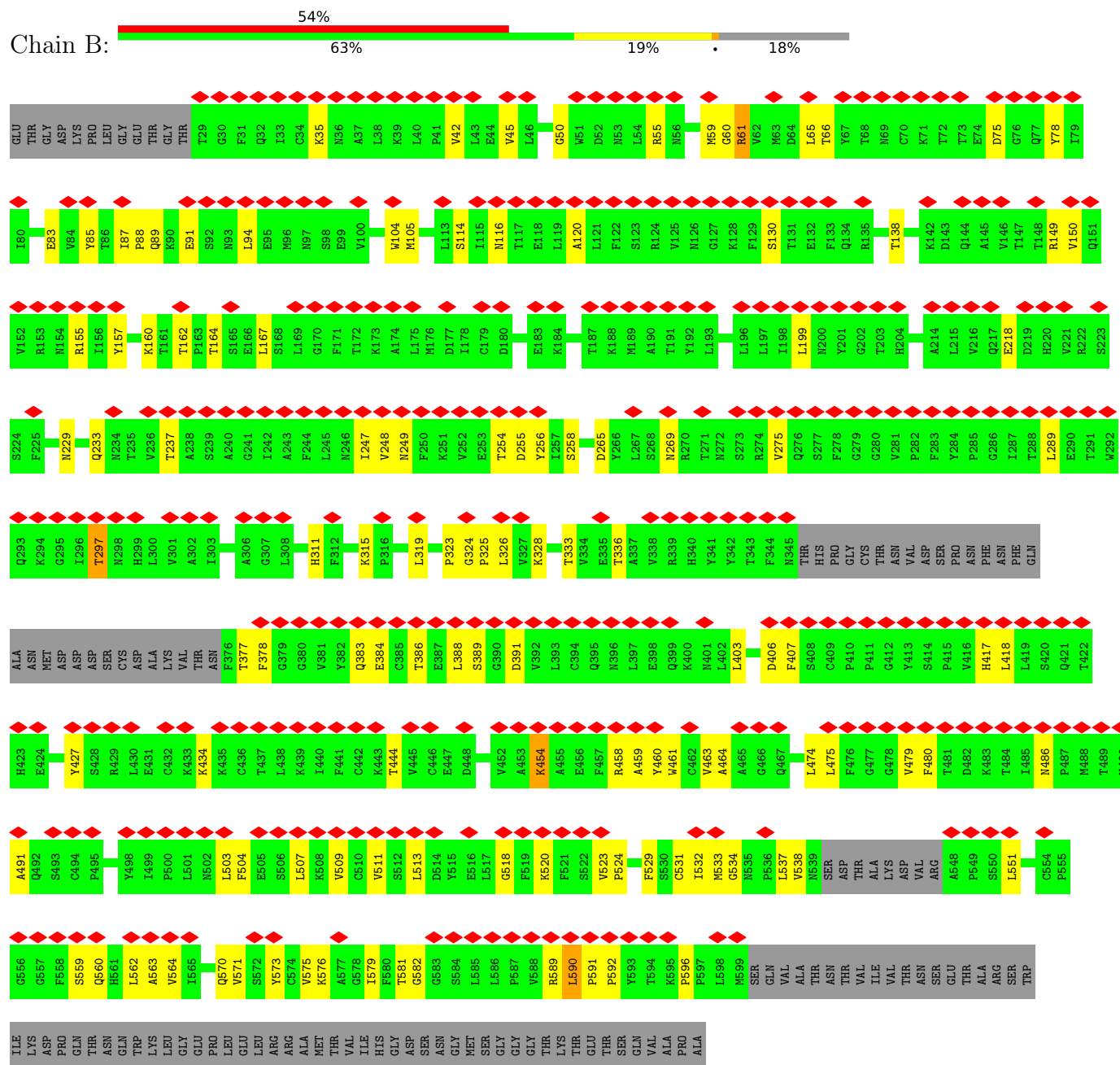
Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			35	24	11	
3	B	1	Total	C	O	0
			35	24	11	
3	C	1	Total	C	O	0
			35	24	11	
3	D	1	Total	C	O	0
			35	24	11	
3	E	1	Total	C	O	0
			35	24	11	
3	F	1	Total	C	O	0
			35	24	11	
3	G	1	Total	C	O	0
			35	24	11	
3	H	1	Total	C	O	0
			35	24	11	
3	I	1	Total	C	O	0
			35	24	11	

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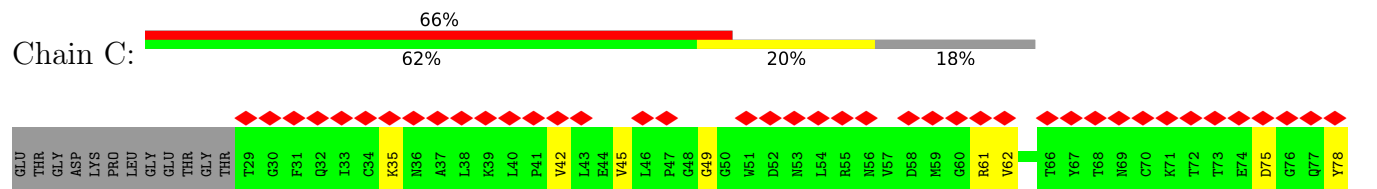
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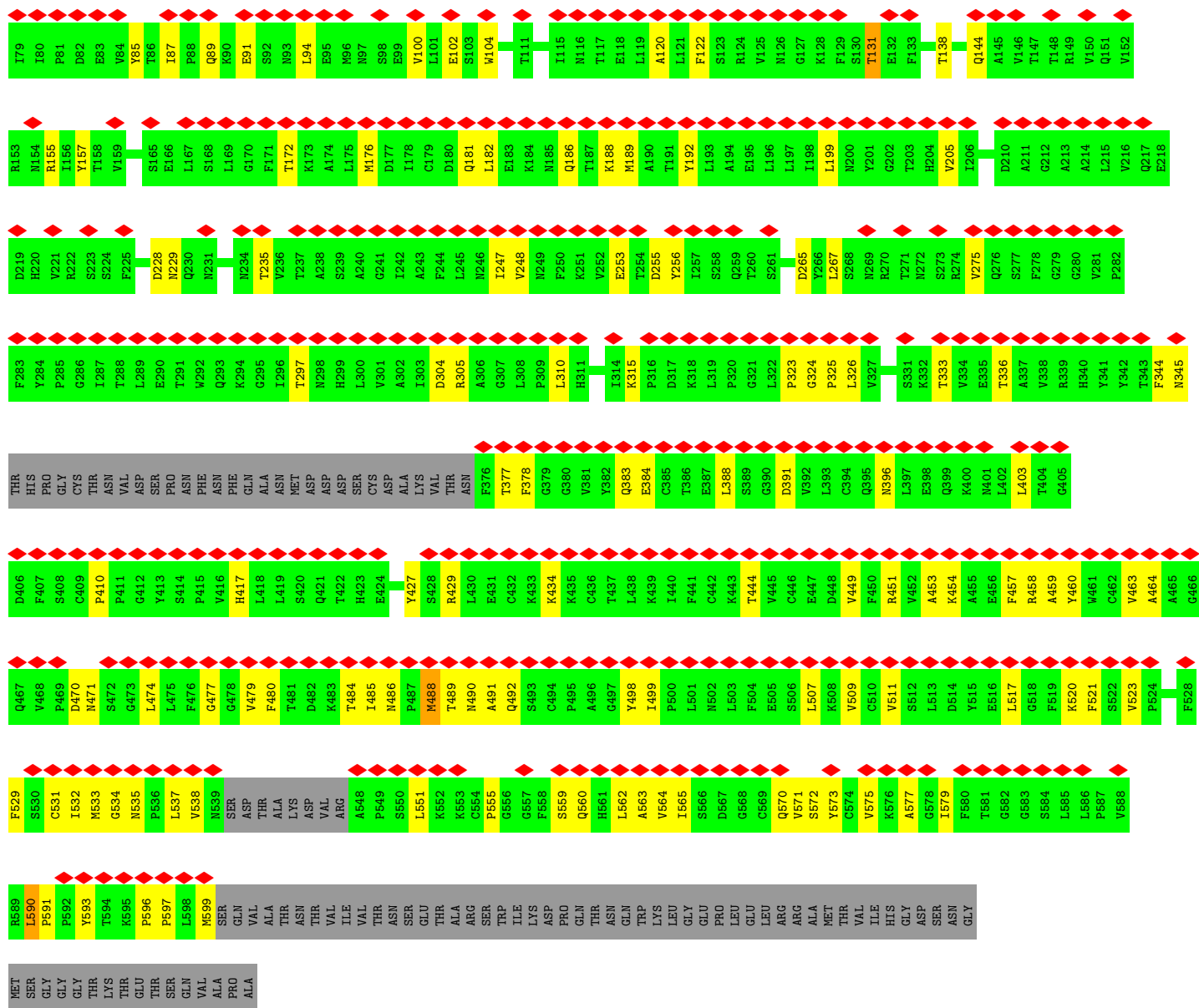
Mol	Chain	Residues	Atoms			AltConf
3	J	1	Total	C	O	0
			35	24	11	
3	K	1	Total	C	O	0
			35	24	11	
3	L	1	Total	C	O	0
			35	24	11	
3	M	1	Total	C	O	0
			35	24	11	
3	N	1	Total	C	O	0
			35	24	11	
3	O	1	Total	C	O	0
			35	24	11	
3	P	1	Total	C	O	0
			35	24	11	

Chain B:

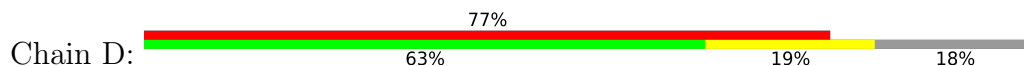


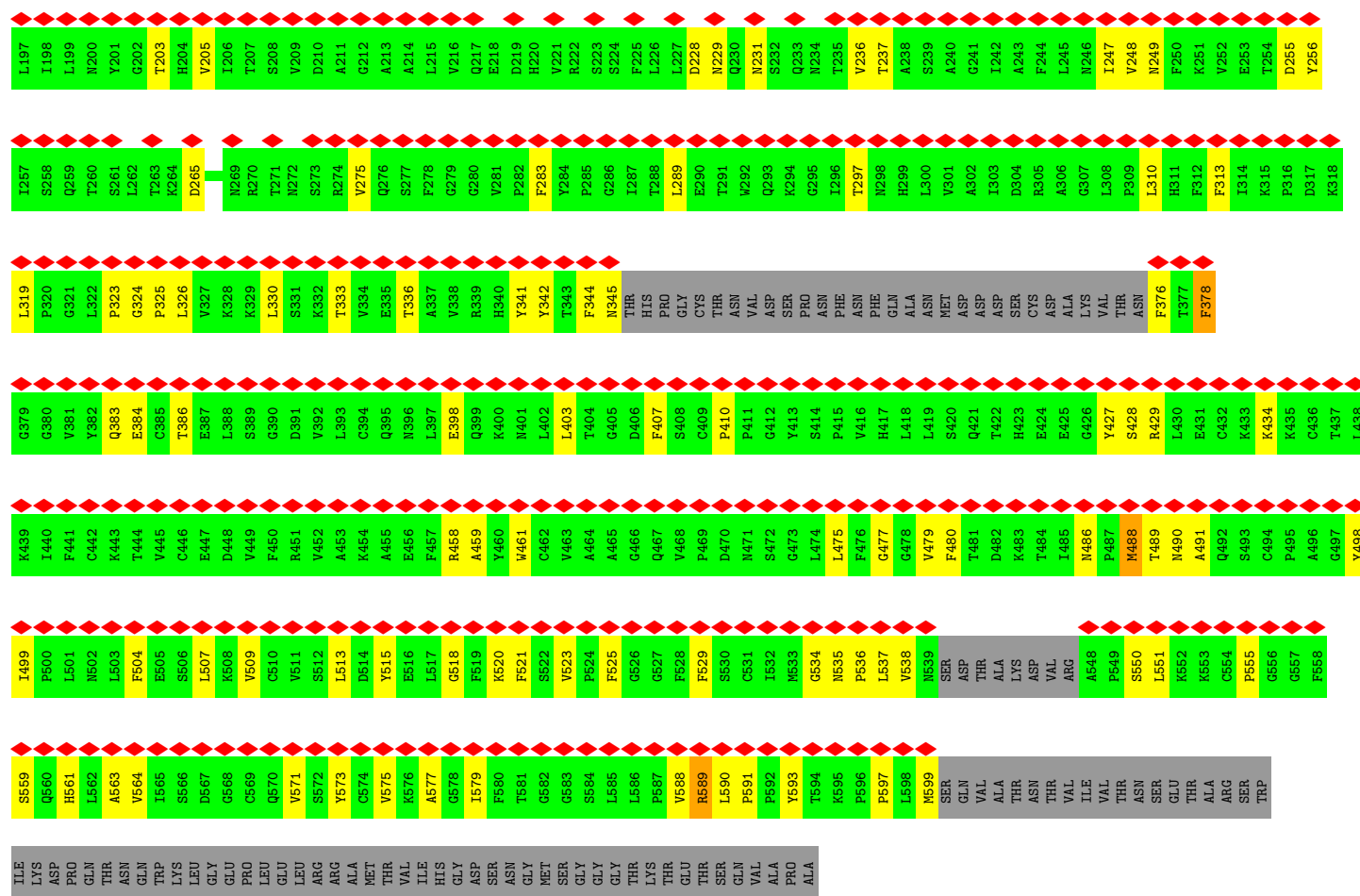
Chain C:



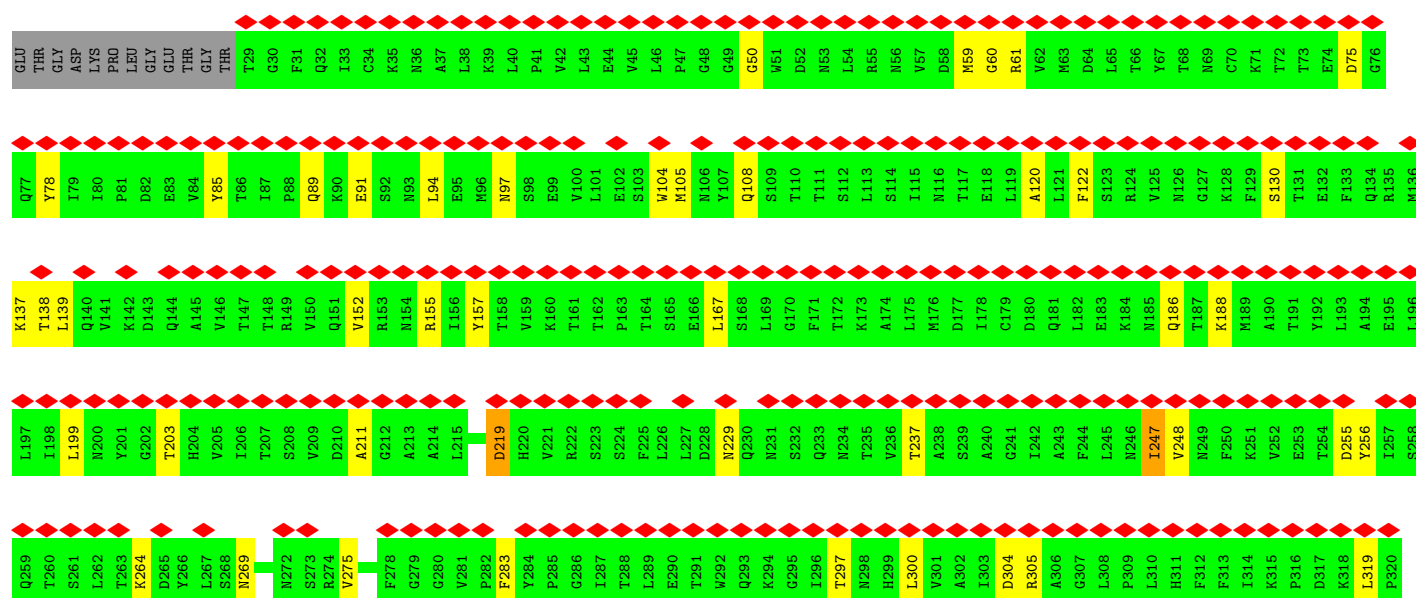


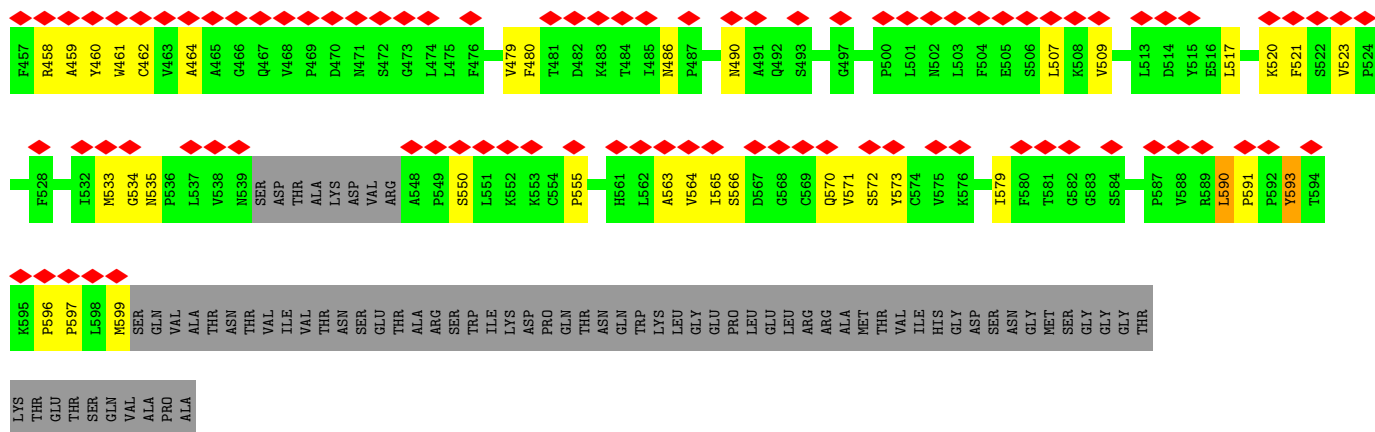
• Molecule 1: Macrophage-expressed gene 1 protein



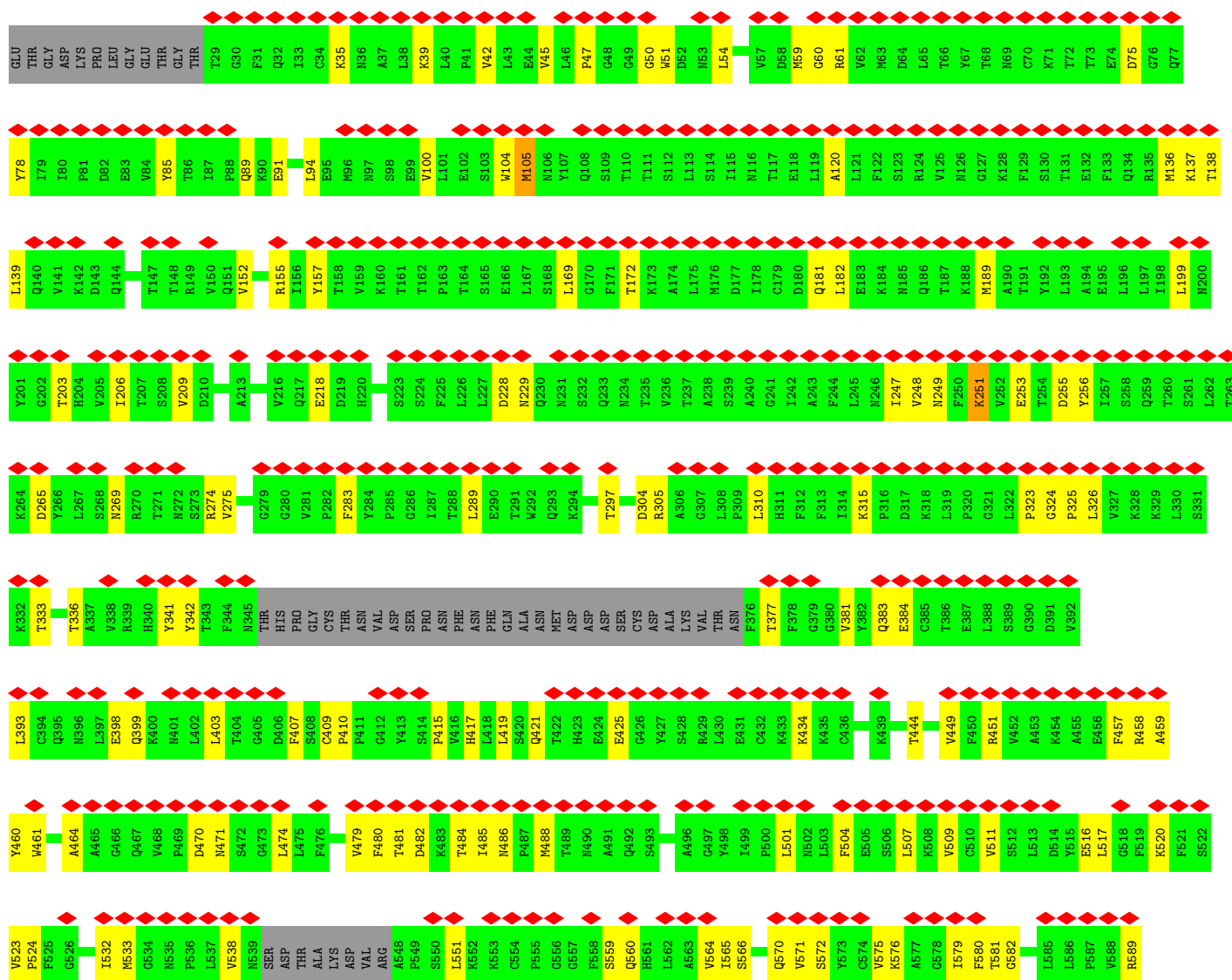


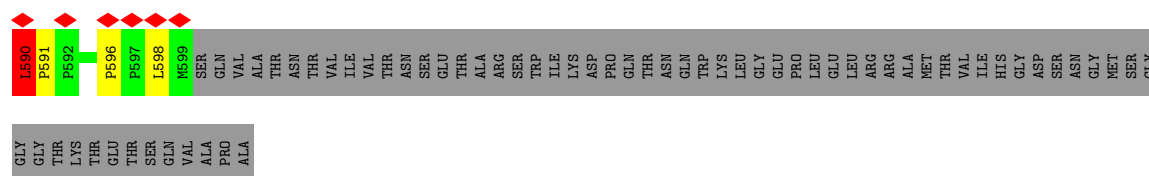
• Molecule 1: Macrophage-expressed gene 1 protein



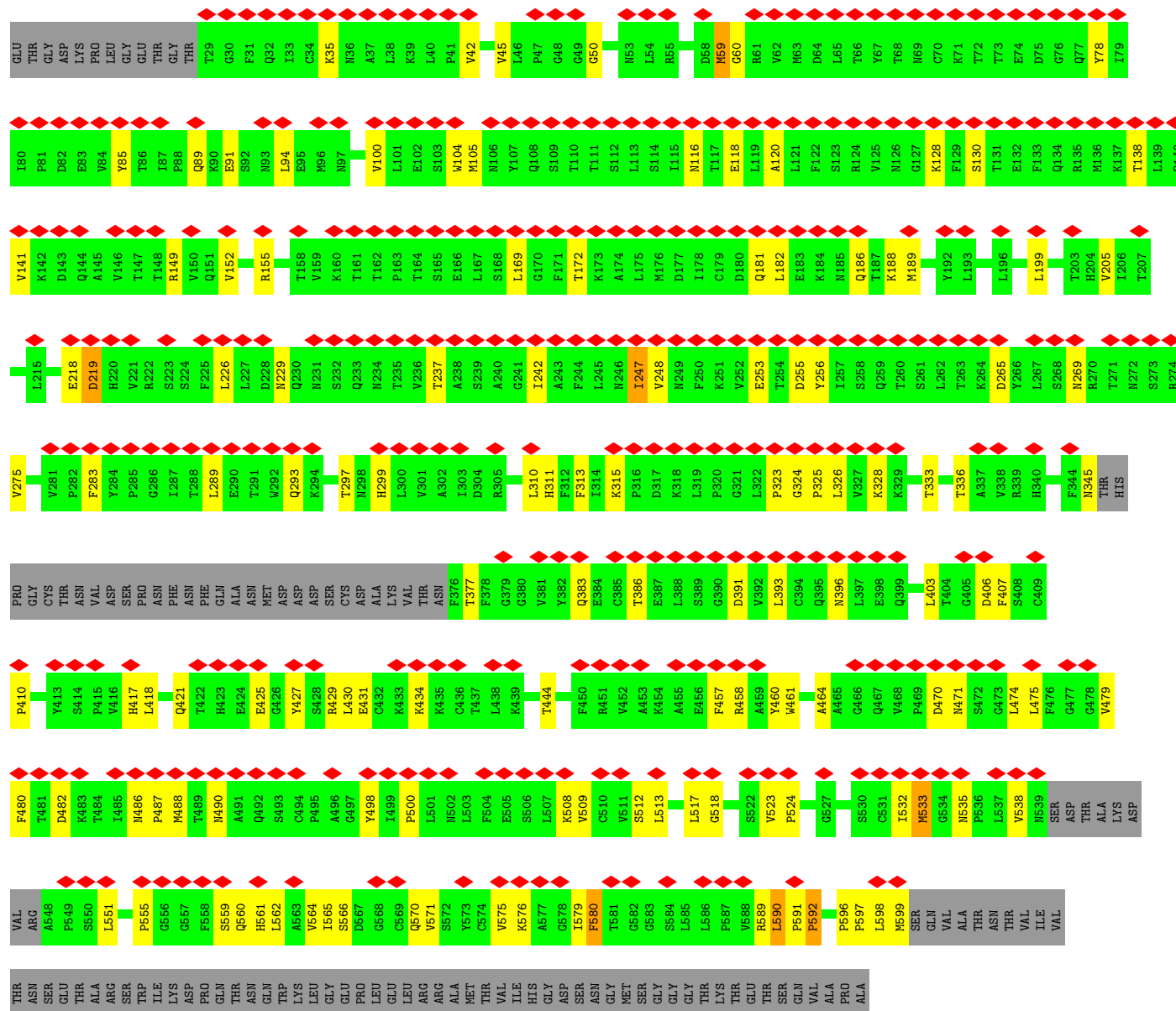


• Molecule 1: Macrophage-expressed gene 1 protein



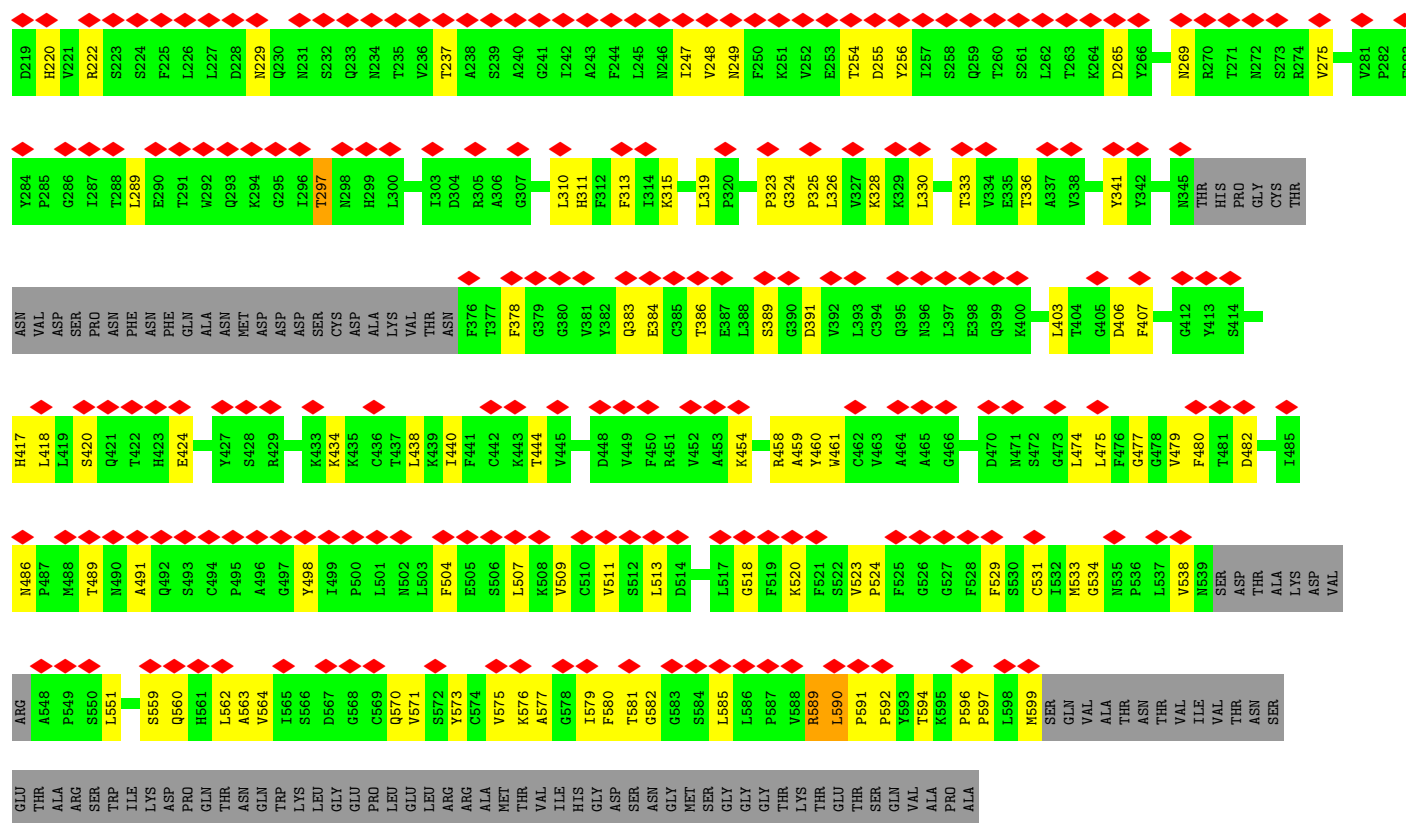


• Molecule 1: Macrophage-expressed gene 1 protein

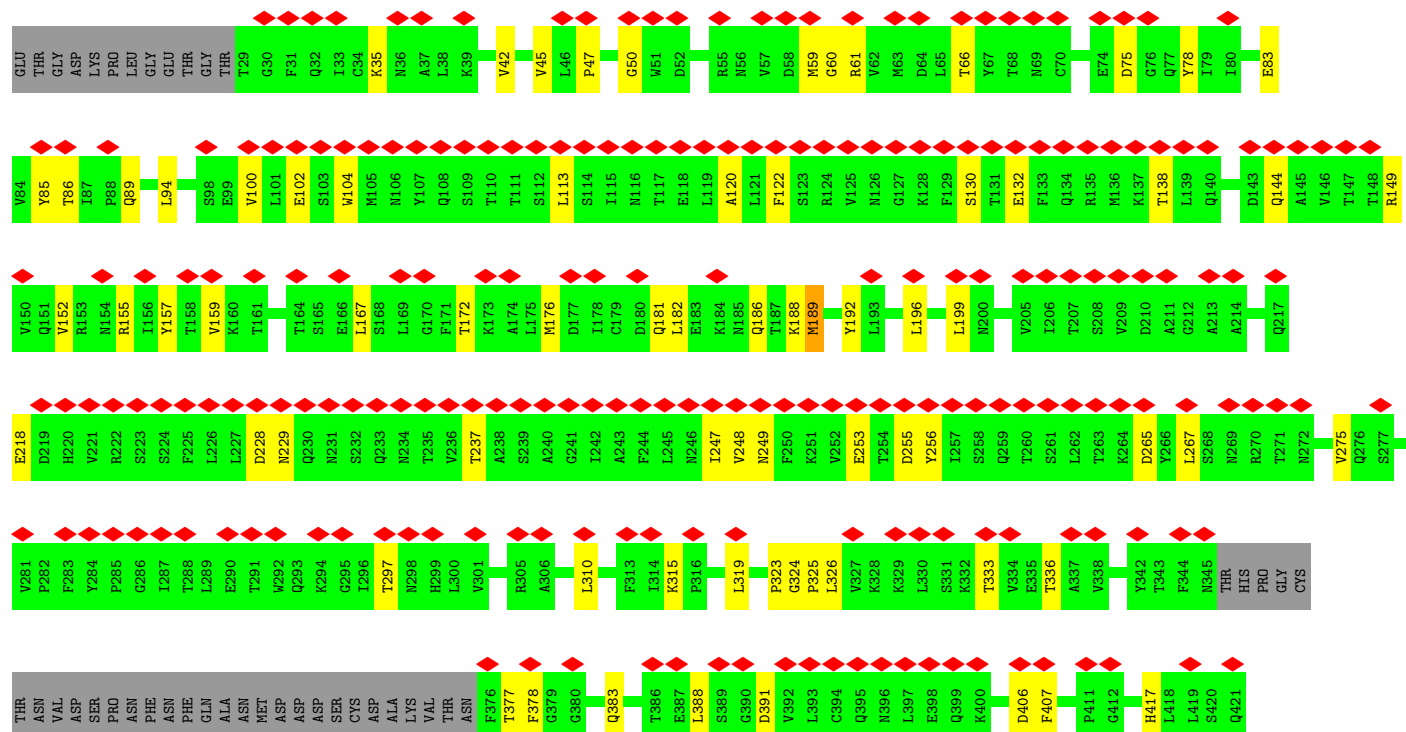


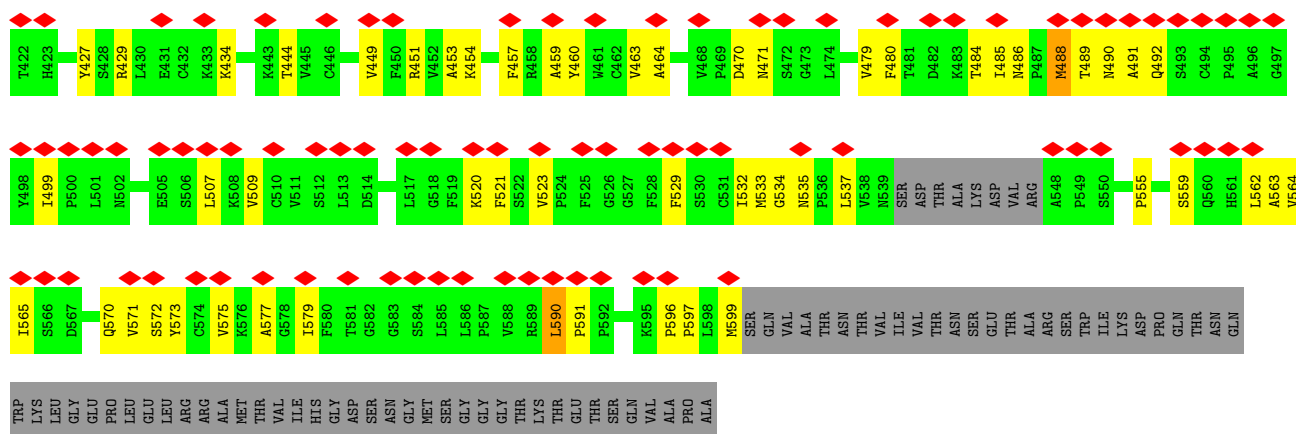
• Molecule 1: Macrophage-expressed gene 1 protein



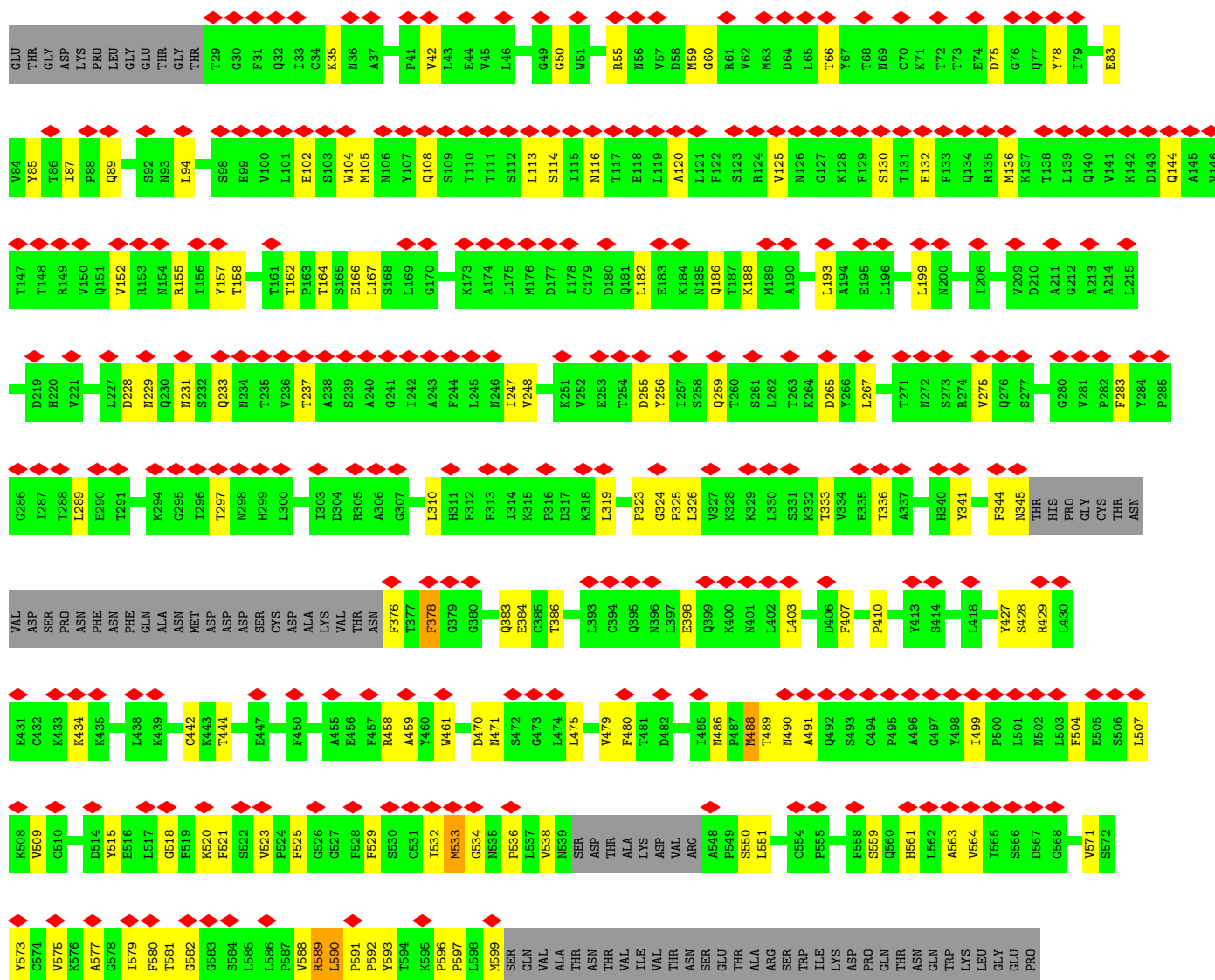
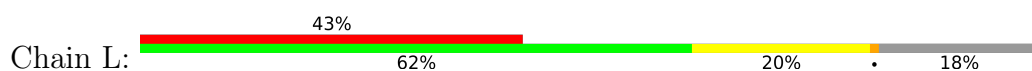


