



Full wwPDB EM Validation Report ⓘ

Jun 1, 2026 – 02:33 PM JST

PDB ID : 9X0Y / pdb_00009x0y
EMDB ID : EMD-66449
Title : Pseudomonas aeruginosa (PAO1) Outer membrane PilQ (Secretin) with SlkA in C14 symmetry
Authors : Kwon, O.; Lee, Y.; Ryu, B.; Yoo, Y.; Chung, J.; Cho, H.
Deposited on : 2025-09-30
Resolution : 2.68 Å(reported)
Based on initial model : .

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.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

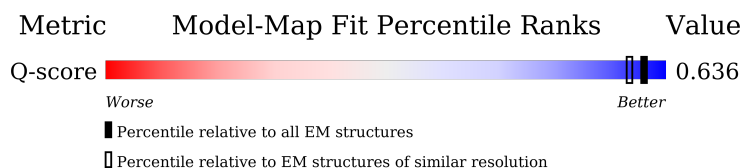
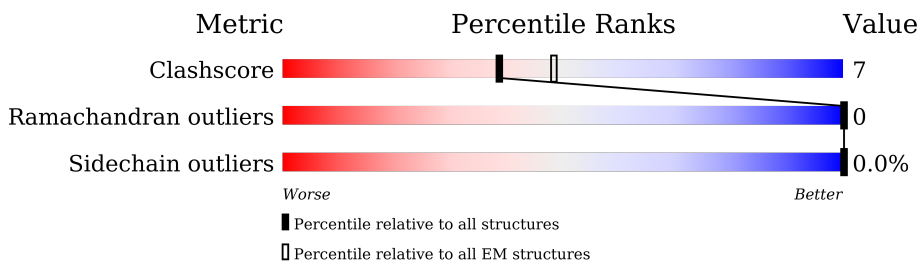
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.68 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.









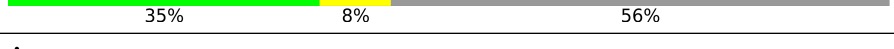
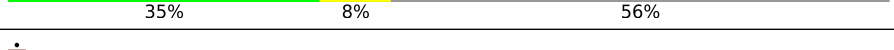
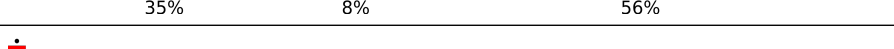
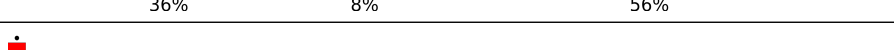

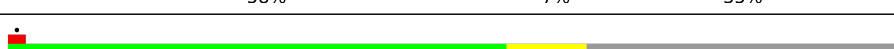


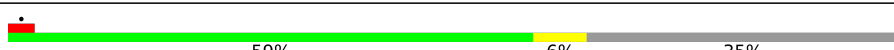





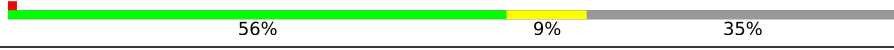



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	9255 (2.18 - 3.18)

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	714	
1	B	714	
1	C	714	
1	D	714	

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Mol	Chain	Length	Quality of chain
1	E	714	
1	F	714	
1	G	714	
1	H	714	
1	I	714	
1	J	714	
1	K	714	
1	L	714	
1	M	714	
1	N	714	
2	O	114	
2	P	114	
2	Q	114	
2	R	114	
2	S	114	
2	T	114	
2	U	114	
2	V	114	
2	W	114	
2	X	114	
2	Y	114	
2	Z	114	
2	a	114	
2	b	114	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 41454 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 Fimbrial assembly protein PilQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	B	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	C	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	D	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	E	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	F	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	G	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	H	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	I	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	J	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	K	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	L	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	M	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		
1	N	311	Total	C	N	O	S	0	0
			2389	1503	413	466	7		

- Molecule 2 is a protein called Multidrug transporter.

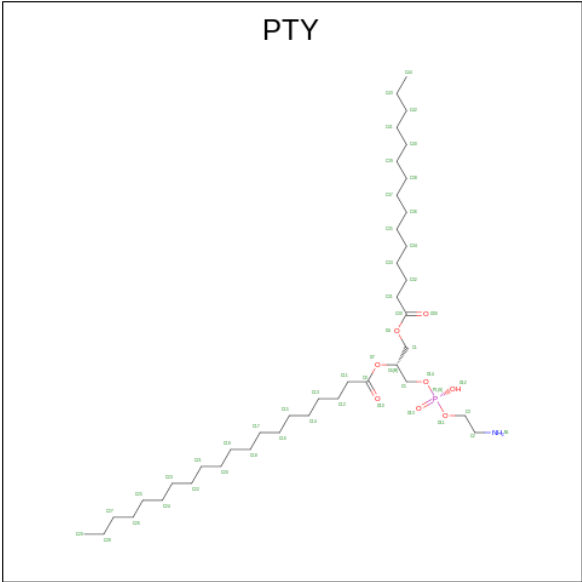
Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	74	Total	C	N	O	S	0	0
			522	340	83	95	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	Q	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	R	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	S	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	T	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	U	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	V	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	W	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	X	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	Y	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	Z	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	a	74	Total	C	N	O	S	0	0
			522	340	83	95	4		
2	b	74	Total	C	N	O	S	0	0
			522	340	83	95	4		

- Molecule 3 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).

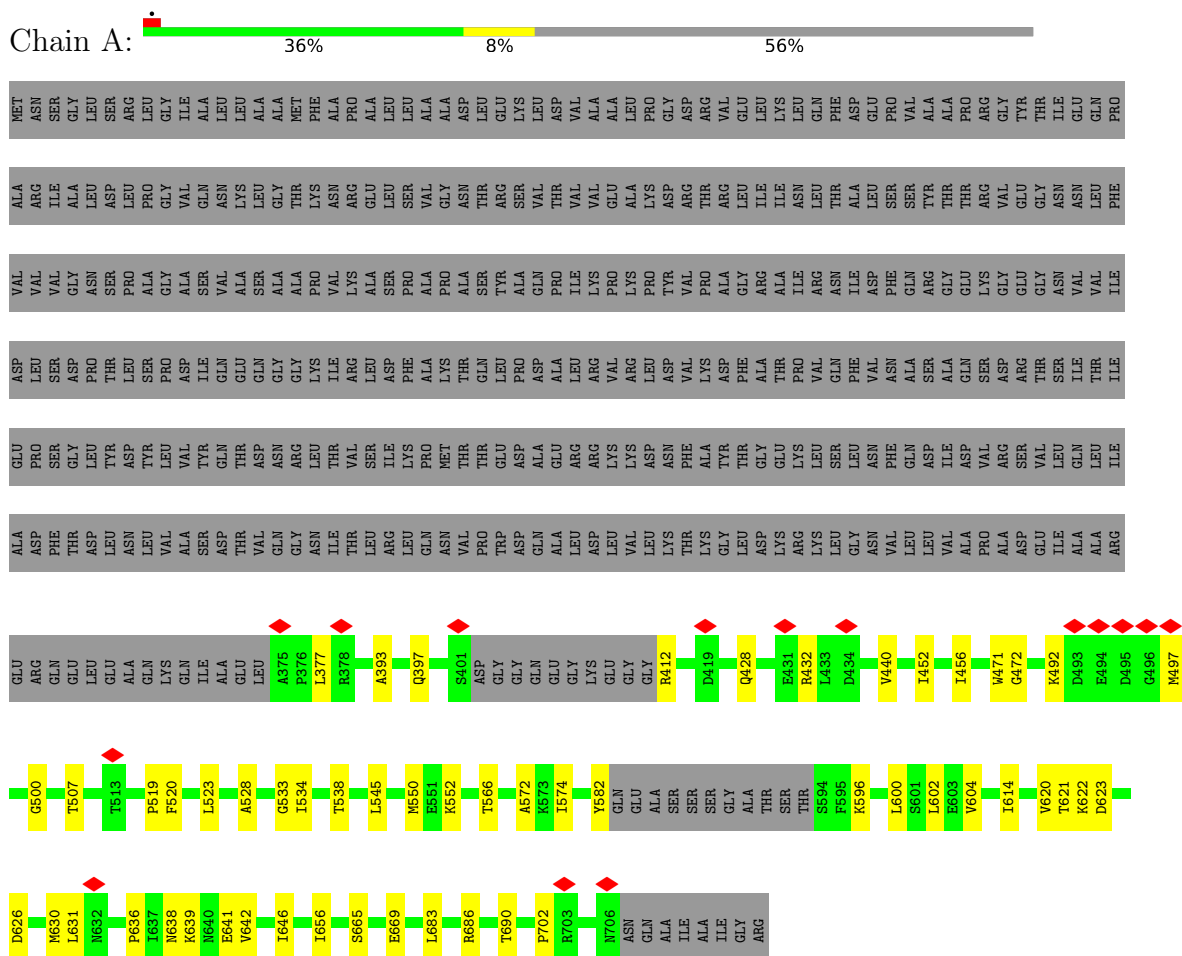


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	B	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	C	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	D	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	E	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	F	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	G	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	I	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	J	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	K	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	L	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

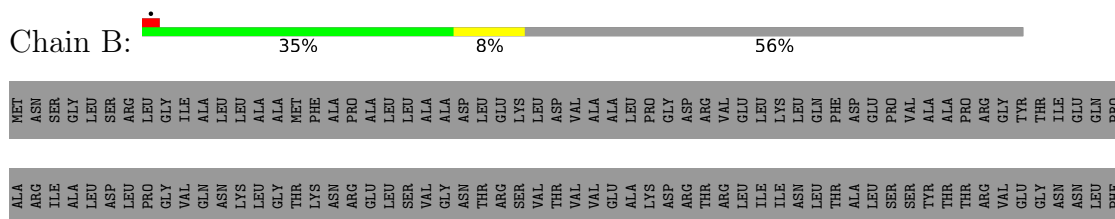
3 Residue-property plots

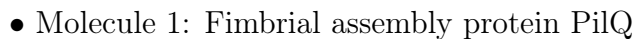
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Fimbrial assembly protein PilQ



• Molecule 1: Fimbrial assembly protein PilQ





M630	G600	GLU	ALA	GLU	ASP	PRO	GLU	ASP	LEU	VAL	ALA	MET
L631	T507	GLN	PHE	GLN	ASP	SER	SER	ILE	ARG	VAL	ARG	ASN
M632	T513	LEU	THR	LEU	THR	GLY	GLY	THR	ASP	GLY	ALA	GLY
P636		GLU	LEU	GLU	LEU	TYR	TYR	THR	SER	PRO	ASP	SER
I637		ALA	ASN	ALA	ASN	ASP	ASP	LEU	LEU	LEU	LEU	ARG
N638	P619	GLN	VAL	GLN	VAL	TYR	TYR	SER	ALA	PRO	PRO	LEU
K639	F520	LYS	VAL	LYS	VAL	VAL	VAL	PRO	GLY	GLY	GLY	ILE
M640	L523	ALA	ILE	ILE	SER	TYR	TYR	ILE	SER	SER	GLN	ALA
E641		ASP	ASP	ASP	ASP	GLN	GLN	GLY	GLY	VAL	ASN	LEU
V642	A528	GLU	THR	GLU	THR	THR	THR	THR	GLY	ALA	LYS	LEU
I646		LEU	THR	LEU	THR	GLN	GLN	GLY	GLY	ALA	ALA	LEU
I656	G533	VAL	GLN	VAL	GLN	ASP	ASP	GLN	SER	SER	LYS	LEU
I656	I634	GLY	ASN	GLY	GLY	ARG	ARG	GLY	GLY	ALA	THR	ALA
S665	T538	ILE	THR	ILE	ASN	THR	THR	THR	ILE	VAL	LYS	PHE
E669	L645	THR	THR	THR	THR	VAL	VAL	ARG	ARG	LYS	ASN	ALA
L674	M550	LEU	ARG	LEU	LEU	ILE	ILE	ASP	ASP	PRO	ALA	ALA
L683	E551	LEU	GLN	GLN	ASN	PRO	PRO	ALA	ALA	VAL	GLY	ALA
L683	K552	ASN	ASN	VAL	VAL	MET	MET	LYS	THR	PRO	GLY	ALA
R686	T566	ASP	VAL	ASP	ASP	THR	THR	THR	THR	ALA	ASN	ASP
D687	A572	GLY	TRP	GLY	TRP	THR	THR	GLN	GLN	SER	THR	LEU
T690	K573	GLN	GLN	GLN	GLN	ASP	ASP	PRO	ALA	ASP	SER	LYS
P702	I574	GLU	GLN	GLU	GLN	ALA	ALA	ALA	ALA	PRO	VAL	LEU
P702		GLY	ALA	GLY	ALA	GLU	GLU	ALA	ALA	PRO	THR	ASP
N706	Y582	LYS	ASP	LYS	ASP	ARG	ARG	ARG	ILE	VAL	VAL	VAL
ASN	GLN	GLU	LEU	GLU	LEU	LYS	LYS	VAL	VAL	ALA	ALA	ALA
GLN	ALA	GLY	VAL	VAL	VAL	LYS	LYS	ARG	ARG	GLY	GLY	ALA
SER	ALA	GLY	LEU	LEU	LEU	ASP	ASP	LEU	LEU	PRO	LYS	PRO
ILE	SER	LEU	LEU	LEU	LEU	ASN	ASN	ASP	ASP	TYR	ASP	GLY
ALA	SER	THR	THR	THR	THR	PHE	PHE	VAL	VAL	ARG	ARG	ASP
ILE	GLY	GLY	LYS	LYS	LYS	TYR	TYR	ASP	ALA	ARG	VAL	VAL
GLY	ALA	THR	ASP	ASP	THR	THR	THR	PHE	GLY	ILE	LEU	LEU
ARG	SER	THR	THR	THR	THR	GLY	GLY	ALA	ALA	ILE	LYS	LYS
						GLU	GLU	THR	THR	ILE	LEU	LEU
						LEU	LEU	THR	THR	ALA	ASP	PHE
						LEU	LEU	GLN	ASN	ARG	LEU	LEU
						LEU	LEU	GLN	ASN	THR	ASN	THR
						LEU	LEU	VAL	PHE	ASP	PRO	GLY
						LEU	LEU	VAL	ASP	THR	VAL	VAL
						LEU	LEU	GLN	ASN	THR	ALA	ALA
						LEU	LEU	ILE	ALA	THR	THR	PRO
						LEU	LEU	GLN	GLY	THR	ARG	ARG
						LEU	LEU	VAL	GLY	VAL	GLY	VAL
						LEU	LEU	ARG	ASP	GLY	GLY	TYR
						LEU	LEU	THR	THR	GLY	ASN	ILE
						LEU	LEU	GLN	ASN	ASN	ASN	GLN
						LEU	LEU	ILE	THR	VAL	VAL	GLN
						LEU	LEU	THR	THR	VAL	VAL	GLN
						LEU	LEU	THR	THR	VAL	VAL	GLN
						LEU	LEU	THR	THR	VAL	VAL	GLN