• Molecule 1: Macrophage-expressed gene 1 protein

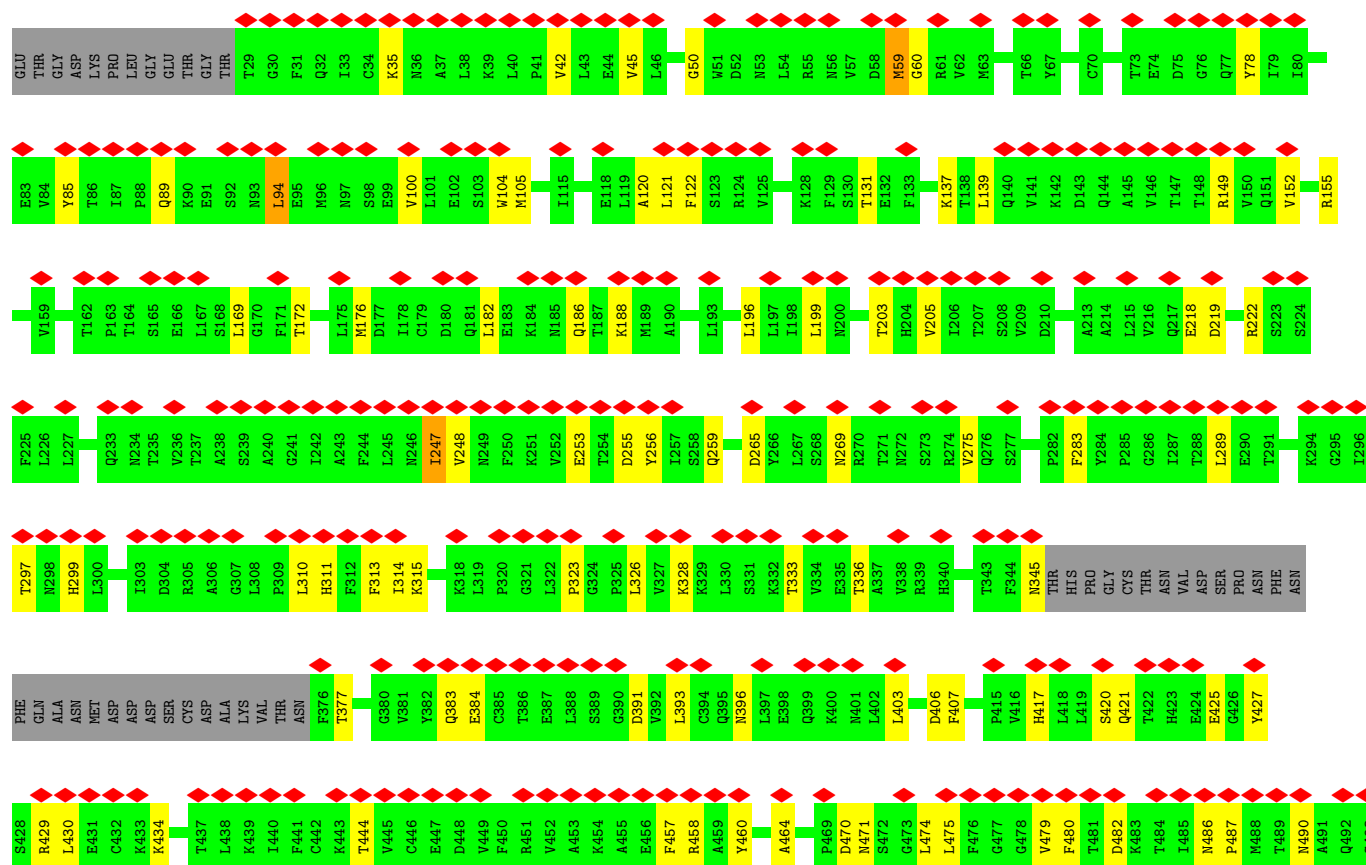


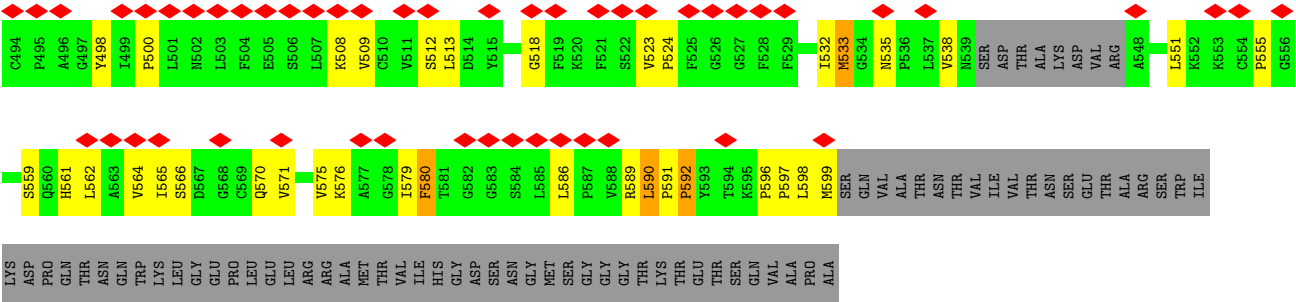


• Molecule 1: Macrophage-expressed gene 1 protein



GLU	THR	GLY	ASP	LYS	PRO	LEU	GLY	GLU	THR	GLY	THR
T29	G30	F31	Q32	I33	C34	K35	N36	K39	L40	P41	V42
								L43	F44	V45	P47
								L46	G48	O49	S50
								W51	D52	N53	D54
								L54	R55	N56	V57
								D58	M59	G60	R61
								D64	L65	T72	D75
								G76	Q77	Y78	P81
								D82	E83	H84	V85





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	116274	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.216	Depositor
Minimum map value	-0.140	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	376.92, 376.92, 376.92	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.047, 1.047, 1.047	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, MA4

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	0.42	0/4238	0.53	0/5752
1	B	0.41	0/4238	0.53	0/5752
1	C	0.41	0/4238	0.52	0/5752
1	D	0.41	0/4238	0.52	0/5752
1	E	0.41	0/4238	0.54	1/5752 (0.0%)
1	F	0.40	0/4238	0.53	0/5752
1	G	0.41	0/4238	0.52	1/5752 (0.0%)
1	H	0.42	0/4238	0.53	1/5752 (0.0%)
1	I	0.42	0/4238	0.53	0/5752
1	J	0.41	0/4238	0.53	0/5752
1	K	0.41	0/4238	0.52	0/5752
1	L	0.41	0/4238	0.53	0/5752
1	M	0.41	0/4238	0.53	1/5752 (0.0%)
1	N	0.40	0/4238	0.52	0/5752
1	O	0.41	0/4238	0.52	0/5752
1	P	0.42	0/4238	0.53	1/5752 (0.0%)
All	All	0.41	0/67808	0.53	5/92032 (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	E	500	PRO	CA-N-CD	-7.91	100.43	111.50
1	M	500	PRO	CA-N-CD	-7.69	100.73	111.50
1	P	592	PRO	CA-N-CD	-5.95	103.16	111.50
1	H	592	PRO	CA-N-CD	-5.94	103.18	111.50
1	G	590	LEU	CA-CB-CG	5.52	128.00	115.30

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	4148	0	4124	94	0
1	B	4148	0	4124	85	0
1	C	4148	0	4124	92	0
1	D	4148	0	4124	86	0
1	E	4148	0	4124	91	0
1	F	4148	0	4124	77	0
1	G	4148	0	4124	94	0
1	H	4148	0	4124	100	0
1	I	4148	0	4124	89	0
1	J	4148	0	4124	88	0
1	K	4148	0	4124	83	0
1	L	4148	0	4124	94	0
1	M	4148	0	4124	93	0
1	N	4148	0	4124	92	0
1	O	4148	0	4124	89	0
1	P	4148	0	4124	90	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
2	K	14	0	13	0	0
2	L	14	0	13	0	0
2	M	14	0	13	0	0
2	N	14	0	13	0	0
2	O	14	0	13	0	0
2	P	14	0	13	0	0
3	A	35	0	44	2	0
3	B	35	0	44	1	0
3	C	35	0	44	2	0
3	D	35	0	44	3	0
3	E	35	0	44	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	35	0	44	1	0
3	G	35	0	44	0	0
3	H	35	0	44	1	0
3	I	35	0	44	1	0
3	J	35	0	44	0	0
3	K	35	0	44	1	0
3	L	35	0	44	5	0
3	M	35	0	44	4	0
3	N	35	0	44	2	0
3	O	35	0	44	1	0
3	P	35	0	44	1	0
All	All	67152	0	66896	1303	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 10.