Chain D:



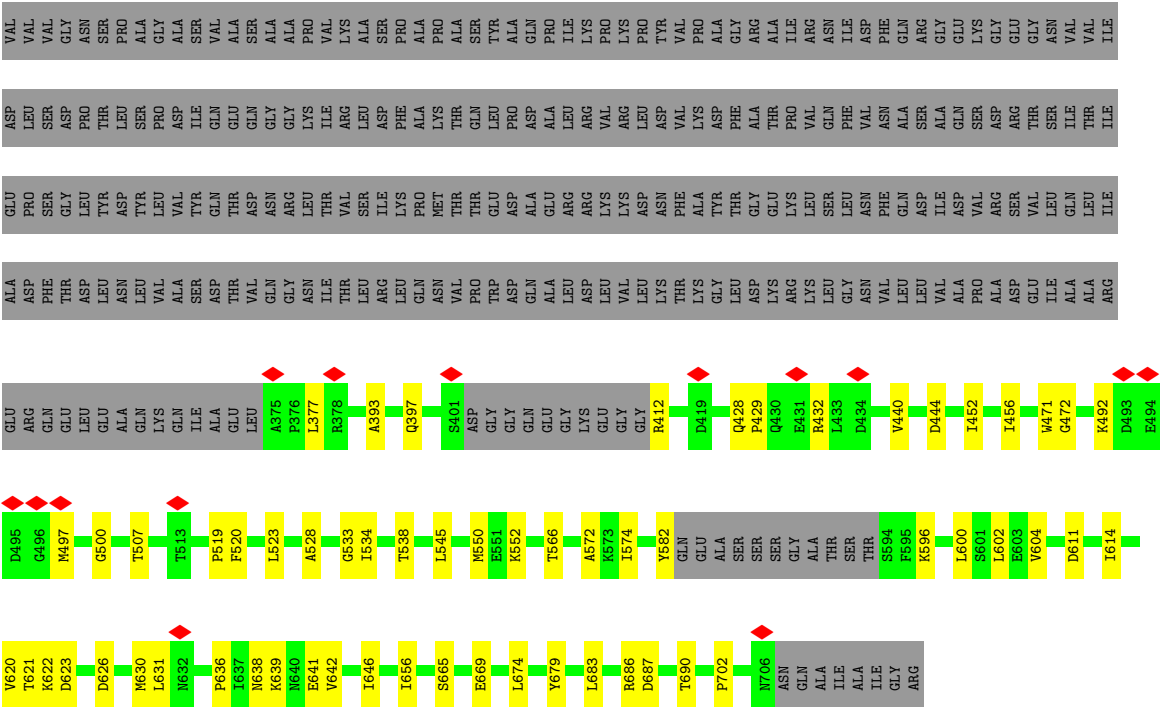
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M630	T513	PHE	ARG	ASP	ASP	ARG	LEU	LEU	SER	VAL	ARG	ASN
L631	S514	THR	GLN	PHE	THR	GLU	GLN	GLY	SER	VAL	ILE	SER
M632	S519	ASP	LEU	LEU	LEU	GLI	LEU	LEU	PRO	ASN	GLY	GLY
P636	F520	ASN	ALA	ASN	LEU	GLU	ALA	GLU	THR	PRO	ASP	SER
M637	L523	LEU	GLN	LEU	GLN	GLN	VAL	GLN	TYR	ASP	LEU	ARG
K638	L543	ALA	ILE	SER	ALA	ASP	VAL	VAL	ASP	GLY	GLY	ILE
K639	A528	ASP	GLU	ASP	THR	GLU	ALA	GLU	GLN	VAL	ASN	ALA
M640	G533	THR	LEU	THR	THR	GLU	THR	THR	GLN	VAL	ASN	LEU
E641	I534	VAL	LEU	VAL	GLN	GLY	GLN	ASN	GLN	SER	GLY	ALA
V642	I534	GLY	ASP	GLY	GLY	P376	ASP	ARG	GLY	ALA	THR	MET
L646	T538	ASN	ASN	ASN	ILE	L377	THR	LEU	ILE	VAL	PRO	PHE
L656	L543	THR	THR	THR	THR	R378	VAL	SER	ARG	LYS	ASN	ALA
S665	D544	LEU	LEU	LEU	LEU	A393	LEU	SER	ILE	ALA	GLU	PRO
S665	L545	ARG	LEU	LEU	LEU	Q397	ILE	ASP	PHE	SER	LEU	LEU
B669	M550	GLN	GLN	GLN	GLN	Q397	PRO	MET	ALA	ALA	VAL	ALA
L674	E551	ASN	ASN	VAL	VAL	S401	THR	THR	LYS	GLY	GLY	ALA
L674	K552	VAL	VAL	VAL	VAL	S401	THR	THR	THR	ALA	ASN	ASP
V679	T566	PRO	PRO	TRP	TRP	GLY	THR	GLU	GLN	SER	THR	GLU
L683	A572	ASP	ASP	GLN	GLN	GLY	ALA	ASP	PRO	ALA	SER	LYS
R686	R573	GLY	GLY	GLN	GLN	GLI	ALA	ALA	ASP	GLN	VAL	LEU
D687	I574	GLY	GLY	GLY	GLY	GLY	GLY	GLY	ALA	PRO	THR	ASP
T690	Y582	LYS	LYS	LEU	LEU	GLY	LEU	ASN	ASP	TYR	ASP	GLY
P702	GLN	THR	THR	THR	THR	R412	THR	ASN	ASP	VAL	ASP	ASP
W706	GLU	LYS	LYS	GLY	GLY	D419	ALA	ALA	VAL	THR	THR	ARG
ASN	SER	GLY	SER	SER	SER	Q428	ASP	THR	PHE	GLY	LEU	GLU
GLN	ALA	ALA	ALA	ALA	ALA	Q428	LEU	ASP	ALA	ARG	ILE	LEU
ILE	THR	SER	THR	THR	THR	R432	LYS	GLY	THR	ALA	ILE	LYS
ILE	THR	THR	THR	THR	THR	L433	ARG	GLY	THR	ALA	ILE	LYS
GLY	S594	THR	THR	THR	THR	D434	LYS	LYS	VAL	ARG	ASN	PHE
ARG	F595	GLY	GLY	GLY	GLY	I452	LEU	LEU	PHE	ASN	THR	GLU
	K596	ASN	ASN	VAL	VAL	I452	ASN	ASN	VAL	ASP	LEU	GLU
	L600	VAL	VAL	VAL	VAL	W471	PHE	ASN	ASN	PHE	SER	PRO
	S601	LEU	LEU	LEU	LEU	G472	GLN	ALA	ALA	THR	VAL	VAL
	L602	LEU	LEU	VAL	VAL	Y483	ILE	SER	SER	ARG	THR	ALA
	E603	VAL	VAL	ALA	ALA	Y483	ALA	ALA	ALA	GLY	THR	ALA
	V604	PRO	PRO	PRO	PRO	K492	GLN	GLN	GLN	LYS	THR	PRO
	D611	ALA	ALA	ALA	ALA	D493	ARG	VAL	SER	GLY	VAL	ARG
	I614	ASP	ASP	ASP	ASP	E494	SER	SER	ARG	GLY	GLY	TYR
	T621	ILE	ILE	ILE	ILE	D495	LEU	LEU	THR	ASN	GLY	ILE
	K622	ALA	ALA	ALA	ALA	G496	GLN	GLN	ILE	VAL	ASN	GLN
						M407	LEU	LEU	THR	VAL	LEU	GLN

Chain E:

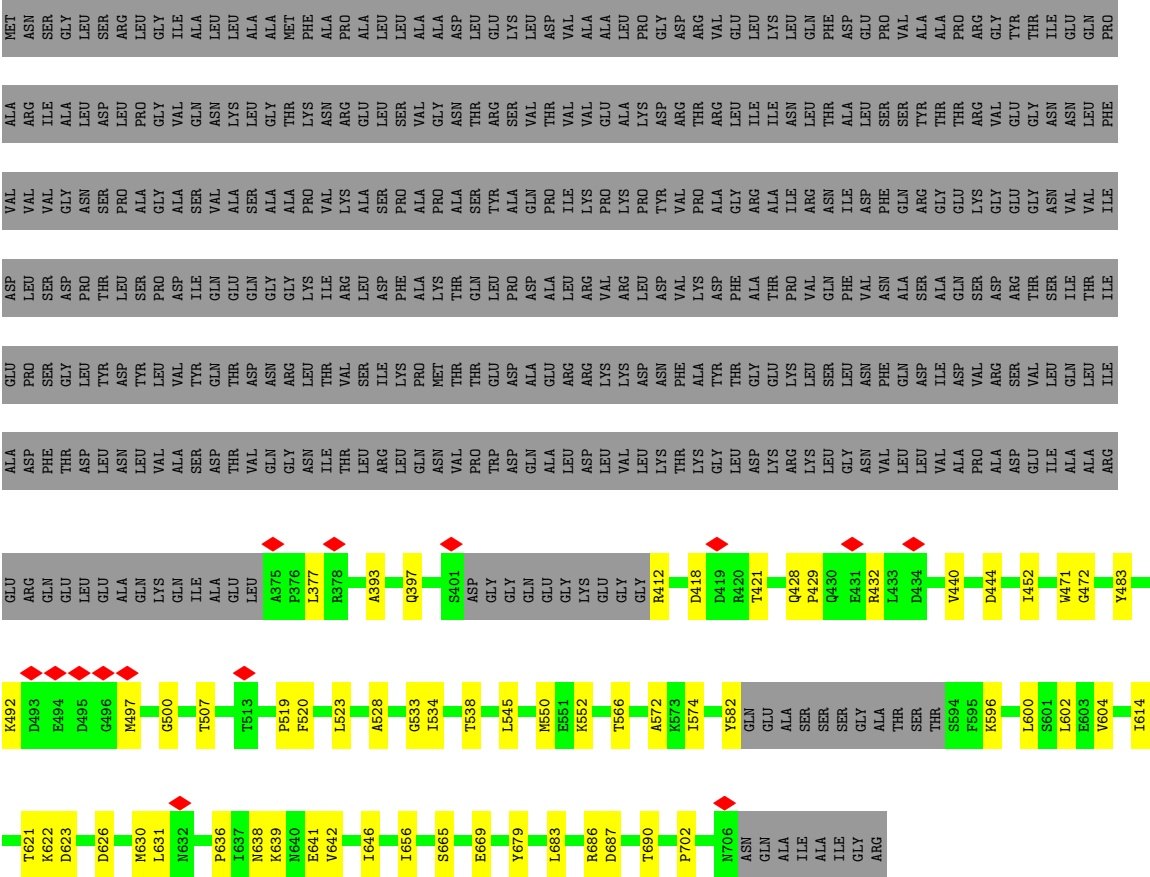
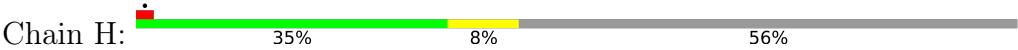