All (1303) 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)
3:C:702:MA4:HO6	3:C:702:MA4:HO60	1.17	0.91
1:K:186:GLN:NE2	1:K:599:MET:SD	2.44	0.89
1:H:186:GLN:NE2	1:H:599:MET:SD	2.48	0.85
1:C:199:LEU:HB2	1:C:591:PRO:HG2	1.58	0.84
1:G:596:PRO:HG3	1:H:315:LYS:HE3	1.61	0.82
1:K:199:LEU:HB2	1:K:591:PRO:HG2	1.61	0.81
1:C:186:GLN:NE2	1:C:599:MET:SD	2.53	0.80
1:K:149:ARG:NH1	1:K:218:GLU:OE2	2.14	0.80
1:M:345:ASN:OD1	1:M:593:TYR:OH	1.99	0.79
1:O:55:ARG:HD3	1:O:590:LEU:HD11	1.65	0.78
1:P:199:LEU:HB2	1:P:591:PRO:HG2	1.64	0.78
1:A:59:MET:O	1:B:85:TYR:OH	2.00	0.78
1:A:85:TYR:OH	1:P:59:MET:O	2.02	0.78
1:M:186:GLN:NE2	1:M:599:MET:SD	2.53	0.78
1:E:345:ASN:OD1	1:E:593:TYR:OH	2.00	0.77
1:O:59:MET:O	1:P:85:TYR:OH	2.02	0.77
1:C:181:GLN:HE21	1:C:189:MET:HB3	1.49	0.77
1:H:59:MET:O	1:I:85:TYR:OH	2.01	0.77
1:N:59:MET:O	1:O:85:TYR:OH	2.01	0.77
1:J:59:MET:O	1:K:85:TYR:OH	2.01	0.77
1:G:59:MET:O	1:H:85:TYR:OH	2.03	0.77
1:P:417:HIS:ND1	1:P:533:MET:SD	2.56	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:59:MET:O	1:F:85:TYR:OH	2.03	0.76
1:I:59:MET:O	1:J:85:TYR:OH	2.02	0.76
1:P:247:ILE:HG13	1:P:248:VAL:HG23	1.66	0.76
1:D:136:MET:HG3	1:D:231:ASN:HB2	1.68	0.76
1:B:59:MET:O	1:C:85:TYR:OH	2.04	0.76
1:H:417:HIS:ND1	1:H:533:MET:SD	2.56	0.76
1:M:199:LEU:HB2	1:M:591:PRO:HG2	1.67	0.76
1:N:199:LEU:HB2	1:N:591:PRO:HG2	1.67	0.75
1:E:199:LEU:HB2	1:E:591:PRO:HG2	1.68	0.75
1:F:59:MET:O	1:G:85:TYR:OH	2.05	0.75
1:F:386:THR:OG1	1:F:458:ARG:NH1	2.21	0.74
1:H:199:LEU:HB2	1:H:591:PRO:HG2	1.68	0.74
1:K:59:MET:O	1:L:85:TYR:OH	2.04	0.74
1:F:323:PRO:HD2	1:F:326:LEU:HD12	1.69	0.74
1:A:186:GLN:NE2	1:A:599:MET:SD	2.60	0.74
1:F:247:ILE:HG12	1:F:248:VAL:HG23	1.68	0.74
1:D:195:GLU:HB3	1:D:591:PRO:HB2	1.68	0.74
1:H:247:ILE:HG13	1:H:248:VAL:HG23	1.69	0.74
1:M:590:LEU:HB2	1:M:591:PRO:CD	2.18	0.74
1:D:59:MET:O	1:E:85:TYR:OH	2.05	0.74
1:M:434:LYS:HG2	1:M:444:THR:HG22	1.69	0.73
1:P:186:GLN:NE2	1:P:599:MET:SD	2.56	0.73
1:E:247:ILE:HG13	1:E:248:VAL:HG23	1.68	0.73
1:L:247:ILE:HG12	1:L:248:VAL:HG23	1.70	0.73
1:E:590:LEU:HB2	1:E:591:PRO:CD	2.18	0.73
1:H:562:LEU:HD22	1:I:499:ILE:HD11	1.70	0.73
1:E:434:LYS:HG2	1:E:444:THR:HG22	1.69	0.73
1:G:323:PRO:HD2	1:G:326:LEU:HD12	1.69	0.73
1:E:590:LEU:HB2	1:E:591:PRO:HD3	1.70	0.73
1:O:323:PRO:HD2	1:O:326:LEU:HD12	1.70	0.73
1:A:417:HIS:ND1	1:A:533:MET:SD	2.60	0.72
1:B:589:ARG:NH2	1:B:590:LEU:O	2.22	0.72
1:M:590:LEU:HB2	1:M:591:PRO:HD3	1.71	0.72
1:A:499:ILE:HD11	1:P:562:LEU:HD22	1.71	0.72
1:H:323:PRO:HD2	1:H:326:LEU:HD12	1.72	0.72
1:N:149:ARG:NH1	1:N:218:GLU:OE2	2.23	0.72
1:M:480:PHE:HB3	1:M:486:ASN:HB2	1.72	0.72
1:L:479:VAL:HB	1:L:507:LEU:HD11	1.72	0.72
1:D:479:VAL:HB	1:D:507:LEU:HD11	1.72	0.71
1:N:323:PRO:HD2	1:N:326:LEU:HD12	1.70	0.71
1:F:149:ARG:NH1	1:F:218:GLU:OE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:59:MET:O	1:N:85:TYR:OH	2.04	0.71
1:C:49:GLY:HA2	1:C:61:ARG:HA	1.70	0.71
1:G:598:LEU:HD22	1:H:328:LYS:HD3	1.71	0.71
1:I:186:GLN:NE2	1:I:599:MET:SD	2.62	0.71
1:L:59:MET:O	1:M:85:TYR:OH	2.04	0.70
1:K:247:ILE:HG12	1:K:248:VAL:HG23	1.73	0.70
1:O:598:LEU:HD22	1:P:328:LYS:HD3	1.71	0.70
1:A:78:TYR:OH	1:A:297:THR:O	2.07	0.70
1:I:199:LEU:HB2	1:I:591:PRO:HG2	1.73	0.70
1:M:323:PRO:HD2	1:M:326:LEU:HD12	1.74	0.70
1:D:247:ILE:HG12	1:D:248:VAL:HG23	1.72	0.70
1:E:479:VAL:HG12	1:E:509:VAL:HG22	1.74	0.70
1:P:323:PRO:HD2	1:P:326:LEU:HD12	1.73	0.70
1:N:247:ILE:HG12	1:N:248:VAL:HG23	1.73	0.70
1:H:598:LEU:HD22	1:I:328:LYS:HD3	1.74	0.70
1:J:589:ARG:NH2	1:J:590:LEU:O	2.25	0.70
1:N:479:VAL:HB	1:N:507:LEU:HD11	1.73	0.70
1:E:480:PHE:HB3	1:E:486:ASN:HB2	1.72	0.70
1:G:78:TYR:OH	1:G:297:THR:O	2.07	0.70
1:N:386:THR:OG1	1:N:458:ARG:NH1	2.24	0.70
1:I:417:HIS:ND1	1:I:533:MET:SD	2.65	0.69
1:D:344:PHE:HB3	1:D:593:TYR:HE1	1.57	0.69
1:D:186:GLN:NE2	1:D:599:MET:SD	2.63	0.69
1:E:428:SER:H	3:E:702:MA4:H601	1.57	0.69
1:L:186:GLN:NE2	1:L:599:MET:SD	2.62	0.69
1:C:247:ILE:HG12	1:C:248:VAL:HG23	1.72	0.69
1:L:89:GLN:OE1	1:L:155:ARG:NH1	2.26	0.69
1:E:323:PRO:HD2	1:E:326:LEU:HD12	1.74	0.68
1:L:323:PRO:HD2	1:L:326:LEU:HD12	1.75	0.68
1:A:328:LYS:HD3	1:P:598:LEU:HD22	1.74	0.68
1:D:323:PRO:HD2	1:D:326:LEU:HD12	1.75	0.68
1:L:199:LEU:HB2	1:L:591:PRO:HG2	1.74	0.68
1:I:532:ILE:HG13	1:I:533:MET:HG3	1.75	0.68
1:M:479:VAL:HG12	1:M:509:VAL:HG22	1.74	0.68
1:I:323:PRO:HD2	1:I:326:LEU:HD12	1.76	0.68
1:M:592:PRO:HD3	1:N:312:PHE:HE1	1.59	0.68
1:A:517:LEU:HA	1:A:520:LYS:HZ2	1.58	0.67
1:O:589:ARG:NH2	1:O:592:PRO:O	2.26	0.67
1:E:344:PHE:HB3	1:E:593:TYR:CZ	2.29	0.67
1:N:517:LEU:HD23	1:N:520:LYS:HE3	1.77	0.67
1:O:78:TYR:OH	1:O:297:THR:O	2.06	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:377:THR:HB	1:O:464:ALA:HB2	1.77	0.67
1:M:344:PHE:HB3	1:M:593:TYR:CZ	2.30	0.67
1:N:89:GLN:OE1	1:N:155:ARG:NH1	2.28	0.67
1:I:559:SER:N	1:I:575:VAL:O	2.22	0.67
1:M:386:THR:OG1	1:M:458:ARG:NH1	2.27	0.66
1:H:523:VAL:HG23	1:H:579:ILE:HD12	1.76	0.66
1:I:517:LEU:HA	1:I:520:LYS:HZ2	1.58	0.66
1:L:592:PRO:HD3	1:M:312:PHE:HE1	1.61	0.66
1:A:323:PRO:HD2	1:A:326:LEU:HD12	1.76	0.66
1:B:89:GLN:OE1	1:B:155:ARG:NH1	2.28	0.66
1:B:559:SER:N	1:B:575:VAL:O	2.25	0.66
1:L:523:VAL:HG23	1:L:579:ILE:HD12	1.78	0.66
1:B:247:ILE:HG22	1:B:248:VAL:HG23	1.77	0.65
1:L:480:PHE:HB3	1:L:486:ASN:HB2	1.78	0.65
1:N:523:VAL:HG23	1:N:579:ILE:HD12	1.77	0.65
1:C:523:VAL:HG23	1:C:579:ILE:HD12	1.78	0.65
1:E:89:GLN:OE1	1:E:155:ARG:NH1	2.29	0.65
1:F:186:GLN:NE2	1:F:599:MET:SD	2.60	0.65
1:M:249:ASN:HB3	1:N:120:ALA:HB3	1.79	0.65
1:D:480:PHE:HB3	1:D:486:ASN:HB2	1.77	0.65
1:J:323:PRO:HD2	1:J:326:LEU:HD12	1.79	0.65
1:P:523:VAL:HG23	1:P:579:ILE:HD12	1.78	0.65
1:G:377:THR:HB	1:G:464:ALA:HB2	1.77	0.65
1:B:323:PRO:HD2	1:B:326:LEU:HD12	1.79	0.64
1:H:589:ARG:NH2	1:H:592:PRO:O	2.29	0.64
1:L:589:ARG:NH2	1:L:590:LEU:O	2.29	0.64
1:F:418:LEU:HA	1:F:533:MET:HE1	1.79	0.64
1:J:480:PHE:HB3	1:J:486:ASN:HB2	1.80	0.64
1:P:188:LYS:HB3	1:P:597:PRO:HB2	1.80	0.64
1:O:94:LEU:HD13	1:O:152:VAL:HG22	1.79	0.64
1:B:149:ARG:NH1	1:B:218:GLU:OE1	2.31	0.64
1:H:434:LYS:HG2	1:H:444:THR:HG22	1.80	0.64
1:H:89:GLN:OE1	1:H:155:ARG:NH1	2.30	0.64
1:C:255:ASP:HB3	1:D:114:SER:HB2	1.80	0.64
1:E:479:VAL:HB	1:E:507:LEU:HD11	1.80	0.64
1:G:590:LEU:HB3	1:G:591:PRO:HD3	1.79	0.63
1:E:386:THR:OG1	1:E:458:ARG:NH1	2.26	0.63
1:J:149:ARG:NH1	1:J:218:GLU:OE2	2.31	0.63
1:P:434:LYS:HG2	1:P:444:THR:HG22	1.80	0.63
1:I:89:GLN:OE1	1:I:155:ARG:NH1	2.31	0.63
1:K:130:SER:HG	1:K:237:THR:HG1	1.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:479:VAL:HB	1:M:507:LEU:HD11	1.81	0.63
1:N:304:ASP:OD1	1:N:305:ARG:N	2.31	0.63
1:P:89:GLN:OE1	1:P:155:ARG:NH1	2.31	0.63
1:A:89:GLN:OE1	1:A:155:ARG:NH1	2.31	0.63
1:M:89:GLN:OE1	1:M:155:ARG:NH1	2.32	0.63
1:N:186:GLN:NE2	1:N:599:MET:SD	2.61	0.63
1:B:529:PHE:HB2	1:B:534:GLY:HA2	1.81	0.63
1:J:434:LYS:HG2	1:J:444:THR:HG22	1.81	0.63
1:B:523:VAL:HG23	1:B:579:ILE:HD12	1.79	0.63
1:K:434:LYS:HG2	1:K:444:THR:HG22	1.81	0.63
1:M:426:GLY:O	3:M:702:MA4:O4	2.16	0.63
1:H:188:LYS:HB3	1:H:597:PRO:HB2	1.81	0.62
1:N:589:ARG:NH2	1:N:590:LEU:O	2.32	0.62
1:G:89:GLN:OE1	1:G:155:ARG:NH1	2.32	0.62
1:J:559:SER:N	1:J:575:VAL:O	2.24	0.62
1:L:87:ILE:HG13	1:L:158:THR:HB	1.82	0.62
1:G:523:VAL:HG23	1:G:579:ILE:HD12	1.82	0.62
1:J:529:PHE:HB2	1:J:534:GLY:HA2	1.81	0.62
1:L:275:VAL:HB	1:M:94:LEU:HB2	1.82	0.62
1:D:564:VAL:HG12	1:D:571:VAL:HB	1.82	0.62
1:C:434:LYS:HG2	1:C:444:THR:HG22	1.81	0.62
1:L:341:TYR:HE1	1:L:590:LEU:HB3	1.65	0.62
1:E:426:GLY:O	3:E:702:MA4:O4	2.17	0.62
1:E:186:GLN:NE2	1:E:599:MET:SD	2.67	0.61
1:L:428:SER:H	3:L:702:MA4:H601	1.65	0.61
1:M:428:SER:H	3:M:702:MA4:H601	1.65	0.61
1:N:502:ASN:OD1	1:N:508:LYS:NZ	2.29	0.61
1:A:304:ASP:OD1	1:A:305:ARG:N	2.33	0.61
1:A:559:SER:N	1:A:575:VAL:O	2.26	0.61
1:I:247:ILE:HG12	1:I:248:VAL:HG23	1.81	0.61
1:P:427:TYR:OH	1:P:429:ARG:NH2	2.33	0.61
1:B:480:PHE:HB3	1:B:486:ASN:HB2	1.82	0.61
1:C:345:ASN:OD1	1:C:593:TYR:OH	2.16	0.61
1:L:564:VAL:HG12	1:L:571:VAL:HB	1.83	0.61
1:A:315:LYS:HE3	1:P:596:PRO:HG3	1.82	0.61
1:I:564:VAL:HG12	1:I:571:VAL:HB	1.81	0.61
1:D:188:LYS:HD3	1:D:597:PRO:HB2	1.83	0.61
1:A:247:ILE:HG12	1:A:248:VAL:HG23	1.83	0.61
1:B:434:LYS:HG2	1:B:444:THR:HG22	1.83	0.61
1:B:199:LEU:HD13	1:B:591:PRO:HD2	1.83	0.61
1:C:304:ASP:OD2	1:C:305:ARG:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:LYS:HG2	1:F:444:THR:HG22	1.83	0.61
1:L:166:GLU:OE1	1:L:166:GLU:N	2.34	0.61
1:A:564:VAL:HG12	1:A:571:VAL:HB	1.83	0.60
1:I:434:LYS:HG2	1:I:444:THR:HG22	1.80	0.60
1:K:253:GLU:HG3	1:L:116:ASN:HB2	1.82	0.60
1:L:589:ARG:NH2	1:L:592:PRO:O	2.30	0.60
1:N:434:LYS:HG2	1:N:444:THR:HG22	1.83	0.60
1:A:434:LYS:HG2	1:A:444:THR:HG22	1.82	0.60
1:M:78:TYR:OH	1:M:297:THR:O	2.10	0.60
1:M:523:VAL:HG23	1:M:579:ILE:HD12	1.83	0.60
1:E:523:VAL:HG23	1:E:579:ILE:HD12	1.83	0.60
1:G:247:ILE:HG22	1:G:248:VAL:HG23	1.83	0.60
1:K:590:LEU:HB2	1:K:591:PRO:HD3	1.83	0.60
1:A:523:VAL:HG23	1:A:579:ILE:HD12	1.82	0.60
1:H:427:TYR:OH	1:H:429:ARG:NH2	2.34	0.60
1:K:532:ILE:HG13	1:K:533:MET:HG2	1.84	0.60
1:H:560:GLN:OE1	1:I:515:TYR:OH	2.13	0.60
1:P:94:LEU:HD13	1:P:152:VAL:HG22	1.84	0.60
1:A:275:VAL:HB	1:B:94:LEU:HB2	1.84	0.60
1:F:55:ARG:HE	1:F:590:LEU:HD21	1.67	0.60
1:P:589:ARG:NH2	1:P:592:PRO:O	2.35	0.60
1:D:75:ASP:OD2	1:D:157:TYR:OH	2.17	0.59
1:J:523:VAL:HG23	1:J:579:ILE:HD12	1.82	0.59
1:C:89:GLN:OE1	1:C:155:ARG:NH1	2.35	0.59
1:N:345:ASN:OD1	1:N:593:TYR:OH	2.20	0.59
1:K:89:GLN:OE1	1:K:155:ARG:NH1	2.35	0.59
1:C:427:TYR:OH	1:C:429:ARG:NH2	2.36	0.59
1:D:166:GLU:OE2	1:D:166:GLU:N	2.35	0.59
1:G:589:ARG:NH2	1:G:590:LEU:O	2.25	0.59
1:K:427:TYR:OH	1:K:429:ARG:NH2	2.36	0.59
1:N:401:ASN:HD21	1:N:410:PRO:HG3	1.68	0.59
1:O:247:ILE:HG22	1:O:248:VAL:HG23	1.83	0.59
1:D:275:VAL:HB	1:E:94:LEU:HB2	1.83	0.59
1:K:47:PRO:O	1:K:61:ARG:NH1	2.35	0.59
1:E:559:SER:N	1:E:575:VAL:O	2.35	0.59
1:O:523:VAL:HG23	1:O:579:ILE:HD12	1.83	0.58
1:F:401:ASN:HD21	1:F:410:PRO:HG3	1.67	0.58
1:A:535:ASN:ND2	1:A:555:PRO:HD3	2.18	0.58
1:A:598:LEU:HD22	1:B:328:LYS:HD3	1.86	0.58
1:E:78:TYR:OH	1:E:297:THR:O	2.09	0.58
1:K:488:MET:HE1	1:K:489:THR:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLY:N	1:E:60:GLY:O	2.25	0.58
1:K:590:LEU:HB2	1:K:591:PRO:CD	2.33	0.58
1:O:131:THR:HG22	1:O:236:VAL:HG22	1.85	0.58
1:D:427:TYR:OH	1:D:429:ARG:NH2	2.36	0.58
1:L:504:PHE:HB2	1:L:507:LEU:HB3	1.86	0.58
1:A:513:LEU:HD12	1:P:562:LEU:HB2	1.86	0.58
1:F:89:GLN:OE1	1:F:155:ARG:NH1	2.37	0.58
1:G:479:VAL:HB	1:G:507:LEU:HD11	1.84	0.58
1:O:249:ASN:HB3	1:P:120:ALA:HB3	1.86	0.58
1:C:75:ASP:OD2	1:C:157:TYR:OH	2.21	0.58
1:I:524:PRO:HG2	1:I:576:LYS:HD2	1.85	0.58
1:J:386:THR:OG1	1:J:458:ARG:NH1	2.30	0.58
1:O:479:VAL:HB	1:O:507:LEU:HD11	1.85	0.58
1:A:562:LEU:HB2	1:B:513:LEU:HD12	1.85	0.58
1:B:275:VAL:HB	1:C:94:LEU:HB2	1.85	0.58
1:I:535:ASN:ND2	1:I:555:PRO:HD3	2.18	0.58
1:C:480:PHE:HB3	1:C:486:ASN:HB2	1.86	0.58
1:I:75:ASP:OD2	1:I:157:TYR:OH	2.22	0.58
1:F:275:VAL:HB	1:G:94:LEU:HB2	1.86	0.58
1:F:523:VAL:HG23	1:F:579:ILE:HD12	1.83	0.58
1:L:538:VAL:HG11	1:L:551:LEU:HB2	1.86	0.58
1:M:138:THR:HB	1:M:229:ASN:HB3	1.85	0.58
1:F:564:VAL:HG12	1:F:571:VAL:HB	1.86	0.57
1:I:275:VAL:HB	1:J:94:LEU:HB2	1.86	0.57
1:N:384:GLU:OE1	1:N:458:ARG:NH2	2.30	0.57
1:P:78:TYR:OH	1:P:297:THR:O	2.17	0.57
1:A:532:ILE:HG13	1:A:533:MET:HG3	1.86	0.57
1:N:421:GLN:OE1	1:N:566:SER:OG	2.17	0.57
1:N:589:ARG:NH2	1:N:592:PRO:O	2.25	0.57
1:B:403:LEU:HD21	1:B:474:LEU:HD21	1.87	0.57
1:M:247:ILE:HG13	1:M:248:VAL:HG23	1.85	0.57
1:A:589:ARG:NH2	1:A:592:PRO:O	2.30	0.57
1:O:570:GLN:NE2	1:O:572:SER:OG	2.37	0.57
1:K:480:PHE:HB3	1:K:486:ASN:HB2	1.86	0.57
1:K:486:ASN:O	1:K:490:ASN:N	2.37	0.57
1:L:344:PHE:HB3	1:L:593:TYR:HE1	1.69	0.57
1:L:427:TYR:OH	1:L:429:ARG:NH2	2.37	0.57
1:L:529:PHE:HB2	1:L:534:GLY:HA2	1.87	0.57
1:B:311:HIS:O	1:B:315:LYS:NZ	2.38	0.57
1:I:598:LEU:HD22	1:J:328:LYS:HD3	1.85	0.57
1:D:403:LEU:HD12	1:D:410:PRO:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:590:LEU:HB3	1:F:591:PRO:HD3	1.87	0.57
1:C:486:ASN:O	1:C:490:ASN:N	2.38	0.56
1:F:596:PRO:HG2	1:G:315:LYS:HE3	1.86	0.56
1:P:377:THR:HB	1:P:464:ALA:HB2	1.87	0.56
1:B:50:GLY:N	1:B:60:GLY:O	2.28	0.56
1:C:590:LEU:HB2	1:C:591:PRO:HD3	1.86	0.56
1:D:529:PHE:HB2	1:D:534:GLY:HA2	1.88	0.56
1:G:181:GLN:NE2	1:G:189:MET:HB3	2.21	0.56
1:G:559:SER:N	1:G:575:VAL:O	2.32	0.56
1:H:559:SER:N	1:H:575:VAL:O	2.32	0.56
1:L:403:LEU:HD12	1:L:410:PRO:HB3	1.87	0.56
1:P:559:SER:N	1:P:575:VAL:O	2.31	0.56
1:H:562:LEU:HB2	1:I:513:LEU:HD12	1.87	0.56
1:M:559:SER:N	1:M:575:VAL:O	2.35	0.56
1:D:89:GLN:OE1	1:D:155:ARG:NH1	2.39	0.56
1:G:532:ILE:HG13	1:G:533:MET:HG2	1.88	0.56
1:K:275:VAL:HB	1:L:94:LEU:HB2	1.88	0.56
1:A:524:PRO:HG2	1:A:576:LYS:HD2	1.86	0.56
1:B:78:TYR:OH	1:B:297:THR:O	2.15	0.56
1:D:538:VAL:HG11	1:D:551:LEU:HB2	1.87	0.56
1:L:344:PHE:CB	1:L:593:TYR:HE1	2.19	0.56
1:M:186:GLN:HG3	1:M:188:LYS:HE2	1.88	0.56
1:I:523:VAL:HG23	1:I:579:ILE:HD12	1.86	0.56
1:N:502:ASN:ND2	1:N:504:PHE:O	2.38	0.56
1:G:479:VAL:HG12	1:G:509:VAL:HG22	1.87	0.56
1:J:275:VAL:HB	1:K:94:LEU:HB2	1.86	0.56
1:J:311:HIS:O	1:J:315:LYS:NZ	2.38	0.56
1:M:304:ASP:OD2	1:M:305:ARG:N	2.38	0.56
1:N:517:LEU:HA	1:N:520:LYS:HE2	1.88	0.56
1:J:89:GLN:O	1:J:91:GLU:HG3	2.05	0.56
1:O:590:LEU:HB2	1:O:591:PRO:CD	2.36	0.56
1:I:480:PHE:HB3	1:I:486:ASN:HB2	1.87	0.56
1:K:75:ASP:OD2	1:K:157:TYR:OH	2.24	0.55
1:N:596:PRO:HG2	1:O:315:LYS:HE3	1.87	0.55
1:O:589:ARG:NH2	1:O:590:LEU:O	2.39	0.55
1:A:480:PHE:HB3	1:A:486:ASN:HB2	1.87	0.55
1:I:484:THR:O	1:I:492:GLN:NE2	2.39	0.55
1:N:479:VAL:HG12	1:N:509:VAL:HG22	1.88	0.55
1:A:94:LEU:HB2	1:P:275:VAL:HB	1.87	0.55
1:O:434:LYS:HG2	1:O:444:THR:HG22	1.88	0.55
1:C:265:ASP:HB2	1:D:104:TRP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:377:THR:HB	1:K:464:ALA:HB2	1.88	0.55
1:K:479:VAL:HG12	1:K:509:VAL:HA	1.89	0.55
1:L:488:MET:HE1	1:L:489:THR:HB	1.88	0.55
1:O:501:LEU:HB3	1:O:509:VAL:HG23	1.89	0.55
1:O:538:VAL:HG11	1:O:551:LEU:HB2	1.87	0.55
1:F:413:TYR:HB3	1:F:462:CYS:HB3	1.89	0.55
1:G:564:VAL:HG12	1:G:571:VAL:HB	1.89	0.55
1:H:377:THR:HB	1:H:464:ALA:HB2	1.87	0.55
1:O:564:VAL:HG12	1:O:571:VAL:HB	1.87	0.55
1:B:389:SER:OG	1:B:454:LYS:N	2.32	0.55
1:B:564:VAL:HG12	1:B:571:VAL:HB	1.87	0.55
1:C:532:ILE:HG13	1:C:533:MET:HG2	1.87	0.55
1:E:304:ASP:OD1	1:E:305:ARG:N	2.40	0.55
1:E:517:LEU:HD23	1:E:520:LYS:HD3	1.89	0.55
1:C:275:VAL:HB	1:D:94:LEU:HB2	1.88	0.55
1:C:488:MET:HE1	1:C:489:THR:HB	1.89	0.55
1:N:199:LEU:HD13	1:N:591:PRO:HD2	1.88	0.55
1:O:381:VAL:HG12	1:O:461:TRP:HA	1.89	0.55
1:P:564:VAL:HG12	1:P:571:VAL:HB	1.89	0.55
1:H:498:TYR:CZ	1:H:512:SER:HB2	2.41	0.55
1:O:383:GLN:HE21	1:O:457:PHE:HB2	1.72	0.55
1:O:479:VAL:HG12	1:O:509:VAL:HG12	1.88	0.55
1:I:596:PRO:HG2	1:J:315:LYS:HE3	1.89	0.55
1:M:255:ASP:HB3	1:N:114:SER:HB2	1.88	0.55
1:M:564:VAL:HG12	1:M:571:VAL:HB	1.89	0.55
1:A:75:ASP:OD2	1:A:157:TYR:OH	2.22	0.54
1:G:51:TRP:HB2	1:G:206:ILE:HD13	1.88	0.54
1:G:249:ASN:HB3	1:H:120:ALA:HB3	1.89	0.54
1:K:529:PHE:HB2	1:K:534:GLY:HA2	1.89	0.54
1:B:35:LYS:HE3	1:B:42:VAL:HG23	1.88	0.54
1:D:504:PHE:HB2	1:D:507:LEU:HB3	1.89	0.54
1:L:386:THR:OG1	1:L:458:ARG:NH1	2.37	0.54
1:P:345:ASN:HD21	1:P:590:LEU:HD12	1.73	0.54
1:C:529:PHE:HB2	1:C:534:GLY:HA2	1.90	0.54
1:E:564:VAL:HG12	1:E:571:VAL:HB	1.89	0.54
1:J:220:HIS:HD2	1:J:222:ARG:HH12	1.55	0.54
1:L:188:LYS:HD3	1:L:597:PRO:HB2	1.89	0.54
1:N:564:VAL:HG12	1:N:571:VAL:HB	1.88	0.54
1:P:498:TYR:CZ	1:P:512:SER:HB2	2.43	0.54
1:G:434:LYS:HG2	1:G:444:THR:HG22	1.88	0.54
1:H:564:VAL:HG12	1:H:571:VAL:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:MET:HG2	1:L:231:ASN:HB2	1.89	0.54
1:H:89:GLN:O	1:H:91:GLU:N	2.40	0.54
1:N:78:TYR:OH	1:N:297:THR:O	2.11	0.54
1:A:228:ASP:OD1	1:A:229:ASN:N	2.40	0.53
1:C:377:THR:HB	1:C:464:ALA:HB2	1.90	0.53
1:E:380:GLY:HA2	1:E:474:LEU:HD21	1.90	0.53
1:G:383:GLN:HE21	1:G:457:PHE:HB2	1.73	0.53
1:G:570:GLN:NE2	1:G:572:SER:OG	2.40	0.53
1:G:590:LEU:HB3	1:G:591:PRO:CD	2.38	0.53
1:G:89:GLN:O	1:G:91:GLU:N	2.42	0.53
1:A:484:THR:O	1:A:492:GLN:NE2	2.40	0.53
1:C:323:PRO:HD2	1:C:326:LEU:HD12	1.90	0.53
1:J:596:PRO:HG2	1:K:315:LYS:HE3	1.90	0.53
1:B:75:ASP:OD2	1:B:157:TYR:OH	2.21	0.53
1:E:563:ALA:HB2	1:E:573:TYR:HD2	1.73	0.53
1:J:504:PHE:HB2	1:J:507:LEU:HB3	1.89	0.53
1:P:396:ASN:OD1	1:P:396:ASN:N	2.41	0.53
1:K:113:LEU:O	1:K:132:GLU:HA	2.09	0.53
1:C:479:VAL:HG12	1:C:509:VAL:HA	1.91	0.53
1:H:199:LEU:HD13	1:H:591:PRO:HD2	1.90	0.53
1:H:396:ASN:N	1:H:396:ASN:OD1	2.41	0.53
1:J:564:VAL:HG12	1:J:571:VAL:HB	1.89	0.53
1:K:323:PRO:HD2	1:K:326:LEU:HD12	1.91	0.53
1:K:570:GLN:NE2	1:K:572:SER:OG	2.41	0.53
1:A:255:ASP:HB3	1:B:114:SER:HB2	1.91	0.53
1:E:398:GLU:HB2	1:E:407:PHE:HZ	1.74	0.53
1:I:89:GLN:O	1:I:91:GLU:HG3	2.09	0.53
1:C:590:LEU:HB2	1:C:591:PRO:CD	2.38	0.53
1:E:344:PHE:HB3	1:E:593:TYR:OH	2.08	0.53
1:F:421:GLN:OE1	1:F:566:SER:OG	2.18	0.53
1:I:589:ARG:NH2	1:I:592:PRO:O	2.31	0.53
1:L:130:SER:HB2	1:L:237:THR:OG1	2.08	0.53
1:O:75:ASP:OD2	1:O:157:TYR:OH	2.25	0.53
1:G:50:GLY:N	1:G:60:GLY:O	2.27	0.53
1:H:486:ASN:O	1:H:490:ASN:N	2.42	0.53
1:C:228:ASP:OD2	1:C:229:ASN:N	2.41	0.52
1:G:484:THR:OG1	1:G:485:ILE:N	2.42	0.52
1:A:42:VAL:HG22	1:A:79:ILE:HB	1.90	0.52
1:C:479:VAL:HB	1:C:507:LEU:HD11	1.90	0.52
1:D:590:LEU:HB3	1:D:591:PRO:HD3	1.91	0.52
1:F:479:VAL:HB	1:F:507:LEU:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:58:ASP:O	1:J:160:LYS:NZ	2.43	0.52
1:J:249:ASN:HB3	1:K:120:ALA:HB3	1.90	0.52
1:P:417:HIS:HA	1:P:460:TYR:CD2	2.45	0.52
1:I:563:ALA:HB2	1:I:573:TYR:HD1	1.74	0.52
1:I:590:LEU:HB2	1:I:591:PRO:CD	2.40	0.52
1:J:389:SER:OG	1:J:454:LYS:N	2.34	0.52
1:A:50:GLY:N	1:A:60:GLY:O	2.38	0.52
1:A:596:PRO:HG2	1:B:315:LYS:HE3	1.89	0.52
1:C:559:SER:N	1:C:575:VAL:O	2.27	0.52
1:H:417:HIS:HA	1:H:460:TYR:CD2	2.45	0.52
1:K:228:ASP:OD1	1:K:229:ASN:N	2.42	0.52
1:M:344:PHE:HB3	1:M:593:TYR:OH	2.09	0.52
1:N:486:ASN:O	1:N:490:ASN:N	2.42	0.52
1:E:427:TYR:OH	1:E:429:ARG:NH2	2.43	0.52
1:G:393:LEU:HD21	1:G:425:GLU:HB3	1.91	0.52
1:A:89:GLN:O	1:A:91:GLU:HG3	2.09	0.52
1:A:138:THR:HB	1:A:229:ASN:HB3	1.92	0.52
1:C:255:ASP:N	1:D:114:SER:O	2.37	0.52
1:C:559:SER:HB3	1:C:577:ALA:HB2	1.92	0.52
1:H:275:VAL:HB	1:I:94:LEU:HB2	1.90	0.52
1:M:50:GLY:N	1:M:60:GLY:O	2.28	0.52
1:F:304:ASP:OD1	1:F:305:ARG:N	2.42	0.52
1:G:75:ASP:OD2	1:G:157:TYR:OH	2.26	0.52
1:K:102:GLU:HG2	1:K:144:GLN:HG2	1.92	0.52
1:F:384:GLU:OE1	1:F:458:ARG:NH2	2.35	0.52
1:I:50:GLY:N	1:I:60:GLY:O	2.27	0.52
1:L:75:ASP:OD2	1:L:157:TYR:OH	2.27	0.52
1:L:559:SER:N	1:L:575:VAL:O	2.40	0.52
1:M:275:VAL:HB	1:N:94:LEU:HB2	1.92	0.52
1:O:524:PRO:HG2	1:O:576:LYS:HD2	1.91	0.52
1:A:383:GLN:HE21	1:A:457:PHE:HB2	1.75	0.52
1:C:188:LYS:HB3	1:C:597:PRO:HB2	1.91	0.52
1:H:78:TYR:OH	1:H:297:THR:O	2.18	0.52
1:K:35:LYS:HE3	1:K:42:VAL:HG23	1.92	0.52
1:A:203:THR:O	1:A:310:LEU:HD22	2.09	0.52
1:F:479:VAL:HG12	1:F:509:VAL:HG22	1.92	0.52
1:G:524:PRO:HG2	1:G:576:LYS:HD2	1.91	0.52
1:H:596:PRO:HG3	1:I:315:LYS:HE3	1.92	0.52
1:I:383:GLN:HE21	1:I:457:PHE:HB2	1.75	0.52
1:K:479:VAL:HB	1:K:507:LEU:HD11	1.92	0.52
1:M:341:TYR:HA	1:M:593:TYR:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:563:ALA:HB2	1:M:573:TYR:HD2	1.75	0.52
1:A:563:ALA:HB2	1:A:573:TYR:HD1	1.75	0.51
1:D:102:GLU:HG2	1:D:144:GLN:HG2	1.92	0.51
1:G:275:VAL:HB	1:H:94:LEU:HB2	1.92	0.51
1:G:560:GLN:HG2	1:H:513:LEU:HD11	1.91	0.51
1:J:50:GLY:N	1:J:60:GLY:O	2.28	0.51
1:J:195:GLU:HB3	1:J:591:PRO:HB2	1.91	0.51
1:J:247:ILE:HG22	1:J:248:VAL:HG23	1.93	0.51
1:A:403:LEU:HD21	1:A:474:LEU:HD21	1.92	0.51
1:B:538:VAL:HG11	1:B:551:LEU:HB2	1.92	0.51
1:I:311:HIS:O	1:I:315:LYS:NZ	2.43	0.51
1:J:35:LYS:HE3	1:J:42:VAL:HG23	1.93	0.51
1:K:265:ASP:HB2	1:L:104:TRP:HB3	1.93	0.51
1:C:35:LYS:HE3	1:C:42:VAL:HG23	1.92	0.51
1:F:480:PHE:HB3	1:F:486:ASN:HB2	1.92	0.51
1:G:580:PHE:HZ	1:H:517:LEU:HD11	1.75	0.51
1:L:344:PHE:HB3	1:L:593:TYR:CE1	2.44	0.51
1:L:434:LYS:HE3	1:L:442:CYS:HB3	1.91	0.51
1:M:417:HIS:HA	1:M:460:TYR:CD2	2.46	0.51
1:N:480:PHE:HB3	1:N:486:ASN:HB2	1.91	0.51
1:F:570:GLN:NE2	1:F:572:SER:OG	2.44	0.51
1:M:421:GLN:OE1	1:M:566:SER:OG	2.20	0.51
1:N:249:ASN:HB3	1:O:120:ALA:HB3	1.92	0.51
1:N:450:PHE:HE1	3:N:702:MA4:H62	1.76	0.51
1:O:54:LEU:HD23	1:O:341:TYR:HE2	1.75	0.51
1:P:199:LEU:HD13	1:P:591:PRO:HD2	1.93	0.51
1:H:532:ILE:HG13	1:H:533:MET:HG3	1.93	0.51
3:L:702:MA4:O60	3:L:702:MA4:O6	2.24	0.51
1:P:532:ILE:HG13	1:P:533:MET:HG3	1.93	0.51
1:D:398:GLU:HB2	1:D:407:PHE:CZ	2.46	0.51
1:E:417:HIS:HA	1:E:460:TYR:CD2	2.45	0.51
1:H:35:LYS:HE3	1:H:42:VAL:HG23	1.93	0.51
3:M:702:MA4:O6	3:M:702:MA4:O60	2.26	0.51
1:O:560:GLN:HG2	1:P:513:LEU:HD11	1.92	0.51
1:E:275:VAL:HB	1:F:94:LEU:HB2	1.92	0.51
1:H:283:PHE:O	1:I:293:GLN:NE2	2.29	0.51
1:K:267:LEU:HB3	1:L:102:GLU:HB2	1.93	0.51
1:C:102:GLU:HG2	1:C:144:GLN:HG2	1.92	0.51
1:C:138:THR:HB	1:C:229:ASN:HB3	1.93	0.51
3:L:702:MA4:H602	3:L:702:MA4:O10	2.10	0.51
1:N:311:HIS:O	1:N:315:LYS:NZ	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:535:ASN:ND2	1:H:555:PRO:HD3	2.26	0.51
1:M:517:LEU:HD23	1:M:520:LYS:HD3	1.93	0.51
1:P:535:ASN:ND2	1:P:555:PRO:HD3	2.26	0.51
1:E:75:ASP:OD2	1:E:157:TYR:OH	2.29	0.51
1:I:589:ARG:O	1:I:590:LEU:HD23	2.10	0.51
1:P:538:VAL:HG21	1:P:551:LEU:H	1.75	0.51
1:H:182:LEU:HD11	1:H:333:THR:HG21	1.93	0.50
1:L:398:GLU:HB2	1:L:407:PHE:CZ	2.46	0.50
1:M:525:PHE:HE1	1:M:573:TYR:HB2	1.76	0.50
1:O:403:LEU:HD12	1:O:410:PRO:HG2	1.93	0.50
1:A:428:SER:N	3:A:702:MA4:O60	2.44	0.50
1:D:175:LEU:HD12	1:D:330:LEU:HD21	1.91	0.50
1:F:89:GLN:O	1:F:91:GLU:HG3	2.11	0.50
1:O:89:GLN:OE1	1:O:155:ARG:NH1	2.44	0.50
1:P:590:LEU:HB2	1:P:591:PRO:HD3	1.92	0.50
1:G:89:GLN:O	1:G:91:GLU:HG3	2.11	0.50
1:H:265:ASP:HB2	1:I:104:TRP:HB3	1.93	0.50
1:H:345:ASN:HD21	1:H:590:LEU:HD12	1.76	0.50
1:P:149:ARG:NH1	1:P:218:GLU:OE2	2.44	0.50
1:E:340:HIS:HD1	1:E:593:TYR:HD2	1.58	0.50
1:J:130:SER:HB2	1:J:237:THR:OG1	2.11	0.50
1:K:463:VAL:HG21	1:K:537:LEU:HD11	1.93	0.50
1:O:565:ILE:HD13	1:O:570:GLN:HA	1.93	0.50
1:D:78:TYR:OH	1:D:297:THR:O	2.19	0.50
1:D:428:SER:H	3:D:702:MA4:C60	2.24	0.50
1:J:188:LYS:HB3	1:J:597:PRO:HB2	1.92	0.50
1:N:418:LEU:HA	1:N:533:MET:HE1	1.94	0.50
1:O:393:LEU:HD21	1:O:425:GLU:HB3	1.93	0.50
1:C:570:GLN:NE2	1:C:572:SER:OG	2.42	0.50
1:E:500:PRO:HD2	1:E:500:PRO:O	2.12	0.50
1:J:417:HIS:NE2	1:J:420:SER:OG	2.30	0.50
1:M:340:HIS:HD1	1:M:593:TYR:HD2	1.58	0.50
1:O:480:PHE:HB3	1:O:486:ASN:HB2	1.94	0.50
1:A:104:TRP:HB3	1:P:265:ASP:HB2	1.93	0.50
1:C:564:VAL:HG12	1:C:571:VAL:HB	1.94	0.50
1:D:386:THR:OG1	1:D:458:ARG:NH1	2.38	0.50
1:G:381:VAL:HG12	1:G:461:TRP:HA	1.93	0.50
1:G:538:VAL:HG11	1:G:551:LEU:HB2	1.92	0.50
1:J:181:GLN:HE21	1:J:189:MET:HB3	1.77	0.50
1:K:564:VAL:HG12	1:K:571:VAL:HB	1.94	0.50
1:H:421:GLN:OE1	1:H:566:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:TYR:OH	1:K:297:THR:O	2.18	0.50
1:A:417:HIS:HA	1:A:460:TYR:CD2	2.48	0.49
1:C:417:HIS:HA	1:C:460:TYR:CD2	2.47	0.49
1:F:249:ASN:HB3	1:G:120:ALA:HB3	1.94	0.49
1:G:565:ILE:HD13	1:G:570:GLN:HA	1.92	0.49
1:K:255:ASP:HB3	1:L:114:SER:HB2	1.94	0.49
1:J:403:LEU:HD21	1:J:474:LEU:HD21	1.94	0.49
1:C:87:ILE:HG22	1:C:89:GLN:HG3	1.94	0.49
1:D:523:VAL:HG23	1:D:579:ILE:HD12	1.94	0.49
1:E:89:GLN:O	1:E:91:GLU:HG3	2.12	0.49
1:E:255:ASP:OD1	1:E:256:TYR:N	2.45	0.49
1:F:486:ASN:O	1:F:490:ASN:N	2.42	0.49
1:G:421:GLN:OE1	1:G:566:SER:OG	2.25	0.49
1:B:388:LEU:HB2	1:B:454:LYS:HG3	1.94	0.49
1:E:525:PHE:HE1	1:E:573:TYR:HB2	1.77	0.49
1:E:596:PRO:HG2	1:F:315:LYS:HE3	1.95	0.49
1:F:55:ARG:HD3	1:F:590:LEU:HD11	1.94	0.49
1:I:199:LEU:HD13	1:I:591:PRO:HD2	1.94	0.49
1:I:479:VAL:HB	1:I:507:LEU:HD11	1.95	0.49
1:J:247:ILE:O	1:K:122:PHE:N	2.43	0.49
1:L:102:GLU:HG2	1:L:144:GLN:HG2	1.94	0.49
1:M:89:GLN:O	1:M:91:GLU:HG3	2.12	0.49
1:G:384:GLU:N	1:G:458:ARG:O	2.45	0.49
1:H:311:HIS:O	1:H:315:LYS:NZ	2.46	0.49
1:K:138:THR:HB	1:K:229:ASN:HB3	1.94	0.49
1:N:598:LEU:HD22	1:O:328:LYS:HD3	1.95	0.49
1:P:486:ASN:O	1:P:490:ASN:N	2.44	0.49
1:I:486:ASN:O	1:I:490:ASN:N	2.45	0.49
1:L:78:TYR:OH	1:L:297:THR:O	2.20	0.49
1:M:570:GLN:NE2	1:M:572:SER:OG	2.46	0.49
1:D:188:LYS:HB3	1:D:597:PRO:HG2	1.94	0.49
1:G:398:GLU:HB2	1:G:407:PHE:CZ	2.48	0.49
1:B:563:ALA:HB2	1:B:573:TYR:HD1	1.77	0.49
1:G:137:LYS:HE2	1:G:139:LEU:HD11	1.95	0.49
1:K:417:HIS:HA	1:K:460:TYR:CD2	2.48	0.49
1:M:427:TYR:OH	1:M:429:ARG:NH2	2.46	0.49
1:N:75:ASP:OD2	1:N:157:TYR:OH	2.23	0.49
1:D:398:GLU:HB2	1:D:407:PHE:HZ	1.78	0.49
1:D:488:MET:HE1	1:D:489:THR:HB	1.95	0.49
1:F:75:ASP:OD2	1:F:157:TYR:OH	2.23	0.49
1:L:188:LYS:HB3	1:L:597:PRO:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:275:VAL:HB	1:O:94:LEU:HB2	1.95	0.49
1:H:255:ASP:OD1	1:H:256:TYR:N	2.46	0.49
1:K:181:GLN:HE22	1:K:189:MET:HG2	1.78	0.49
1:L:559:SER:HB3	1:L:577:ALA:HB2	1.95	0.49
1:O:517:LEU:HA	1:O:520:LYS:HZ2	1.77	0.49
1:D:341:TYR:O	1:D:345:ASN:ND2	2.45	0.48
1:D:563:ALA:HB2	1:D:573:TYR:HD2	1.77	0.48
1:I:403:LEU:HD21	1:I:474:LEU:HD21	1.95	0.48
1:B:255:ASP:OD1	1:B:256:TYR:N	2.46	0.48
1:C:383:GLN:HE21	1:C:457:PHE:HB2	1.78	0.48
1:F:417:HIS:HA	1:F:460:TYR:CD2	2.47	0.48
1:L:486:ASN:O	1:L:490:ASN:N	2.47	0.48
1:P:311:HIS:O	1:P:315:LYS:NZ	2.42	0.48
1:B:89:GLN:O	1:B:91:GLU:HG3	2.14	0.48
1:B:269:ASN:HB2	1:C:100:VAL:HB	1.96	0.48
1:D:249:ASN:HB3	1:E:120:ALA:HB3	1.95	0.48
1:H:524:PRO:HG2	1:H:576:LYS:HD2	1.94	0.48
1:H:538:VAL:HG21	1:H:551:LEU:H	1.78	0.48
1:I:249:ASN:HB3	1:J:120:ALA:HB3	1.96	0.48
1:J:269:ASN:HB2	1:K:100:VAL:HB	1.95	0.48
1:J:538:VAL:HG11	1:J:551:LEU:HB2	1.95	0.48
1:C:463:VAL:HG21	1:C:537:LEU:HD11	1.95	0.48
1:J:386:THR:HG1	1:J:458:ARG:HH12	1.55	0.48
1:M:398:GLU:HB2	1:M:407:PHE:HZ	1.78	0.48
1:N:565:ILE:HD13	1:N:570:GLN:HA	1.96	0.48
1:O:275:VAL:HB	1:P:94:LEU:HB2	1.96	0.48
1:O:559:SER:N	1:O:575:VAL:O	2.33	0.48
1:A:293:GLN:NE2	1:P:283:PHE:O	2.29	0.48
1:F:199:LEU:HD13	1:F:591:PRO:HD2	1.95	0.48
1:G:383:GLN:HA	1:G:459:ALA:HA	1.94	0.48
1:G:516:GLU:HB2	1:G:520:LYS:HZ1	1.79	0.48
1:H:89:GLN:O	1:H:91:GLU:HG3	2.13	0.48
1:J:417:HIS:HA	1:J:460:TYR:CD2	2.48	0.48
1:L:398:GLU:HB2	1:L:407:PHE:HZ	1.78	0.48
1:N:417:HIS:HA	1:N:460:TYR:HD2	1.78	0.48
1:O:398:GLU:HB2	1:O:407:PHE:CZ	2.48	0.48
1:B:386:THR:HG1	1:B:458:ARG:HH12	1.56	0.48
1:E:333:THR:O	1:E:336:THR:HG22	2.13	0.48
1:E:474:LEU:HD22	1:E:511:VAL:HG11	1.95	0.48
1:J:563:ALA:HB2	1:J:573:TYR:HD1	1.77	0.48
1:A:479:VAL:HB	1:A:507:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:ILE:HD12	1:C:492:GLN:HG3	1.96	0.48
1:E:188:LYS:HB3	1:E:597:PRO:HB2	1.96	0.48
1:F:517:LEU:HD23	1:F:520:LYS:HD3	1.95	0.48
1:G:517:LEU:HA	1:G:520:LYS:HZ2	1.78	0.48
1:O:421:GLN:OE1	1:O:566:SER:OG	2.25	0.48
1:P:524:PRO:HG2	1:P:576:LYS:HD2	1.94	0.48
1:A:406:ASP:OD1	1:A:407:PHE:N	2.44	0.48
1:E:341:TYR:HA	1:E:593:TYR:HE2	1.78	0.48
1:G:35:LYS:HE3	1:G:42:VAL:HG23	1.95	0.48
1:G:403:LEU:HD12	1:G:410:PRO:HG2	1.94	0.48
1:H:500:PRO:HA	1:H:509:VAL:O	2.12	0.48
1:M:596:PRO:HG2	1:N:315:LYS:HE3	1.96	0.48
1:P:182:LEU:HD11	1:P:333:THR:HG21	1.96	0.48
1:J:424:GLU:HG2	1:J:454:LYS:HG3	1.96	0.48
1:M:563:ALA:HB2	1:M:573:TYR:CD2	2.48	0.48
1:O:311:HIS:O	1:O:315:LYS:NZ	2.47	0.48
1:B:233:GLN:HA	1:B:258:SER:O	2.14	0.48
1:B:417:HIS:HA	1:B:460:TYR:CD2	2.49	0.48
1:E:563:ALA:HB2	1:E:573:TYR:CD2	2.49	0.48
1:L:536:PRO:HA	1:L:550:SER:HA	1.96	0.48
1:M:333:THR:O	1:M:336:THR:HG22	2.13	0.48
1:B:590:LEU:HB2	1:B:591:PRO:CD	2.43	0.47
1:G:480:PHE:HB3	1:G:486:ASN:HB2	1.96	0.47
1:M:269:ASN:HB2	1:N:100:VAL:HB	1.96	0.47
1:M:484:THR:O	1:M:492:GLN:NE2	2.46	0.47
1:M:500:PRO:HD2	1:M:500:PRO:O	2.13	0.47
1:O:199:LEU:HD13	1:O:591:PRO:HD2	1.96	0.47
1:A:255:ASP:N	1:B:114:SER:O	2.37	0.47
1:B:418:LEU:HD12	1:B:461:TRP:CD1	2.49	0.47
1:C:192:TYR:CE1	1:C:596:PRO:HG3	2.50	0.47
1:I:417:HIS:HA	1:I:460:TYR:CD2	2.49	0.47
1:K:172:THR:O	1:K:176:MET:HG3	2.13	0.47
1:O:403:LEU:HD11	1:O:474:LEU:HG	1.95	0.47
1:O:403:LEU:HD21	1:O:474:LEU:HD21	1.96	0.47
1:E:484:THR:O	1:E:492:GLN:NE2	2.47	0.47
1:J:66:THR:OG1	1:J:83:GLU:OE2	2.22	0.47
1:O:35:LYS:HE3	1:O:42:VAL:HG23	1.95	0.47
1:C:396:ASN:N	1:C:396:ASN:OD1	2.46	0.47
1:D:486:ASN:O	1:D:490:ASN:N	2.47	0.47
1:D:559:SER:HB3	1:D:577:ALA:HB2	1.96	0.47
1:E:559:SER:HB3	1:E:577:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:589:ARG:NH2	1:J:592:PRO:O	2.47	0.47
1:M:75:ASP:OD2	1:M:157:TYR:OH	2.28	0.47
1:O:137:LYS:HE2	1:O:139:LEU:HD11	1.96	0.47
1:P:421:GLN:OE1	1:P:566:SER:OG	2.26	0.47
1:A:589:ARG:O	1:A:590:LEU:HD23	2.15	0.47
1:C:172:THR:O	1:C:176:MET:HG3	2.14	0.47
1:F:535:ASN:HD22	1:F:555:PRO:HD3	1.80	0.47
1:J:562:LEU:HD22	1:K:499:ILE:HD11	1.96	0.47
1:N:138:THR:HB	1:N:229:ASN:HB3	1.96	0.47
1:N:534:GLY:HA3	1:N:550:SER:C	2.35	0.47
1:O:484:THR:OG1	1:O:485:ILE:N	2.47	0.47
1:P:500:PRO:HA	1:P:509:VAL:O	2.15	0.47
1:A:122:PHE:N	1:P:247:ILE:O	2.38	0.47
1:L:162:THR:HG22	1:L:164:THR:H	1.80	0.47
1:N:590:LEU:HB2	1:N:591:PRO:CD	2.44	0.47
1:O:218:GLU:OE1	1:O:274:ARG:NH2	2.39	0.47
1:O:517:LEU:HD23	1:O:520:LYS:NZ	2.29	0.47
1:B:130:SER:HB2	1:B:237:THR:OG1	2.15	0.47
1:D:162:THR:HG22	1:D:164:THR:H	1.80	0.47
1:E:75:ASP:OD1	1:E:75:ASP:N	2.46	0.47
1:E:186:GLN:NE2	1:E:599:MET:HA	2.30	0.47
3:E:702:MA4:O6	3:E:702:MA4:O60	2.27	0.47
1:F:565:ILE:HD13	1:F:570:GLN:HA	1.96	0.47
1:G:47:PRO:O	1:G:61:ARG:NH1	2.46	0.47
1:I:265:ASP:HB2	1:J:104:TRP:HB3	1.97	0.47
1:J:78:TYR:OH	1:J:297:THR:O	2.17	0.47
1:J:255:ASP:OD1	1:J:256:TYR:N	2.46	0.47
1:K:559:SER:HB3	1:K:577:ALA:HB2	1.95	0.47
1:L:35:LYS:HE3	1:L:42:VAL:HG23	1.97	0.47
1:P:314:ILE:O	1:P:315:LYS:HD3	2.14	0.47
1:P:590:LEU:HB2	1:P:591:PRO:CD	2.44	0.47
1:B:138:THR:HB	1:B:229:ASN:HB3	1.97	0.47
1:B:406:ASP:OD1	1:B:407:PHE:N	2.44	0.47
1:L:233:GLN:HG3	1:L:259:GLN:HG2	1.97	0.47
1:L:563:ALA:HB2	1:L:573:TYR:HD2	1.80	0.47
1:M:529:PHE:HB2	1:M:534:GLY:HA2	1.97	0.47
1:O:75:ASP:OD1	1:O:75:ASP:N	2.48	0.47
1:O:590:LEU:HB2	1:O:591:PRO:HD3	1.96	0.47
1:C:383:GLN:HA	1:C:459:ALA:HA	1.97	0.47
1:E:94:LEU:HD13	1:E:152:VAL:HG22	1.97	0.47
1:H:487:PRO:HB2	1:H:580:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:428:SER:N	3:I:702:MA4:O60	2.48	0.47
1:I:517:LEU:HD23	1:I:520:LYS:NZ	2.30	0.47
1:J:418:LEU:HD12	1:J:461:TRP:CD1	2.49	0.47
1:P:255:ASP:OD1	1:P:256:TYR:N	2.47	0.47
1:P:393:LEU:HD21	1:P:425:GLU:HB3	1.97	0.47
1:K:255:ASP:OD1	1:K:256:TYR:N	2.48	0.47
1:L:475:LEU:HD12	1:L:518:GLY:HA3	1.96	0.47
1:B:333:THR:O	1:B:336:THR:HG22	2.15	0.46
1:C:427:TYR:HA	3:C:702:MA4:H501	1.97	0.46
1:D:265:ASP:HB2	1:E:104:TRP:HB3	1.97	0.46
1:O:47:PRO:O	1:O:61:ARG:NH1	2.45	0.46
1:A:315:LYS:HE3	1:P:596:PRO:CG	2.45	0.46
1:G:403:LEU:HD21	1:G:474:LEU:HD21	1.97	0.46
1:G:481:THR:OG1	1:G:484:THR:HG22	2.14	0.46
1:G:516:GLU:O	1:G:520:LYS:HG2	2.15	0.46
1:L:345:ASN:OD1	1:L:593:TYR:OH	2.33	0.46
1:M:341:TYR:HA	1:M:593:TYR:CE2	2.50	0.46
1:H:289:LEU:HD23	1:H:289:LEU:HA	1.77	0.46
1:O:169:LEU:O	1:O:172:THR:OG1	2.31	0.46
1:O:516:GLU:HB2	1:O:520:LYS:HZ1	1.80	0.46
1:P:35:LYS:HE3	1:P:42:VAL:HG23	1.97	0.46
1:B:61:ARG:HD3	1:B:65:LEU:HG	1.97	0.46
1:B:596:PRO:HG2	1:C:315:LYS:HE3	1.97	0.46
1:C:565:ILE:HD13	1:C:570:GLN:HA	1.97	0.46
1:F:333:THR:O	1:F:336:THR:HG22	2.16	0.46
1:H:149:ARG:NH1	1:H:218:GLU:OE2	2.47	0.46
1:J:333:THR:O	1:J:336:THR:HG22	2.15	0.46
1:J:531:CYS:HB3	1:J:570:GLN:H	1.80	0.46
1:K:485:ILE:HD12	1:K:492:GLN:HG3	1.97	0.46
1:N:417:HIS:HA	1:N:460:TYR:CD2	2.50	0.46
1:P:487:PRO:HB2	1:P:580:PHE:CE1	2.50	0.46
1:A:486:ASN:O	1:A:490:ASN:N	2.45	0.46
1:D:341:TYR:CE1	1:D:591:PRO:HD3	2.51	0.46
1:E:589:ARG:HD2	1:E:589:ARG:HA	1.60	0.46
3:E:702:MA4:H602	3:E:702:MA4:O10	2.14	0.46
1:F:403:LEU:HD12	1:F:410:PRO:HG2	1.96	0.46
1:K:50:GLY:N	1:K:60:GLY:O	2.31	0.46
1:K:559:SER:N	1:K:575:VAL:O	2.27	0.46
1:L:113:LEU:O	1:L:132:GLU:HA	2.15	0.46
1:L:333:THR:O	1:L:336:THR:HG22	2.15	0.46
1:N:333:THR:O	1:N:336:THR:HG22	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:413:TYR:HB3	1:N:462:CYS:HB3	1.97	0.46
1:A:253:GLU:HG3	1:B:116:ASN:HB2	1.98	0.46
1:G:517:LEU:HD23	1:G:520:LYS:HZ2	1.81	0.46
1:K:523:VAL:HG23	1:K:579:ILE:HD12	1.96	0.46
1:M:264:LYS:HE3	1:N:105:MET:HE2	1.97	0.46
1:N:516:GLU:O	1:N:520:LYS:HG2	2.15	0.46
1:D:475:LEU:HD12	1:D:518:GLY:HA3	1.97	0.46
1:D:536:PRO:HA	1:D:550:SER:HA	1.97	0.46
1:F:387:GLU:HG2	1:F:394:CYS:SG	2.56	0.46
1:F:534:GLY:HA3	1:F:550:SER:C	2.36	0.46
1:H:498:TYR:CE2	1:H:512:SER:HB2	2.51	0.46
1:H:538:VAL:HG11	1:H:551:LEU:HB2	1.98	0.46
1:L:376:PHE:HB2	1:L:525:PHE:O	2.15	0.46
1:M:131:THR:HG23	1:M:236:VAL:HG22	1.98	0.46
1:O:104:TRP:HD1	1:O:105:MET:N	2.14	0.46
1:D:35:LYS:HE3	1:D:42:VAL:HG23	1.97	0.46
1:D:188:LYS:HB3	1:D:597:PRO:HB2	1.98	0.46
1:E:138:THR:HB	1:E:229:ASN:HB3	1.97	0.46
1:E:570:GLN:NE2	1:E:572:SER:OG	2.48	0.46
1:F:341:TYR:HE1	1:F:590:LEU:HB3	1.80	0.46
1:J:406:ASP:OD1	1:J:407:PHE:N	2.44	0.46
1:K:383:GLN:HA	1:K:459:ALA:HA	1.97	0.46
1:L:120:ALA:HA	1:L:125:VAL:O	2.16	0.46
1:O:383:GLN:HA	1:O:459:ALA:HA	1.97	0.46
1:P:289:LEU:HD23	1:P:289:LEU:HA	1.77	0.46
1:P:538:VAL:HG11	1:P:551:LEU:HB2	1.98	0.46
1:D:131:THR:HG22	1:D:236:VAL:HG22	1.96	0.46
1:D:333:THR:O	1:D:336:THR:HG22	2.16	0.46
1:H:104:TRP:HD1	1:H:105:MET:N	2.14	0.46
1:H:393:LEU:HD21	1:H:425:GLU:HB3	1.97	0.46
1:M:503:LEU:HD23	1:M:507:LEU:HD23	1.97	0.46
1:N:570:GLN:NE2	1:N:572:SER:OG	2.48	0.46
1:P:498:TYR:CE2	1:P:512:SER:HB2	2.51	0.46
1:A:182:LEU:HD11	1:A:333:THR:HG21	1.98	0.46
1:A:538:VAL:HG11	1:A:551:LEU:HB2	1.98	0.46
1:E:421:GLN:OE1	1:E:566:SER:OG	2.22	0.46
1:E:486:ASN:HB3	1:E:491:ALA:O	2.16	0.46
1:E:535:ASN:HD22	1:E:555:PRO:HD3	1.80	0.46
1:F:389:SER:OG	1:F:453:ALA:HA	2.16	0.46
1:G:403:LEU:HD11	1:G:474:LEU:HG	1.96	0.46
1:G:517:LEU:HD23	1:G:520:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:383:GLN:HE21	1:K:457:PHE:HB2	1.80	0.46
1:K:427:TYR:HA	3:K:702:MA4:H501	1.99	0.46
1:B:504:PHE:HB2	1:B:507:LEU:HB3	1.97	0.45
1:C:265:ASP:N	1:D:104:TRP:O	2.45	0.45
1:D:255:ASP:OD1	1:D:256:TYR:N	2.48	0.45
1:F:377:THR:HB	1:F:464:ALA:HB2	1.98	0.45
1:M:228:ASP:OD1	1:M:229:ASN:N	2.49	0.45
1:B:531:CYS:HB3	1:B:570:GLN:H	1.81	0.45
1:F:104:TRP:HD1	1:F:105:MET:N	2.15	0.45
1:F:417:HIS:HA	1:F:460:TYR:HD2	1.81	0.45
1:F:418:LEU:HD12	1:F:461:TRP:CD1	2.51	0.45
1:I:57:VAL:HG22	1:J:160:LYS:HZ1	1.82	0.45
1:J:138:THR:HB	1:J:229:ASN:HB3	1.97	0.45
1:M:385:CYS:SG	1:M:397:LEU:HD22	2.56	0.45
1:N:47:PRO:O	1:N:61:ARG:NH1	2.50	0.45
1:N:590:LEU:HB2	1:N:591:PRO:HD3	1.99	0.45
1:A:100:VAL:HB	1:P:269:ASN:HB2	1.98	0.45
1:I:538:VAL:HG11	1:I:551:LEU:HB2	1.98	0.45
1:L:188:LYS:HB3	1:L:597:PRO:HG2	1.98	0.45
1:L:434:LYS:HD3	1:L:444:THR:HG22	1.98	0.45
1:M:535:ASN:HD22	1:M:555:PRO:HD3	1.82	0.45
1:A:44:GLU:HB2	1:B:88:PRO:HG2	1.99	0.45
1:A:251:LYS:NZ	1:A:253:GLU:HG2	2.31	0.45
1:E:529:PHE:HB2	1:E:534:GLY:HA2	1.98	0.45
1:H:253:GLU:HG3	1:I:116:ASN:HB2	1.98	0.45
1:I:182:LEU:HD11	1:I:333:THR:HG21	1.98	0.45
1:P:104:TRP:HD1	1:P:105:MET:N	2.15	0.45
1:A:517:LEU:HD23	1:A:520:LYS:NZ	2.31	0.45
1:C:489:THR:HG23	1:C:491:ALA:H	1.82	0.45
1:D:378:PHE:CE2	1:D:461:TRP:HE3	2.34	0.45
1:E:385:CYS:SG	1:E:397:LEU:HD22	2.57	0.45
3:F:702:MA4:H612	3:F:702:MA4:H312	1.61	0.45
1:G:209:VAL:HG12	1:G:305:ARG:HB3	1.99	0.45
1:K:565:ILE:HD13	1:K:570:GLN:HA	1.97	0.45
1:L:378:PHE:CE2	1:L:461:TRP:HE3	2.34	0.45
1:O:203:THR:O	1:O:310:LEU:HB2	2.16	0.45
1:B:167:LEU:HD12	1:B:319:LEU:HD21	1.97	0.45
1:H:475:LEU:HD12	1:H:518:GLY:HA3	1.99	0.45
1:I:403:LEU:HD12	1:I:410:PRO:HG2	1.99	0.45
1:O:588:VAL:HG12	1:O:588:VAL:O	2.17	0.45
1:C:78:TYR:OH	1:C:297:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:399:GLN:H	1:G:407:PHE:HE1	1.65	0.45
1:G:474:LEU:HD13	1:G:511:VAL:HG11	1.99	0.45
1:I:599:MET:SD	1:I:599:MET:N	2.89	0.45
1:N:530:SER:H	1:N:533:MET:HB3	1.82	0.45
1:B:562:LEU:HD22	1:C:499:ILE:HD11	1.97	0.45
1:E:211:ALA:HB1	1:E:300:LEU:HD13	1.99	0.45
1:G:75:ASP:OD1	1:G:75:ASP:N	2.49	0.45
1:G:104:TRP:HD1	1:G:105:MET:N	2.15	0.45
1:H:188:LYS:HB3	1:H:597:PRO:CB	2.47	0.45
1:M:94:LEU:HD13	1:M:152:VAL:HG22	1.99	0.45
1:M:589:ARG:HD2	1:M:589:ARG:HA	1.59	0.45
1:C:590:LEU:CB	1:C:591:PRO:HD3	2.46	0.45
1:I:94:LEU:C	1:I:95:GLU:OE1	2.55	0.45
1:I:304:ASP:OD1	1:I:305:ARG:N	2.50	0.45
1:J:486:ASN:HB3	1:J:491:ALA:O	2.17	0.45
1:O:516:GLU:O	1:O:520:LYS:HG2	2.16	0.45
1:P:475:LEU:HD12	1:P:518:GLY:HA3	1.98	0.45
1:A:167:LEU:HD12	1:A:319:LEU:HD21	1.99	0.45
1:B:199:LEU:HB2	1:B:591:PRO:HG2	1.98	0.45
1:G:449:VAL:HG11	1:G:451:ARG:HE	1.82	0.45
1:K:485:ILE:HD11	1:K:491:ALA:HA	1.99	0.45
1:M:559:SER:HB3	1:M:577:ALA:HB2	1.97	0.45
1:N:387:GLU:HG2	1:N:394:CYS:SG	2.57	0.45
1:P:565:ILE:HD13	1:P:570:GLN:HA	1.99	0.45
1:A:403:LEU:HD12	1:A:410:PRO:HG2	1.98	0.44
1:G:470:ASP:HA	1:G:471:ASN:HA	1.68	0.44
1:H:596:PRO:CG	1:I:315:LYS:HE3	2.47	0.44
1:K:188:LYS:HB3	1:K:597:PRO:HB2	1.98	0.44
1:N:172:THR:O	1:N:176:MET:HG2	2.17	0.44
1:P:406:ASP:OD1	1:P:407:PHE:N	2.49	0.44
1:A:131:THR:HA	1:A:235:THR:O	2.16	0.44
1:D:588:VAL:HB	1:D:590:LEU:HD23	1.99	0.44
1:E:488:MET:HE1	1:E:489:THR:HB	1.99	0.44
1:H:169:LEU:O	1:H:172:THR:OG1	2.31	0.44
1:J:592:PRO:HB2	1:J:594:THR:O	2.17	0.44
1:L:434:LYS:HD2	1:L:434:LYS:HA	1.73	0.44
1:P:480:PHE:HB3	1:P:486:ASN:HB2	1.98	0.44
1:B:383:GLN:HA	1:B:459:ALA:HA	1.98	0.44
1:B:391:ASP:OD1	1:B:391:ASP:N	2.50	0.44
1:F:381:VAL:HG12	1:F:461:TRP:HA	1.99	0.44
1:L:265:ASP:HB2	1:M:104:TRP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:417:HIS:HA	1:O:460:TYR:CD2	2.52	0.44
1:P:203:THR:O	1:P:310:LEU:HB2	2.16	0.44
1:B:486:ASN:HB3	1:B:491:ALA:O	2.18	0.44
1:G:218:GLU:OE1	1:G:274:ARG:NH2	2.38	0.44
1:H:299:HIS:HB3	1:I:90:LYS:HD2	1.99	0.44
1:I:205:VAL:HB	1:I:313:PHE:CE2	2.53	0.44
1:J:167:LEU:HD12	1:J:319:LEU:HD21	1.99	0.44
1:K:333:THR:O	1:K:336:THR:HG22	2.17	0.44
1:M:486:ASN:HB3	1:M:491:ALA:O	2.17	0.44
1:N:381:VAL:HG12	1:N:461:TRP:HA	1.99	0.44
1:B:55:ARG:HE	1:B:590:LEU:HD11	1.82	0.44
1:E:130:SER:HB2	1:E:237:THR:OG1	2.17	0.44
1:E:376:PHE:CE1	1:E:537:LEU:HD13	2.53	0.44
1:I:289:LEU:HA	1:I:289:LEU:HD23	1.71	0.44
1:J:581:THR:OG1	1:J:582:GLY:N	2.50	0.44
1:O:182:LEU:HD11	1:O:333:THR:HG21	1.97	0.44
1:B:66:THR:OG1	1:B:83:GLU:OE2	2.24	0.44
1:F:269:ASN:HB2	1:G:100:VAL:HB	1.99	0.44
1:H:269:ASN:HB2	1:I:100:VAL:HB	2.00	0.44
1:J:205:VAL:HB	1:J:313:PHE:CE2	2.53	0.44
1:L:520:LYS:HG3	1:L:521:PHE:CD2	2.52	0.44
1:L:581:THR:OG1	1:L:582:GLY:N	2.51	0.44
1:A:162:THR:HG22	1:A:164:THR:H	1.83	0.44
1:A:421:GLN:OE1	1:A:566:SER:OG	2.30	0.44
1:C:255:ASP:OD1	1:C:256:TYR:N	2.49	0.44
1:C:535:ASN:HD22	1:C:555:PRO:HD3	1.82	0.44
1:E:324:GLY:N	1:E:325:PRO:HD2	2.33	0.44
1:F:78:TYR:OH	1:F:297:THR:O	2.23	0.44
1:G:417:HIS:HA	1:G:460:TYR:CD2	2.52	0.44
1:G:581:THR:OG1	1:G:582:GLY:N	2.50	0.44
1:H:333:THR:O	1:H:336:THR:HG22	2.18	0.44
1:H:383:GLN:HE21	1:H:457:PHE:HB2	1.82	0.44
1:H:479:VAL:HG12	1:H:509:VAL:HA	1.98	0.44
1:E:585:LEU:HD13	1:F:51:TRP:CD1	2.53	0.44
1:H:480:PHE:HB3	1:H:486:ASN:HB2	1.99	0.44
1:H:565:ILE:HD13	1:H:570:GLN:HA	2.00	0.44
1:J:384:GLU:N	1:J:458:ARG:O	2.49	0.44
1:N:104:TRP:HD1	1:N:105:MET:N	2.15	0.44
1:N:389:SER:OG	1:N:453:ALA:HA	2.18	0.44
1:O:419:LEU:HD23	1:O:504:PHE:HE1	1.81	0.44
1:P:403:LEU:HD21	1:P:474:LEU:HD21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:GLU:N	1:A:95:GLU:OE1	2.51	0.44
1:A:205:VAL:HB	1:A:313:PHE:CE2	2.52	0.44
1:A:249:ASN:HB3	1:B:120:ALA:HB3	2.00	0.44
1:A:477:GLY:HA3	1:A:498:TYR:CE2	2.53	0.44
1:A:482:ASP:OD1	1:A:482:ASP:N	2.49	0.44
1:B:524:PRO:HG2	1:B:576:LYS:HD2	2.00	0.44
1:C:333:THR:O	1:C:336:THR:HG22	2.18	0.44
1:E:592:PRO:HD3	1:F:312:PHE:HE1	1.83	0.44
1:H:487:PRO:HB2	1:H:580:PHE:HE1	1.83	0.44
1:I:590:LEU:HB2	1:I:591:PRO:HD3	1.99	0.44
1:J:538:VAL:HG21	1:J:551:LEU:H	1.83	0.44
1:K:489:THR:HG23	1:K:491:ALA:H	1.82	0.44
1:K:590:LEU:CB	1:K:591:PRO:HD3	2.48	0.44
1:L:383:GLN:HA	1:L:459:ALA:HA	2.00	0.44
3:M:702:MA4:H602	3:M:702:MA4:O10	2.18	0.44
1:O:449:VAL:HG11	1:O:451:ARG:HE	1.82	0.44
1:A:599:MET:SD	1:A:599:MET:N	2.91	0.43
1:B:474:LEU:HD13	1:B:511:VAL:HG11	2.00	0.43
1:D:130:SER:HB2	1:D:237:THR:OG1	2.17	0.43
1:D:247:ILE:O	1:E:122:PHE:N	2.45	0.43
1:I:247:ILE:O	1:J:122:PHE:N	2.42	0.43
1:I:255:ASP:HB3	1:J:114:SER:HB2	1.99	0.43
1:K:449:VAL:HG11	1:K:451:ARG:HE	1.83	0.43
1:L:267:LEU:HB3	1:M:102:GLU:HB3	2.00	0.43
1:M:203:THR:HG21	1:M:342:TYR:HE2	1.83	0.43
1:O:399:GLN:H	1:O:407:PHE:HE1	1.65	0.43
1:D:383:GLN:HA	1:D:459:ALA:HA	2.00	0.43
1:E:503:LEU:HD23	1:E:507:LEU:HD23	2.00	0.43
1:F:195:GLU:HB3	1:F:591:PRO:HB2	1.99	0.43
1:H:138:THR:HB	1:H:229:ASN:HB3	2.00	0.43
1:H:406:ASP:OD1	1:H:407:PHE:N	2.48	0.43
1:J:265:ASP:HB2	1:K:104:TRP:HB3	2.01	0.43
1:J:383:GLN:HA	1:J:459:ALA:HA	1.99	0.43
1:L:596:PRO:HG2	1:M:315:LYS:HE3	2.00	0.43
1:M:186:GLN:HA	1:M:188:LYS:NZ	2.33	0.43
1:O:304:ASP:OD2	1:O:305:ARG:N	2.52	0.43
1:P:417:HIS:HA	1:P:460:TYR:HD2	1.83	0.43
1:C:391:ASP:N	1:C:391:ASP:OD1	2.52	0.43
1:C:562:LEU:HD22	1:D:499:ILE:HD11	2.00	0.43
1:F:105:MET:HE2	1:F:105:MET:HB2	1.86	0.43
1:F:517:LEU:HA	1:F:520:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:563:ALA:HB2	1:I:573:TYR:CD1	2.53	0.43
1:K:599:MET:SD	1:K:599:MET:N	2.92	0.43
1:N:427:TYR:OH	1:N:429:ARG:NH2	2.51	0.43
1:A:116:ASN:HB2	1:P:253:GLU:HG3	2.00	0.43
1:D:376:PHE:HB2	1:D:525:PHE:O	2.18	0.43
1:E:341:TYR:HA	1:E:593:TYR:CE2	2.53	0.43
1:E:387:GLU:HG2	1:E:394:CYS:SG	2.59	0.43
1:F:383:GLN:HA	1:F:459:ALA:HA	2.00	0.43
1:H:417:HIS:HA	1:H:460:TYR:HD2	1.83	0.43
1:J:477:GLY:HA3	1:J:498:TYR:CE2	2.54	0.43
1:K:94:LEU:HD13	1:K:152:VAL:HG22	1.99	0.43
1:K:192:TYR:CZ	1:K:596:PRO:HG3	2.54	0.43
1:M:58:ASP:HB2	1:N:87:ILE:HG12	2.00	0.43
1:N:255:ASP:OD1	1:N:256:TYR:N	2.52	0.43
1:P:333:THR:O	1:P:336:THR:HG22	2.17	0.43
1:B:324:GLY:N	1:B:325:PRO:HD2	2.33	0.43
1:D:520:LYS:HG3	1:D:521:PHE:CD2	2.53	0.43
1:D:559:SER:N	1:D:575:VAL:O	2.42	0.43
1:E:219:ASP:OD2	1:E:219:ASP:N	2.51	0.43
1:I:162:THR:HG22	1:I:164:THR:H	1.84	0.43
1:K:192:TYR:CE1	1:K:596:PRO:HG3	2.52	0.43
1:L:75:ASP:OD1	1:L:75:ASP:N	2.49	0.43
1:P:590:LEU:CB	1:P:591:PRO:HD3	2.47	0.43
1:A:469:PRO:O	1:A:472:SER:OG	2.27	0.43
1:B:265:ASP:HB2	1:C:104:TRP:HB3	1.99	0.43
1:B:475:LEU:HD12	1:B:518:GLY:HA3	2.00	0.43
1:E:524:PRO:HG2	1:E:576:LYS:HD2	2.01	0.43
1:J:330:LEU:HD12	1:J:330:LEU:HA	1.84	0.43
1:J:341:TYR:CE1	1:J:591:PRO:HD3	2.53	0.43
1:L:324:GLY:N	1:L:325:PRO:HD2	2.33	0.43
1:M:536:PRO:HA	1:M:550:SER:HA	2.00	0.43
1:N:94:LEU:HD13	1:N:152:VAL:HG22	1.99	0.43
1:N:403:LEU:HD12	1:N:410:PRO:HG2	2.01	0.43
1:P:589:ARG:O	1:P:590:LEU:HD13	2.17	0.43
1:A:192:TYR:CZ	1:A:596:PRO:HG3	2.54	0.43
1:E:167:LEU:HD12	1:E:319:LEU:HD21	2.01	0.43
1:G:269:ASN:HB2	1:H:100:VAL:HB	2.00	0.43
1:H:597:PRO:O	1:H:599:MET:HE1	2.18	0.43
1:I:255:ASP:OD1	1:I:256:TYR:N	2.52	0.43
1:I:482:ASP:OD1	1:I:482:ASP:N	2.49	0.43
1:J:391:ASP:OD1	1:J:391:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:105:MET:HE2	1:M:105:MET:HB2	1.83	0.43
1:M:376:PHE:CE1	1:M:537:LEU:HD13	2.53	0.43
1:M:470:ASP:HA	1:M:471:ASN:HA	1.70	0.43
1:N:269:ASN:HB2	1:O:100:VAL:HB	2.01	0.43
1:O:52:ASP:OD2	1:O:55:ARG:HG3	2.19	0.43
1:O:324:GLY:N	1:O:325:PRO:HD2	2.34	0.43
1:G:333:THR:O	1:G:336:THR:HG22	2.19	0.43
1:H:403:LEU:HB2	1:H:410:PRO:HG3	2.01	0.43
1:I:474:LEU:HD13	1:I:511:VAL:HG11	2.00	0.43
1:M:387:GLU:HG2	1:M:394:CYS:SG	2.58	0.43
1:A:265:ASP:HB2	1:B:104:TRP:HB3	2.00	0.43
1:D:275:VAL:HG11	1:D:283:PHE:CD1	2.54	0.43
1:G:324:GLY:N	1:G:325:PRO:HD2	2.34	0.43
1:J:524:PRO:HG2	1:J:576:LYS:HD2	2.01	0.43
1:L:94:LEU:HD13	1:L:152:VAL:HG22	2.01	0.43
1:O:333:THR:O	1:O:336:THR:HG22	2.18	0.43
1:A:58:ASP:O	1:B:160:LYS:HE3	2.19	0.43
1:A:489:THR:HG23	1:A:491:ALA:H	1.83	0.43
1:C:427:TYR:HE1	1:C:453:ALA:HB2	1.84	0.43
1:C:531:CYS:SG	1:C:532:ILE:HG23	2.59	0.43
1:C:563:ALA:HB2	1:C:573:TYR:HD2	1.83	0.43
1:H:590:LEU:CB	1:H:591:PRO:HD3	2.49	0.43
1:I:251:LYS:NZ	1:I:253:GLU:HG2	2.34	0.43
1:K:391:ASP:OD1	1:K:391:ASP:N	2.51	0.43
1:L:384:GLU:N	1:L:458:ARG:O	2.51	0.43
1:L:479:VAL:HG12	1:L:509:VAL:HG22	2.01	0.43
1:M:423:HIS:ND1	1:M:505:GLU:OE2	2.52	0.43
1:N:344:PHE:HD2	1:N:593:TYR:HH	1.66	0.43
1:O:406:ASP:OD1	1:O:407:PHE:N	2.51	0.43
1:P:383:GLN:HE21	1:P:457:PHE:HB2	1.84	0.43
1:P:470:ASP:HA	1:P:471:ASN:HA	1.73	0.43
1:G:409:CYS:HB2	1:G:415:PRO:HG3	2.00	0.42
1:M:427:TYR:HE1	1:M:453:ALA:HB2	1.84	0.42
1:N:418:LEU:HB3	1:N:459:ALA:O	2.19	0.42
1:N:590:LEU:CB	1:N:591:PRO:HD3	2.48	0.42
1:P:391:ASP:OD1	1:P:391:ASP:N	2.52	0.42
1:C:474:LEU:HD13	1:C:511:VAL:HG11	2.01	0.42
1:D:167:LEU:HD12	1:D:319:LEU:HD21	2.02	0.42
1:D:324:GLY:N	1:D:325:PRO:HD2	2.34	0.42
1:D:333:THR:HA	1:D:336:THR:HG22	2.01	0.42
1:E:427:TYR:HE1	1:E:453:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:228:ASP:OD1	1:G:229:ASN:N	2.51	0.42
1:M:324:GLY:N	1:M:325:PRO:HD2	2.33	0.42
1:M:345:ASN:OD1	1:M:345:ASN:N	2.52	0.42
1:B:150:VAL:HG11	1:B:289:LEU:HD11	2.01	0.42
1:B:427:TYR:HA	3:B:702:MA4:H501	2.00	0.42
1:F:47:PRO:O	1:F:61:ARG:NH1	2.52	0.42
1:G:381:VAL:HG23	1:G:501:LEU:HD22	2.01	0.42
1:H:391:ASP:N	1:H:391:ASP:OD1	2.52	0.42
1:H:430:LEU:HD12	3:H:702:MA4:H322	2.02	0.42
1:H:589:ARG:O	1:H:590:LEU:HD13	2.19	0.42
1:I:489:THR:HG23	1:I:491:ALA:H	1.85	0.42
1:I:560:GLN:NE2	1:J:513:LEU:HD11	2.34	0.42
1:M:89:GLN:O	1:M:91:GLU:N	2.53	0.42
1:N:409:CYS:HB2	1:N:415:PRO:HG3	2.02	0.42
1:D:205:VAL:HB	1:D:313:PHE:CE2	2.55	0.42
1:F:340:HIS:HE1	1:F:593:TYR:HD1	1.65	0.42
1:G:54:LEU:HD23	1:G:341:TYR:HE2	1.84	0.42
1:L:275:VAL:HG11	1:L:283:PHE:CD1	2.54	0.42
1:M:289:LEU:HD23	1:M:289:LEU:HA	1.83	0.42
1:A:199:LEU:HB2	1:A:591:PRO:HG2	2.00	0.42
1:B:249:ASN:HB3	1:C:120:ALA:HB3	2.00	0.42
1:C:131:THR:HA	1:C:235:THR:O	2.19	0.42
1:E:255:ASP:HB3	1:F:114:SER:HB2	2.02	0.42
1:G:54:LEU:HD13	1:G:54:LEU:HA	1.90	0.42
1:H:403:LEU:HD21	1:H:474:LEU:HD21	2.01	0.42
1:L:105:MET:HE1	3:L:702:MA4:H322	2.01	0.42
1:P:384:GLU:OE1	1:P:458:ARG:NH2	2.40	0.42
1:P:535:ASN:HD22	1:P:555:PRO:HD3	1.84	0.42
1:C:485:ILE:HD11	1:C:491:ALA:HA	2.00	0.42
1:D:66:THR:OG1	1:D:83:GLU:OE2	2.24	0.42
1:E:105:MET:HE2	1:E:105:MET:HB2	1.87	0.42
1:G:169:LEU:O	1:G:172:THR:OG1	2.32	0.42
1:G:419:LEU:HD23	1:G:504:PHE:HE1	1.84	0.42
1:K:388:LEU:HD12	1:K:454:LYS:HG2	2.02	0.42
1:L:532:ILE:HG13	1:L:533:MET:HG3	2.01	0.42
1:L:589:ARG:O	1:L:590:LEU:HD13	2.20	0.42
1:N:535:ASN:HD22	1:N:555:PRO:HD3	1.84	0.42
1:O:209:VAL:HG12	1:O:305:ARG:HB3	2.01	0.42
1:C:470:ASP:HA	1:C:471:ASN:HA	1.76	0.42
1:F:55:ARG:NE	1:F:590:LEU:HD21	2.34	0.42
1:F:188:LYS:HB3	1:F:597:PRO:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:535:ASN:HD22	1:H:555:PRO:HD3	1.83	0.42
1:I:192:TYR:CZ	1:I:596:PRO:HG3	2.55	0.42
1:I:418:LEU:HB2	1:I:461:TRP:HD1	1.84	0.42
1:I:477:GLY:HA3	1:I:498:TYR:CE2	2.55	0.42
1:N:87:ILE:HG22	1:N:89:GLN:HG3	2.02	0.42
1:O:269:ASN:HB2	1:P:100:VAL:HB	2.01	0.42
1:P:188:LYS:HB3	1:P:597:PRO:CB	2.47	0.42
1:A:341:TYR:OH	1:A:590:LEU:HD13	2.18	0.42
1:A:428:SER:H	3:A:702:MA4:C60	2.32	0.42
1:F:172:THR:O	1:F:176:MET:HG2	2.20	0.42
1:G:94:LEU:HD13	1:G:152:VAL:HG22	2.01	0.42
1:H:50:GLY:N	1:H:60:GLY:O	2.27	0.42
1:I:529:PHE:HZ	1:I:560:GLN:HG3	1.85	0.42
1:J:289:LEU:HD23	1:J:289:LEU:HA	1.75	0.42
1:K:406:ASP:OD1	1:K:407:PHE:N	2.47	0.42
1:K:563:ALA:HB2	1:K:573:TYR:HD1	1.84	0.42
1:M:167:LEU:HD12	1:M:319:LEU:HD21	2.01	0.42
1:P:430:LEU:HD12	3:P:702:MA4:H322	2.02	0.42
1:A:474:LEU:HD13	1:A:511:VAL:HG11	2.01	0.42
1:B:55:ARG:NE	1:B:590:LEU:HD11	2.35	0.42
1:B:581:THR:OG1	1:B:582:GLY:N	2.51	0.42
1:C:267:LEU:HB3	1:D:102:GLU:HB3	2.02	0.42
1:C:384:GLU:N	1:C:458:ARG:O	2.49	0.42
1:C:403:LEU:HD12	1:C:410:PRO:HG2	2.01	0.42
1:E:381:VAL:HG12	1:E:461:TRP:HA	2.01	0.42
1:F:255:ASP:OD1	1:F:256:TYR:N	2.52	0.42
1:G:304:ASP:OD2	1:G:305:ARG:N	2.53	0.42
1:G:398:GLU:HB2	1:G:407:PHE:HZ	1.84	0.42
1:H:324:GLY:N	1:H:325:PRO:HD2	2.35	0.42
1:H:470:ASP:HA	1:H:471:ASN:HA	1.73	0.42
1:I:590:LEU:CB	1:I:591:PRO:HD3	2.50	0.42
1:L:588:VAL:O	1:L:588:VAL:HG23	2.20	0.42
1:N:171:PHE:CE1	1:N:197:LEU:HD11	2.55	0.42
3:N:702:MA4:O10	3:N:702:MA4:H602	2.20	0.42
1:O:142:LYS:HB3	1:O:225:PHE:HB3	2.02	0.42
1:A:104:TRP:HD1	1:A:105:MET:N	2.18	0.42
1:B:162:THR:HG22	1:B:164:THR:H	1.85	0.42
1:D:117:THR:HB	1:D:129:PHE:HB3	2.02	0.42
1:D:434:LYS:HD2	1:D:434:LYS:HA	1.89	0.42
1:F:563:ALA:HB2	1:F:573:TYR:CD2	2.55	0.42
1:J:55:ARG:NE	1:J:590:LEU:HD11	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:324:GLY:N	1:J:325:PRO:HD2	2.35	0.42
1:J:438:LEU:O	1:J:440:ILE:HG22	2.20	0.42
1:L:427:TYR:HA	3:L:702:MA4:H501	2.01	0.42
1:M:277:SER:O	1:N:91:GLU:HA	2.20	0.42
1:M:406:ASP:OD1	1:M:407:PHE:N	2.53	0.42
1:N:54:LEU:HD13	1:N:54:LEU:HA	1.89	0.42
1:N:324:GLY:N	1:N:325:PRO:HD2	2.35	0.42
1:N:340:HIS:CE1	1:N:593:TYR:HD1	2.37	0.42
1:P:169:LEU:O	1:P:172:THR:OG1	2.32	0.42
1:P:172:THR:O	1:P:176:MET:HG3	2.19	0.42
1:D:228:ASP:OD1	1:D:229:ASN:N	2.52	0.41
1:F:340:HIS:CE1	1:F:593:TYR:HD1	2.38	0.41
1:F:418:LEU:HB3	1:F:459:ALA:O	2.20	0.41
1:H:430:LEU:HD22	1:H:431:GLU:N	2.35	0.41
1:I:333:THR:O	1:I:336:THR:HG22	2.20	0.41
1:M:186:GLN:NE2	1:M:599:MET:HA	2.35	0.41
1:M:517:LEU:HA	1:M:520:LYS:HG2	2.02	0.41
1:N:182:LEU:HD11	1:N:333:THR:HG21	2.02	0.41
1:N:430:LEU:HD22	1:N:431:GLU:N	2.35	0.41
1:O:481:THR:OG1	1:O:484:THR:HG22	2.19	0.41
1:A:534:GLY:HA2	1:A:552:LYS:HG2	2.02	0.41
1:C:449:VAL:HG11	1:C:451:ARG:HE	1.85	0.41
1:F:324:GLY:N	1:F:325:PRO:HD2	2.35	0.41
1:G:138:THR:HB	1:G:229:ASN:HB3	2.02	0.41
1:J:220:HIS:CD2	1:J:222:ARG:HH12	2.37	0.41
1:K:86:THR:HG22	1:K:159:VAL:HG22	2.02	0.41
1:K:535:ASN:HD22	1:K:555:PRO:HD3	1.84	0.41
1:O:199:LEU:HB2	1:O:591:PRO:HG2	2.01	0.41
1:O:384:GLU:N	1:O:458:ARG:O	2.48	0.41
1:O:409:CYS:HB2	1:O:415:PRO:HG3	2.02	0.41
1:O:428:SER:O	3:O:702:MA4:H212	2.20	0.41
1:A:55:ARG:HE	1:A:590:LEU:HD21	1.85	0.41
1:B:589:ARG:O	1:B:590:LEU:HD23	2.20	0.41
1:C:520:LYS:HG3	1:C:521:PHE:CD2	2.55	0.41
1:D:479:VAL:HG12	1:D:509:VAL:HG22	2.02	0.41
1:E:137:LYS:HE2	1:E:139:LEU:HD11	2.02	0.41
1:E:203:THR:HG21	1:E:342:TYR:HE2	1.85	0.41
1:F:54:LEU:HD23	1:F:341:TYR:HE2	1.85	0.41
1:G:251:LYS:HG2	1:H:118:GLU:HB2	2.03	0.41
1:G:265:ASP:HB2	1:H:104:TRP:HB3	2.02	0.41
1:H:130:SER:HB2	1:H:237:THR:OG1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:482:ASP:OD1	1:H:482:ASP:N	2.52	0.41
1:I:95:GLU:OE1	1:I:95:GLU:N	2.53	0.41
1:I:488:MET:HE1	1:I:489:THR:HB	2.02	0.41
1:K:66:THR:OG1	1:K:83:GLU:OE2	2.26	0.41
1:M:381:VAL:HG12	1:M:461:TRP:HA	2.02	0.41
1:N:470:ASP:HA	1:N:471:ASN:HA	1.76	0.41
1:A:172:THR:O	1:A:176:MET:HG2	2.20	0.41
1:C:344:PHE:CD2	1:C:593:TYR:CE2	3.08	0.41
1:C:388:LEU:HD12	1:C:454:LYS:HG2	2.02	0.41
1:C:417:HIS:HA	1:C:460:TYR:HD2	1.84	0.41
1:C:484:THR:O	1:C:492:GLN:NE2	2.53	0.41
1:D:535:ASN:HD21	1:D:537:LEU:HB2	1.86	0.41
1:D:535:ASN:HD22	1:D:555:PRO:HD3	1.86	0.41
1:F:289:LEU:HD23	1:F:289:LEU:HA	1.77	0.41
1:G:199:LEU:HD13	1:G:591:PRO:HD2	2.03	0.41
1:H:403:LEU:HD11	1:H:474:LEU:HG	2.02	0.41
1:J:475:LEU:HD12	1:J:518:GLY:HA3	2.03	0.41
1:B:289:LEU:HA	1:B:289:LEU:HD23	1.75	0.41
1:C:89:GLN:O	1:C:91:GLU:HG3	2.21	0.41
1:C:253:GLU:HG3	1:D:116:ASN:HB2	2.01	0.41
1:D:589:ARG:HD2	1:D:589:ARG:HA	1.74	0.41
1:D:590:LEU:HB3	1:D:591:PRO:CD	2.50	0.41
1:E:386:THR:HG1	1:E:458:ARG:HH12	1.61	0.41
1:G:136:MET:HE3	1:G:136:MET:HB3	1.96	0.41
1:I:54:LEU:HD23	1:I:341:TYR:HE2	1.85	0.41
1:J:482:ASP:N	1:J:482:ASP:OD1	2.53	0.41
1:L:247:ILE:O	1:M:122:PHE:N	2.51	0.41
1:N:209:VAL:HG12	1:N:305:ARG:HB3	2.01	0.41
1:P:137:LYS:HE2	1:P:139:LEU:HD11	2.01	0.41
1:P:479:VAL:HG12	1:P:509:VAL:HA	2.01	0.41
1:P:482:ASP:N	1:P:482:ASP:OD1	2.52	0.41
1:A:90:LYS:HD2	1:P:299:HIS:HB3	2.02	0.41
1:C:62:VAL:HG21	1:C:205:VAL:HG22	2.02	0.41
1:C:324:GLY:N	1:C:325:PRO:HD2	2.35	0.41
1:D:94:LEU:HD13	1:D:152:VAL:HG22	2.00	0.41
1:D:489:THR:HG23	1:D:491:ALA:H	1.85	0.41
1:G:482:ASP:OD1	1:G:482:ASP:N	2.54	0.41
1:I:172:THR:O	1:I:176:MET:HG2	2.21	0.41
1:K:427:TYR:HE1	1:K:453:ALA:HB2	1.84	0.41
1:K:520:LYS:HG3	1:K:521:PHE:CD2	2.56	0.41
1:N:219:ASP:N	1:N:219:ASP:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:507:LEU:HD22	1:O:564:VAL:HB	2.03	0.41
1:B:589:ARG:NH2	1:B:592:PRO:O	2.40	0.41
1:D:477:GLY:HA3	1:D:498:TYR:CE2	2.56	0.41
3:D:702:MA4:H112	3:D:702:MA4:H201	1.88	0.41
1:E:413:TYR:HB3	1:E:462:CYS:HB3	2.03	0.41
1:G:105:MET:HE2	1:G:105:MET:HB2	1.89	0.41
1:G:182:LEU:HD11	1:G:333:THR:HG21	2.02	0.41
1:I:255:ASP:N	1:J:114:SER:O	2.45	0.41
1:J:479:VAL:HG12	1:J:509:VAL:HA	2.03	0.41
1:K:562:LEU:HD22	1:L:499:ILE:HD11	2.03	0.41
1:L:228:ASP:OD1	1:L:229:ASN:N	2.53	0.41
1:L:489:THR:HG23	1:L:491:ALA:H	1.85	0.41
1:M:486:ASN:O	1:M:490:ASN:N	2.54	0.41
1:N:560:GLN:O	1:N:561:HIS:ND1	2.53	0.41
1:A:59:MET:HG3	1:A:200:ASN:O	2.21	0.41
1:A:189:MET:HG2	1:A:597:PRO:HG2	2.03	0.41
1:D:138:THR:HB	1:D:229:ASN:HB3	2.03	0.41
1:E:264:LYS:HE3	1:F:105:MET:HE2	2.02	0.41
1:E:419:LEU:HD23	1:E:504:PHE:HE1	1.86	0.41
1:F:228:ASP:N	1:F:228:ASP:OD1	2.54	0.41
1:G:203:THR:HG21	1:G:342:TYR:HE2	1.86	0.41
1:I:299:HIS:HB3	1:J:90:LYS:HD2	2.02	0.41
1:J:162:THR:HG22	1:J:164:THR:H	1.86	0.41
1:K:182:LEU:HA	1:K:182:LEU:HD23	1.75	0.41
1:L:193:LEU:HD12	1:L:193:LEU:HA	1.94	0.41
1:O:381:VAL:HG23	1:O:501:LEU:HD22	2.03	0.41
1:O:563:ALA:HB2	1:O:573:TYR:HD2	1.84	0.41
1:P:487:PRO:HB2	1:P:580:PHE:HE1	1.86	0.41
1:A:87:ILE:HA	1:A:88:PRO:HD3	1.90	0.41
1:A:475:LEU:HD12	1:A:518:GLY:HA3	2.03	0.41
1:B:87:ILE:HA	1:B:88:PRO:HD3	1.92	0.41
1:B:384:GLU:N	1:B:458:ARG:O	2.53	0.41
1:B:463:VAL:HG21	1:B:537:LEU:HD11	2.03	0.41
1:B:531:CYS:SG	1:B:532:ILE:HG23	2.60	0.41
1:B:596:PRO:CG	1:C:315:LYS:HE3	2.51	0.41
1:C:538:VAL:HG11	1:C:551:LEU:HB2	2.02	0.41
1:D:289:LEU:HA	1:D:289:LEU:HD23	1.77	0.41
1:D:384:GLU:N	1:D:458:ARG:O	2.53	0.41
1:E:486:ASN:O	1:E:490:ASN:N	2.53	0.41
1:F:175:LEU:HD23	1:F:175:LEU:HA	1.91	0.41
1:H:94:LEU:HD13	1:H:152:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:386:THR:OG1	1:H:458:ARG:NH1	2.34	0.41
1:H:418:LEU:HD12	1:H:461:TRP:CD1	2.56	0.41
1:I:345:ASN:N	1:I:345:ASN:OD1	2.54	0.41
1:I:585:LEU:HD13	1:J:51:TRP:CD1	2.56	0.41
1:J:590:LEU:CB	1:J:591:PRO:CD	2.99	0.41
1:K:249:ASN:HB3	1:L:120:ALA:HB3	2.03	0.41
1:K:324:GLY:N	1:K:325:PRO:HD2	2.35	0.41
1:L:66:THR:OG1	1:L:83:GLU:OE2	2.23	0.41
1:M:275:VAL:HG11	1:M:283:PHE:CD1	2.56	0.41
1:N:345:ASN:OD1	1:N:345:ASN:N	2.54	0.41
1:O:162:THR:HG22	1:O:164:THR:H	1.86	0.41
1:O:470:ASP:HA	1:O:471:ASN:HA	1.66	0.41
1:P:121:LEU:HB3	1:P:122:PHE:CD2	2.56	0.41
1:P:403:LEU:HD11	1:P:474:LEU:HG	2.03	0.41
1:P:417:HIS:NE2	1:P:420:SER:OG	2.44	0.41
1:A:54:LEU:HD23	1:A:341:TYR:HE2	1.86	0.41
1:A:427:TYR:CE1	1:A:453:ALA:HB2	2.56	0.41
1:D:203:THR:HG21	1:D:342:TYR:HE1	1.85	0.41
1:F:219:ASP:N	1:F:219:ASP:OD1	2.54	0.41
1:H:219:ASP:N	1:H:219:ASP:OD1	2.54	0.41
1:L:182:LEU:HD11	1:L:333:THR:HG21	2.02	0.41
1:B:247:ILE:O	1:C:122:PHE:N	2.46	0.40
1:C:477:GLY:HA3	1:C:498:TYR:CE2	2.56	0.40
1:E:97:ASN:N	1:E:97:ASN:OD1	2.54	0.40
1:E:345:ASN:OD1	1:E:345:ASN:N	2.54	0.40
1:F:75:ASP:N	1:F:75:ASP:OD1	2.52	0.40
1:F:115:ILE:O	1:F:130:SER:HA	2.21	0.40
1:G:283:PHE:O	1:H:293:GLN:NE2	2.33	0.40
1:H:141:VAL:HG22	1:H:226:LEU:HD13	2.04	0.40
1:I:141:VAL:HG22	1:I:226:LEU:HD13	2.03	0.40
1:K:470:ASP:HB3	1:K:471:ASN:OD1	2.21	0.40
1:L:50:GLY:N	1:L:60:GLY:O	2.32	0.40
1:L:55:ARG:HD3	1:L:590:LEU:HD21	2.03	0.40
1:L:289:LEU:HA	1:L:289:LEU:HD23	1.78	0.40
1:L:470:ASP:HA	1:L:471:ASN:HA	1.77	0.40
1:N:533:MET:HG2	1:N:534:GLY:O	2.22	0.40
1:N:589:ARG:O	1:N:590:LEU:HD13	2.22	0.40
1:O:384:GLU:OE1	1:O:458:ARG:NH2	2.39	0.40
1:O:420:SER:HB3	1:O:458:ARG:HG2	2.03	0.40
1:P:50:GLY:N	1:P:60:GLY:O	2.28	0.40
1:P:222:ARG:HE	1:P:222:ARG:HB3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:VAL:HG12	1:B:509:VAL:HA	2.03	0.40
1:C:517:LEU:HA	1:C:520:LYS:HG2	2.03	0.40
1:D:55:ARG:HD3	1:D:590:LEU:HD21	2.03	0.40
1:G:253:GLU:HG3	1:H:116:ASN:HB2	2.04	0.40
1:H:118:GLU:HG2	1:H:128:LYS:HG2	2.04	0.40
1:H:181:GLN:HE21	1:H:189:MET:CB	2.34	0.40
1:J:150:VAL:HG11	1:J:289:LEU:HD11	2.01	0.40
1:J:474:LEU:HD13	1:J:511:VAL:HG11	2.03	0.40
1:J:486:ASN:ND2	1:J:489:THR:HG22	2.36	0.40
1:M:384:GLU:OE1	1:M:458:ARG:NH2	2.42	0.40
1:M:520:LYS:HG3	1:M:521:PHE:CD2	2.57	0.40
1:A:289:LEU:HD23	1:A:289:LEU:HA	1.71	0.40
1:B:377:THR:HB	1:B:464:ALA:HB2	2.03	0.40
1:C:344:PHE:CD2	1:C:593:TYR:HE2	2.39	0.40
1:C:560:GLN:HG2	1:D:513:LEU:HD11	2.03	0.40
1:E:269:ASN:HB2	1:F:100:VAL:HB	2.02	0.40
1:E:427:TYR:HA	3:E:702:MA4:H501	2.03	0.40
1:G:255:ASP:OD1	1:G:256:TYR:N	2.54	0.40
1:G:289:LEU:HA	1:G:289:LEU:HD23	1.80	0.40
1:H:205:VAL:HB	1:H:313:PHE:CE2	2.56	0.40
1:K:167:LEU:HD12	1:K:319:LEU:HD21	2.03	0.40
1:L:167:LEU:HD12	1:L:319:LEU:HD21	2.04	0.40
1:L:563:ALA:HB2	1:L:573:TYR:CD2	2.55	0.40
1:M:419:LEU:HD23	1:M:504:PHE:HE2	1.86	0.40
1:N:378:PHE:HB2	1:N:525:PHE:HD2	1.86	0.40
1:O:482:ASP:N	1:O:482:ASP:OD1	2.53	0.40
1:P:205:VAL:HB	1:P:313:PHE:CE2	2.56	0.40
1:B:503:LEU:HD13	1:B:503:LEU:O	2.22	0.40
1:B:529:PHE:HZ	1:B:560:GLN:HG3	1.86	0.40
1:D:345:ASN:ND2	1:D:593:TYR:OH	2.52	0.40
1:E:581:THR:OG1	1:E:582:GLY:N	2.55	0.40
1:F:171:PHE:CE1	1:F:197:LEU:HD11	2.56	0.40
1:I:42:VAL:HG22	1:I:79:ILE:HB	2.03	0.40
1:K:484:THR:O	1:K:492:GLN:NE2	2.55	0.40
1:L:255:ASP:OD1	1:L:256:TYR:N	2.54	0.40
1:N:54:LEU:HD23	1:N:341:TYR:HE2	1.87	0.40
1:O:398:GLU:HB2	1:O:407:PHE:HZ	1.86	0.40
1:A:57:VAL:HG13	1:A:59:MET:CE	2.52	0.40
1:A:378:PHE:HB2	1:A:525:PHE:HD2	1.87	0.40
1:A:590:LEU:CB	1:A:591:PRO:CD	3.00	0.40
1:B:538:VAL:HG21	1:B:551:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:LEU:HD23	1:C:182:LEU:HA	1.75	0.40
1:C:470:ASP:HB3	1:C:471:ASN:OD1	2.21	0.40
3:D:702:MA4:H612	3:D:702:MA4:H312	1.90	0.40
1:E:275:VAL:HG11	1:E:283:PHE:CD1	2.56	0.40
1:I:181:GLN:OE1	1:I:189:MET:HB2	2.21	0.40
1:J:529:PHE:HZ	1:J:560:GLN:HG3	1.85	0.40
1:J:559:SER:HB3	1:J:577:ALA:HB2	2.04	0.40
1:M:524:PRO:HG2	1:M:576:LYS:HD2	2.03	0.40
1:N:488:MET:HE3	1:N:489:THR:HB	2.03	0.40
1:N:581:THR:OG1	1:N:582:GLY:N	2.54	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 PDB entries followed by that with respect to all EM entries.

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	527/648 (81%)	508 (96%)	18 (3%)	1 (0%)	47	79
1	B	527/648 (81%)	505 (96%)	21 (4%)	1 (0%)	47	79
1	C	527/648 (81%)	505 (96%)	21 (4%)	1 (0%)	47	79
1	D	527/648 (81%)	512 (97%)	15 (3%)	0	100	100
1	E	527/648 (81%)	504 (96%)	22 (4%)	1 (0%)	47	79
1	F	527/648 (81%)	501 (95%)	25 (5%)	1 (0%)	47	79
1	G	527/648 (81%)	506 (96%)	20 (4%)	1 (0%)	47	79
1	H	527/648 (81%)	502 (95%)	24 (5%)	1 (0%)	47	79
1	I	527/648 (81%)	507 (96%)	19 (4%)	1 (0%)	47	79
1	J	527/648 (81%)	505 (96%)	21 (4%)	1 (0%)	47	79
1	K	527/648 (81%)	502 (95%)	24 (5%)	1 (0%)	47	79
1	L	527/648 (81%)	511 (97%)	15 (3%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	527/648 (81%)	507 (96%)	19 (4%)	1 (0%)	47	79
1	N	527/648 (81%)	505 (96%)	21 (4%)	1 (0%)	47	79
1	O	527/648 (81%)	507 (96%)	19 (4%)	1 (0%)	47	79
1	P	527/648 (81%)	504 (96%)	22 (4%)	1 (0%)	47	79
All	All	8432/10368 (81%)	8091 (96%)	326 (4%)	15 (0%)	50	79

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	590	LEU
1	B	590	LEU
1	C	590	LEU
1	E	590	LEU
1	F	590	LEU
1	G	590	LEU
1	H	590	LEU
1	I	590	LEU
1	J	590	LEU
1	K	590	LEU
1	L	590	LEU
1	M	590	LEU
1	N	590	LEU
1	O	590	LEU
1	P	590	LEU

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 PDB entries followed by that with respect to all EM entries.