ALA	GLU	ASP	VAL	ALA	MET
ALA	PRO	LEU	VAL	ALA	ASN
PHE	SER	SER	SER	ILE	ASN
THR	GLY	ASP	VAL	ILE	GLY
LEU	LEU	PRO	GLY	LEU	LEU
ASN	TYR	THR	SER	ASP	SER
LEU	ASP	LEU	PRO	LEU	ARG
LEU	TYR	SER	ALA	PRO	LEU
VAL	LEU	PRO	GLY	GLY	GLY
ALA	VAL	ASP	ALA	VAL	ILE
SER	TYR	ILE	SER	GLN	ALA
ASP	GLN	GLN	VAL	ASN	LEU
THR	THR	GLU	ALA	LYS	LEU
GLN	ASP	GLN	SER	LEU	ALA
VAL	ASN	GLY	SER	GLY	ALA
GLN	ASN	GLY	ALA	THR	ALA
GLY	ARG	GLY	ALA	MET	PHE
ASN	LEU	LYS	PRO	LYS	PHE
ILE	THR	ILE	VAL	ASN	ALA
THR	VAL	ARG	LYS	ARG	PRO
LEU	SER	LEU	ALA	GLU	ALA
ARG	ILE	ASP	ALA	LEU	ALA
LEU	LYS	PHE	PRO	SER	LEU
LEU	PRO	ALA	ALA	VAL	ALA
GLN	MET	LYS	PRO	GLY	ALA
VAL	THR	THR	ALA	ASN	ASP
VAL	THR	GLN	SER	THR	LEU
TRP	GLU	LEU	SER	ARG	GLU
ASP	ASP	PRO	ALA	SER	LYS
GLN	ALA	ASP	GLN	VAL	LEU
ALA	GLU	ALA	PRO	THR	ASP
LEU	ARG	LEU	ILE	VAL	VAL
ASP	ARG	ARG	LYS	VAL	ALA
VAL	LYS	VAL	PRO	GLU	ALA
VAL	LYS	ARG	LYS	LEU	LEU
LEU	ASP	LEU	PRO	LYS	PRO
LYS	ASN	ASP	TYR	ASP	GLY
THR	PHE	VAL	VAL	ARG	ASP
LYS	ALA	LYS	PRO	THR	ARG
GLY	TYR	ASP	ALA	ARG	VAL
ASP	THR	PHE	GLY	LEU	GLU
LEU	GLY	ALA	ARG	ILE	LEU
LYS	GLU	THR	ALA	ILE	LYS
ARG	LYS	PRO	ILE	ASN	LEU
LYS	LEU	VAL	ARG	LEU	LEU
LEU	SER	GLN	ASN	THR	PHE
GLY	LEU	PHE	ILE	ALA	ASP
ASN	ASN	VAL	ASP	LEU	GLU
VAL	PHE	ASN	PHE	SER	PRO
LEU	GLN	ALA	VAL	SER	VAL
LEU	ASP	SER	ARG	TYR	ALA
VAL	ILE	ALA	GLY	THR	ALA
ALA	ASP	GLN	GLU	THR	PRO
PRO	VAL	SER	LYS	ARG	ARG
ASP	ARG	THR	GLY	VAL	GLY
GLU	VAL	ARG	GLU	GLU	TYR
ILE	LEU	SER	ASN	ASN	ILE
ALA	GLN	ILE	VAL	ASN	GLU
ALA	LEU	THR	VAL	LEU	GLN
ALA	THR	THR	VAL	THR	ALA





● Molecule 1: Fimbrial assembly protein PilQ



Chain I:

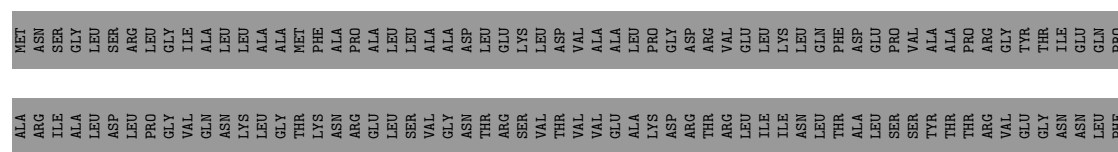


K492	I614	ALA	GLU	GLY	ASP	ALA	GLU	ASP	PRO	GLY	ASP	LEU	VAL	ALA	MET
D493	T621	PHE	ARG	GLN	THR	THR	GLY	THR	GLY	GLY	SER	SER	VAL	ARG	ASN
E494	D623	THR	GLU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	ASP	ASP	ASN	ILE	GLY
D495	D623	LEU	GLU	GLU	LEU	LEU	GLY	LEU	TYR	THR	THR	LEU	SER	LEU	SER
G496	D626	ALA	ALA	ALA	ASN	ASN	ALA	ASN	ASP	ASP	LEU	LEU	PRO	LEU	ARG
M497	D630	THR	GLN	GLN	VAL	VAL	GLN	VAL	TYR	TYR	SER	SER	ALA	LEU	LEU
G500	M630	VAL	LYS	LYS	VAL	VAL	VAL	VAL	LEU	PRO	ASP	GLY	GLY	GLY	ILE
T507	M631	SER	ILE	ILE	SER	ALA	GLN	ASP	TYR	TYR	ILE	GLN	VAL	GLN	ALA
T513	M632	THR	GLU	GLU	THR	THR	THR	THR	THR	THR	GLY	GLY	VAL	ASN	LEU
A375	P636	VAL	LEU	LEU	VAL	GLN	ASP	ASN	ASP	ASP	GLN	GLY	SER	LYS	LEU
P376	I637	GLN	A375	A375	GLN	GLN	ASN	GLY	THR	THR	GLY	GLY	ALA	THR	ALA
F520	M638	ASN	P376	P376	ASN	GLY	ARG	ARG	LEU	LEU	GLY	GLY	ALA	LYS	THR
K377	K639	ILE	L377	L377	ILE	ILE	THR	THR	THR	THR	ILE	ILE	VAL	PRO	THR
R378	M640	THR	R378	R378	THR	THR	VAL	VAL	VAL	VAL	ARG	ARG	LYS	VAL	ALA
A393	V642	LEU	A393	A393	LEU	LEU	SER	SER	SER	SER	LEU	LEU	ALA	GLY	ALA
A528	V646	LEU	ILE	ILE	ARG	ILE	ARG	ILE	LYS	PHE	PHE	PHE	ALA	VAL	PRO
G533	I646	GLN	Q397	Q397	GLN	PRO	PRO	PRO	PRO	ASP	ASP	GLN	VAL	GLY	ASN
I534	I656	ASN	S401	S401	ASN	GLN	MET	MET	LYS	LYS	THR	THR	PRO	GLY	ALA
T338	S665	VAL	ASP	ASP	VAL	VAL	THR	THR	THR	THR	THR	GLN	ASN	ASN	ASP
L543	E669	PRO	GLY	GLY	TRP	TRP	THR	THR	GLY	GLY	LEU	SER	SER	THR	LEU
D544	L674	GLN	GLY	GLN	GLN	GLN	ALA	ALA	ALA	ASP	ASP	GLN	VAL	VAL	LYS
L545	L674	GLY	GLY	GLY	ALA	ALA	GLY	GLY	GLY	ALA	ALA	PRO	VAL	THR	ASP
M550	L683	LEU	LYS	LYS	LEU	LEU	ARG	ARG	ARG	ARG	VAL	ILE	VAL	VAL	VAL
E551	R686	GLU	GLY	GLY	LEU	LEU	GLY	GLY	VAL	VAL	ARG	LYS	GLY	GLY	ALA
K552	D687	GLY	GLY	GLY	LEU	LEU	ASN	ASN	LYS	LYS	LEU	PRO	LYS	ALA	LEU
T566	T690	LYS	R412	R412	LYS	LYS	ASN	ASP	ASP	ASP	VAL	TYR	ARG	ASP	GLY
A572	P702	THR	D418	D418	THR	THR	PHE	VAL	VAL	VAL	ARG	ARG	THR	ASP	GLY
R573	M706	LYS	D419	D419	LYS	LYS	ALA	ALA	ALA	ASP	LYS	PRO	THR	THR	ARG
I574	ASN	GLY	R420	R420	GLY	GLY	TYR	TYR	TYR	ASP	ASP	ALA	ARG	ARG	VAL
Y552	GLN	ASP	T421	T421	ASP	ASP	GLY	GLY	GLY	ALA	ALA	ARG	ILE	ILE	LEU
GLN	ALA	LYS	Q428	Q428	LYS	ARG	GLU	GLU	GLU	THR	THR	ALA	ILE	ILE	LYS
GLU	GLY	ARG	P429	P429	LYS	LYS	LYS	LEU	LEU	PRO	PRO	ILE	ASN	ASN	LEU
ALA	ILE	LEU	Q430	Q430	LEU	LEU	SER	SER	SER	VAL	VAL	ARG	THR	THR	LEU
SER	ALA	LEU	E431	E431	GLY	LEU	LEU	PHE	PHE	ASP	ASP	ILE	ALA	ALA	PHE
SER	ILE	SER	R432	R432	ASN	ASN	ASN	VAL	VAL	ASN	ASN	PHE	GLN	GLN	SER
ILE	GLY	GLY	L433	L433	VAL	LEU	PHE	GLN	GLN	ALA	ALA	VAL	ARG	SER	LEU
GLY	ARG	ALA	D434	D434	LEU	LEU	LEU	GLN	ASP	ALA	ALA	GLY	THR	THR	GLY
THR	THR	THR	V440	V440	VAL	VAL	VAL	ILE	ILE	ALA	ALA	GLY	THR	THR	ARG
SER	THR	SER	D444	D444	ALA	PRO	PRO	ALA	VAL	VAL	VAL	GLN	THR	VAL	ARG
S594	F595	THR	Y442	Y442	ALA	ALA	ARG	ARG	ARG	ASP	ASP	GLY	VAL	VAL	GLY
F595	K596	THR	I452	I452	ASP	ASP	VAL	VAL	SER	ARG	ARG	THR	GLY	GLY	THR
K596	L600	GLU	W471	W471	GLU	ILE	SER	SER	LEU	THR	THR	ILE	ASN	ASN	ILE
L600	S601	ILE	G472	G472	ILE	ALA	GLN	GLN	LEU	ILE	ILE	GLN	ASN	ASN	THR
S601	L602	ALA			ALA	ALA	LEU	LEU	THR	THR	THR	THR	GLN	GLN	PRO
L602		ASP			ASP	ASP	THR	THR	THR	THR	THR	THR	THR	THR	THR

Chain J:

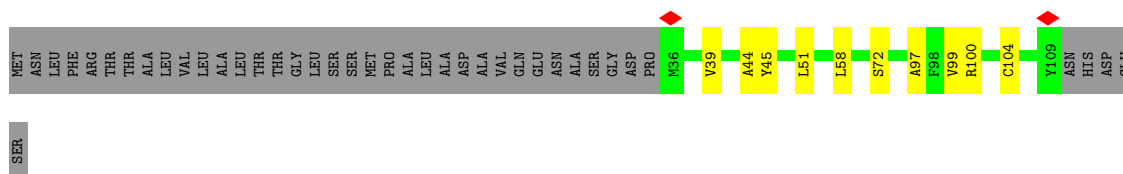


ALA	GLU	ASP	VAL	ALA	MET
PRO	PRO	LEU	VAL	ARG	ASN
SER	SER	SER	VAL	ILE	ASN
GLY	GLY	ASP	GLY	ALA	GLY
LEU	LEU	PRO	ASN	LEU	LEU
TYR	TYR	THR	SER	ASP	SER
ASP	ASP	LEU	PRO	LEU	ARG
TYR	TYR	SER	ALA	PRO	LEU
LEU	LEU	PRO	GLY	GLY	GLY
VAL	VAL	ASP	ALA	VAL	ILE
VAL	VAL	ILE	SER	GLN	ALA
TYR	TYR	ILE	SER	ASN	LEU
GLN	GLN	GLN	VAL	VAL	ALA
THR	THR	GLU	ALA	LYS	LEU
ASP	ASP	GLN	SER	LEU	ALA
ASN	ASN	GLY	ALA	GLY	ALA
GLY	ARG	GLY	ALA	THR	MET
ASN	LEU	LYS	PRO	LYS	PHE
LEU	THR	ILE	VAL	VAL	ALA
THR	VAL	ARG	LYS	ARG	PRO
SER	SER	LEU	ALA	GLU	ALA
ARG	ILE	ASP	SER	LEU	LEU
LYS	LYS	PHE	PRO	SER	LEU
PRO	PRO	ALA	ALA	VAL	ALA
MET	MET	LYS	PRO	GLY	ALA
THR	THR	THR	ALA	ASN	ASP
THR	GLU	GLN	SER	THR	GLU
GLU	GLU	LEU	TYR	ARG	LYS
ASP	ASP	PRO	ALA	SER	LYS
ALA	ALA	ASP	GLN	VAL	LEU
GLU	GLU	ALA	PRO	THR	ASP
ARG	ARG	LEU	ILE	VAL	ALA
ARG	LYS	ARG	LYS	VAL	ALA
LYS	LYS	VAL	PRO	GLU	ALA
VAL	VAL	ARG	LYS	ALA	LEU
LEU	LEU	ASP	PRO	LYS	PRO
LYS	ASN	ASP	TYR	ASP	GLY
THR	PHE	VAL	VAL	ARG	ASP
LYS	TYR	LYS	PRO	THR	ARG
GLY	TYR	ASP	ALA	ARG	VAL
LEU	THR	PHE	GLY	LEU	LEU
ASP	GLY	ALA	ARG	ILE	LEU
LYS	GLU	THR	ALA	ILE	LYS
ARG	LYS	PRO	ILE	ASN	LEU
LYS	SER	VAL	ARG	LEU	LEU
LEU	SER	GLN	ASN	THR	PHE
GLY	LEU	PHE	ILE	ALA	ASP
ASN	ASN	VAL	ASP	LEU	GLU
VAL	PHE	ASN	PHE	SER	PRO
LEU	GLN	ALA	GLN	SER	VAL
LEU	ASP	SER	ARG	TYR	ALA
VAL	ILE	ALA	GLY	THR	ALA
ALA	ASP	GLN	LYS	ARG	PRO
PRO	ARG	SER	GLY	VAL	GLY
ASP	SER	ARG	GLU	GLY	TYR
GLU	VAL	THR	GLY	GLY	ILE
ILE	LEU	SER	ASN	ASN	ILE
ALA	GLN	ILE	VAL	VAL	GLU
ALA	LEU	THR	ILE	LEU	ASN
ALA	THR	ILE	THR	VAL	GLN
ALA	THR	ILE	THR	THR	PHE

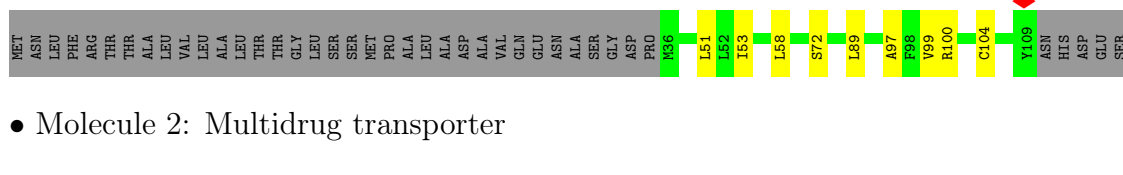




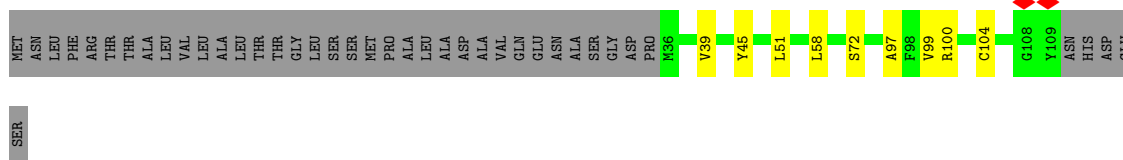




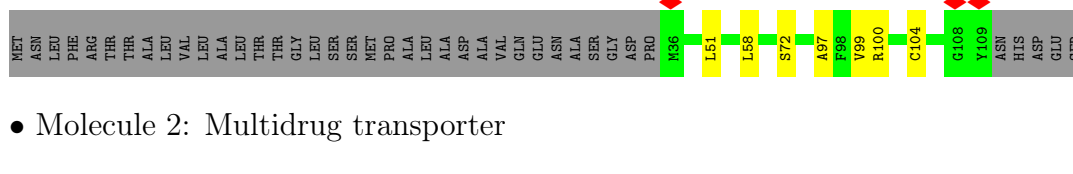
- Molecule 2: Multidrug transporter



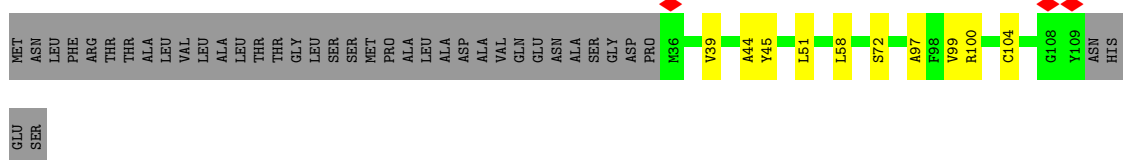
- Molecule 2: Multidrug transporter



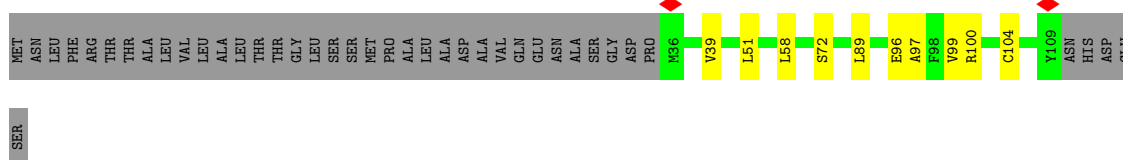
- Molecule 2: Multidrug transporter



- Molecule 2: Multidrug transporter

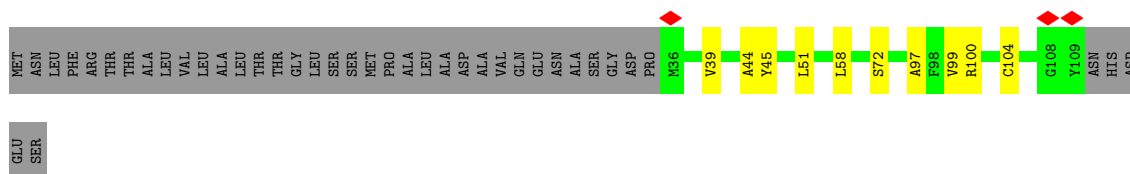


- Molecule 2: Multidrug transporter



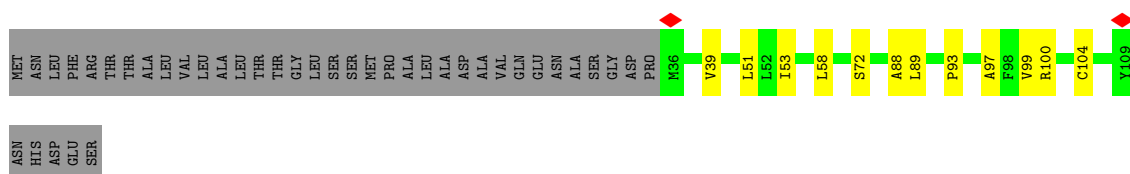
- Molecule 2: Multidrug transporter

Chain W: 



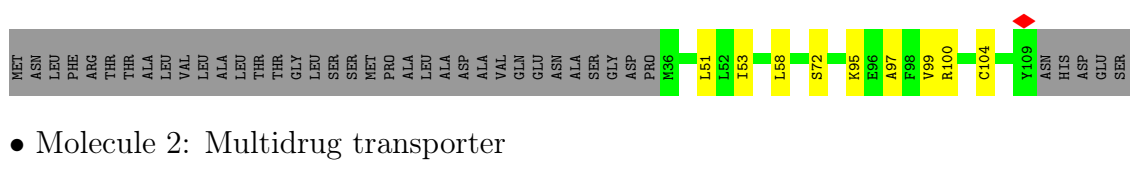
- Molecule 2: Multidrug transporter

Chain X: 



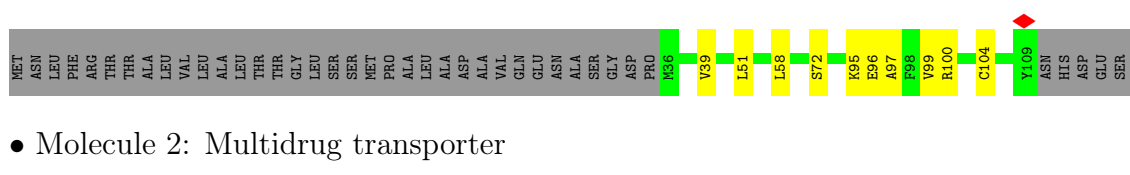
- Molecule 2: Multidrug transporter

Chain Y: 



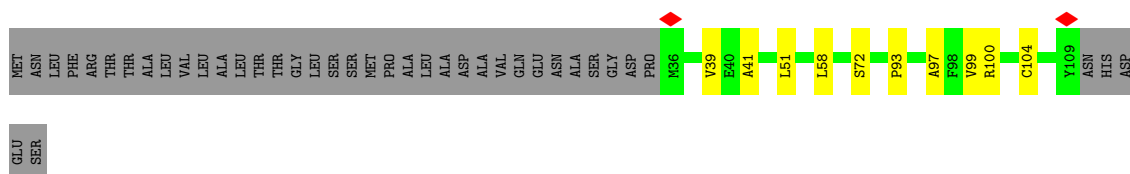
- Molecule 2: Multidrug transporter

Chain Z: 



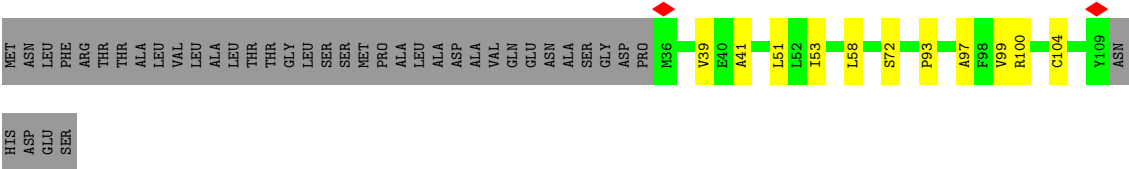
- Molecule 2: Multidrug transporter

Chain a: 



- Molecule 2: Multidrug transporter

Chain b: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63311	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.1	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.466	Depositor
Minimum map value	-0.837	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.045	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	413.1, 413.1, 413.1	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.81, 0.81, 0.81	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	0/2425	0.36	0/3282
1	B	0.15	0/2425	0.36	0/3282
1	C	0.15	0/2425	0.36	0/3282
1	D	0.15	0/2425	0.36	0/3282
1	E	0.15	0/2425	0.36	0/3282
1	F	0.15	0/2425	0.36	0/3282
1	G	0.15	0/2425	0.36	0/3282
1	H	0.15	0/2425	0.36	0/3282
1	I	0.15	0/2425	0.36	0/3282
1	J	0.15	0/2425	0.36	0/3282
1	K	0.15	0/2425	0.36	0/3282
1	L	0.15	0/2425	0.36	0/3282
1	M	0.15	0/2425	0.36	0/3282
1	N	0.15	0/2425	0.36	0/3282
2	O	0.42	0/533	0.54	0/728
2	P	0.42	0/533	0.54	0/728
2	Q	0.42	0/533	0.55	0/728
2	R	0.42	0/533	0.55	0/728
2	S	0.42	0/533	0.54	0/728
2	T	0.42	0/533	0.54	0/728
2	U	0.42	0/533	0.55	0/728
2	V	0.42	0/533	0.54	0/728
2	W	0.42	0/533	0.54	0/728
2	X	0.42	0/533	0.54	0/728
2	Y	0.42	0/533	0.54	0/728
2	Z	0.42	0/533	0.55	0/728
2	a	0.42	0/533	0.54	0/728
2	b	0.42	0/533	0.54	0/728
All	All	0.22	0/41412	0.40	0/56140

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2389	0	2422	40	0
1	B	2389	0	2422	44	0
1	C	2389	0	2422	40	0
1	D	2389	0	2422	44	0
1	E	2389	0	2422	43	0
1	F	2389	0	2422	44	0
1	G	2389	0	2422	45	0
1	H	2389	0	2422	45	0
1	I	2389	0	2422	46	0
1	J	2389	0	2422	41	0
1	K	2389	0	2422	41	0
1	L	2389	0	2422	44	0
1	M	2389	0	2422	44	0
1	N	2389	0	2422	42	0
2	O	522	0	532	6	0
2	P	522	0	532	7	0
2	Q	522	0	532	10	0
2	R	522	0	532	7	0
2	S	522	0	532	7	0
2	T	522	0	532	5	0
2	U	522	0	532	9	0
2	V	522	0	532	8	0
2	W	522	0	532	10	0
2	X	522	0	532	12	0
2	Y	522	0	532	8	0
2	Z	522	0	532	10	0
2	a	522	0	532	10	0
2	b	522	0	532	10	0
3	A	50	0	79	3	0
3	B	50	0	79	1	0
3	C	50	0	79	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	50	0	79	2	0
3	E	50	0	79	2	0
3	F	50	0	79	1	0
3	G	50	0	79	2	0
3	H	50	0	79	3	0
3	I	50	0	79	2	0
3	J	50	0	79	1	0
3	K	50	0	79	3	0
3	L	50	0	79	2	0
3	M	50	0	79	2	0
3	N	50	0	79	1	0
All	All	41454	0	42462	610	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 7.