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	469/566 (83%)	465 (99%)	4 (1%)	78	88
1	B	469/566 (83%)	460 (98%)	9 (2%)	57	75
1	C	469/566 (83%)	464 (99%)	5 (1%)	73	85
1	D	469/566 (83%)	462 (98%)	7 (2%)	65	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	469/566 (83%)	462 (98%)	7 (2%)	65	80
1	F	469/566 (83%)	461 (98%)	8 (2%)	60	78
1	G	469/566 (83%)	463 (99%)	6 (1%)	69	82
1	H	469/566 (83%)	458 (98%)	11 (2%)	50	70
1	I	469/566 (83%)	464 (99%)	5 (1%)	73	85
1	J	469/566 (83%)	453 (97%)	16 (3%)	37	61
1	K	469/566 (83%)	463 (99%)	6 (1%)	69	82
1	L	469/566 (83%)	460 (98%)	9 (2%)	57	75
1	M	469/566 (83%)	465 (99%)	4 (1%)	78	88
1	N	469/566 (83%)	462 (98%)	7 (2%)	65	80
1	O	469/566 (83%)	464 (99%)	5 (1%)	73	85
1	P	469/566 (83%)	456 (97%)	13 (3%)	43	65
All	All	7504/9056 (83%)	7382 (98%)	122 (2%)	64	79

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	LEU
1	A	251	LYS
1	A	310	LEU
1	A	488	MET
1	B	45	VAL
1	B	61	ARG
1	B	105	MET
1	B	254	THR
1	B	297	THR
1	B	378	PHE
1	B	454	LYS
1	B	520	LYS
1	B	533	MET
1	C	45	VAL
1	C	131	THR
1	C	310	LEU
1	C	378	PHE
1	C	488	MET
1	D	108	GLN
1	D	310	LEU
1	D	378	PHE

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Mol	Chain	Res	Type
1	D	488	MET
1	D	515	TYR
1	D	561	HIS
1	D	589	ARG
1	E	61	ARG
1	E	108	GLN
1	E	219	ASP
1	E	247	ILE
1	E	378	PHE
1	E	423	HIS
1	E	585	LEU
1	F	45	VAL
1	F	105	MET
1	F	189	MET
1	F	219	ASP
1	F	310	LEU
1	F	378	PHE
1	F	521	PHE
1	F	593	TYR
1	G	39	LYS
1	G	45	VAL
1	G	105	MET
1	G	251	LYS
1	G	310	LEU
1	G	488	MET
1	H	45	VAL
1	H	59	MET
1	H	219	ASP
1	H	242	ILE
1	H	247	ILE
1	H	310	LEU
1	H	488	MET
1	H	508	LYS
1	H	533	MET
1	H	561	HIS
1	H	580	PHE
1	I	45	VAL
1	I	196	LEU
1	I	251	LYS
1	I	488	MET
1	I	515	TYR
1	J	45	VAL

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Mol	Chain	Res	Type
1	J	55	ARG
1	J	95	GLU
1	J	105	MET
1	J	189	MET
1	J	196	LEU
1	J	254	THR
1	J	297	THR
1	J	310	LEU
1	J	378	PHE
1	J	520	LYS
1	J	533	MET
1	J	580	PHE
1	J	585	LEU
1	J	589	ARG
1	J	599	MET
1	K	45	VAL
1	K	189	MET
1	K	196	LEU
1	K	310	LEU
1	K	378	PHE
1	K	488	MET
1	L	108	GLN
1	L	310	LEU
1	L	378	PHE
1	L	488	MET
1	L	515	TYR
1	L	533	MET
1	L	561	HIS
1	L	580	PHE
1	L	589	ARG
1	M	105	MET
1	M	310	LEU
1	M	378	PHE
1	M	423	HIS
1	N	45	VAL
1	N	94	LEU
1	N	219	ASP
1	N	247	ILE
1	N	259	GLN
1	N	520	LYS
1	N	521	PHE
1	O	45	VAL

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Mol	Chain	Res	Type
1	O	105	MET
1	O	251	LYS
1	O	488	MET
1	O	561	HIS
1	P	45	VAL
1	P	59	MET
1	P	94	LEU
1	P	131	THR
1	P	196	LEU
1	P	219	ASP
1	P	247	ILE
1	P	259	GLN
1	P	508	LYS
1	P	533	MET
1	P	561	HIS
1	P	580	PHE
1	P	586	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	134	GLN
1	A	234	ASN
1	A	259	GLN
1	A	276	GLN
1	A	340	HIS
1	A	383	GLN
1	A	467	GLN
1	B	32	GLN
1	B	467	GLN
1	C	32	GLN
1	C	181	GLN
1	C	276	GLN
1	C	311	HIS
1	C	467	GLN
1	D	32	GLN
1	D	181	GLN
1	D	276	GLN
1	D	311	HIS
1	D	401	ASN
1	D	467	GLN

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Mol	Chain	Res	Type
1	D	570	GLN
1	E	32	GLN
1	E	234	ASN
1	E	276	GLN
1	E	401	ASN
1	E	467	GLN
1	E	570	GLN
1	F	32	GLN
1	F	234	ASN
1	F	259	GLN
1	F	276	GLN
1	F	311	HIS
1	F	340	HIS
1	F	401	ASN
1	F	467	GLN
1	F	486	ASN
1	F	570	GLN
1	G	32	GLN
1	G	234	ASN
1	G	276	GLN
1	G	340	HIS
1	G	383	GLN
1	G	401	ASN
1	G	467	GLN
1	G	570	GLN
1	H	134	GLN
1	H	181	GLN
1	H	234	ASN
1	H	276	GLN
1	H	311	HIS
1	H	340	HIS
1	H	467	GLN
1	I	234	ASN
1	I	276	GLN
1	I	340	HIS
1	I	383	GLN
1	I	467	GLN
1	J	32	GLN
1	J	89	GLN
1	J	181	GLN
1	J	220	HIS
1	J	467	GLN

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Mol	Chain	Res	Type
1	K	32	GLN
1	K	276	GLN
1	K	311	HIS
1	K	467	GLN
1	K	570	GLN
1	L	32	GLN
1	L	181	GLN
1	L	276	GLN
1	L	311	HIS
1	L	401	ASN
1	L	467	GLN
1	L	570	GLN
1	M	32	GLN
1	M	234	ASN
1	M	276	GLN
1	M	311	HIS
1	M	401	ASN
1	M	467	GLN
1	M	570	GLN
1	N	32	GLN
1	N	234	ASN
1	N	276	GLN
1	N	401	ASN
1	N	467	GLN
1	N	570	GLN
1	O	32	GLN
1	O	234	ASN
1	O	276	GLN
1	O	340	HIS
1	O	383	GLN
1	O	401	ASN
1	O	467	GLN
1	O	570	GLN
1	P	32	GLN
1	P	77	GLN
1	P	234	ASN
1	P	276	GLN
1	P	340	HIS
1	P	467	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

32 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	NAG	L	701	1	14,14,15	0.56	0	17,19,21	0.42	0
2	NAG	F	701	1	14,14,15	0.57	0	17,19,21	0.43	0
3	MA4	B	702	-	37,37,37	0.14	0	50,50,50	0.36	0
2	NAG	O	701	1	14,14,15	0.51	0	17,19,21	0.41	0
3	MA4	H	702	-	37,37,37	0.15	0	50,50,50	0.37	0
3	MA4	M	702	-	37,37,37	0.15	0	50,50,50	0.36	0
3	MA4	L	702	-	37,37,37	0.15	0	50,50,50	0.37	0
3	MA4	K	702	-	37,37,37	0.15	0	50,50,50	0.38	0
2	NAG	N	701	1	14,14,15	0.55	0	17,19,21	0.42	0
2	NAG	D	701	1	14,14,15	0.55	0	17,19,21	0.42	0
2	NAG	P	701	1	14,14,15	0.54	0	17,19,21	0.42	0
3	MA4	P	702	-	37,37,37	0.16	0	50,50,50	0.37	0
2	NAG	J	701	1	14,14,15	0.53	0	17,19,21	0.42	0
2	NAG	G	701	1	14,14,15	0.51	0	17,19,21	0.41	0
2	NAG	C	701	1	14,14,15	0.60	1 (7%)	17,19,21	0.44	0
2	NAG	M	701	1	14,14,15	0.68	1 (7%)	17,19,21	0.44	0
3	MA4	E	702	-	37,37,37	0.15	0	50,50,50	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MA4	G	702	-	37,37,37	0.12	0	50,50,50	0.17	0
3	MA4	D	702	-	37,37,37	0.15	0	50,50,50	0.40	0
3	MA4	O	702	-	37,37,37	0.12	0	50,50,50	0.17	0
3	MA4	F	702	-	37,37,37	0.16	0	50,50,50	0.37	0
3	MA4	A	702	-	37,37,37	0.15	0	50,50,50	0.33	0
2	NAG	I	701	1	14,14,15	0.51	0	17,19,21	0.43	0
2	NAG	A	701	1	14,14,15	0.48	0	17,19,21	0.42	0
2	NAG	K	701	1	14,14,15	0.57	0	17,19,21	0.44	0
3	MA4	I	702	-	37,37,37	0.12	0	50,50,50	0.18	0
3	MA4	N	702	-	37,37,37	0.16	0	50,50,50	0.38	0
3	MA4	J	702	-	37,37,37	0.15	0	50,50,50	0.36	0
2	NAG	H	701	1	14,14,15	0.54	0	17,19,21	0.42	0
2	NAG	B	701	1	14,14,15	0.51	0	17,19,21	0.42	0
3	MA4	C	702	-	37,37,37	0.15	0	50,50,50	0.37	0
2	NAG	E	701	1	14,14,15	0.64	1 (7%)	17,19,21	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	L	701	1	-	1/6/23/26	0/1/1/1
2	NAG	F	701	1	-	2/6/23/26	0/1/1/1
3	MA4	B	702	-	-	8/18/66/66	0/3/3/3
2	NAG	O	701	1	-	2/6/23/26	0/1/1/1
3	MA4	H	702	-	-	12/18/66/66	0/3/3/3
3	MA4	M	702	-	-	9/18/66/66	0/3/3/3
3	MA4	L	702	-	-	12/18/66/66	0/3/3/3
3	MA4	K	702	-	-	10/18/66/66	0/3/3/3
2	NAG	N	701	1	-	1/6/23/26	0/1/1/1
2	NAG	D	701	1	-	1/6/23/26	0/1/1/1
2	NAG	P	701	1	-	2/6/23/26	0/1/1/1
3	MA4	P	702	-	-	10/18/66/66	0/3/3/3
2	NAG	J	701	1	-	2/6/23/26	0/1/1/1
2	NAG	G	701	1	-	1/6/23/26	0/1/1/1
2	NAG	C	701	1	-	2/6/23/26	0/1/1/1
2	NAG	M	701	1	-	1/6/23/26	0/1/1/1
3	MA4	E	702	-	-	9/18/66/66	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MA4	G	702	-	-	8/18/66/66	0/3/3/3
3	MA4	D	702	-	-	11/18/66/66	0/3/3/3
3	MA4	O	702	-	-	8/18/66/66	0/3/3/3
3	MA4	F	702	-	-	10/18/66/66	0/3/3/3
3	MA4	A	702	-	-	12/18/66/66	0/3/3/3
2	NAG	I	701	1	-	2/6/23/26	0/1/1/1
2	NAG	A	701	1	-	2/6/23/26	0/1/1/1
2	NAG	K	701	1	-	2/6/23/26	0/1/1/1
3	MA4	I	702	-	-	7/18/66/66	0/3/3/3
3	MA4	N	702	-	-	11/18/66/66	0/3/3/3
3	MA4	J	702	-	-	8/18/66/66	0/3/3/3
2	NAG	H	701	1	-	1/6/23/26	0/1/1/1
2	NAG	B	701	1	-	2/6/23/26	0/1/1/1
3	MA4	C	702	-	-	10/18/66/66	0/3/3/3
2	NAG	E	701	1	-	1/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	701	NAG	O5-C1	-2.24	1.40	1.43
2	E	701	NAG	O5-C1	-2.17	1.40	1.43
2	C	701	NAG	O5-C1	-2.01	1.40	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (180) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	MA4	C20-C10-O10-C11
3	A	702	MA4	O50-C10-O10-C11
3	B	702	MA4	C20-C10-O10-C11
3	B	702	MA4	O50-C10-O10-C11
3	C	702	MA4	O50-C10-O10-C11
3	C	702	MA4	C21-C11-O10-C10
3	D	702	MA4	C20-C10-O10-C11
3	D	702	MA4	O50-C10-O10-C11
3	E	702	MA4	O50-C10-O10-C11
3	F	702	MA4	O50-C10-O10-C11

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Mol	Chain	Res	Type	Atoms
3	G	702	MA4	O50-C10-O10-C11
3	G	702	MA4	C21-C11-O10-C10
3	H	702	MA4	O50-C10-O10-C11
3	I	702	MA4	O50-C10-O10-C11
3	I	702	MA4	C21-C11-O10-C10
3	J	702	MA4	C20-C10-O10-C11
3	J	702	MA4	O50-C10-O10-C11
3	K	702	MA4	O50-C10-O10-C11
3	K	702	MA4	C21-C11-O10-C10
3	L	702	MA4	O50-C10-O10-C11
3	L	702	MA4	C21-C11-O10-C10
3	M	702	MA4	O50-C10-O10-C11
3	N	702	MA4	C20-C10-O10-C11
3	N	702	MA4	O50-C10-O10-C11
3	O	702	MA4	O50-C10-O10-C11
3	O	702	MA4	C21-C11-O10-C10
3	P	702	MA4	C20-C10-O10-C11
3	P	702	MA4	O50-C10-O10-C11
3	A	702	MA4	O50-C50-C60-O60
3	B	702	MA4	O50-C50-C60-O60
3	F	702	MA4	O50-C50-C60-O60
3	N	702	MA4	C40-C50-C60-O60
3	J	702	MA4	O50-C50-C60-O60
3	L	702	MA4	C40-C50-C60-O60
3	H	702	MA4	O5-C5-C6-O6
3	H	702	MA4	C4-C5-C6-O6
3	H	702	MA4	C40-C50-C60-O60
3	J	702	MA4	C40-C50-C60-O60
3	G	702	MA4	O50-C50-C60-O60
3	L	702	MA4	O50-C50-C60-O60
3	O	702	MA4	O50-C50-C60-O60
3	A	702	MA4	C40-C50-C60-O60
3	D	702	MA4	O50-C50-C60-O60
3	I	702	MA4	O50-C50-C60-O60
3	B	702	MA4	C40-C50-C60-O60
3	C	702	MA4	O50-C50-C60-O60
3	K	702	MA4	O50-C50-C60-O60
3	N	702	MA4	O50-C50-C60-O60
3	F	702	MA4	C40-C50-C60-O60
3	I	702	MA4	C40-C50-C60-O60
3	K	702	MA4	C40-C50-C60-O60
3	D	702	MA4	C40-C50-C60-O60

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Mol	Chain	Res	Type	Atoms
3	H	702	MA4	C20-C10-O10-C11
3	M	702	MA4	C20-C10-O10-C11
3	P	702	MA4	C41-C51-C61-C12
3	C	702	MA4	C40-C50-C60-O60
3	F	702	MA4	C31-C41-C51-C61
3	A	702	MA4	O5-C5-C6-O6
3	H	702	MA4	O50-C50-C60-O60
3	G	702	MA4	C40-C50-C60-O60
3	O	702	MA4	C40-C50-C60-O60
3	H	702	MA4	C41-C51-C61-C12
3	M	702	MA4	C41-C51-C61-C12
3	F	702	MA4	C41-C51-C61-C12
3	B	702	MA4	O10-C11-C21-C31
3	M	702	MA4	O10-C11-C21-C31
3	A	702	MA4	O10-C11-C21-C31
3	P	702	MA4	C11-C21-C31-C41
3	J	702	MA4	O10-C11-C21-C31
3	H	702	MA4	O10-C11-C21-C31
3	E	702	MA4	O10-C11-C21-C31
3	F	702	MA4	O10-C11-C21-C31
3	O	702	MA4	C4-C5-C6-O6
3	H	702	MA4	C11-C21-C31-C41
3	N	702	MA4	O10-C11-C21-C31
3	G	702	MA4	C20-C10-O10-C11
3	I	702	MA4	C20-C10-O10-C11
3	O	702	MA4	C20-C10-O10-C11
3	F	702	MA4	C11-C21-C31-C41
3	C	702	MA4	C22-C12-C61-C51
3	F	702	MA4	C22-C12-C61-C51
3	M	702	MA4	C22-C12-C61-C51
3	M	702	MA4	C62-C12-C61-C51
3	N	702	MA4	C62-C12-C61-C51
3	C	702	MA4	C11-C21-C31-C41
3	D	702	MA4	C11-C21-C31-C41
3	E	702	MA4	C41-C51-C61-C12
3	N	702	MA4	C41-C51-C61-C12
3	E	702	MA4	C62-C12-C61-C51
3	H	702	MA4	C22-C12-C61-C51
3	K	702	MA4	C22-C12-C61-C51
3	N	702	MA4	C22-C12-C61-C51
3	P	702	MA4	C62-C12-C61-C51
3	C	702	MA4	C20-C10-O10-C11

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Mol	Chain	Res	Type	Atoms
3	F	702	MA4	C20-C10-O10-C11
3	L	702	MA4	C20-C10-O10-C11
3	A	702	MA4	C22-C12-C61-C51
3	E	702	MA4	O50-C50-C60-O60
3	K	702	MA4	C11-C21-C31-C41
3	P	702	MA4	O50-C50-C60-O60
3	M	702	MA4	C11-C21-C31-C41
3	A	702	MA4	C4-C5-C6-O6
3	E	702	MA4	C21-C31-C41-C51
3	O	702	MA4	O5-C5-C6-O6
3	C	702	MA4	C62-C12-C61-C51
3	D	702	MA4	C22-C12-C61-C51
3	D	702	MA4	C62-C12-C61-C51
3	E	702	MA4	C22-C12-C61-C51
3	H	702	MA4	C62-C12-C61-C51
3	P	702	MA4	C22-C12-C61-C51
3	L	702	MA4	C21-C31-C41-C51
3	G	702	MA4	C4-C5-C6-O6
3	P	702	MA4	C40-C50-C60-O60
3	I	702	MA4	O10-C11-C21-C31
3	F	702	MA4	C62-C12-C61-C51
3	K	702	MA4	C62-C12-C61-C51
3	M	702	MA4	O50-C50-C60-O60
3	E	702	MA4	C20-C10-O10-C11
3	K	702	MA4	C20-C10-O10-C11
3	B	702	MA4	C22-C12-C61-C51
3	D	702	MA4	O5-C1-O1-C40
3	A	702	MA4	C62-C12-C61-C51
3	B	702	MA4	C62-C12-C61-C51
3	A	702	MA4	C21-C11-O10-C10
3	B	702	MA4	C21-C11-O10-C10
3	J	702	MA4	C21-C11-O10-C10
3	J	702	MA4	C62-C12-C61-C51
3	L	702	MA4	C62-C12-C61-C51
3	P	702	MA4	O10-C11-C21-C31
3	K	702	MA4	O10-C11-C21-C31
3	M	702	MA4	C31-C41-C51-C61
3	L	702	MA4	C22-C12-C61-C51
3	E	702	MA4	C31-C41-C51-C61
3	J	702	MA4	C22-C12-C61-C51
3	O	702	MA4	C41-C51-C61-C12
3	L	702	MA4	C11-C21-C31-C41

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Mol	Chain	Res	Type	Atoms
3	G	702	MA4	C41-C51-C61-C12
3	C	702	MA4	C31-C41-C51-C61
3	H	702	MA4	C31-C41-C51-C61
3	G	702	MA4	O5-C5-C6-O6
3	D	702	MA4	C31-C41-C51-C61
2	H	701	NAG	C3-C2-N2-C7
2	O	701	NAG	C4-C5-C6-O6
3	D	702	MA4	C2-C1-O1-C40
3	N	702	MA4	C31-C41-C51-C61
3	N	702	MA4	O5-C5-C6-O6
3	A	702	MA4	O5-C1-O1-C40
3	L	702	MA4	O5-C1-O1-C40
3	C	702	MA4	O10-C11-C21-C31
3	N	702	MA4	C11-C21-C31-C41
3	I	702	MA4	C62-C12-C61-C51
3	A	702	MA4	C2-C1-O1-C40
3	K	702	MA4	C31-C41-C51-C61
2	A	701	NAG	C3-C2-N2-C7
2	B	701	NAG	C3-C2-N2-C7
2	C	701	NAG	C3-C2-N2-C7
2	D	701	NAG	C3-C2-N2-C7
2	E	701	NAG	C3-C2-N2-C7
2	F	701	NAG	C3-C2-N2-C7
2	G	701	NAG	C3-C2-N2-C7
2	I	701	NAG	C3-C2-N2-C7
2	J	701	NAG	C3-C2-N2-C7
2	K	701	NAG	C3-C2-N2-C7
2	L	701	NAG	C3-C2-N2-C7
2	M	701	NAG	C3-C2-N2-C7
2	N	701	NAG	C3-C2-N2-C7
2	O	701	NAG	C3-C2-N2-C7
2	P	701	NAG	C3-C2-N2-C7
3	L	702	MA4	C2-C1-O1-C40
3	D	702	MA4	C21-C31-C41-C51
2	C	701	NAG	C1-C2-N2-C7
2	F	701	NAG	C1-C2-N2-C7
3	L	702	MA4	O5-C5-C6-O6
3	P	702	MA4	C21-C31-C41-C51
2	A	701	NAG	C1-C2-N2-C7
2	B	701	NAG	C1-C2-N2-C7
2	I	701	NAG	C1-C2-N2-C7
2	J	701	NAG	C1-C2-N2-C7

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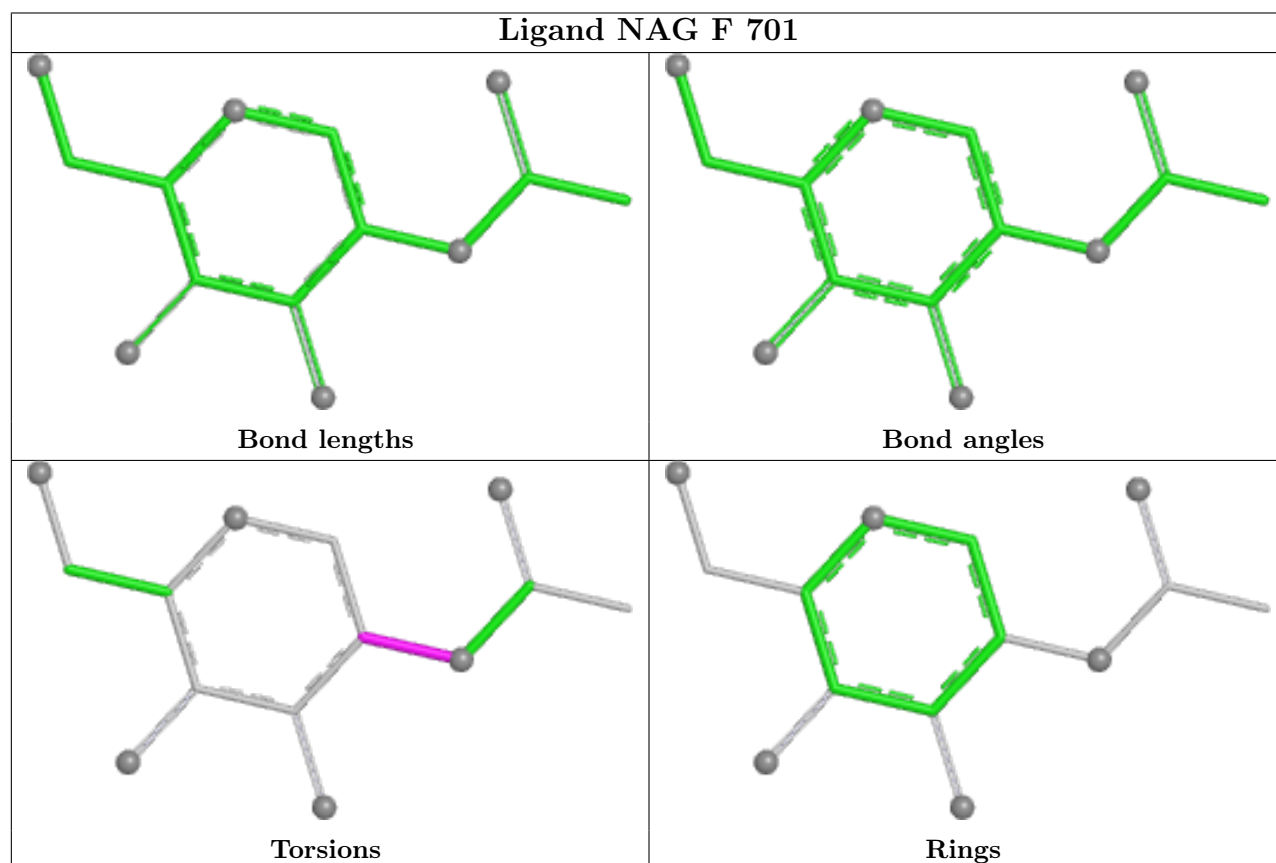
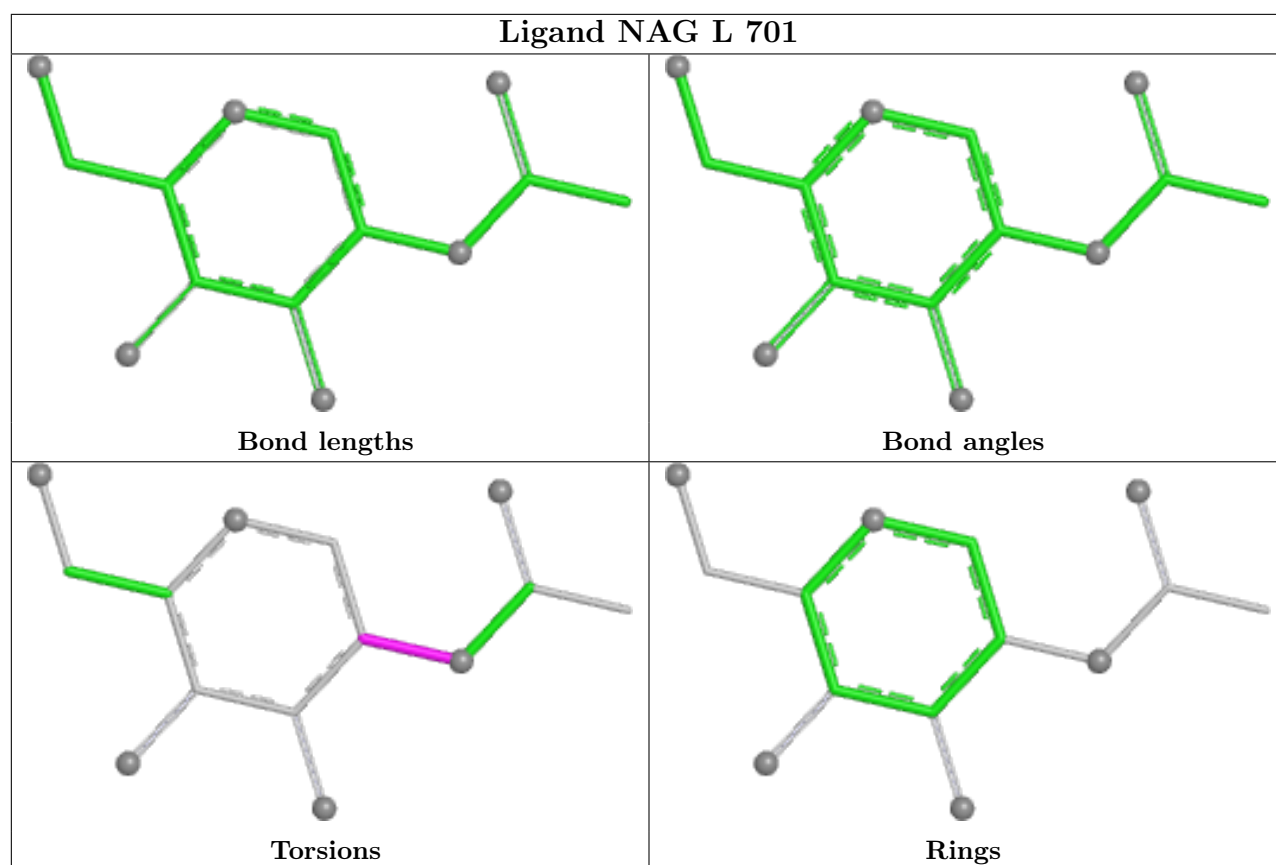
Mol	Chain	Res	Type	Atoms
2	K	701	NAG	C1-C2-N2-C7
2	P	701	NAG	C1-C2-N2-C7

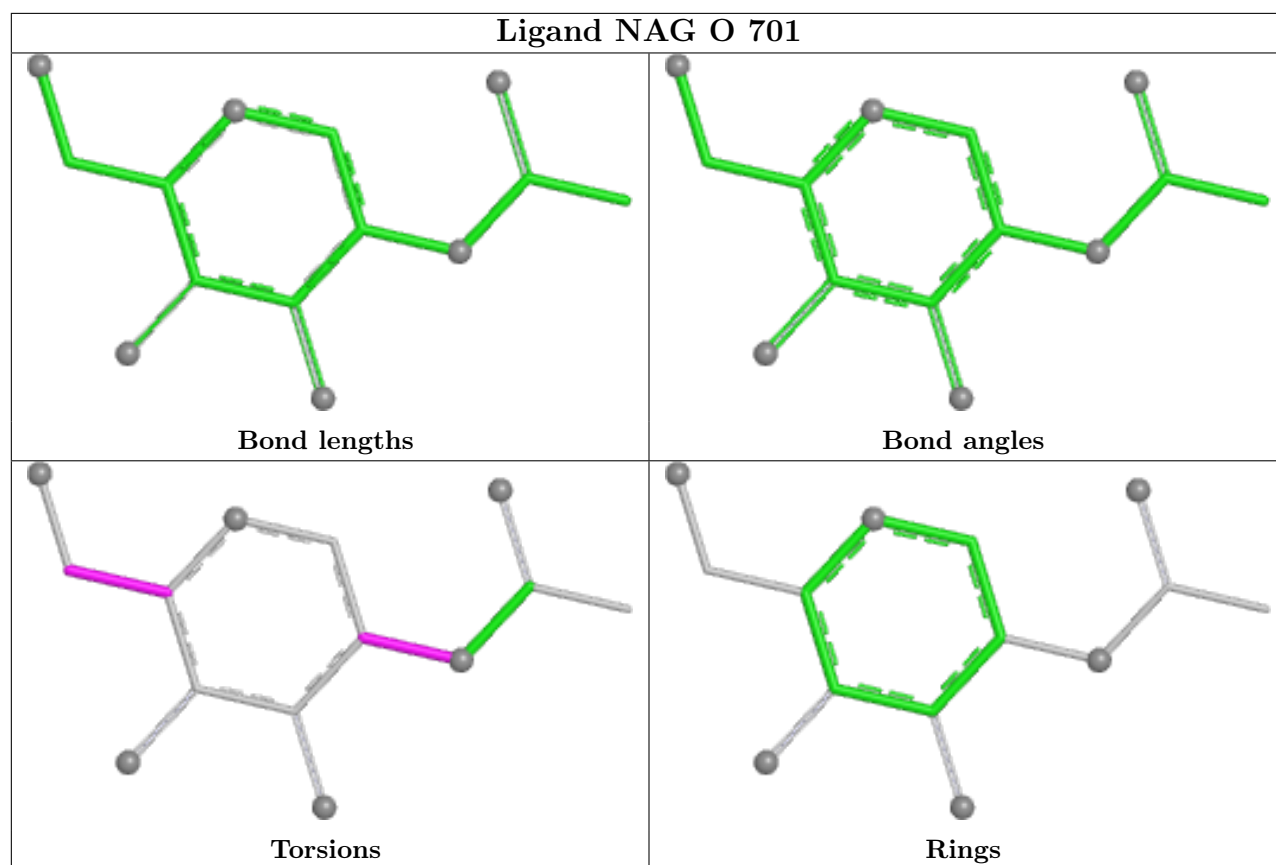
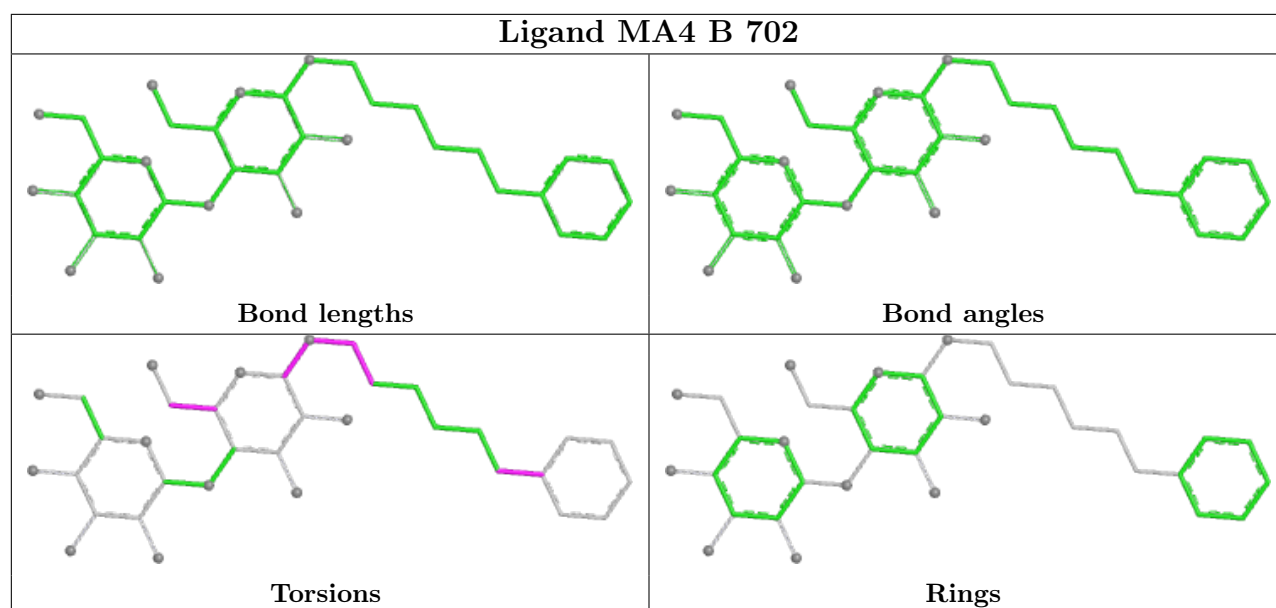
There are no ring outliers.