All (610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:51:LEU:HD11	2:X:72:SER:HB3	1.58	0.85
2:V:51:LEU:HD11	2:W:72:SER:HB3	1.56	0.85
2:Z:51:LEU:HD11	2:a:72:SER:HB3	1.68	0.75
2:T:51:LEU:HD11	2:U:72:SER:HB3	1.70	0.74
1:M:497:MET:HE3	1:M:497:MET:HA	1.71	0.73
1:L:497:MET:HE3	1:L:497:MET:HA	1.71	0.73
1:N:497:MET:HE3	1:N:497:MET:HA	1.71	0.73
1:J:497:MET:HE3	1:J:497:MET:HA	1.71	0.73
1:K:497:MET:HE3	1:K:497:MET:HA	1.71	0.73
1:A:497:MET:HE3	1:A:497:MET:HA	1.71	0.73
1:I:497:MET:HE3	1:I:497:MET:HA	1.71	0.73
1:H:497:MET:HE3	1:H:497:MET:HA	1.71	0.73
1:B:497:MET:HA	1:B:497:MET:HE3	1.71	0.72
1:G:497:MET:HE3	1:G:497:MET:HA	1.71	0.72
2:Q:51:LEU:HD11	2:R:72:SER:HB3	1.72	0.72
2:U:51:LEU:HD11	2:V:72:SER:HB3	1.70	0.72
1:C:497:MET:HE3	1:C:497:MET:HA	1.71	0.72
1:F:497:MET:HE3	1:F:497:MET:HA	1.71	0.72
1:E:497:MET:HE3	1:E:497:MET:HA	1.71	0.72
1:D:497:MET:HE3	1:D:497:MET:HA	1.71	0.72
2:P:51:LEU:HD11	2:Q:72:SER:HB3	1.73	0.71
2:O:51:LEU:HD11	2:P:72:SER:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:51:LEU:HD11	2:Z:72:SER:HB3	1.74	0.69
2:S:51:LEU:HD11	2:T:72:SER:HB3	1.76	0.68
1:G:432:ARG:HG3	1:G:432:ARG:HH11	1.58	0.68
1:F:432:ARG:HG3	1:F:432:ARG:HH11	1.58	0.68
1:C:432:ARG:HG3	1:C:432:ARG:HH11	1.58	0.68
1:B:432:ARG:HG3	1:B:432:ARG:HH11	1.58	0.68
1:H:432:ARG:HG3	1:H:432:ARG:HH11	1.58	0.67
1:E:432:ARG:HH11	1:E:432:ARG:HG3	1.58	0.67
1:L:432:ARG:HG3	1:L:432:ARG:HH11	1.58	0.67
1:M:432:ARG:HG3	1:M:432:ARG:HH11	1.58	0.67
1:D:432:ARG:HG3	1:D:432:ARG:HH11	1.58	0.67
1:N:432:ARG:HG3	1:N:432:ARG:HH11	1.58	0.67
1:K:432:ARG:HG3	1:K:432:ARG:HH11	1.58	0.67
1:J:432:ARG:HH11	1:J:432:ARG:HG3	1.58	0.67
2:a:51:LEU:HD11	2:b:72:SER:HB3	1.78	0.66
1:A:432:ARG:HG3	1:A:432:ARG:HH11	1.58	0.66
1:L:452:ILE:HG21	1:L:604:VAL:HG11	1.77	0.66
1:I:432:ARG:HG3	1:I:432:ARG:HH11	1.58	0.66
1:K:452:ILE:HG21	1:K:604:VAL:HG11	1.77	0.66
1:M:452:ILE:HG21	1:M:604:VAL:HG11	1.77	0.66
1:E:452:ILE:HG21	1:E:604:VAL:HG11	1.77	0.66
1:D:452:ILE:HG21	1:D:604:VAL:HG11	1.77	0.66
1:J:452:ILE:HG21	1:J:604:VAL:HG11	1.77	0.66
1:F:452:ILE:HG21	1:F:604:VAL:HG11	1.77	0.66
1:N:452:ILE:HG21	1:N:604:VAL:HG11	1.77	0.66
1:I:452:ILE:HG21	1:I:604:VAL:HG11	1.77	0.65
1:C:452:ILE:HG21	1:C:604:VAL:HG11	1.77	0.65
1:A:452:ILE:HG21	1:A:604:VAL:HG11	1.77	0.65
1:G:452:ILE:HG21	1:G:604:VAL:HG11	1.77	0.65
1:H:452:ILE:HG21	1:H:604:VAL:HG11	1.77	0.65
1:B:452:ILE:HG21	1:B:604:VAL:HG11	1.77	0.65
1:I:621:THR:HG22	1:I:641:GLU:HG3	1.79	0.65
1:H:621:THR:HG22	1:H:641:GLU:HG3	1.79	0.64
1:J:621:THR:HG22	1:J:641:GLU:HG3	1.79	0.64
1:F:621:THR:HG22	1:F:641:GLU:HG3	1.79	0.64
1:G:621:THR:HG22	1:G:641:GLU:HG3	1.79	0.64
1:E:621:THR:HG22	1:E:641:GLU:HG3	1.79	0.64
1:D:621:THR:HG22	1:D:641:GLU:HG3	1.79	0.64
1:K:621:THR:HG22	1:K:641:GLU:HG3	1.80	0.64
1:C:621:THR:HG22	1:C:641:GLU:HG3	1.79	0.64
2:R:51:LEU:HD11	2:S:72:SER:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:100:ARG:HD2	2:U:104:CYS:O	1.98	0.63
1:L:621:THR:HG22	1:L:641:GLU:HG3	1.79	0.63
2:T:100:ARG:HD2	2:T:104:CYS:O	1.99	0.63
2:P:100:ARG:HD2	2:P:104:CYS:O	1.99	0.63
2:Z:100:ARG:HD2	2:Z:104:CYS:O	1.99	0.63
2:O:100:ARG:HD2	2:O:104:CYS:O	1.99	0.63
2:Q:100:ARG:HD2	2:Q:104:CYS:O	1.99	0.63
2:Y:100:ARG:HD2	2:Y:104:CYS:O	1.99	0.63
1:B:621:THR:HG22	1:B:641:GLU:HG3	1.79	0.63
2:a:100:ARG:HD2	2:a:104:CYS:O	1.99	0.63
2:V:100:ARG:HD2	2:V:104:CYS:O	1.99	0.63
1:M:621:THR:HG22	1:M:641:GLU:HG3	1.79	0.63
2:X:100:ARG:HD2	2:X:104:CYS:O	1.99	0.62
1:A:621:THR:HG22	1:A:641:GLU:HG3	1.79	0.62
2:S:100:ARG:HD2	2:S:104:CYS:O	1.99	0.62
1:N:621:THR:HG22	1:N:641:GLU:HG3	1.79	0.62
2:b:100:ARG:HD2	2:b:104:CYS:O	1.99	0.62
2:R:100:ARG:HD2	2:R:104:CYS:O	1.99	0.62
2:W:100:ARG:HD2	2:W:104:CYS:O	1.99	0.62
1:J:393:ALA:O	1:J:397:GLN:HG2	2.00	0.61
1:K:393:ALA:O	1:K:397:GLN:HG2	2.00	0.61
1:E:393:ALA:O	1:E:397:GLN:HG2	2.00	0.61
1:N:393:ALA:O	1:N:397:GLN:HG2	2.00	0.61
1:D:393:ALA:O	1:D:397:GLN:HG2	2.00	0.61
1:L:393:ALA:O	1:L:397:GLN:HG2	2.00	0.61
1:A:393:ALA:O	1:A:397:GLN:HG2	2.00	0.61
1:F:393:ALA:O	1:F:397:GLN:HG2	2.00	0.61
1:C:393:ALA:O	1:C:397:GLN:HG2	2.00	0.61
1:I:393:ALA:O	1:I:397:GLN:HG2	2.00	0.61
1:M:393:ALA:O	1:M:397:GLN:HG2	2.00	0.61
1:G:393:ALA:O	1:G:397:GLN:HG2	2.00	0.60
1:B:393:ALA:O	1:B:397:GLN:HG2	2.00	0.60
1:H:393:ALA:O	1:H:397:GLN:HG2	2.00	0.60
1:N:665:SER:HB3	1:N:690:THR:HG22	1.85	0.59
1:B:665:SER:HB3	1:B:690:THR:HG22	1.85	0.59
1:M:665:SER:HB3	1:M:690:THR:HG22	1.85	0.59
1:J:428:GLN:HB3	1:J:432:ARG:HB2	1.85	0.59
1:A:665:SER:HB3	1:A:690:THR:HG22	1.85	0.59
1:I:428:GLN:HB3	1:I:432:ARG:HB2	1.85	0.59
1:K:428:GLN:HB3	1:K:432:ARG:HB2	1.85	0.59
1:H:428:GLN:HB3	1:H:432:ARG:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:665:SER:HB3	1:K:690:THR:HG22	1.85	0.58
1:L:428:GLN:HB3	1:L:432:ARG:HB2	1.85	0.58
1:L:665:SER:HB3	1:L:690:THR:HG22	1.85	0.58
1:C:665:SER:HB3	1:C:690:THR:HG22	1.85	0.58
1:G:428:GLN:HB3	1:G:432:ARG:HB2	1.85	0.58
1:M:428:GLN:HB3	1:M:432:ARG:HB2	1.85	0.58
1:F:428:GLN:HB3	1:F:432:ARG:HB2	1.85	0.58
1:J:665:SER:HB3	1:J:690:THR:HG22	1.85	0.58
1:D:665:SER:HB3	1:D:690:THR:HG22	1.85	0.58
1:E:428:GLN:HB3	1:E:432:ARG:HB2	1.85	0.58
1:D:428:GLN:HB3	1:D:432:ARG:HB2	1.85	0.58
1:I:665:SER:HB3	1:I:690:THR:HG22	1.85	0.58
1:C:428:GLN:HB3	1:C:432:ARG:HB2	1.85	0.57
1:N:428:GLN:HB3	1:N:432:ARG:HB2	1.85	0.57
1:A:428:GLN:HB3	1:A:432:ARG:HB2	1.85	0.57
1:B:428:GLN:HB3	1:B:432:ARG:HB2	1.85	0.57
1:E:665:SER:HB3	1:E:690:THR:HG22	1.85	0.57
1:G:665:SER:HB3	1:G:690:THR:HG22	1.85	0.57
1:H:665:SER:HB3	1:H:690:THR:HG22	1.85	0.57
1:F:665:SER:HB3	1:F:690:THR:HG22	1.85	0.57
2:O:72:SER:HB3	2:b:51:LEU:HD11	1.86	0.56
2:X:51:LEU:HD11	2:Y:72:SER:HB3	1.91	0.53
1:A:614:ILE:HD13	1:A:702:PRO:HB2	1.91	0.53
1:J:432:ARG:HG3	1:J:432:ARG:NH1	2.24	0.53
1:J:614:ILE:HD13	1:J:702:PRO:HB2	1.91	0.53
1:C:614:ILE:HD13	1:C:702:PRO:HB2	1.91	0.52
1:H:432:ARG:HG3	1:H:432:ARG:NH1	2.24	0.52
1:I:432:ARG:HG3	1:I:432:ARG:NH1	2.24	0.52
1:I:642:VAL:HB	1:J:574:ILE:HD12	1.91	0.52
1:I:614:ILE:HD13	1:I:702:PRO:HB2	1.91	0.52
1:H:642:VAL:HB	1:I:574:ILE:HD12	1.91	0.52
1:K:432:ARG:HG3	1:K:432:ARG:NH1	2.24	0.52
1:N:623:ASP:HA	1:N:638:ASN:O	2.10	0.52
1:A:623:ASP:HA	1:A:638:ASN:O	2.10	0.52
1:C:669:GLU:CD	1:C:686:ARG:HH21	2.18	0.52
1:D:623:ASP:HA	1:D:638:ASN:O	2.10	0.52
1:D:669:GLU:CD	1:D:686:ARG:HH21	2.18	0.52
1:G:642:VAL:HB	1:H:574:ILE:HD12	1.91	0.52
1:N:432:ARG:HG3	1:N:432:ARG:NH1	2.24	0.52
1:A:432:ARG:HG3	1:A:432:ARG:NH1	2.24	0.52
1:A:566:THR:HB	1:A:572:ALA:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:ASP:HA	1:C:638:ASN:O	2.10	0.52
1:I:566:THR:HB	1:I:572:ALA:HB2	1.92	0.52
1:I:623:ASP:HA	1:I:638:ASN:O	2.10	0.52
1:L:432:ARG:HG3	1:L:432:ARG:NH1	2.24	0.52
1:A:574:ILE:HD12	1:N:642:VAL:HB	1.91	0.52
1:B:669:GLU:CD	1:B:686:ARG:HH21	2.18	0.52
1:F:566:THR:HB	1:F:572:ALA:HB2	1.92	0.52
1:F:614:ILE:HD13	1:F:702:PRO:HB2	1.91	0.52
1:H:566:THR:HB	1:H:572:ALA:HB2	1.92	0.52
1:H:623:ASP:HA	1:H:638:ASN:O	2.10	0.52
1:J:623:ASP:HA	1:J:638:ASN:O	2.10	0.52
1:K:642:VAL:HB	1:L:574:ILE:HD12	1.91	0.52
1:M:432:ARG:HG3	1:M:432:ARG:NH1	2.24	0.52
1:M:623:ASP:HA	1:M:638:ASN:O	2.10	0.52
1:A:600:LEU:HD13	1:A:622:LYS:HG3	1.92	0.52
1:A:642:VAL:HB	1:B:574:ILE:HD12	1.91	0.52
1:B:432:ARG:HG3	1:B:432:ARG:NH1	2.24	0.52
1:B:642:VAL:HB	1:C:574:ILE:HD12	1.91	0.52
1:C:566:THR:HB	1:C:572:ALA:HB2	1.92	0.52
1:E:669:GLU:CD	1:E:686:ARG:HH21	2.18	0.52
1:F:642:VAL:HB	1:G:574:ILE:HD12	1.91	0.52
1:G:614:ILE:HD13	1:G:702:PRO:HB2	1.91	0.52
1:J:642:VAL:HB	1:K:574:ILE:HD12	1.91	0.52
1:K:600:LEU:HD13	1:K:622:LYS:HG3	1.92	0.52
1:K:614:ILE:HD13	1:K:702:PRO:HB2	1.91	0.52
1:M:566:THR:HB	1:M:572:ALA:HB2	1.92	0.52
1:N:566:THR:HB	1:N:572:ALA:HB2	1.92	0.52
1:N:669:GLU:CD	1:N:686:ARG:HH21	2.17	0.52
1:C:600:LEU:HD13	1:C:622:LYS:HG3	1.92	0.52
1:D:566:THR:HB	1:D:572:ALA:HB2	1.92	0.52
1:E:642:VAL:HB	1:F:574:ILE:HD12	1.91	0.52
1:G:566:THR:HB	1:G:572:ALA:HB2	1.92	0.52
1:M:600:LEU:HD13	1:M:622:LYS:HG3	1.92	0.52
1:B:614:ILE:HD13	1:B:702:PRO:HB2	1.91	0.52
1:C:432:ARG:HG3	1:C:432:ARG:NH1	2.24	0.52
1:E:614:ILE:HD13	1:E:702:PRO:HB2	1.91	0.52
1:J:566:THR:HB	1:J:572:ALA:HB2	1.92	0.52
1:K:566:THR:HB	1:K:572:ALA:HB2	1.92	0.52
1:L:566:THR:HB	1:L:572:ALA:HB2	1.92	0.52
1:M:669:GLU:CD	1:M:686:ARG:HH21	2.18	0.52
1:A:669:GLU:CD	1:A:686:ARG:HH21	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:THR:HB	1:B:572:ALA:HB2	1.92	0.52
1:I:600:LEU:HD13	1:I:622:LYS:HG3	1.92	0.52
1:L:642:VAL:HB	1:M:574:ILE:HD12	1.91	0.52
1:M:614:ILE:HD13	1:M:702:PRO:HB2	1.91	0.52
2:Q:45:TYR:CD2	3:K:801:PTY:H201	2.45	0.51
1:B:623:ASP:HA	1:B:638:ASN:O	2.10	0.51
1:C:626:ASP:HB3	1:C:636:PRO:HG2	1.92	0.51
1:D:600:LEU:HD13	1:D:622:LYS:HG3	1.92	0.51
1:D:626:ASP:HB3	1:D:636:PRO:HG2	1.92	0.51
1:E:623:ASP:HA	1:E:638:ASN:O	2.10	0.51
1:L:600:LEU:HD13	1:L:622:LYS:HG3	1.92	0.51
1:M:642:VAL:HB	1:N:574:ILE:HD12	1.91	0.51
1:N:614:ILE:HD13	1:N:702:PRO:HB2	1.91	0.51
1:B:600:LEU:HD13	1:B:622:LYS:HG3	1.92	0.51
1:E:566:THR:HB	1:E:572:ALA:HB2	1.92	0.51
1:E:600:LEU:HD13	1:E:622:LYS:HG3	1.92	0.51
1:J:600:LEU:HD13	1:J:622:LYS:HG3	1.92	0.51
1:E:626:ASP:HB3	1:E:636:PRO:HG2	1.92	0.51
1:F:669:GLU:CD	1:F:686:ARG:HH21	2.18	0.51
1:G:623:ASP:HA	1:G:638:ASN:O	2.10	0.51
1:H:600:LEU:HD13	1:H:622:LYS:HG3	1.92	0.51
1:H:614:ILE:HD13	1:H:702:PRO:HB2	1.91	0.51
1:H:669:GLU:CD	1:H:686:ARG:HH21	2.18	0.51
1:L:623:ASP:HA	1:L:638:ASN:O	2.10	0.51
1:N:600:LEU:HD13	1:N:622:LYS:HG3	1.92	0.51
2:P:58:LEU:HB3	2:P:97:ALA:HB2	1.93	0.51
2:R:58:LEU:HB3	2:R:97:ALA:HB2	1.93	0.51
2:S:58:LEU:HB3	2:S:97:ALA:HB2	1.93	0.51
1:F:600:LEU:HD13	1:F:622:LYS:HG3	1.92	0.51
1:F:626:ASP:HB3	1:F:636:PRO:HG2	1.92	0.51
1:A:523:LEU:HD22	1:A:669:GLU:HB3	1.93	0.51
2:O:58:LEU:HB3	2:O:97:ALA:HB2	1.93	0.51
2:b:58:LEU:HB3	2:b:97:ALA:HB2	1.93	0.51
1:C:642:VAL:HB	1:D:574:ILE:HD12	1.91	0.51
1:D:432:ARG:HG3	1:D:432:ARG:NH1	2.25	0.51
1:N:523:LEU:HD22	1:N:669:GLU:HB3	1.93	0.51
2:Q:58:LEU:HB3	2:Q:97:ALA:HB2	1.93	0.51
1:B:626:ASP:HB3	1:B:636:PRO:HG2	1.92	0.51
1:D:642:VAL:HB	1:E:574:ILE:HD12	1.91	0.51
1:G:626:ASP:HB3	1:G:636:PRO:HG2	1.92	0.51
1:J:669:GLU:CD	1:J:686:ARG:HH21	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:614:ILE:HD13	1:L:702:PRO:HB2	1.91	0.51
1:L:669:GLU:CD	1:L:686:ARG:HH21	2.18	0.51
2:T:58:LEU:HB3	2:T:97:ALA:HB2	1.93	0.51
2:a:58:LEU:HB3	2:a:97:ALA:HB2	1.93	0.51
1:B:523:LEU:HD22	1:B:669:GLU:HB3	1.93	0.51
1:D:614:ILE:HD13	1:D:702:PRO:HB2	1.91	0.51
1:E:528:ALA:HA	1:E:550:MET:HB2	1.93	0.51
1:G:528:ALA:HA	1:G:550:MET:HB2	1.93	0.51
1:G:600:LEU:HD13	1:G:622:LYS:HG3	1.92	0.51
1:H:626:ASP:HB3	1:H:636:PRO:HG2	1.92	0.51
1:I:669:GLU:CD	1:I:686:ARG:HH21	2.18	0.51
1:A:626:ASP:HB3	1:A:636:PRO:HG2	1.92	0.51
1:K:623:ASP:HA	1:K:638:ASN:O	2.10	0.51
2:Z:58:LEU:HB3	2:Z:97:ALA:HB2	1.93	0.51
1:B:528:ALA:HA	1:B:550:MET:HB2	1.93	0.51
1:C:523:LEU:HD22	1:C:669:GLU:HB3	1.93	0.51
1:E:432:ARG:HG3	1:E:432:ARG:NH1	2.24	0.51
1:K:669:GLU:CD	1:K:686:ARG:HH21	2.18	0.51
1:M:523:LEU:HD22	1:M:669:GLU:HB3	1.93	0.51
1:D:528:ALA:HA	1:D:550:MET:HB2	1.93	0.51
2:U:58:LEU:HB3	2:U:97:ALA:HB2	1.93	0.50
2:Y:58:LEU:HB3	2:Y:97:ALA:HB2	1.93	0.50
1:F:623:ASP:HA	1:F:638:ASN:O	2.10	0.50
1:G:669:GLU:CD	1:G:686:ARG:HH21	2.18	0.50
1:I:626:ASP:HB3	1:I:636:PRO:HG2	1.92	0.50
1:J:626:ASP:HB3	1:J:636:PRO:HG2	1.92	0.50
1:H:528:ALA:HA	1:H:550:MET:HB2	1.93	0.50
1:N:626:ASP:HB3	1:N:636:PRO:HG2	1.92	0.50
2:a:39:VAL:HG22	1:H:687:ASP:HB3	1.93	0.50
1:J:528:ALA:HA	1:J:550:MET:HB2	1.93	0.50
1:K:626:ASP:HB3	1:K:636:PRO:HG2	1.92	0.50
1:C:528:ALA:HA	1:C:550:MET:HB2	1.93	0.50
1:L:523:LEU:HD22	1:L:669:GLU:HB3	1.93	0.50
2:V:58:LEU:HB3	2:V:97:ALA:HB2	1.93	0.50
2:X:58:LEU:HB3	2:X:97:ALA:HB2	1.93	0.50
1:F:432:ARG:HG3	1:F:432:ARG:NH1	2.24	0.50
1:M:626:ASP:HB3	1:M:636:PRO:HG2	1.92	0.50
1:N:528:ALA:HA	1:N:550:MET:HB2	1.93	0.50
2:W:58:LEU:HB3	2:W:97:ALA:HB2	1.93	0.50
2:X:39:VAL:HG22	1:E:687:ASP:HB3	1.93	0.50
1:D:523:LEU:HD22	1:D:669:GLU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:626:ASP:HB3	1:L:636:PRO:HG2	1.92	0.50
1:I:528:ALA:HA	1:I:550:MET:HB2	1.93	0.50
1:L:528:ALA:HA	1:L:550:MET:HB2	1.93	0.50
1:C:533:GLY:C	1:C:534:ILE:HD13	2.38	0.49
1:F:528:ALA:HA	1:F:550:MET:HB2	1.93	0.49
1:B:533:GLY:C	1:B:534:ILE:HD13	2.38	0.49
1:D:533:GLY:C	1:D:534:ILE:HD13	2.38	0.49
1:E:533:GLY:C	1:E:534:ILE:HD13	2.38	0.49
1:G:432:ARG:HG3	1:G:432:ARG:NH1	2.24	0.49
1:F:500:GLY:HA2	1:G:538:THR:O	2.13	0.49
1:G:523:LEU:HD22	1:G:669:GLU:HB3	1.93	0.49
1:F:533:GLY:C	1:F:534:ILE:HD13	2.38	0.49
1:H:533:GLY:C	1:H:534:ILE:HD13	2.38	0.49
1:I:523:LEU:HD22	1:I:669:GLU:HB3	1.93	0.49
1:G:533:GLY:C	1:G:534:ILE:HD13	2.38	0.49
1:H:523:LEU:HD22	1:H:669:GLU:HB3	1.93	0.49
1:M:500:GLY:HA2	1:N:538:THR:O	2.13	0.49
1:D:500:GLY:HA2	1:E:538:THR:O	2.13	0.49
1:E:500:GLY:HA2	1:F:538:THR:O	2.13	0.49
1:F:523:LEU:HD22	1:F:669:GLU:HB3	1.93	0.49
1:I:533:GLY:C	1:I:534:ILE:HD13	2.38	0.49
1:J:523:LEU:HD22	1:J:669:GLU:HB3	1.93	0.49
1:L:500:GLY:HA2	1:M:538:THR:O	2.13	0.49
1:A:533:GLY:C	1:A:534:ILE:HD13	2.38	0.49
2:b:39:VAL:HG22	1:I:687:ASP:HB3	1.94	0.49
1:K:500:GLY:HA2	1:L:538:THR:O	2.13	0.49
1:A:500:GLY:HA2	1:B:538:THR:O	2.13	0.49
1:A:528:ALA:HA	1:A:550:MET:HB2	1.93	0.49
1:H:500:GLY:HA2	1:I:538:THR:O	2.13	0.49
1:K:523:LEU:HD22	1:K:669:GLU:HB3	1.93	0.49
1:K:528:ALA:HA	1:K:550:MET:HB2	1.93	0.49
1:C:500:GLY:HA2	1:D:538:THR:O	2.13	0.49
1:E:523:LEU:HD22	1:E:669:GLU:HB3	1.93	0.49
1:F:471:TRP:O	1:F:520:PHE:N	2.46	0.49
1:I:500:GLY:HA2	1:J:538:THR:O	2.13	0.49
1:A:471:TRP:O	1:A:520:PHE:N	2.46	0.48
1:B:500:GLY:HA2	1:C:538:THR:O	2.13	0.48
1:G:500:GLY:HA2	1:H:538:THR:O	2.14	0.48
1:H:471:TRP:O	1:H:520:PHE:N	2.46	0.48
1:J:500:GLY:HA2	1:K:538:THR:O	2.13	0.48
1:J:533:GLY:C	1:J:534:ILE:HD13	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:471:TRP:O	1:M:520:PHE:N	2.46	0.48
1:K:533:GLY:C	1:K:534:ILE:HD13	2.38	0.48
2:Q:45:TYR:CZ	3:K:801:PTY:H221	2.49	0.48
2:Z:99:VAL:HG12	2:Z:99:VAL:O	2.14	0.48
2:a:99:VAL:HG12	2:a:99:VAL:O	2.14	0.48
1:E:471:TRP:O	1:E:520:PHE:N	2.46	0.48
1:L:471:TRP:O	1:L:520:PHE:N	2.46	0.48
1:M:528:ALA:HA	1:M:550:MET:HB2	1.93	0.48
1:A:538:THR:O	1:N:500:GLY:HA2	2.14	0.48
1:A:639:LYS:HB3	1:A:639:LYS:HE3	1.55	0.48
2:U:39:VAL:HG22	1:B:687:ASP:HB3	1.95	0.48
2:U:99:VAL:HG12	2:U:99:VAL:O	2.14	0.48
2:b:99:VAL:HG12	2:b:99:VAL:O	2.14	0.48
1:B:639:LYS:HB3	1:B:639:LYS:HE3	1.55	0.48
1:L:533:GLY:C	1:L:534:ILE:HD13	2.38	0.48
2:W:99:VAL:O	2:W:99:VAL:HG12	2.14	0.48
2:Y:99:VAL:HG12	2:Y:99:VAL:O	2.14	0.48
1:M:533:GLY:C	1:M:534:ILE:HD13	2.38	0.48
1:N:533:GLY:C	1:N:534:ILE:HD13	2.38	0.48
1:D:471:TRP:O	1:D:520:PHE:N	2.46	0.48
2:O:99:VAL:HG12	2:O:99:VAL:O	2.14	0.48
1:C:471:TRP:O	1:C:520:PHE:N	2.46	0.48
1:I:471:TRP:O	1:I:520:PHE:N	2.46	0.48
1:J:471:TRP:O	1:J:520:PHE:N	2.46	0.48
1:K:471:TRP:O	1:K:520:PHE:N	2.46	0.48
1:N:471:TRP:O	1:N:520:PHE:N	2.46	0.48
1:G:471:TRP:O	1:G:520:PHE:N	2.46	0.48
2:P:99:VAL:HG12	2:P:99:VAL:O	2.14	0.47
2:S:99:VAL:HG12	2:S:99:VAL:O	2.14	0.47
2:X:99:VAL:HG12	2:X:99:VAL:O	2.14	0.47
2:V:99:VAL:HG12	2:V:99:VAL:O	2.14	0.47
1:H:412:ARG:HG2	1:I:377:LEU:HD21	1.97	0.47
1:J:639:LYS:HE3	1:J:639:LYS:HB3	1.55	0.47
2:Q:99:VAL:HG12	2:Q:99:VAL:O	2.14	0.47
1:B:471:TRP:O	1:B:520:PHE:N	2.46	0.47
1:D:412:ARG:HG2	1:E:377:LEU:HD21	1.97	0.47
3:H:801:PTY:H242	1:I:683:LEU:HD11	1.97	0.47
3:J:801:PTY:H242	1:K:683:LEU:HD11	1.97	0.47
3:I:801:PTY:H242	1:J:683:LEU:HD11	1.97	0.47
3:K:801:PTY:H242	1:L:683:LEU:HD11	1.97	0.47
2:R:99:VAL:O	2:R:99:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:99:VAL:HG12	2:T:99:VAL:O	2.14	0.47
3:L:801:PTY:H242	1:M:683:LEU:HD11	1.97	0.47
1:E:412:ARG:HG2	1:F:377:LEU:HD21	1.97	0.47
3:F:801:PTY:H242	1:G:683:LEU:HD11	1.97	0.47
3:G:801:PTY:H242	1:H:683:LEU:HD11	1.97	0.47
1:J:412:ARG:HG2	1:K:377:LEU:HD21	1.97	0.47
3:M:801:PTY:H242	1:N:683:LEU:HD11	1.97	0.47
1:A:412:ARG:HG2	1:B:377:LEU:HD21	1.97	0.46
2:W:51:LEU:HD21	2:X:72:SER:HB3	1.97	0.46
1:C:412:ARG:HG2	1:D:377:LEU:HD21	1.97	0.46
1:A:683:LEU:HD11	3:N:801:PTY:H242	1.97	0.46
3:E:801:PTY:H242	1:F:683:LEU:HD11	1.97	0.46
1:F:412:ARG:HG2	1:G:377:LEU:HD21	1.98	0.46
1:I:472:GLY:HA2	1:I:519:PRO:HA	1.98	0.46
1:N:472:GLY:HA2	1:N:519:PRO:HA	1.98	0.46
3:A:801:PTY:H201	2:U:45:TYR:CD2	2.51	0.46
1:K:412:ARG:HG2	1:L:377:LEU:HD21	1.97	0.46
1:M:418:ASP:OD2	1:M:421:THR:OG1	2.30	0.46
3:A:801:PTY:H242	1:B:683:LEU:HD11	1.97	0.46
1:F:693:LYS:HB2	1:F:693:LYS:HE3	1.75	0.46
1:K:472:GLY:HA2	1:K:519:PRO:HA	1.98	0.46
1:L:412:ARG:HG2	1:M:377:LEU:HD21	1.97	0.46
1:L:472:GLY:HA2	1:L:519:PRO:HA	1.98	0.46
2:W:44:ALA:HB1	2:X:89:LEU:HD23	1.98	0.46
1:B:472:GLY:HA2	1:B:519:PRO:HA	1.98	0.46
3:C:801:PTY:H242	1:D:683:LEU:HD11	1.97	0.46
3:D:801:PTY:H242	1:E:683:LEU:HD11	1.97	0.46
1:G:412:ARG:HG2	1:H:377:LEU:HD21	1.98	0.46
1:G:472:GLY:HA2	1:G:519:PRO:HA	1.98	0.46
1:K:492:LYS:HB2	1:K:507:THR:HG21	1.98	0.46
1:I:412:ARG:HG2	1:J:377:LEU:HD21	1.98	0.46
1:B:412:ARG:HG2	1:C:377:LEU:HD21	1.98	0.46
3:B:801:PTY:H242	1:C:683:LEU:HD11	1.97	0.46
1:I:492:LYS:HB2	1:I:507:THR:HG21	1.98	0.46
1:J:492:LYS:HB2	1:J:507:THR:HG21	1.98	0.46
1:L:674:LEU:HD23	1:L:674:LEU:HA	1.81	0.46
1:M:492:LYS:HB2	1:M:507:THR:HG21	1.98	0.46
1:E:471:TRP:CE2	1:E:545:LEU:HD13	2.52	0.45
1:F:471:TRP:CE2	1:F:545:LEU:HD13	2.52	0.45
1:G:471:TRP:CE2	1:G:545:LEU:HD13	2.51	0.45
1:H:471:TRP:CE2	1:H:545:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:GLY:HA2	1:H:519:PRO:HA	1.98	0.45
1:I:471:TRP:CE2	1:I:545:LEU:HD13	2.51	0.45
1:J:418:ASP:OD2	1:J:421:THR:OG1	2.30	0.45
1:L:471:TRP:CE2	1:L:545:LEU:HD13	2.52	0.45
1:M:639:LYS:HE3	1:M:639:LYS:HB3	1.55	0.45
1:K:471:TRP:CE2	1:K:545:LEU:HD13	2.52	0.45
1:L:492:LYS:HB2	1:L:507:THR:HG21	1.98	0.45
1:M:471:TRP:CE2	1:M:545:LEU:HD13	2.52	0.45
1:F:472:GLY:HA2	1:F:519:PRO:HA	1.98	0.45
1:J:471:TRP:CE2	1:J:545:LEU:HD13	2.52	0.45
1:A:472:GLY:HA2	1:A:519:PRO:HA	1.98	0.45
1:D:472:GLY:HA2	1:D:519:PRO:HA	1.98	0.45
1:K:418:ASP:OD2	1:K:421:THR:OG1	2.30	0.45
1:M:412:ARG:HG2	1:N:377:LEU:HD21	1.98	0.45
1:N:471:TRP:CE2	1:N:545:LEU:HD13	2.52	0.45
1:N:492:LYS:HB2	1:N:507:THR:HG21	1.98	0.45
1:A:471:TRP:CE2	1:A:545:LEU:HD13	2.52	0.45
2:Q:39:VAL:HG22	1:L:687:ASP:HB3	1.99	0.45
1:D:471:TRP:CE2	1:D:545:LEU:HD13	2.52	0.45
1:G:492:LYS:HB2	1:G:507:THR:HG21	1.98	0.45
1:H:492:LYS:HB2	1:H:507:THR:HG21	1.98	0.45
1:J:472:GLY:HA2	1:J:519:PRO:HA	1.98	0.45
1:M:472:GLY:HA2	1:M:519:PRO:HA	1.98	0.45
2:W:45:TYR:CD2	3:C:801:PTY:H201	2.52	0.45
1:C:472:GLY:HA2	1:C:519:PRO:HA	1.98	0.45
1:E:472:GLY:HA2	1:E:519:PRO:HA	1.98	0.45
1:A:492:LYS:HB2	1:A:507:THR:HG21	1.98	0.45
2:Z:51:LEU:HD23	2:Z:51:LEU:HA	1.85	0.45
1:B:471:TRP:CE2	1:B:545:LEU:HD13	2.52	0.45
1:C:471:TRP:CE2	1:C:545:LEU:HD13	2.52	0.45
1:I:646:ILE:HD13	1:I:656:ILE:HG22	1.99	0.45
1:L:418:ASP:OD2	1:L:421:THR:OG1	2.30	0.45
1:H:646:ILE:HD13	1:H:656:ILE:HG22	1.99	0.45
1:I:418:ASP:OD2	1:I:421:THR:OG1	2.30	0.45
1:K:639:LYS:HB3	1:K:639:LYS:HE3	1.55	0.45
1:A:377:LEU:HD21	1:N:412:ARG:HG2	1.98	0.44
1:J:646:ILE:HD13	1:J:656:ILE:HG22	1.99	0.44
1:B:492:LYS:HB2	1:B:507:THR:HG21	1.98	0.44
1:F:492:LYS:HB2	1:F:507:THR:HG21	1.98	0.44
1:K:646:ILE:HD13	1:K:656:ILE:HG22	1.99	0.44
1:C:674:LEU:HD23	1:C:674:LEU:HA	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:492:LYS:HB2	1:E:507:THR:HG21	1.98	0.44
1:L:646:ILE:HD13	1:L:656:ILE:HG22	1.99	0.44
2:V:39:VAL:HG22	1:C:687:ASP:HB3	1.98	0.44
2:Z:39:VAL:HG22	1:G:687:ASP:HB3	1.98	0.44
1:D:492:LYS:HB2	1:D:507:THR:HG21	1.98	0.44
1:E:639:LYS:HE3	1:E:639:LYS:HB3	1.55	0.44
1:F:639:LYS:HB3	1:F:639:LYS:HE3	1.55	0.44
1:G:646:ILE:HD13	1:G:656:ILE:HG22	1.99	0.44
1:G:674:LEU:HD23	1:G:674:LEU:HA	1.81	0.44
1:A:646:ILE:HD13	1:A:656:ILE:HG22	1.99	0.44
1:B:646:ILE:HD13	1:B:656:ILE:HG22	1.99	0.44
1:C:492:LYS:HB2	1:C:507:THR:HG21	1.98	0.44
1:E:611:ASP:OD1	1:E:611:ASP:N	2.45	0.44
1:E:646:ILE:HD13	1:E:656:ILE:HG22	1.99	0.44
1:H:639:LYS:HE3	1:H:639:LYS:HB3	1.55	0.44
1:K:669:GLU:HG3	1:L:552:LYS:HG3	2.00	0.44
2:W:39:VAL:HG22	1:D:687:ASP:HB3	1.99	0.43
1:C:646:ILE:HD13	1:C:656:ILE:HG22	1.99	0.43
1:M:646:ILE:HD13	1:M:656:ILE:HG22	1.99	0.43
1:N:646:ILE:HD13	1:N:656:ILE:HG22	1.99	0.43