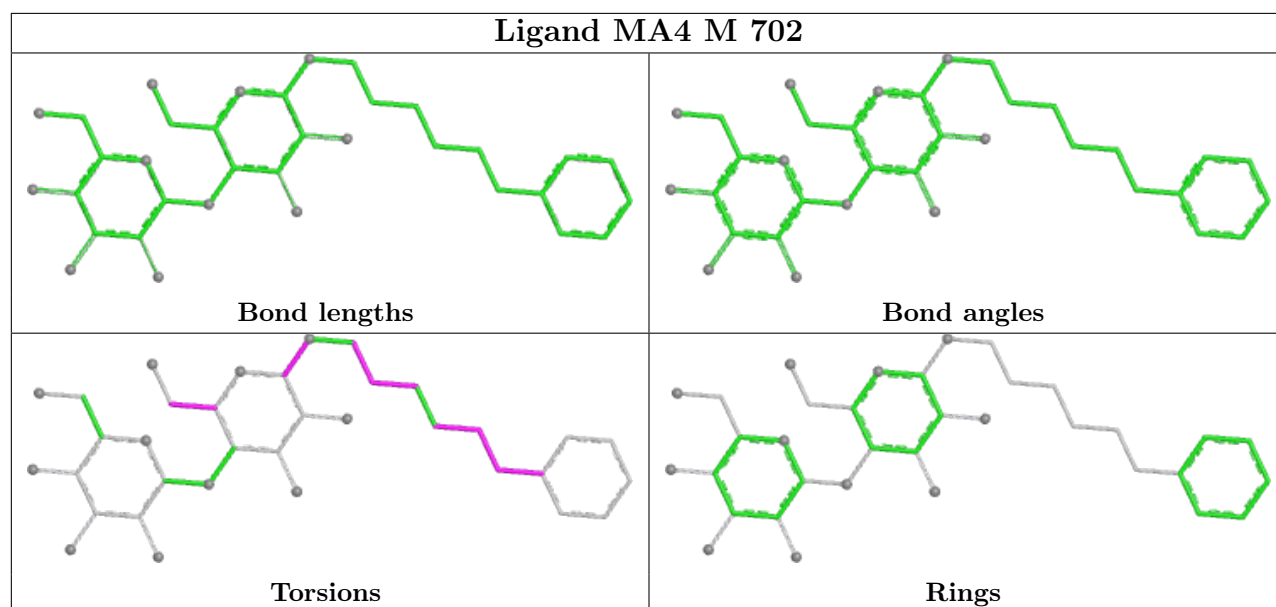
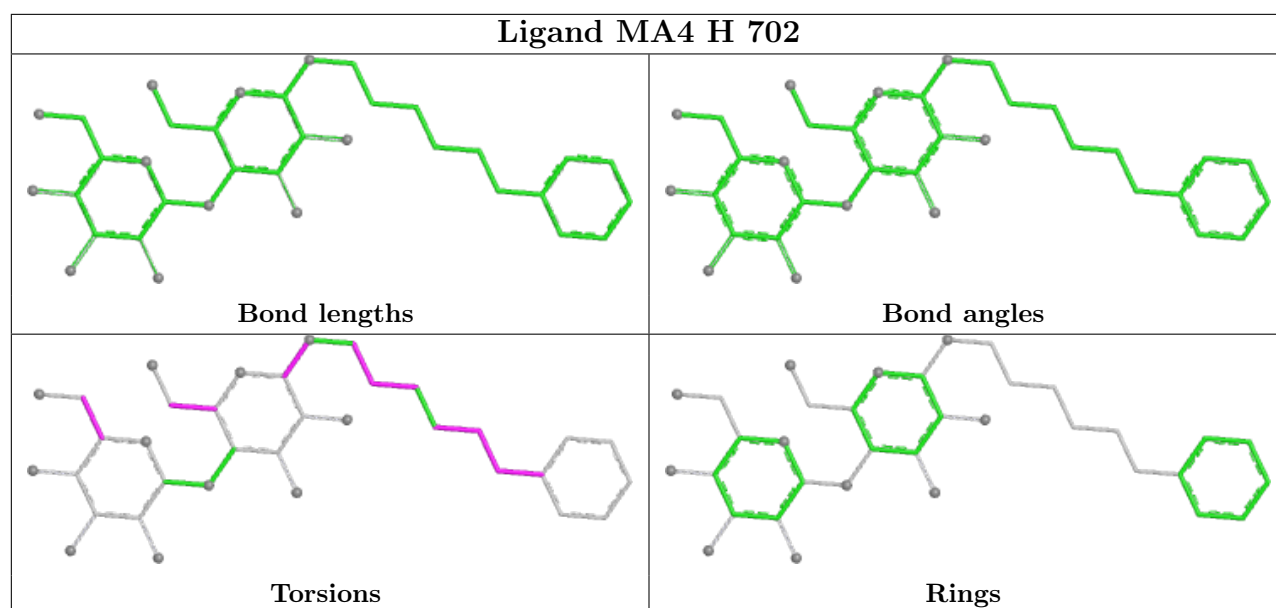
14 monomers are involved in 30 short contacts:

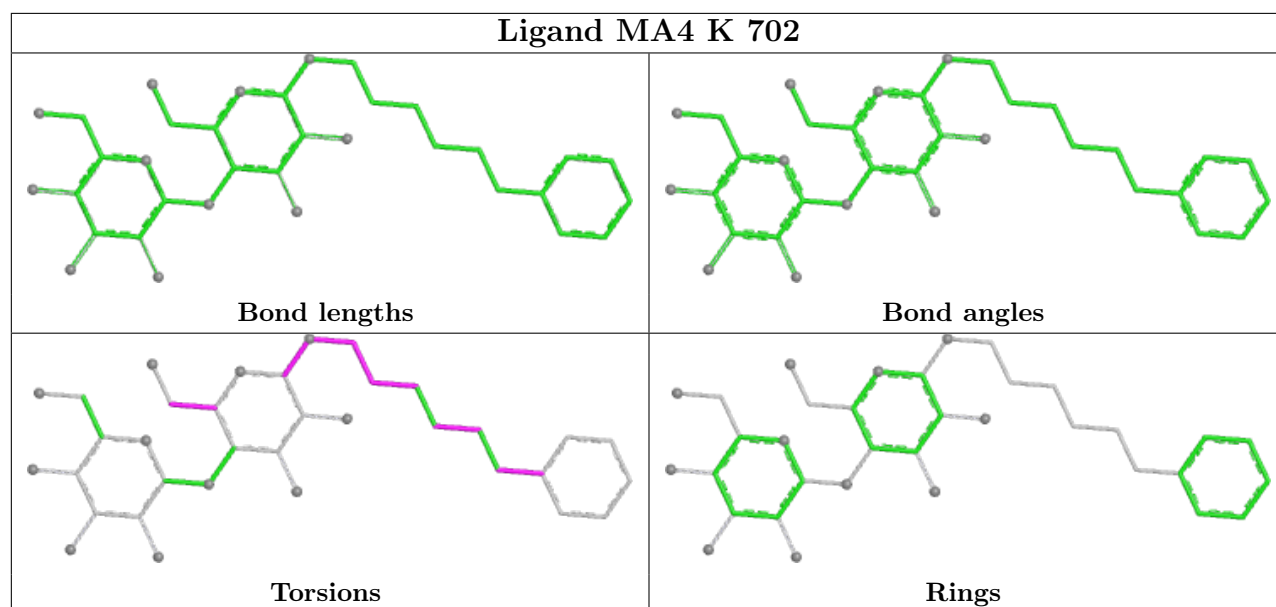
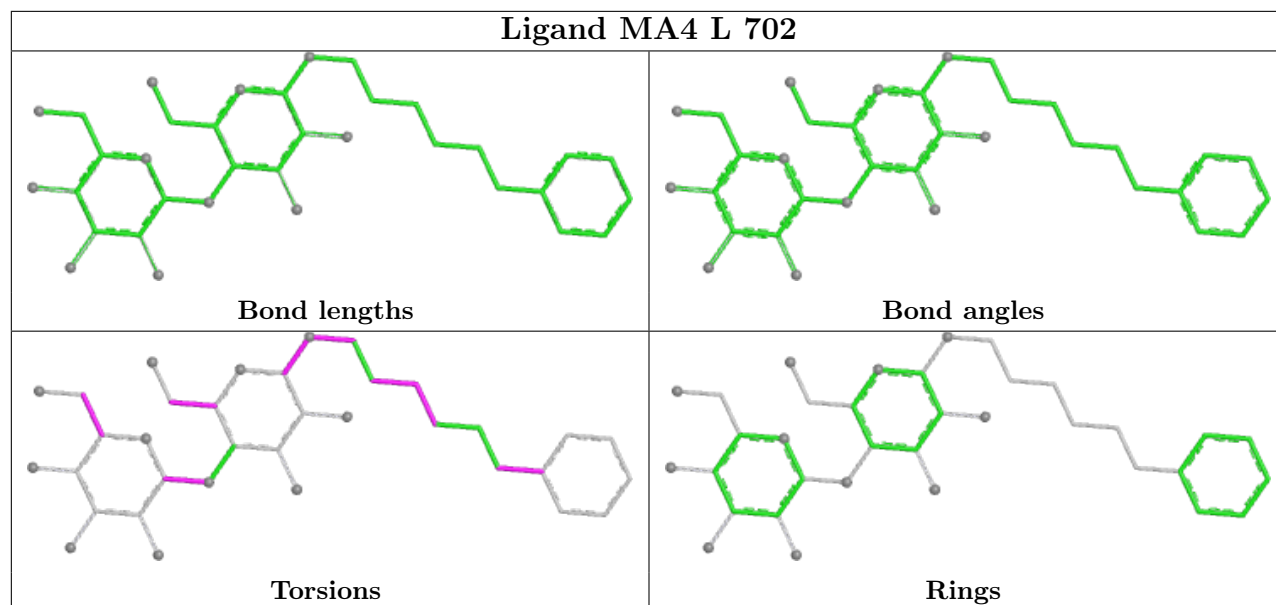
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	MA4	1	0
3	H	702	MA4	1	0
3	M	702	MA4	4	0
3	L	702	MA4	5	0
3	K	702	MA4	1	0
3	P	702	MA4	1	0
3	E	702	MA4	5	0
3	D	702	MA4	3	0
3	O	702	MA4	1	0
3	F	702	MA4	1	0
3	A	702	MA4	2	0
3	I	702	MA4	1	0
3	N	702	MA4	2	0
3	C	702	MA4	2	0

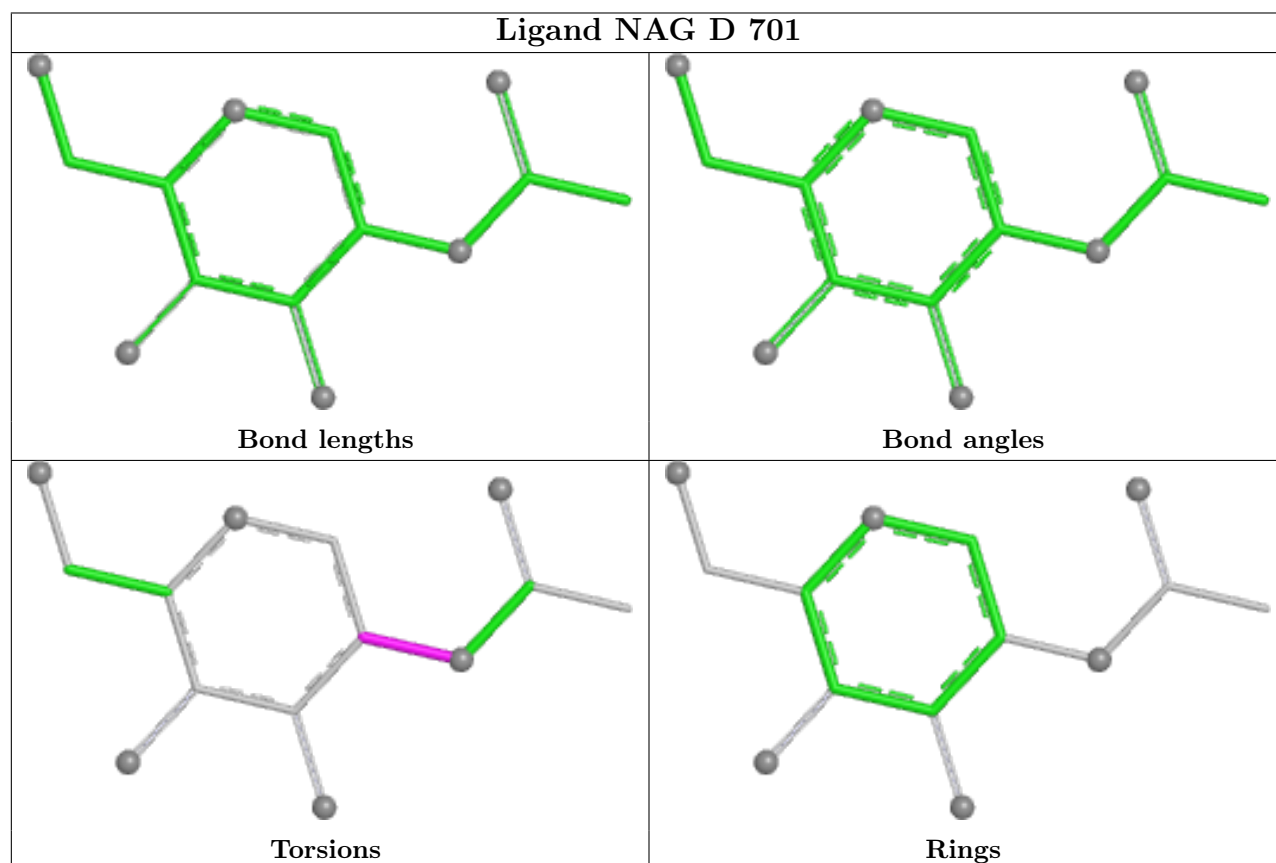
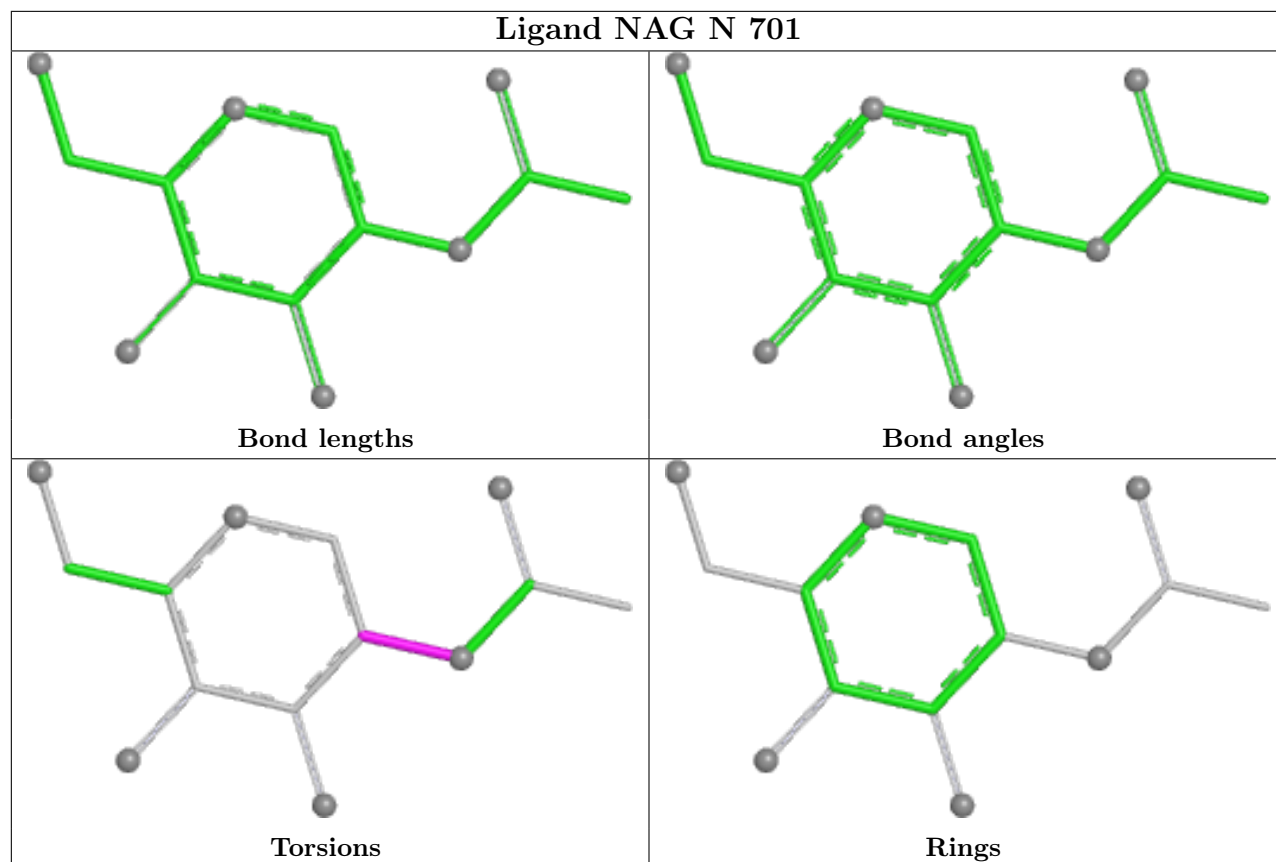
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

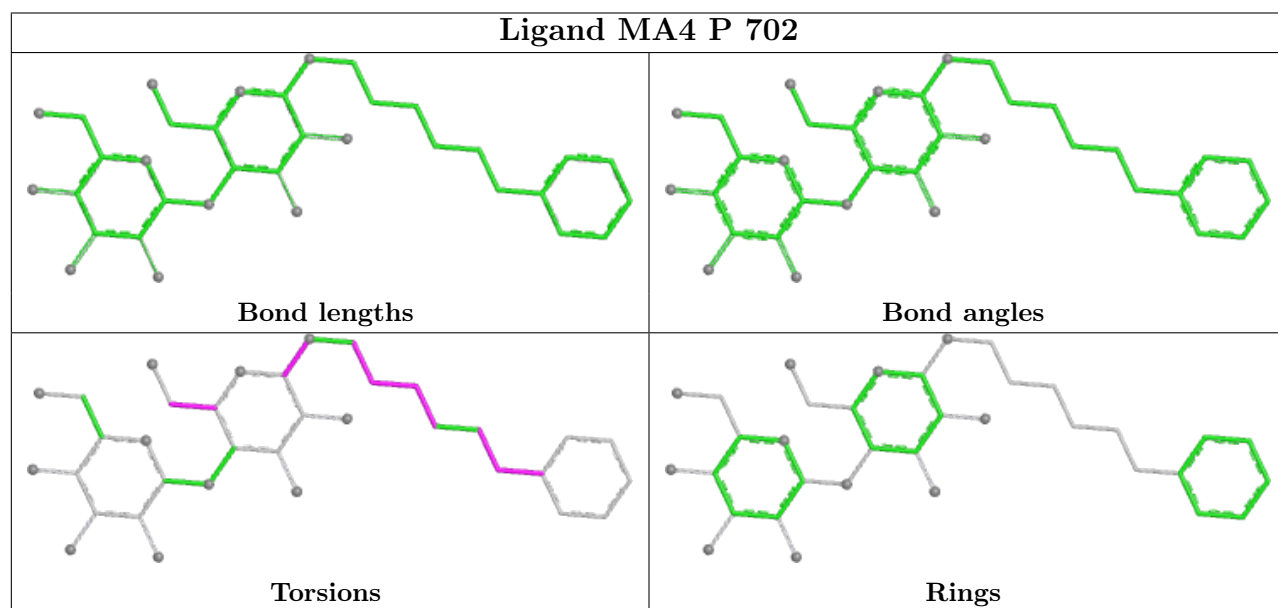
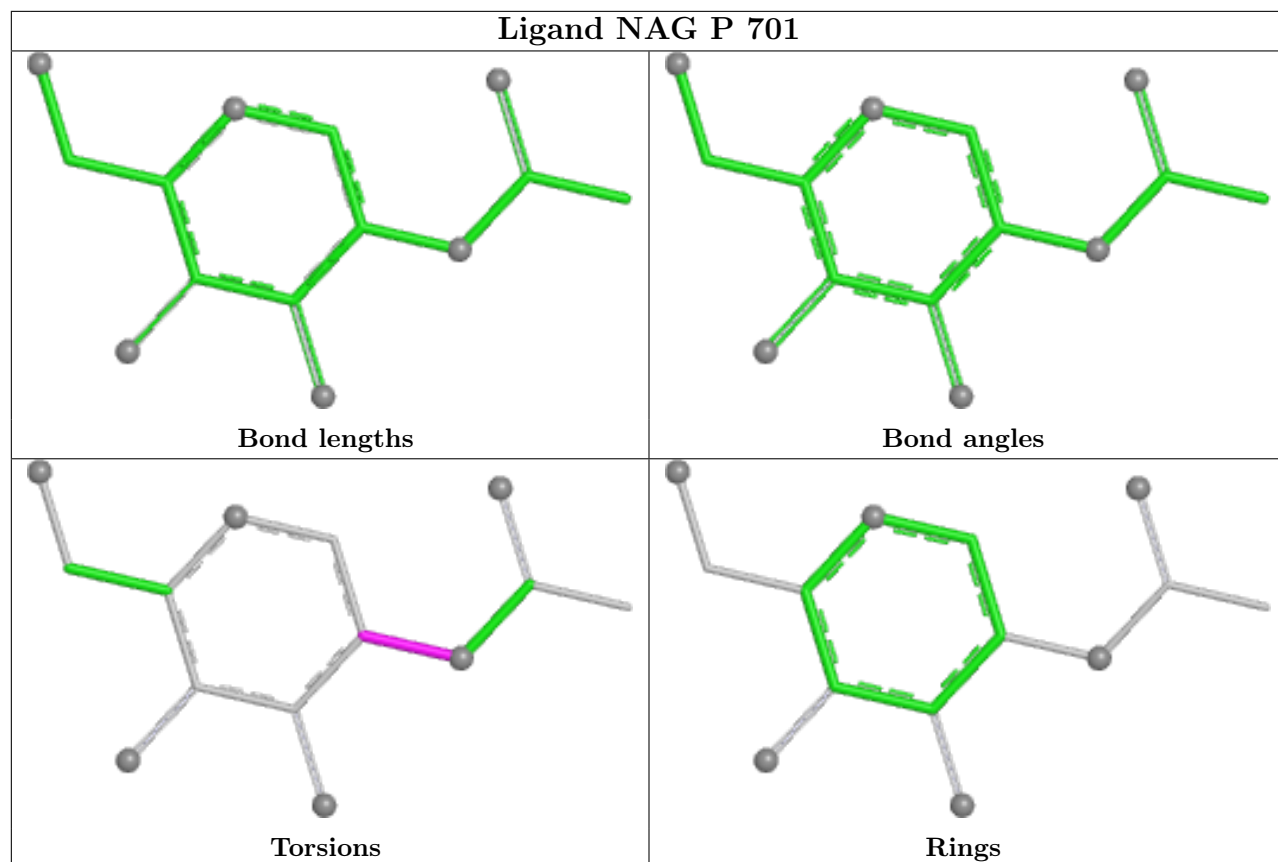


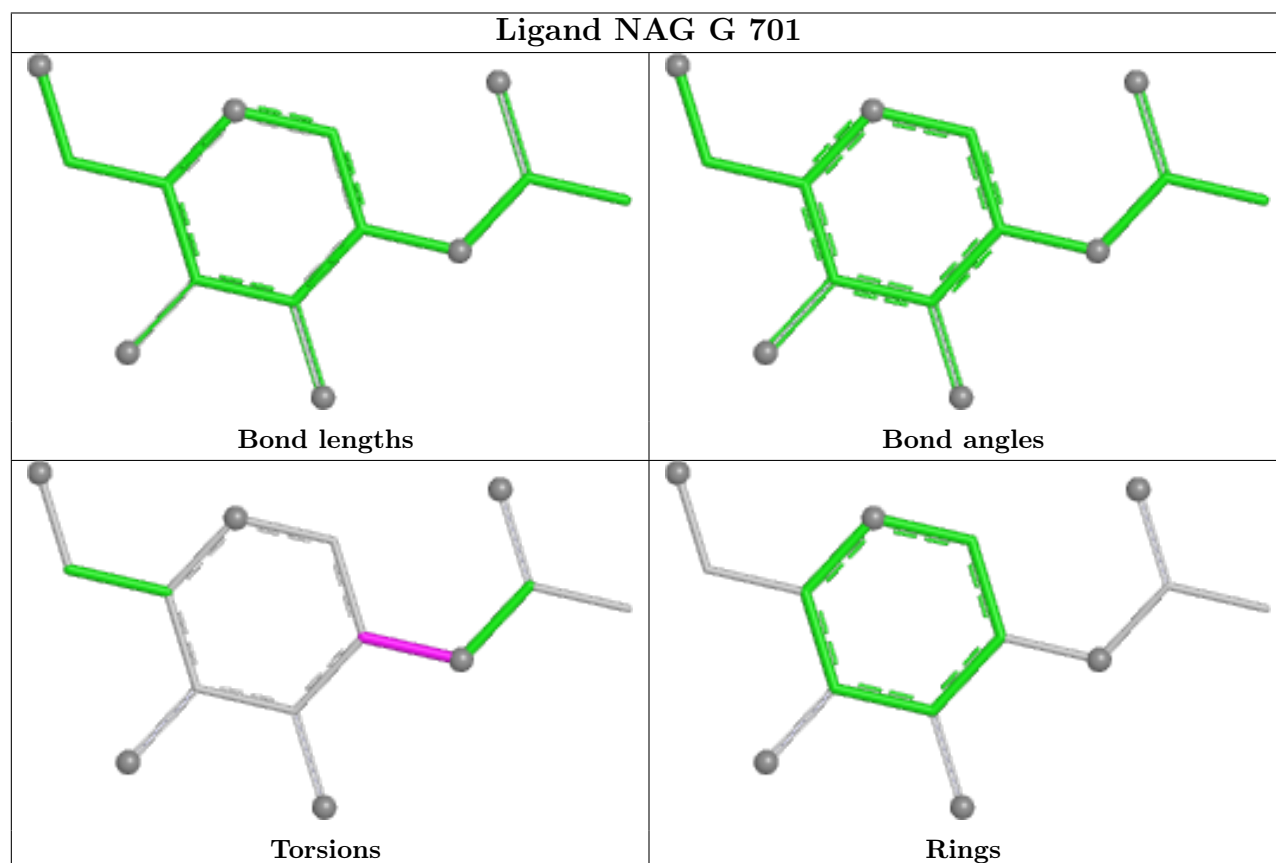
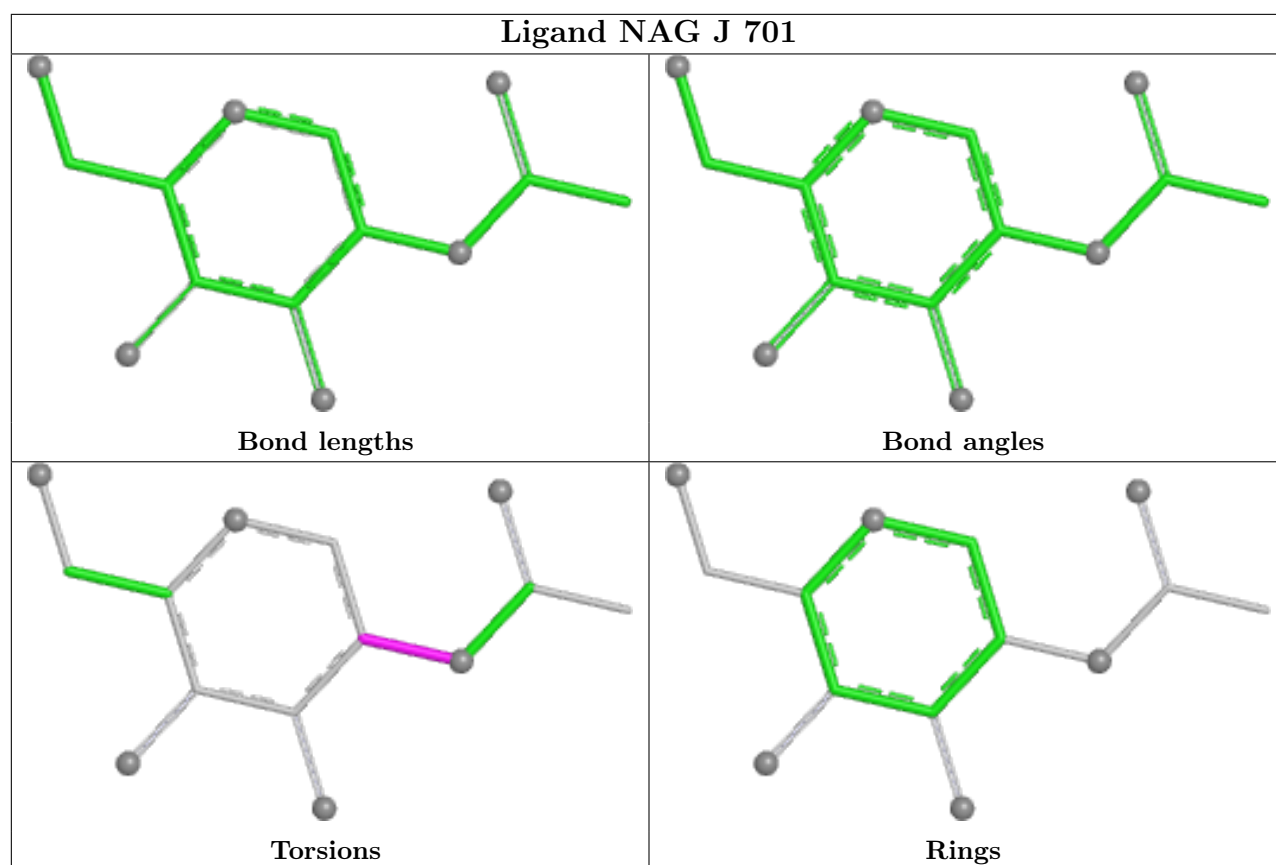


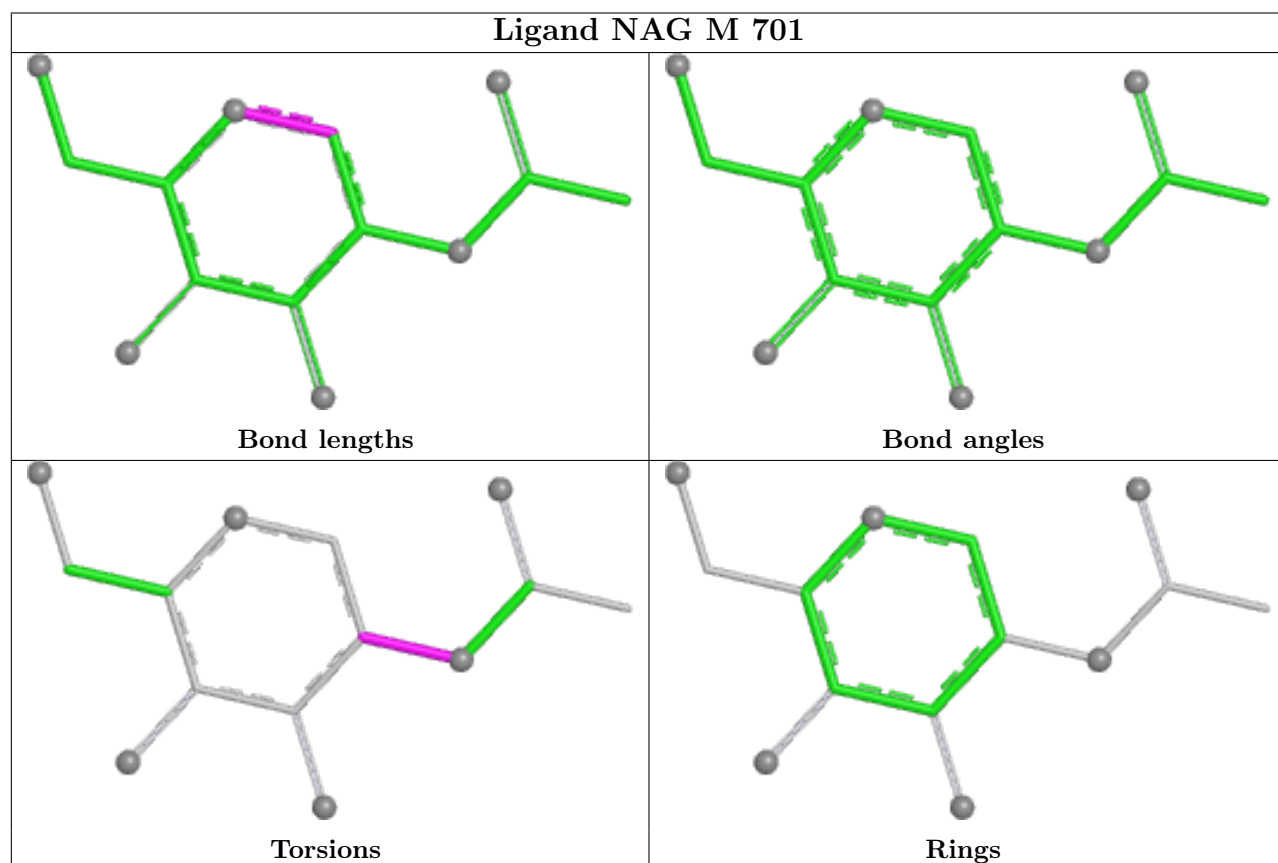
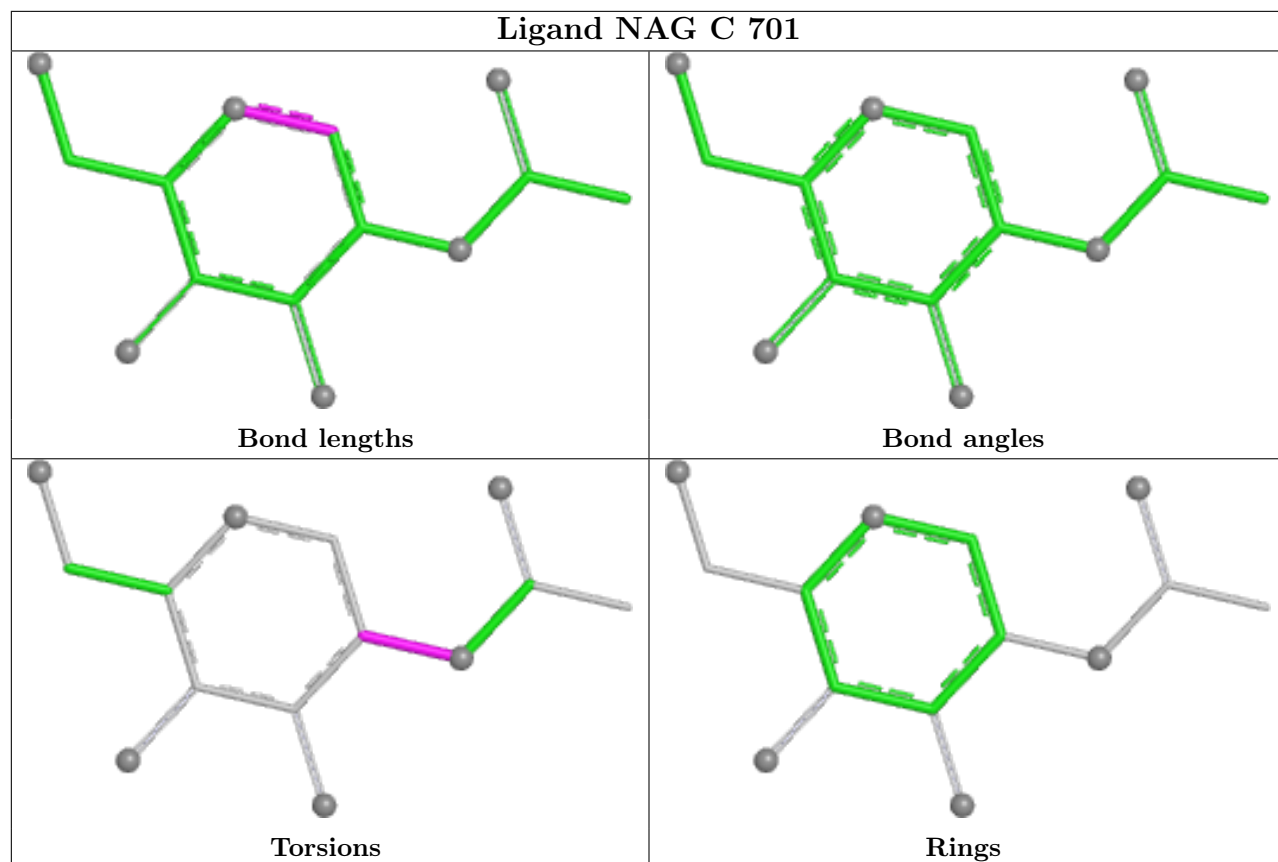


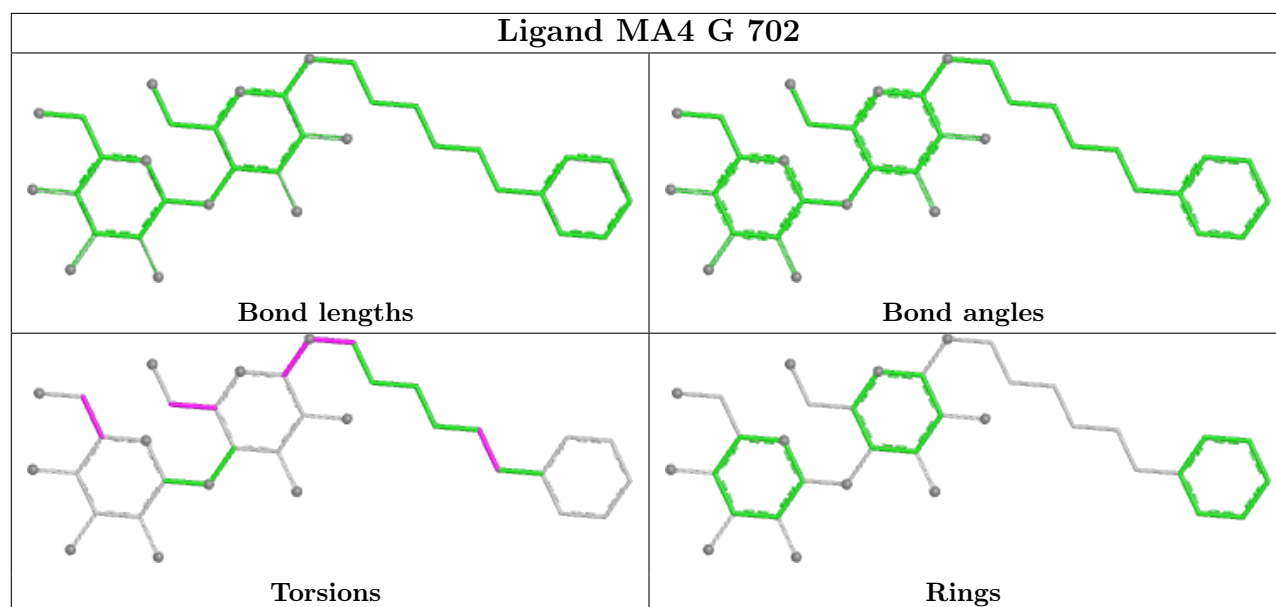
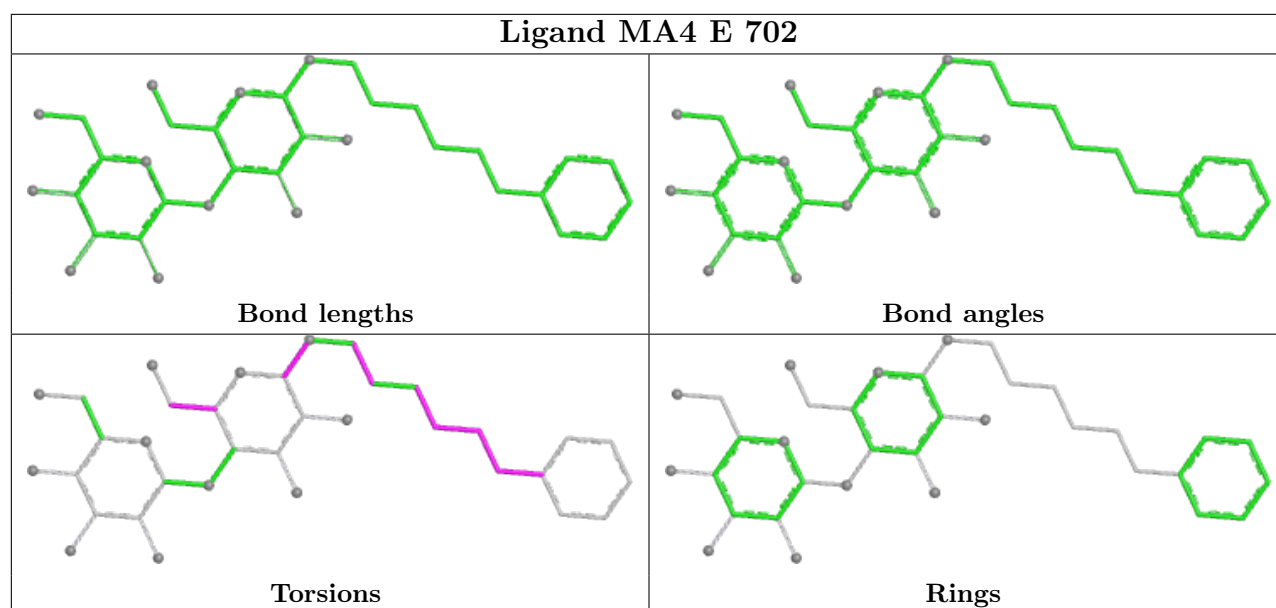