1:D:646:ILE:HD13	1:D:656:ILE:HG22	1.99	0.43
1:G:611:ASP:OD1	1:G:611:ASP:N	2.46	0.43
1:A:552:LYS:HG3	1:N:669:GLU:HG3	2.00	0.43
2:O:53:ILE:HD12	3:I:801:PTY:H132	2.01	0.43
1:E:674:LEU:HD23	1:E:674:LEU:HA	1.81	0.43
1:I:674:LEU:HD23	1:I:674:LEU:HA	1.81	0.43
1:A:646:ILE:CD1	1:A:656:ILE:HG22	2.49	0.43
1:F:646:ILE:HD13	1:F:656:ILE:HG22	1.99	0.43
1:N:674:LEU:HD23	1:N:674:LEU:HA	1.80	0.43
1:D:639:LYS:HE3	1:D:639:LYS:HB3	1.55	0.43
1:H:631:LEU:HD22	1:I:630:MET:HE1	2.01	0.43
2:Y:51:LEU:HD23	2:Y:51:LEU:HA	1.85	0.43
1:E:646:ILE:CD1	1:E:656:ILE:HG22	2.49	0.43
1:F:646:ILE:CD1	1:F:656:ILE:HG22	2.49	0.43
1:G:639:LYS:HE3	1:G:639:LYS:HB3	1.55	0.43
1:M:543:LEU:HD12	1:M:543:LEU:HA	1.89	0.43
1:N:646:ILE:CD1	1:N:656:ILE:HG22	2.49	0.43
1:B:646:ILE:CD1	1:B:656:ILE:HG22	2.49	0.43
1:E:631:LEU:HD22	1:F:630:MET:HE1	2.01	0.43
1:F:574:ILE:HG22	1:F:602:LEU:HB3	2.01	0.43
1:H:483:TYR:OH	1:I:544:ASP:OD1	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:631:LEU:HD22	1:M:630:MET:HE1	2.01	0.43
1:D:631:LEU:HD22	1:E:630:MET:HE1	2.01	0.43
1:M:669:GLU:HG3	1:N:552:LYS:HG3	2.01	0.43
2:V:96:GLU:OE1	1:B:678:PRO:HD2	2.19	0.43
1:D:646:ILE:CD1	1:D:656:ILE:HG22	2.49	0.43
1:G:574:ILE:HG22	1:G:602:LEU:HB3	2.01	0.43
1:G:631:LEU:HD22	1:H:630:MET:HE1	2.01	0.43
1:H:574:ILE:HG22	1:H:602:LEU:HB3	2.01	0.43
1:I:574:ILE:HG22	1:I:602:LEU:HB3	2.01	0.43
1:I:631:LEU:HD22	1:J:630:MET:HE1	2.01	0.43
1:A:631:LEU:HD22	1:B:630:MET:HE1	2.01	0.43
2:Q:44:ALA:HB1	2:R:89:LEU:HD23	2.01	0.43
1:B:669:GLU:HG3	1:C:552:LYS:HG3	2.01	0.43
1:C:646:ILE:CD1	1:C:656:ILE:HG22	2.49	0.43
1:E:574:ILE:HG22	1:E:602:LEU:HB3	2.01	0.43
1:G:646:ILE:CD1	1:G:656:ILE:HG22	2.49	0.43
1:J:631:LEU:HD22	1:K:630:MET:HE1	2.01	0.43
1:B:631:LEU:HD22	1:C:630:MET:HE1	2.01	0.42
1:C:631:LEU:HD22	1:D:630:MET:HE1	2.01	0.42
1:E:693:LYS:HB2	1:E:693:LYS:HE3	1.75	0.42
1:F:631:LEU:HD22	1:G:630:MET:HE1	2.01	0.42
1:H:669:GLU:HG3	1:I:552:LYS:HG3	2.00	0.42
1:J:574:ILE:HG22	1:J:602:LEU:HB3	2.01	0.42
1:J:611:ASP:OD1	1:J:611:ASP:N	2.46	0.42
1:K:631:LEU:HD22	1:L:630:MET:HE1	2.01	0.42
1:M:574:ILE:HG22	1:M:602:LEU:HB3	2.01	0.42
1:A:630:MET:HE1	1:N:631:LEU:HD22	2.01	0.42
1:D:669:GLU:HG3	1:E:552:LYS:HG3	2.00	0.42
1:H:418:ASP:OD2	1:H:421:THR:OG1	2.30	0.42
1:L:574:ILE:HG22	1:L:602:LEU:HB3	2.01	0.42
1:M:646:ILE:CD1	1:M:656:ILE:HG22	2.49	0.42
2:U:44:ALA:HB1	2:V:89:LEU:HD23	2.01	0.42
2:a:41:ALA:HB3	3:G:801:PTY:HC51	2.01	0.42
2:b:53:ILE:HD12	3:H:801:PTY:H132	2.02	0.42
1:I:669:GLU:HG3	1:J:552:LYS:HG3	2.01	0.42
1:K:574:ILE:HG22	1:K:602:LEU:HB3	2.01	0.42
1:L:483:TYR:OH	1:M:544:ASP:OD1	2.31	0.42
1:M:631:LEU:HD22	1:N:630:MET:HE1	2.01	0.42
2:a:51:LEU:HD23	2:a:51:LEU:HA	1.85	0.42
2:b:93:PRO:HG3	1:H:679:TYR:CE2	2.55	0.42
1:H:646:ILE:CD1	1:H:656:ILE:HG22	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:574:ILE:HG22	1:N:602:LEU:HB3	2.01	0.42
1:A:574:ILE:HG22	1:A:602:LEU:HB3	2.01	0.42
1:A:669:GLU:HG3	1:B:552:LYS:HG3	2.00	0.42
1:D:574:ILE:HG22	1:D:602:LEU:HB3	2.01	0.42
1:J:669:GLU:HG3	1:K:552:LYS:HG3	2.01	0.42
1:B:574:ILE:HG22	1:B:602:LEU:HB3	2.01	0.42
1:C:574:ILE:HG22	1:C:602:LEU:HB3	2.01	0.42
1:D:483:TYR:OH	1:E:544:ASP:OD1	2.31	0.42
1:L:669:GLU:HG3	1:M:552:LYS:HG3	2.01	0.42
2:P:51:LEU:HD21	2:Q:72:SER:HB3	2.02	0.42
1:I:639:LYS:HE3	1:I:639:LYS:HB3	1.55	0.42
1:I:646:ILE:CD1	1:I:656:ILE:HG22	2.49	0.42
2:W:44:ALA:HB2	2:X:88:ALA:O	2.19	0.42
1:J:646:ILE:CD1	1:J:656:ILE:HG22	2.49	0.42
2:P:39:VAL:HG22	1:K:687:ASP:HB3	2.01	0.42
2:Z:51:LEU:HD21	2:a:72:SER:HB3	2.01	0.42
1:K:646:ILE:CD1	1:K:656:ILE:HG22	2.49	0.42
1:L:646:ILE:CD1	1:L:656:ILE:HG22	2.49	0.42
2:X:53:ILE:HD12	3:D:801:PTY:H132	2.02	0.42
1:L:639:LYS:HB3	1:L:639:LYS:HE3	1.55	0.42
2:X:51:LEU:HD23	2:X:51:LEU:HA	1.85	0.41
1:G:669:GLU:HG3	1:H:552:LYS:HG3	2.01	0.41
2:Z:95:LYS:HA	2:Z:95:LYS:HD3	1.96	0.41
1:F:669:GLU:HG3	1:G:552:LYS:HG3	2.01	0.41
1:M:674:LEU:HD23	1:M:674:LEU:HA	1.81	0.41
2:X:93:PRO:HG3	1:D:679:TYR:CE2	2.55	0.41
1:C:669:GLU:HG3	1:D:552:LYS:HG3	2.01	0.41
1:M:456:ILE:HD11	1:M:620:VAL:HG12	2.03	0.41
1:N:639:LYS:HB3	1:N:639:LYS:HE3	1.55	0.41
3:A:801:PTY:H221	2:U:45:TYR:CZ	2.55	0.41
1:N:456:ILE:HD11	1:N:620:VAL:HG12	2.03	0.41
1:D:674:LEU:HD23	1:D:674:LEU:HA	1.80	0.41
1:I:483:TYR:OH	1:J:544:ASP:OD1	2.32	0.41
1:K:440:VAL:O	1:K:444:ASP:HB3	2.21	0.41
1:L:456:ILE:HD11	1:L:620:VAL:HG12	2.03	0.41
1:A:456:ILE:HD11	1:A:620:VAL:HG12	2.03	0.41
1:F:523:LEU:HB3	1:F:686:ARG:HB2	2.03	0.41
1:J:582:TYR:CE1	1:J:596:LYS:HB2	2.56	0.41
2:R:53:ILE:HD12	3:L:801:PTY:H132	2.03	0.41
1:E:669:GLU:HG3	1:F:552:LYS:HG3	2.01	0.41
1:I:582:TYR:CE1	1:I:596:LYS:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:582:TYR:CE1	1:K:596:LYS:HB2	2.56	0.41
1:L:582:TYR:CE1	1:L:596:LYS:HB2	2.56	0.41
1:M:440:VAL:O	1:M:444:ASP:HB3	2.21	0.41
1:N:523:LEU:HB3	1:N:686:ARG:HB2	2.03	0.41
2:b:41:ALA:HB3	3:H:801:PTY:HC51	2.02	0.41
1:B:440:VAL:O	1:B:444:ASP:HB3	2.21	0.41
1:C:440:VAL:O	1:C:444:ASP:HB3	2.21	0.41
1:D:543:LEU:HD12	1:D:543:LEU:HA	1.89	0.41
1:D:611:ASP:OD1	1:D:611:ASP:N	2.46	0.41
1:F:440:VAL:O	1:F:444:ASP:HB3	2.21	0.41
1:F:582:TYR:CE1	1:F:596:LYS:HB2	2.56	0.41
1:G:582:TYR:CE1	1:G:596:LYS:HB2	2.56	0.41
1:H:582:TYR:CE1	1:H:596:LYS:HB2	2.56	0.41
1:I:440:VAL:O	1:I:444:ASP:HB3	2.21	0.41
1:K:456:ILE:HD11	1:K:620:VAL:HG12	2.03	0.41
1:L:523:LEU:HB3	1:L:686:ARG:HB2	2.02	0.41
1:M:582:TYR:CE1	1:M:596:LYS:HB2	2.56	0.41
1:A:582:TYR:CE1	1:A:596:LYS:HB2	2.56	0.41
1:I:543:LEU:HD12	1:I:543:LEU:HA	1.89	0.41
1:N:440:VAL:O	1:N:444:ASP:HB3	2.21	0.41
1:B:582:TYR:CE1	1:B:596:LYS:HB2	2.56	0.40
1:C:582:TYR:CE1	1:C:596:LYS:HB2	2.56	0.40
1:E:582:TYR:CE1	1:E:596:LYS:HB2	2.56	0.40
1:F:543:LEU:HD12	1:F:543:LEU:HA	1.90	0.40
1:H:440:VAL:O	1:H:444:ASP:HB3	2.21	0.40
1:I:523:LEU:HB3	1:I:686:ARG:HB2	2.02	0.40
1:M:523:LEU:HB3	1:M:686:ARG:HB2	2.03	0.40
1:N:582:TYR:CE1	1:N:596:LYS:HB2	2.56	0.40
2:Y:53:ILE:HD12	3:E:801:PTY:H132	2.03	0.40
1:C:639:LYS:HE3	1:C:639:LYS:HB3	1.55	0.40
1:D:523:LEU:HB3	1:D:686:ARG:HB2	2.03	0.40
1:E:440:VAL:O	1:E:444:ASP:HB3	2.21	0.40
1:G:523:LEU:HB3	1:G:686:ARG:HB2	2.03	0.40
1:J:456:ILE:HD11	1:J:620:VAL:HG12	2.03	0.40
2:S:39:VAL:HG22	1:N:687:ASP:HB3	2.03	0.40
2:S:45:TYR:CD2	3:M:801:PTY:H201	2.56	0.40
2:a:93:PRO:HG3	1:G:679:TYR:CE2	2.56	0.40
1:B:456:ILE:HD11	1:B:620:VAL:HG12	2.03	0.40
1:B:523:LEU:HB3	1:B:686:ARG:HB2	2.02	0.40
1:D:582:TYR:CE1	1:D:596:LYS:HB2	2.56	0.40
1:H:523:LEU:HB3	1:H:686:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:429:PRO:HD2	1:I:432:ARG:HG3	2.04	0.40
1:A:523:LEU:HB3	1:A:686:ARG:HB2	2.03	0.40
2:Z:96:GLU:OE1	1:F:678:PRO:HD2	2.22	0.40
2:b:93:PRO:HG3	1:H:679:TYR:CZ	2.56	0.40
1:F:429:PRO:HD2	1:F:432:ARG:HG3	2.04	0.40
1:F:674:LEU:HD23	1:F:674:LEU:HA	1.81	0.40
1:G:429:PRO:HD2	1:G:432:ARG:HG3	2.04	0.40
1:G:456:ILE:HD11	1:G:620:VAL:HG12	2.03	0.40
1:H:429:PRO:HD2	1:H:432:ARG:HG3	2.04	0.40
1:A:440:VAL:HG21	1:B:382:ILE:HG21	2.04	0.40
2:Y:95:LYS:HA	2:Y:95:LYS:HD3	1.97	0.40
1:B:611:ASP:OD1	1:B:611:ASP:N	2.45	0.40
1:G:440:VAL:O	1:G:444:ASP:HB3	2.21	0.40
1:L:670:LYS:HB2	1:L:675:GLY:HA3	2.04	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	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	B	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	C	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	D	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	E	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	F	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	G	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	H	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	I	305/714 (43%)	298 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	K	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	L	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	M	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
1	N	305/714 (43%)	298 (98%)	7 (2%)	0	100	100
2	O	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	P	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	Q	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	R	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	S	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	T	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	U	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	V	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	W	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	X	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	Y	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	Z	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	a	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
2	b	72/114 (63%)	71 (99%)	1 (1%)	0	100	100
All	All	5278/11592 (46%)	5166 (98%)	112 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	266/595 (45%)	266 (100%)	0	100	100
1	B	266/595 (45%)	265 (100%)	1 (0%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	266/595 (45%)	265 (100%)	1 (0%)	84	93
1	D	266/595 (45%)	266 (100%)	0	100	100
1	E	266/595 (45%)	266 (100%)	0	100	100
1	F	266/595 (45%)	266 (100%)	0	100	100
1	G	266/595 (45%)	266 (100%)	0	100	100
1	H	266/595 (45%)	266 (100%)	0	100	100
1	I	266/595 (45%)	266 (100%)	0	100	100
1	J	266/595 (45%)	266 (100%)	0	100	100
1	K	266/595 (45%)	266 (100%)	0	100	100
1	L	266/595 (45%)	266 (100%)	0	100	100
1	M	266/595 (45%)	266 (100%)	0	100	100
1	N	266/595 (45%)	266 (100%)	0	100	100
2	O	52/84 (62%)	52 (100%)	0	100	100
2	P	52/84 (62%)	52 (100%)	0	100	100
2	Q	52/84 (62%)	52 (100%)	0	100	100
2	R	52/84 (62%)	52 (100%)	0	100	100
2	S	52/84 (62%)	52 (100%)	0	100	100
2	T	52/84 (62%)	52 (100%)	0	100	100
2	U	52/84 (62%)	52 (100%)	0	100	100
2	V	52/84 (62%)	52 (100%)	0	100	100
2	W	52/84 (62%)	52 (100%)	0	100	100
2	X	52/84 (62%)	52 (100%)	0	100	100
2	Y	52/84 (62%)	52 (100%)	0	100	100
2	Z	52/84 (62%)	52 (100%)	0	100	100
2	a	52/84 (62%)	52 (100%)	0	100	100
2	b	52/84 (62%)	52 (100%)	0	100	100
All	All	4452/9506 (47%)	4450 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
1	B	623	ASP
1	C	623	ASP