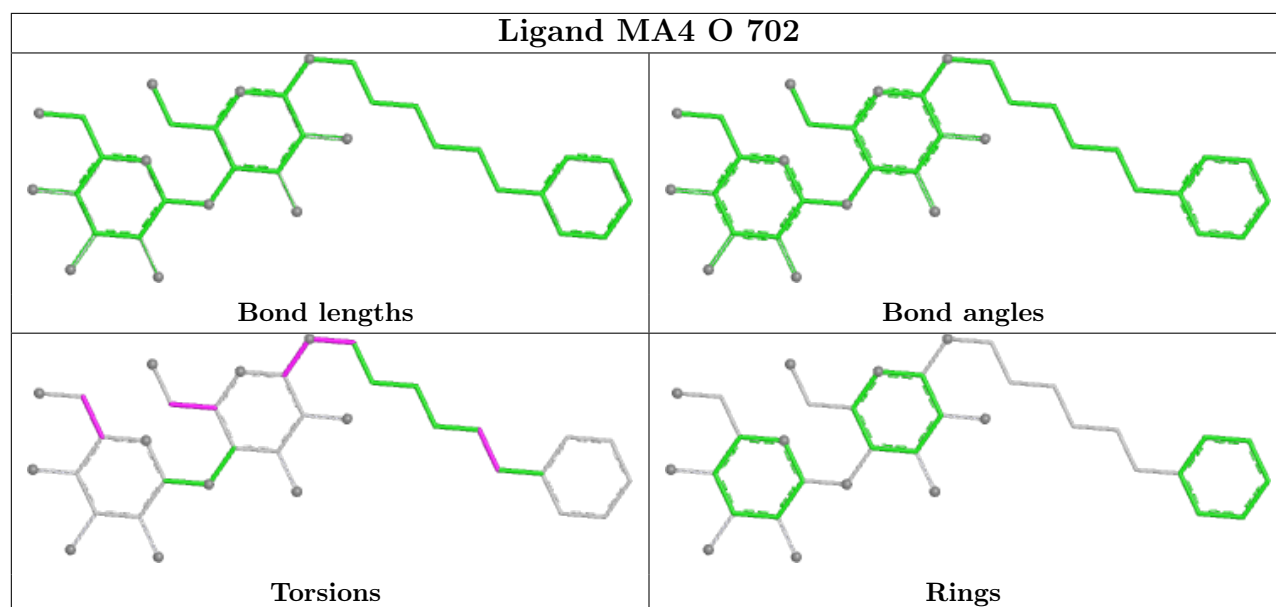
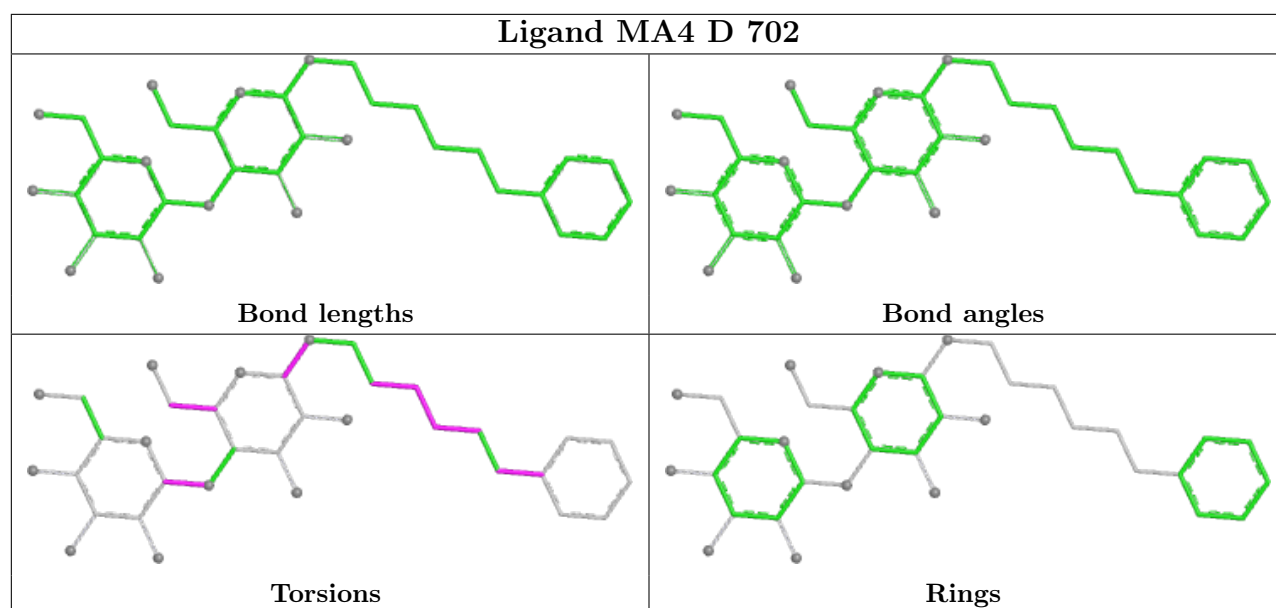


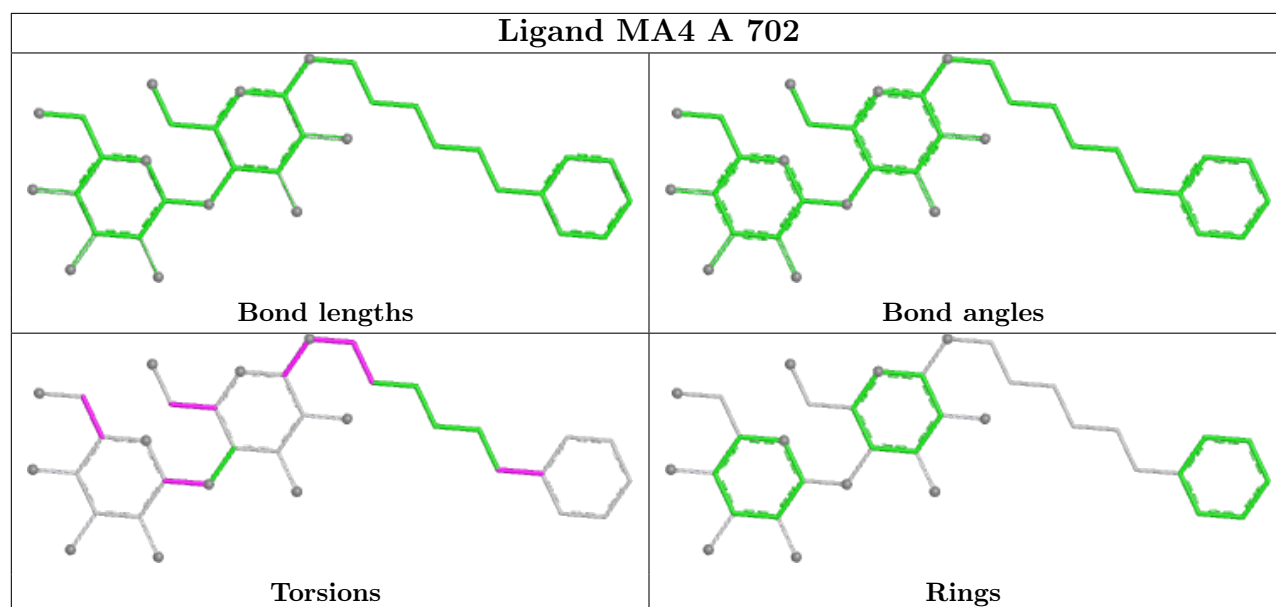
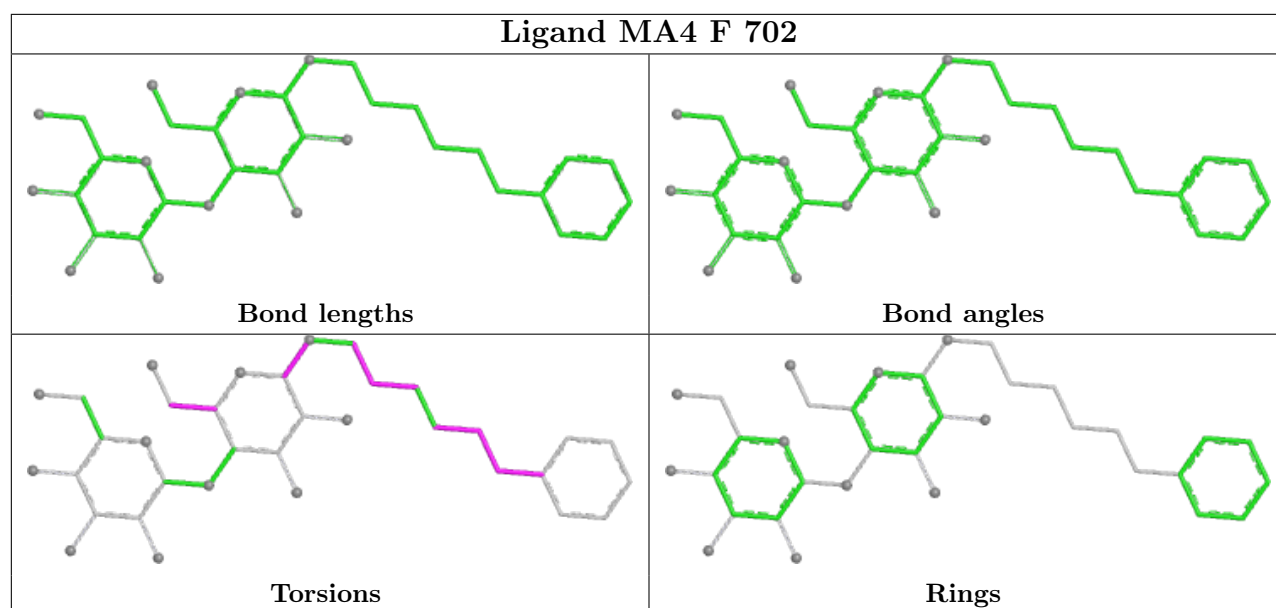


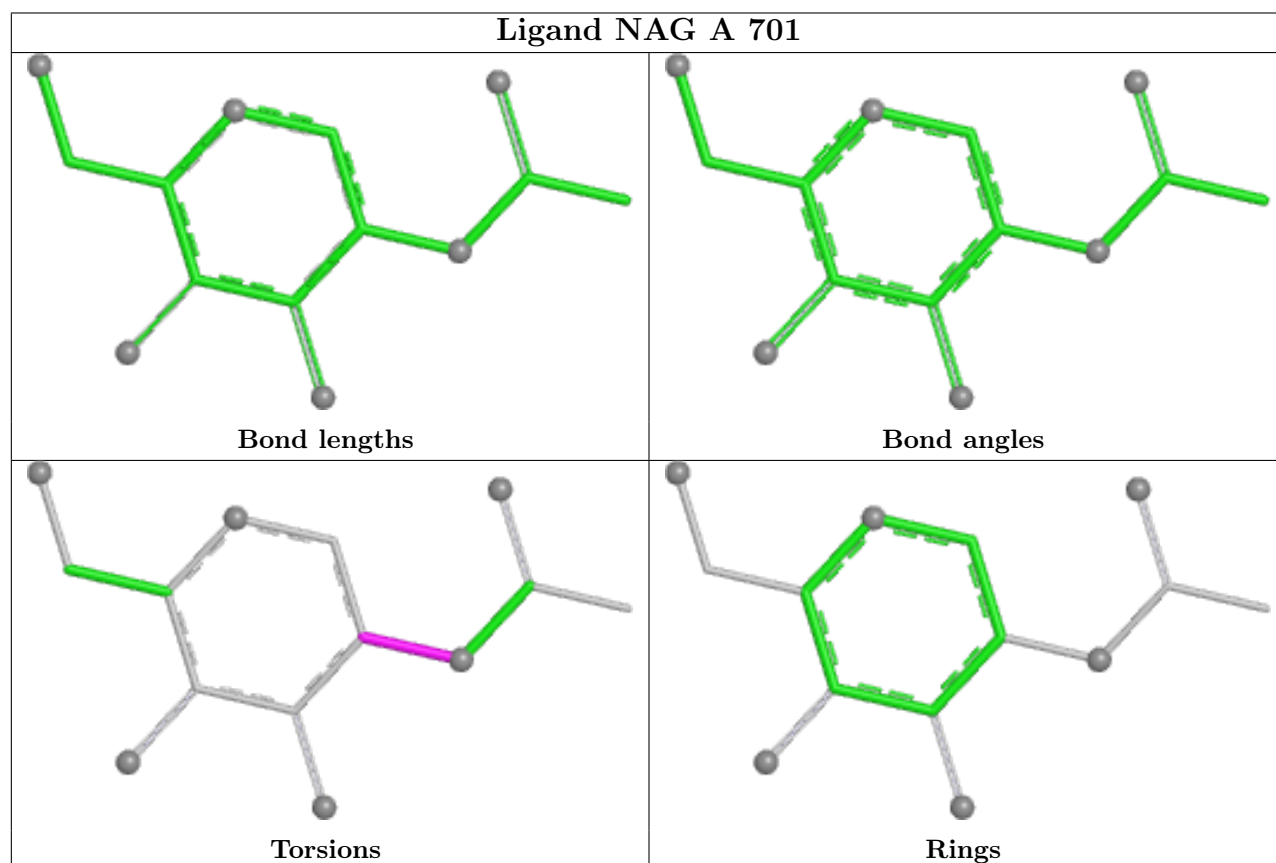
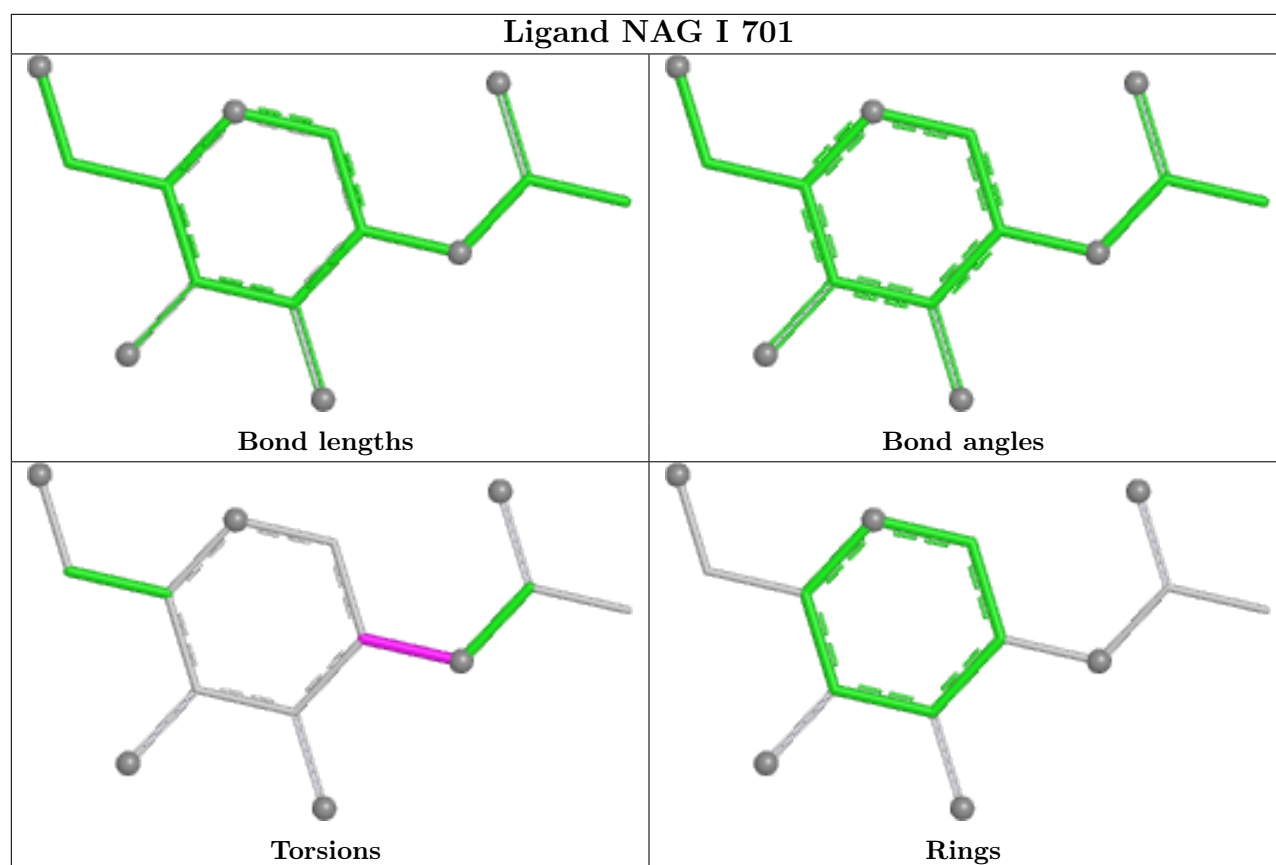


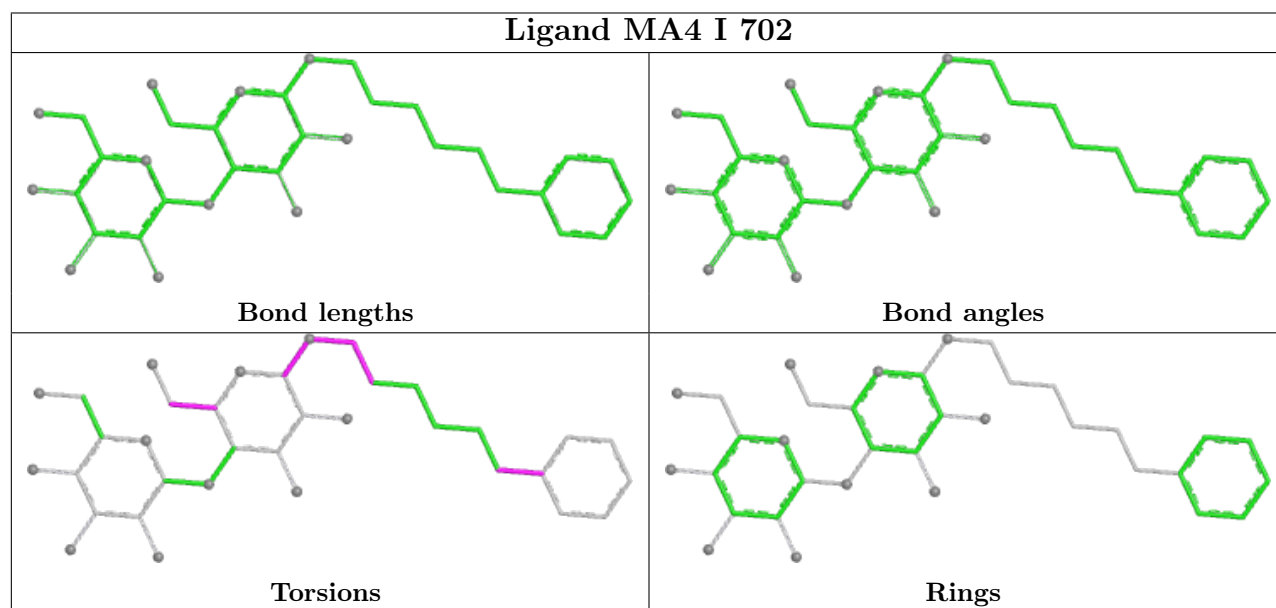
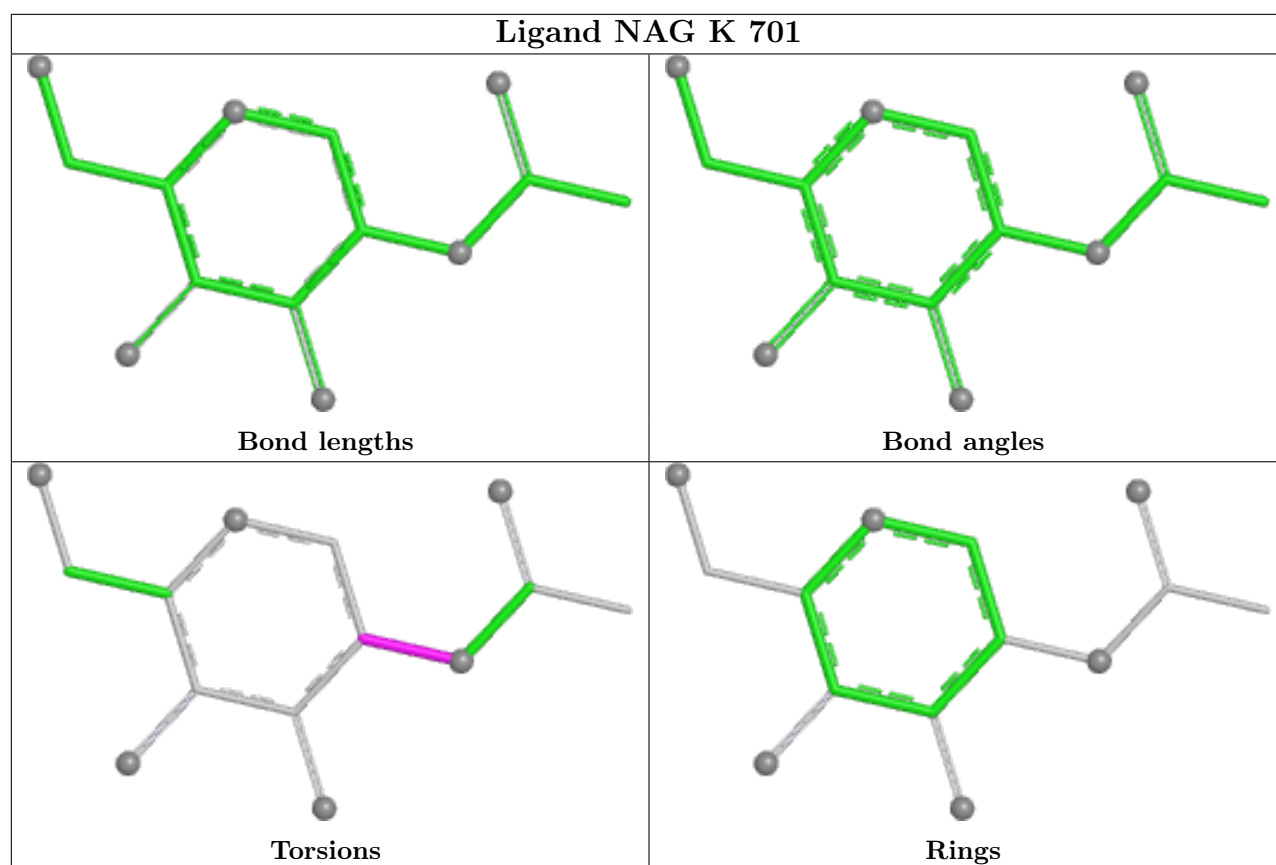


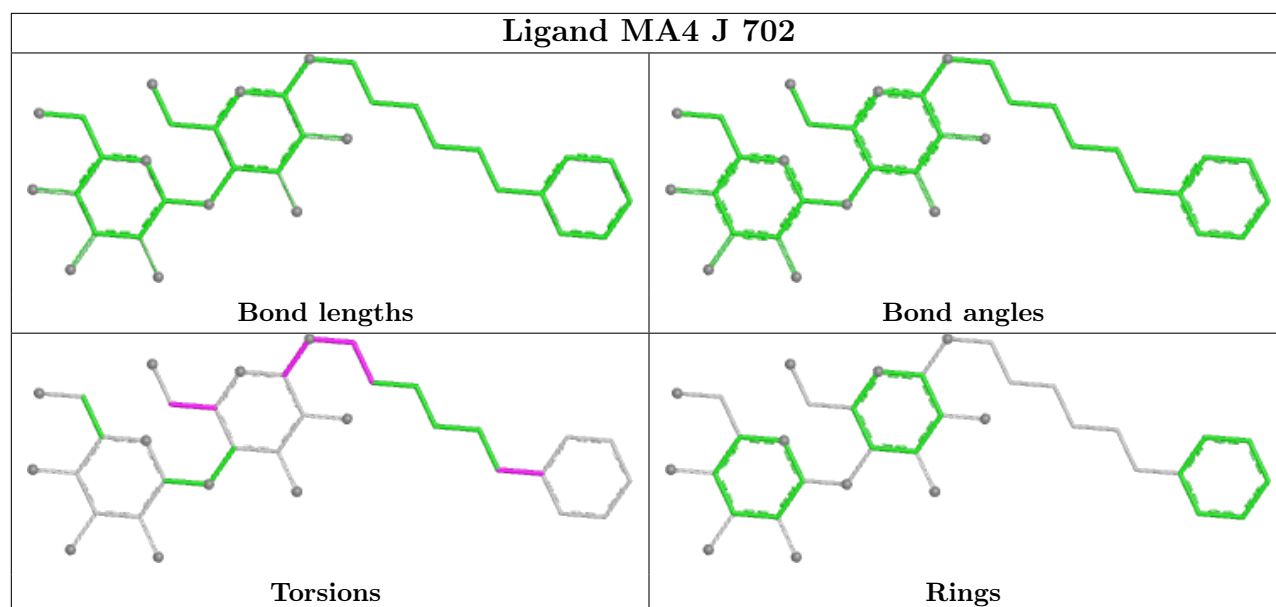
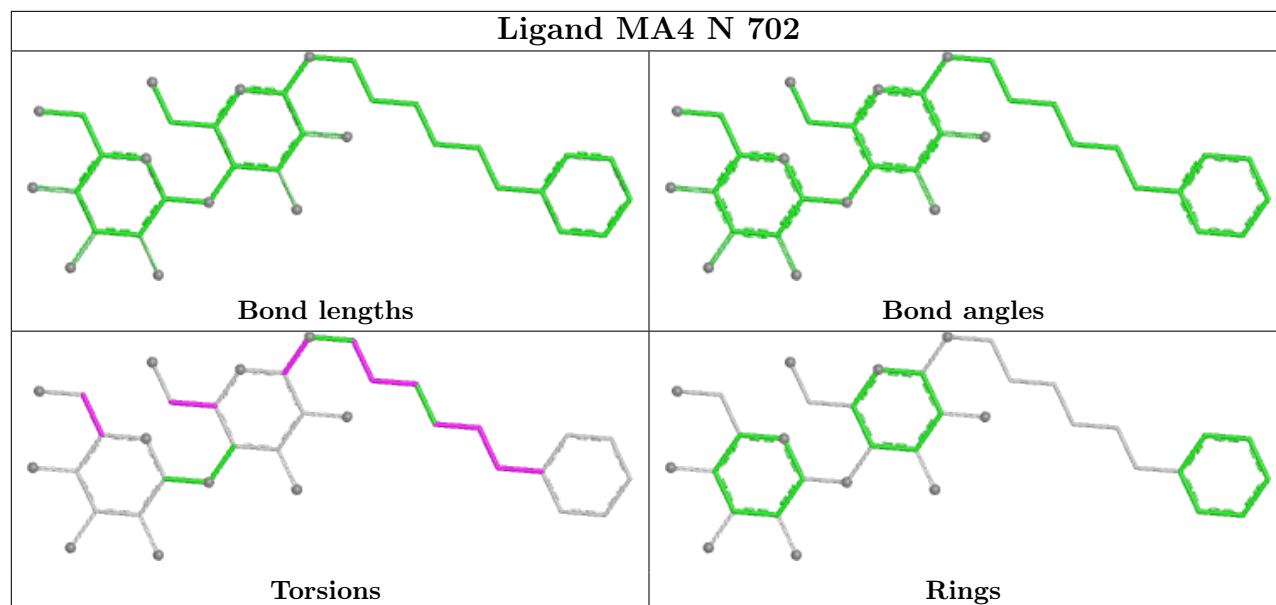


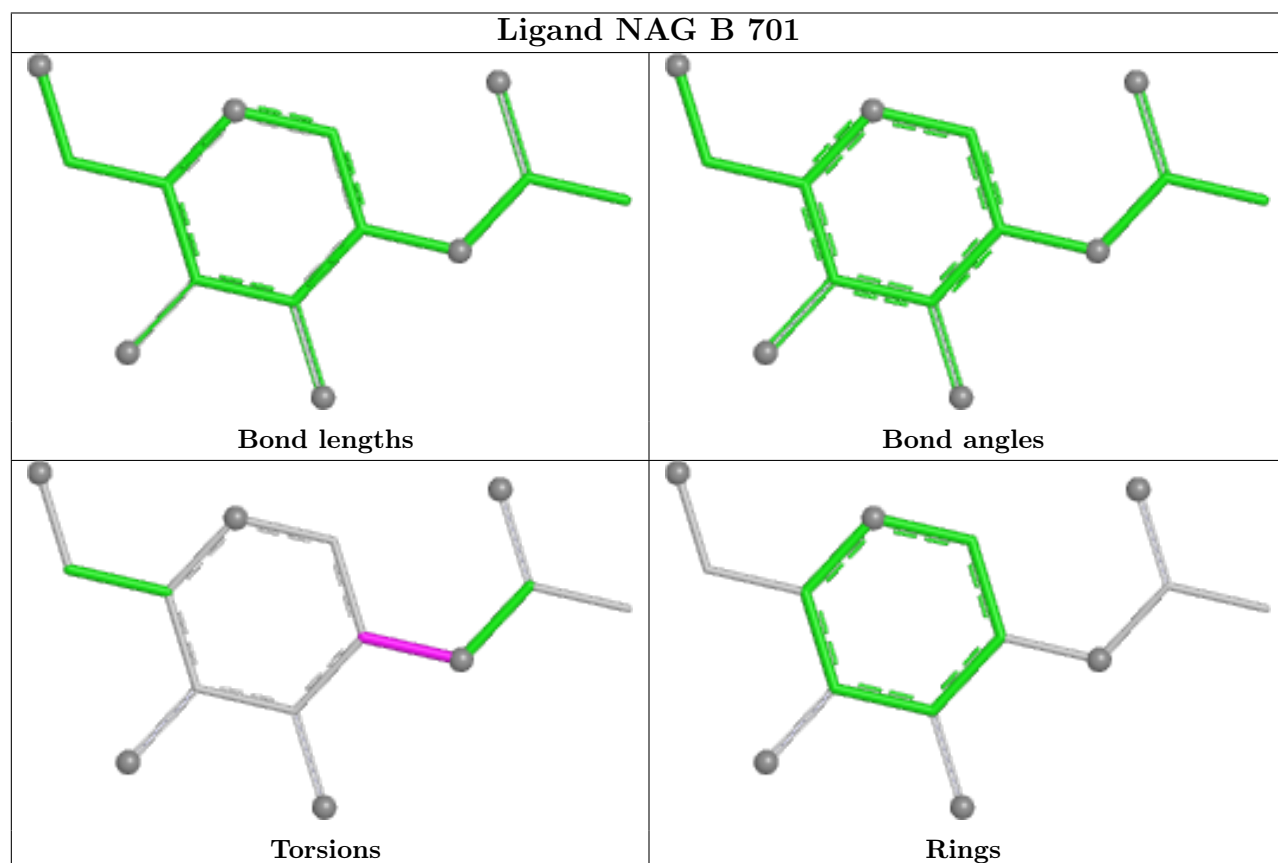
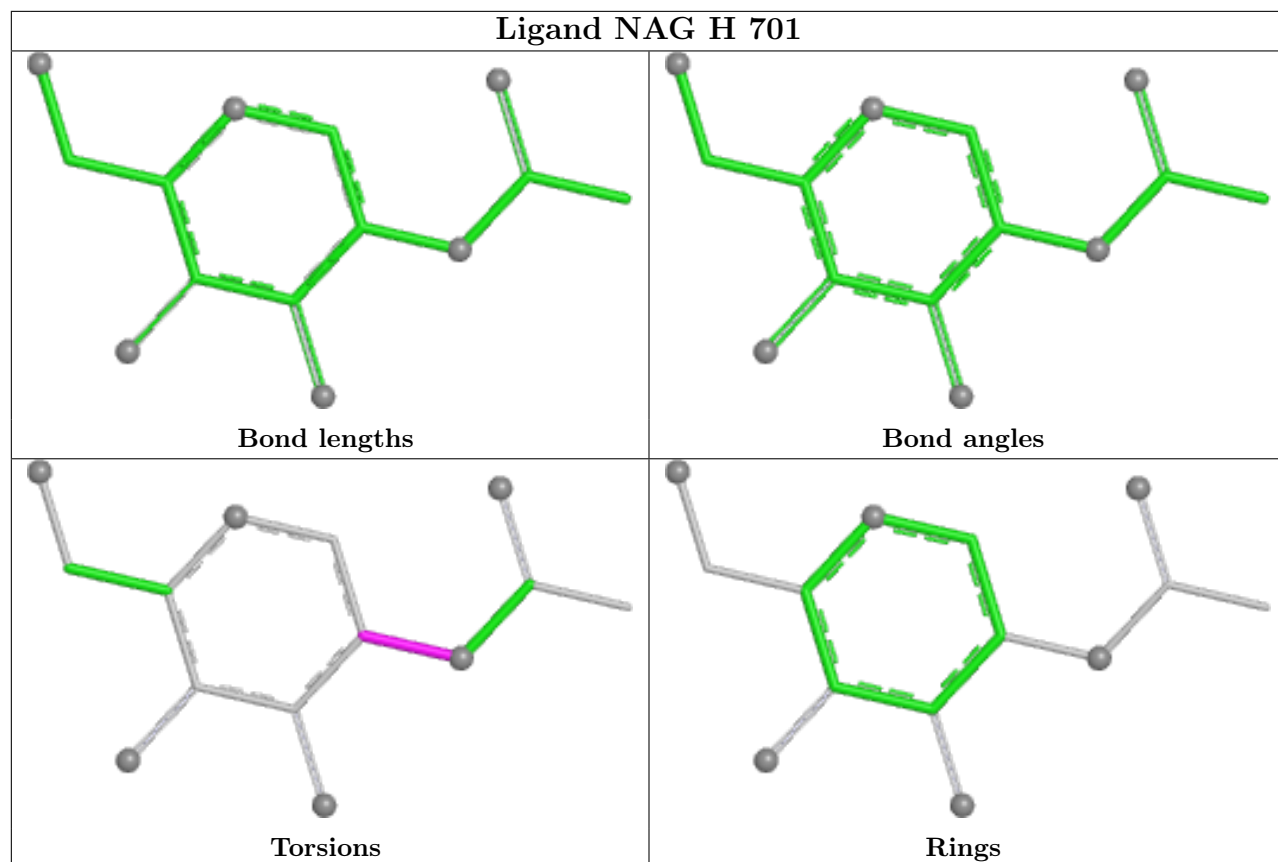


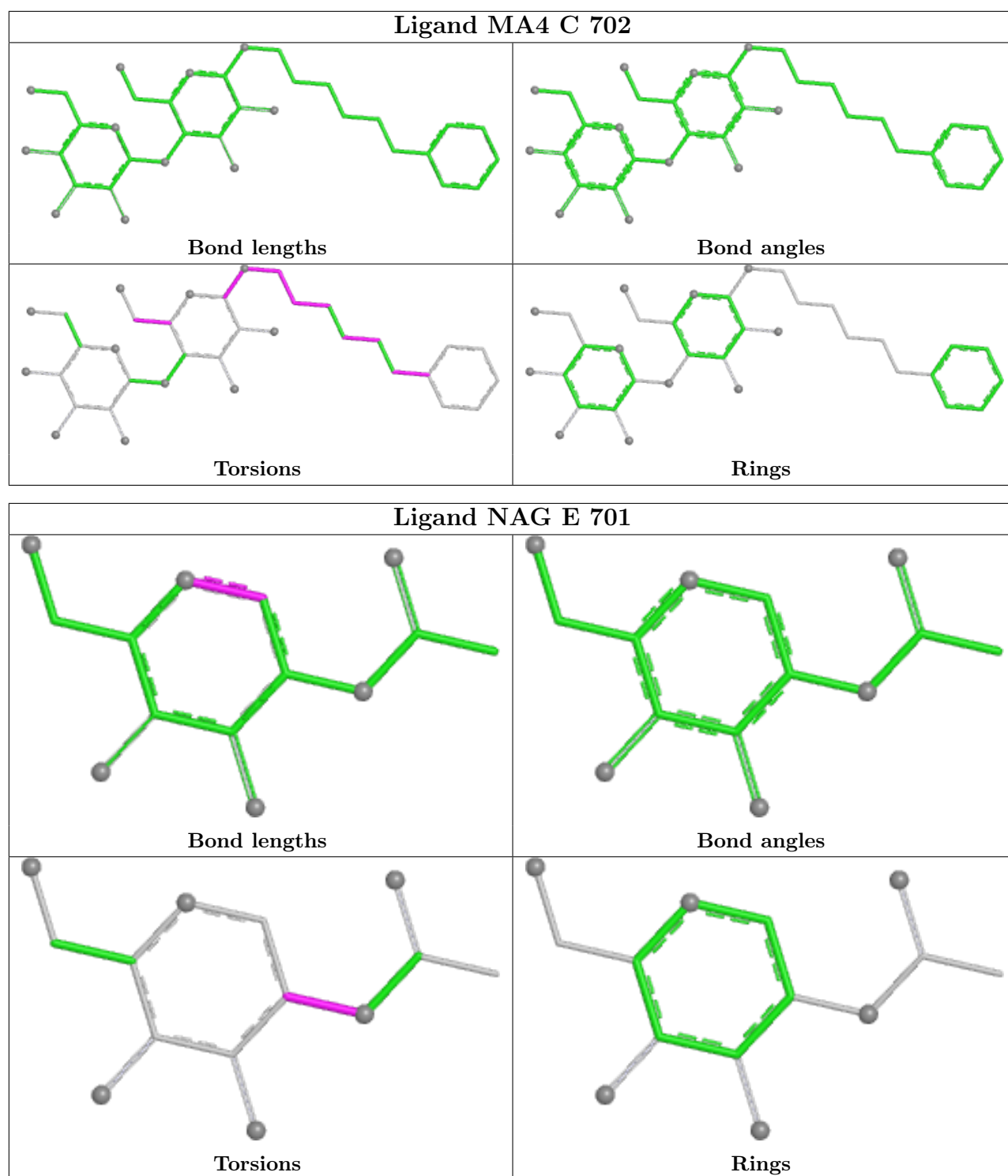












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

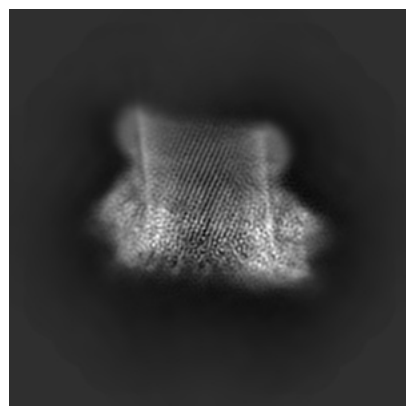
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15086. These allow visual inspection of the internal detail of the map and identification of artifacts.

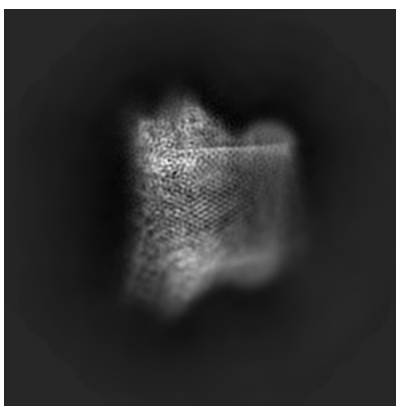
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

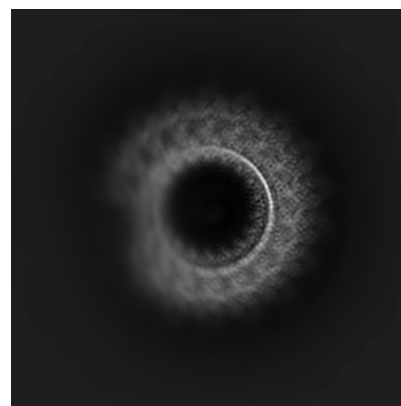
6.1.1 Primary map



X

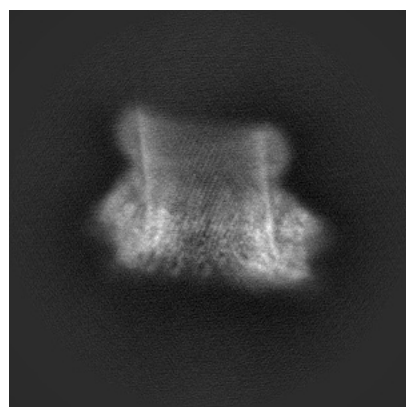


Y

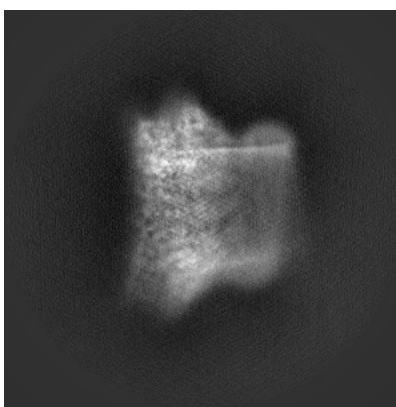


Z

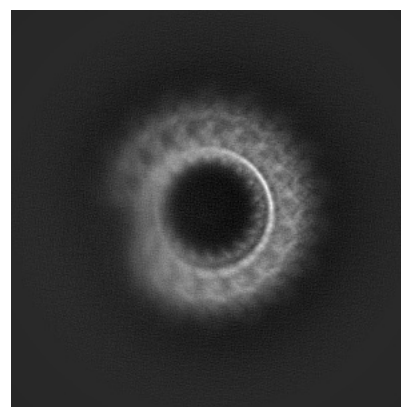
6.1.2 Raw map



X



Y

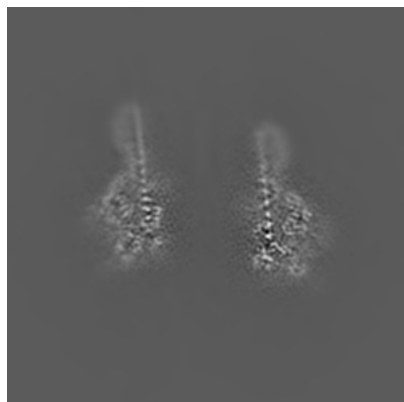


Z

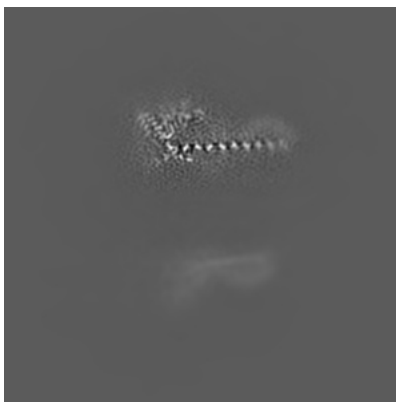
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

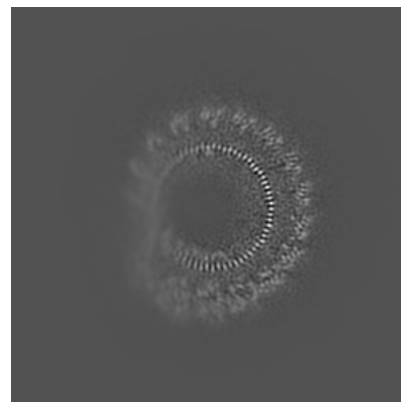
6.2.1 Primary map



X Index: 180



Y Index: 180

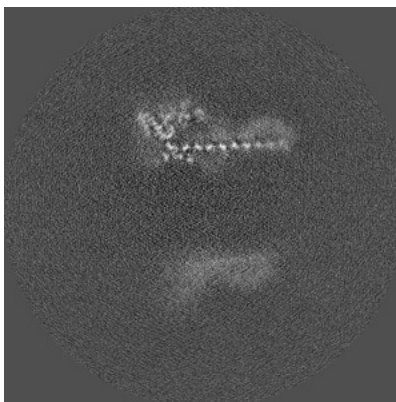


Z Index: 180

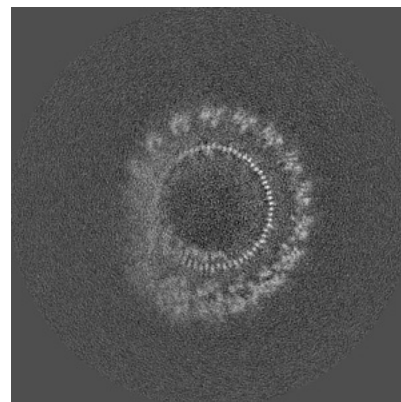
6.2.2 Raw map



X Index: 180



Y Index: 180

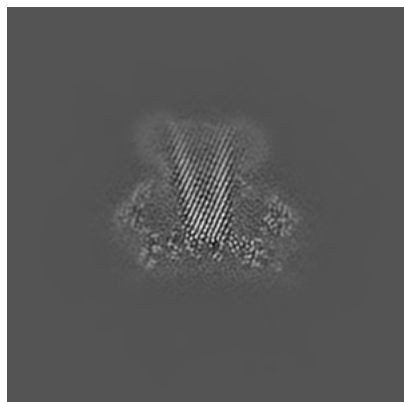


Z Index: 180

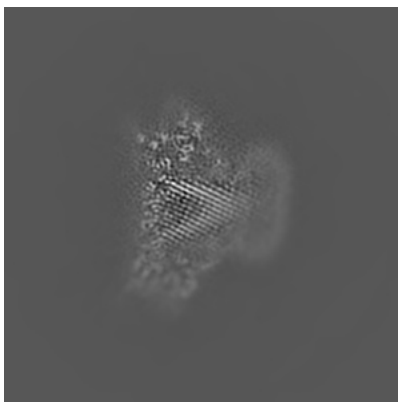
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

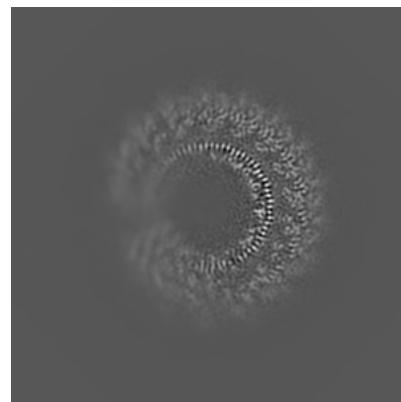
6.3.1 Primary map



X Index: 232

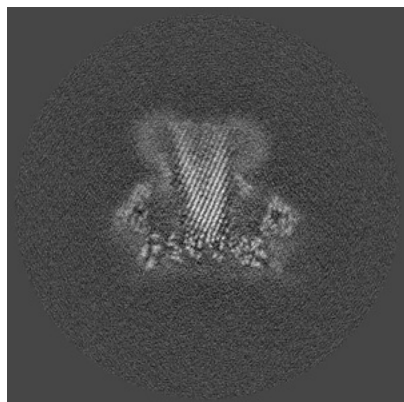


Y Index: 232

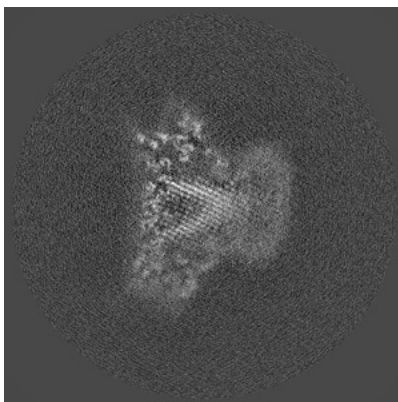


Z Index: 163

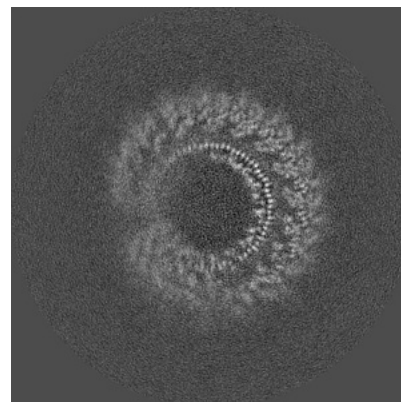
6.3.2 Raw map



X Index: 233



Y Index: 232

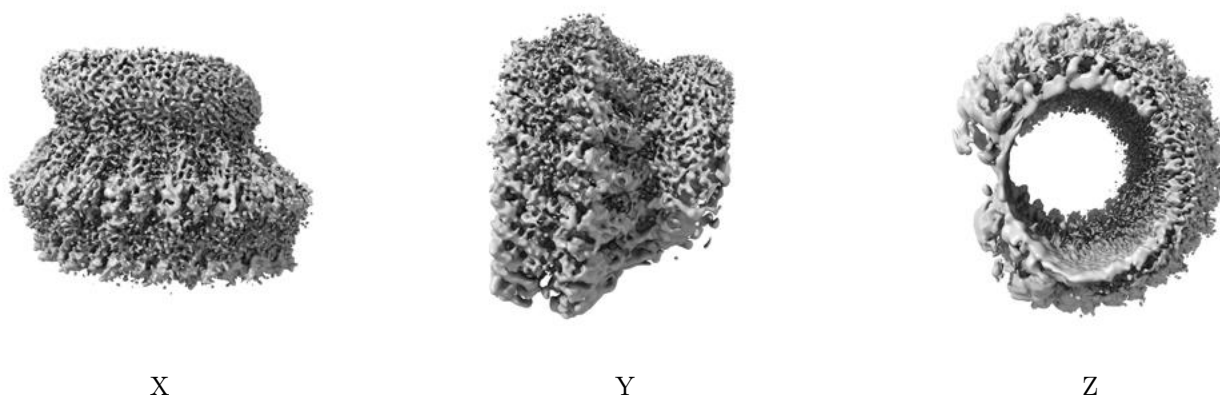


Z Index: 163

The images above show the largest variance slices of the map in three orthogonal directions.

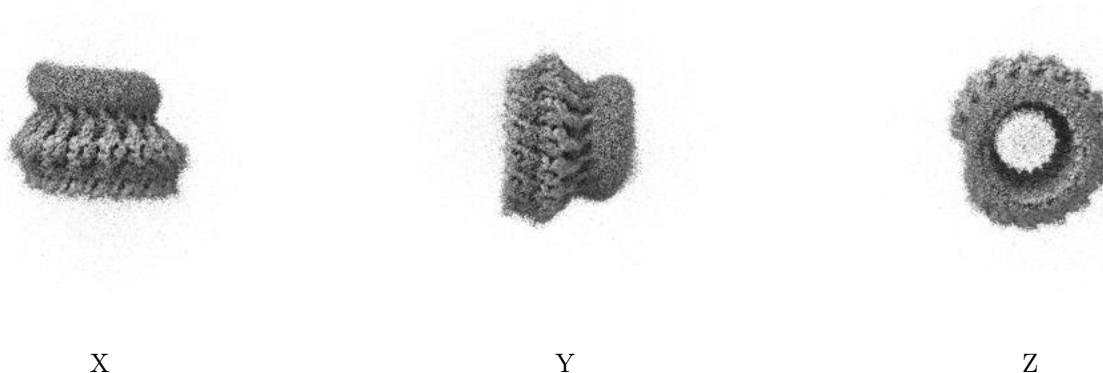
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

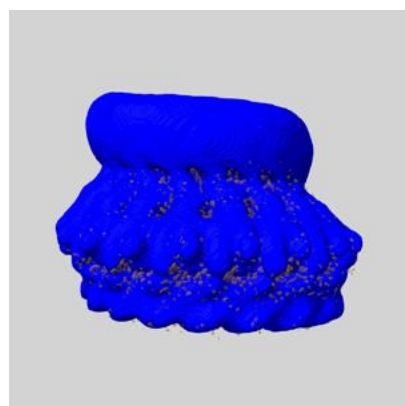
6.5 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

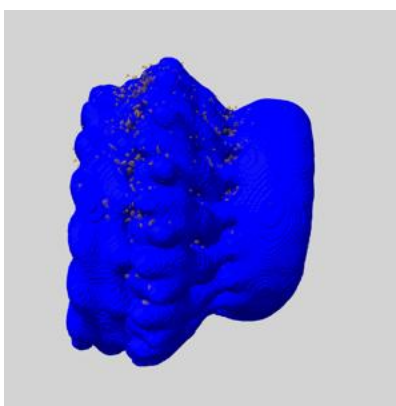
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

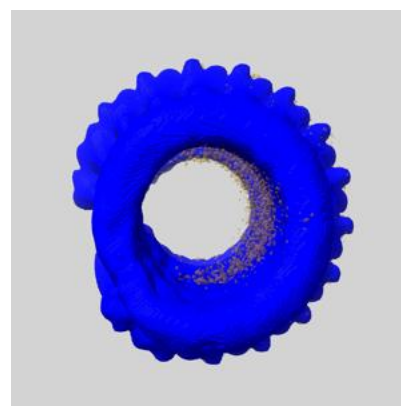
6.5.1 emd_15086_msk_1.map [i](#)



X



Y

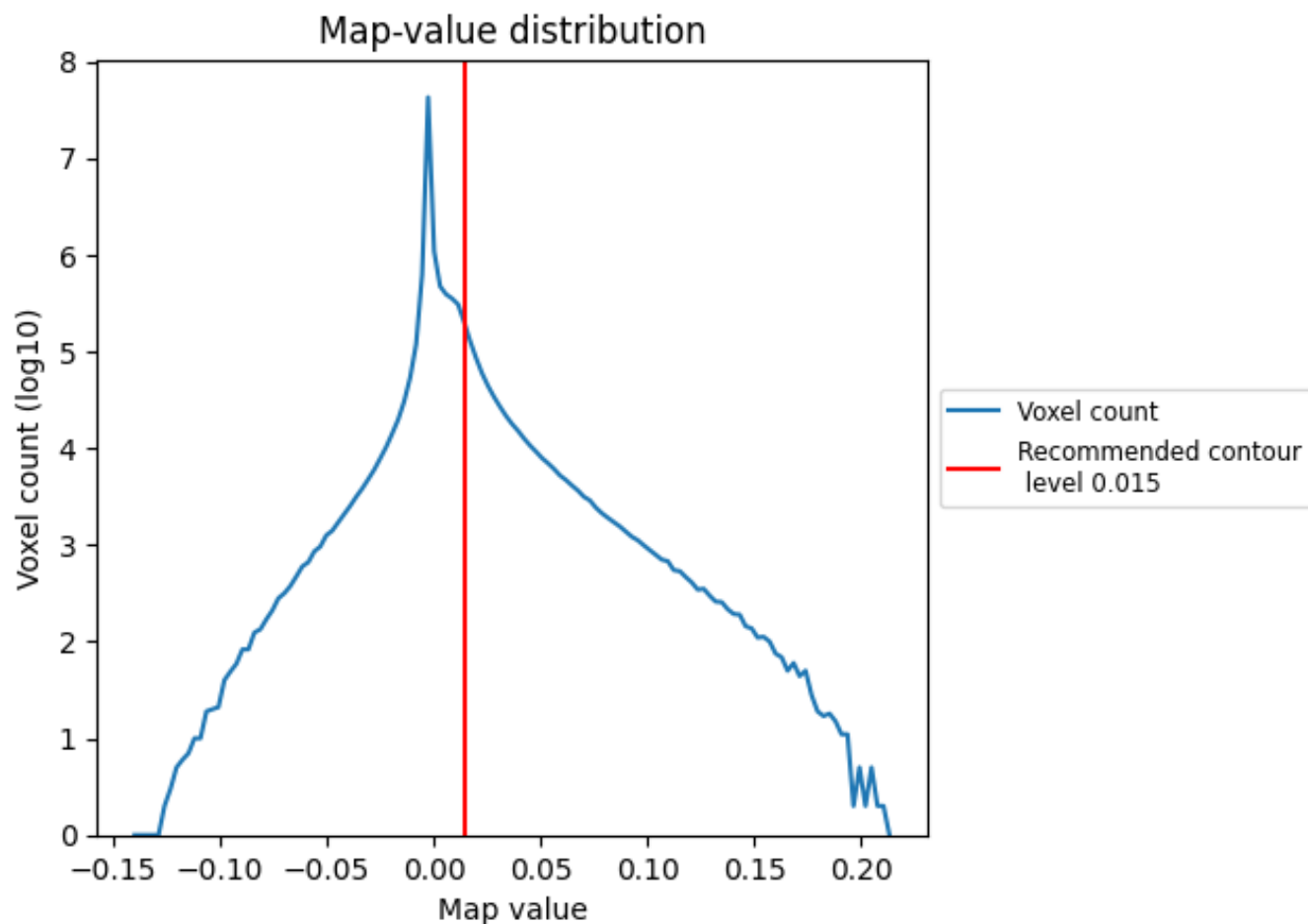


Z

7 Map analysis [i](#)

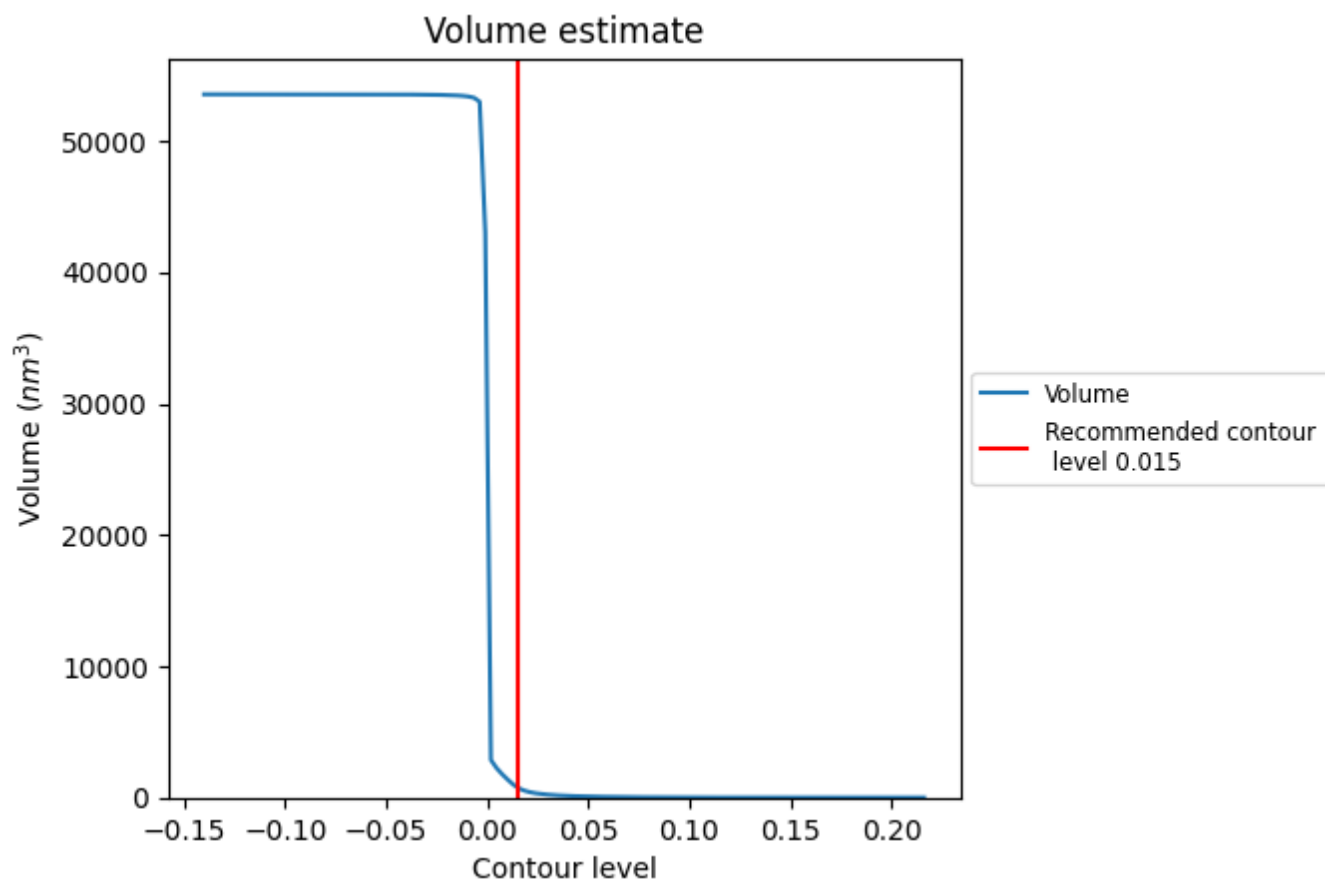
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

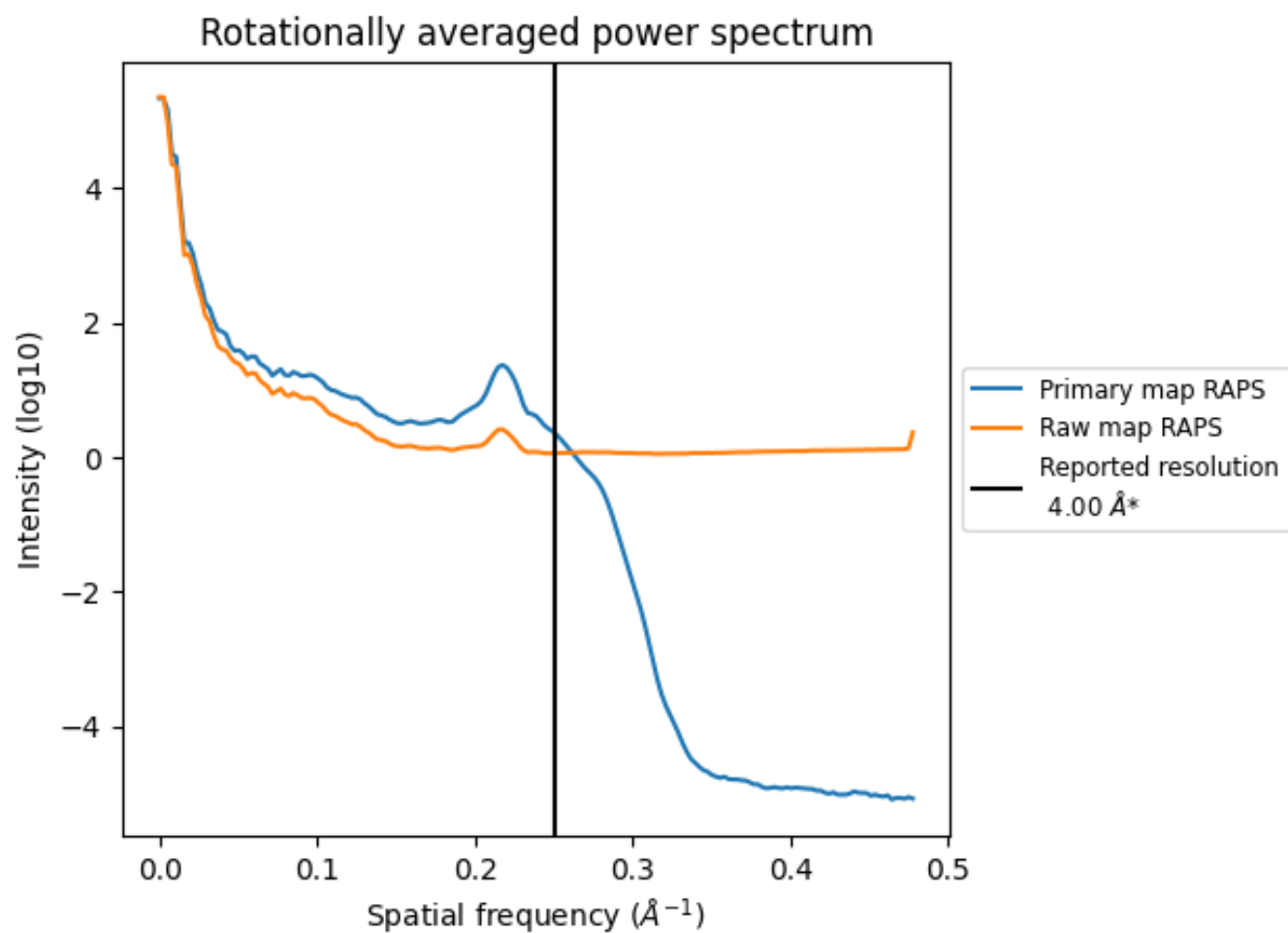
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 780 nm^3 ; this corresponds to an approximate mass of 705 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

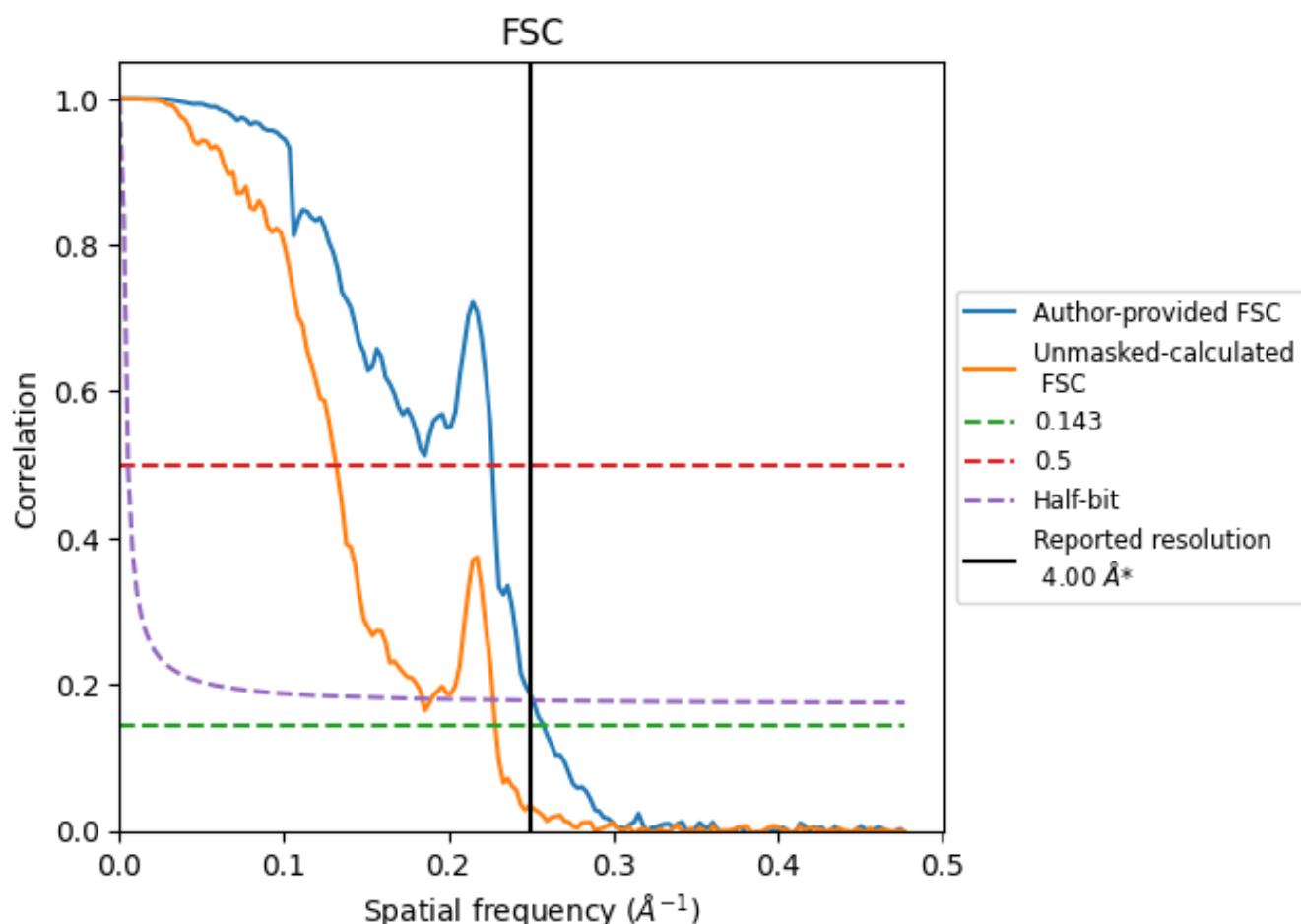


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

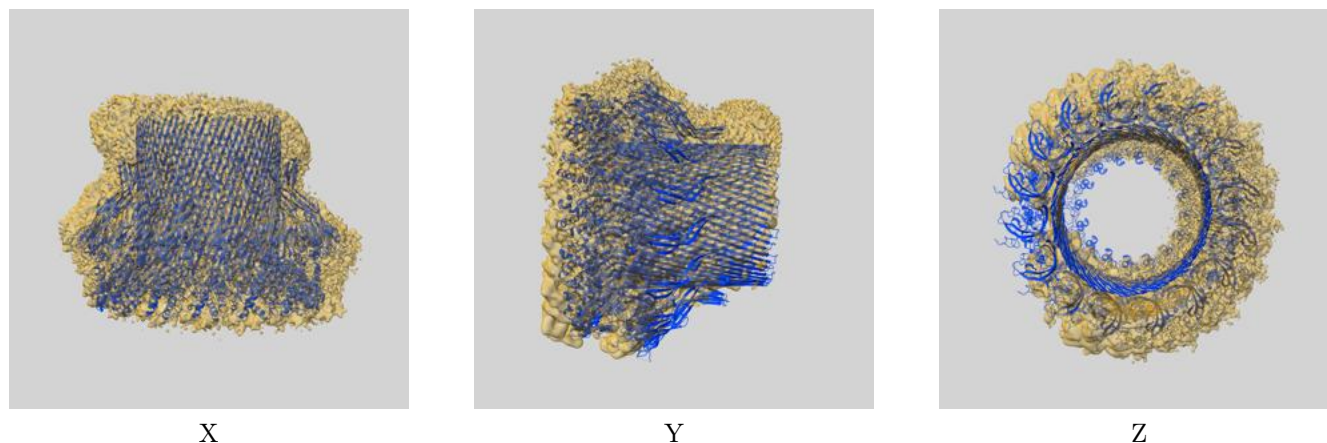
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	3.88	4.41	3.98
Unmasked-calculated*	4.38	7.59	5.43

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

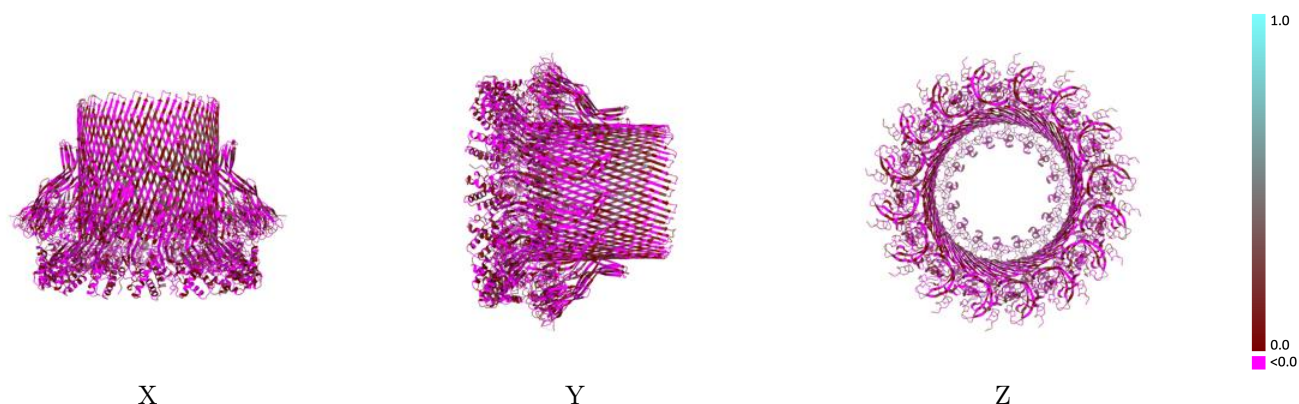
This section contains information regarding the fit between EMDB map EMD-15086 and PDB model 8A1S. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



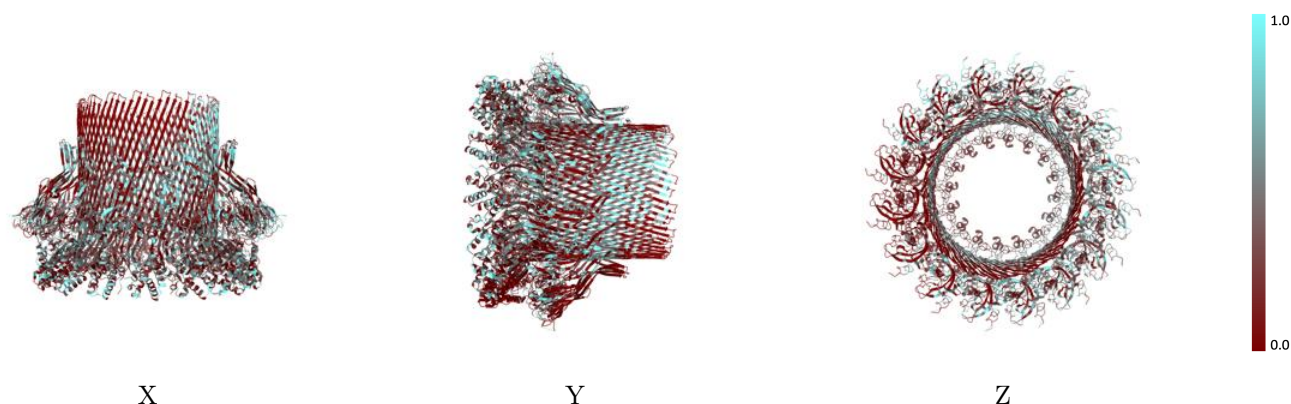
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



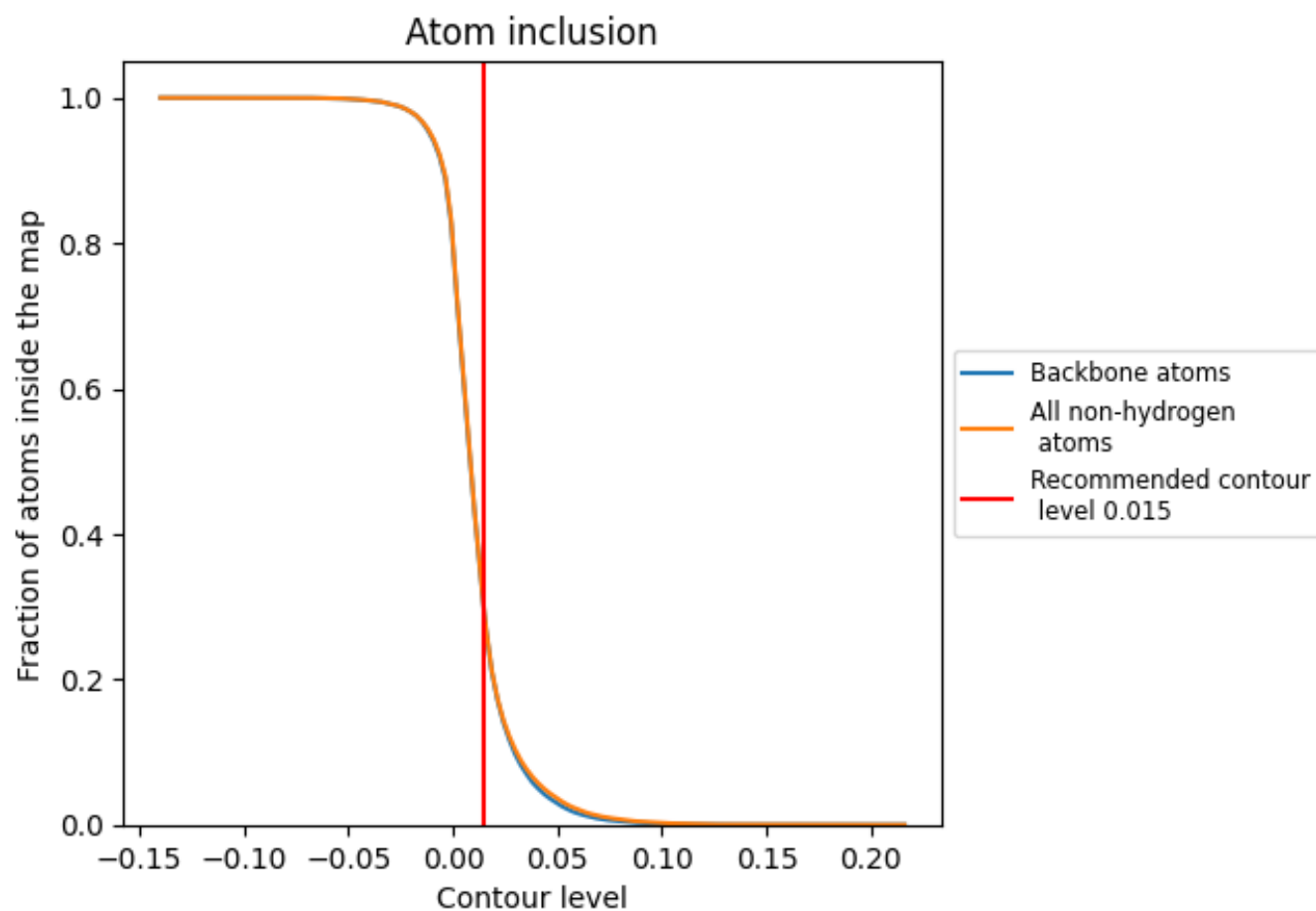
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).



































9.4 Atom inclusion [i](#)



At the recommended contour level, 29% of all backbone atoms, 29% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2902	 -0.0030
A	 0.3381	 0.0020
B	 0.2903	 -0.0010
C	 0.1599	 0.0190
D	 0.0613	 -0.0090
E	 0.1403	 -0.0090
F	 0.1806	 -0.0240
G	 0.2350	 -0.0150
H	 0.2825	 -0.0060
I	 0.3096	 0.0020
J	 0.3383	 -0.0070
K	 0.3683	 -0.0050
L	 0.3902	 -0.0050
M	 0.4062	 0.0080
N	 0.3835	 -0.0090
O	 0.4006	 0.0010
P	 0.3584	 0.0060