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

Mol	Chain	Res	Type
1	A	546	GLN
1	A	555	ASN
1	A	612	ASN
1	B	546	GLN
1	B	612	ASN
1	C	546	GLN
1	C	555	ASN
1	C	612	ASN
1	D	546	GLN
1	D	612	ASN
1	E	546	GLN
1	E	612	ASN
1	F	546	GLN
1	F	612	ASN
1	G	546	GLN
1	G	612	ASN
1	H	546	GLN
1	H	612	ASN
1	I	546	GLN
1	I	612	ASN
1	J	546	GLN
1	J	612	ASN
1	K	546	GLN
1	K	612	ASN
1	L	546	GLN
1	L	612	ASN
1	M	546	GLN
1	M	612	ASN
1	N	546	GLN
1	N	612	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	PTY	A	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	H	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	I	801	-	49,49,49	0.45	0	52,54,54	0.41	0
3	PTY	J	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	D	801	-	49,49,49	0.45	0	52,54,54	0.41	0
3	PTY	F	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	G	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	N	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	M	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	C	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	K	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	E	801	-	49,49,49	0.45	0	52,54,54	0.41	0
3	PTY	B	801	-	49,49,49	0.46	0	52,54,54	0.41	0
3	PTY	L	801	-	49,49,49	0.46	0	52,54,54	0.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PTY	A	801	-	-	12/53/53/53	-
3	PTY	H	801	-	-	12/53/53/53	-
3	PTY	I	801	-	-	12/53/53/53	-
3	PTY	J	801	-	-	12/53/53/53	-
3	PTY	D	801	-	-	12/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PTY	F	801	-	-	12/53/53/53	-
3	PTY	G	801	-	-	12/53/53/53	-
3	PTY	N	801	-	-	12/53/53/53	-
3	PTY	M	801	-	-	13/53/53/53	-
3	PTY	C	801	-	-	12/53/53/53	-
3	PTY	K	801	-	-	12/53/53/53	-
3	PTY	E	801	-	-	12/53/53/53	-
3	PTY	B	801	-	-	12/53/53/53	-
3	PTY	L	801	-	-	13/53/53/53	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (170) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	PTY	O30-C30-O4-C1
3	B	801	PTY	O30-C30-O4-C1
3	C	801	PTY	O30-C30-O4-C1
3	D	801	PTY	O30-C30-O4-C1
3	E	801	PTY	O30-C30-O4-C1
3	F	801	PTY	O30-C30-O4-C1
3	G	801	PTY	O30-C30-O4-C1
3	H	801	PTY	O30-C30-O4-C1
3	I	801	PTY	O30-C30-O4-C1
3	J	801	PTY	O30-C30-O4-C1
3	K	801	PTY	O30-C30-O4-C1
3	L	801	PTY	O30-C30-O4-C1
3	M	801	PTY	O30-C30-O4-C1
3	N	801	PTY	O30-C30-O4-C1
3	A	801	PTY	C31-C30-O4-C1
3	B	801	PTY	C31-C30-O4-C1
3	C	801	PTY	C31-C30-O4-C1
3	D	801	PTY	C31-C30-O4-C1
3	E	801	PTY	C31-C30-O4-C1
3	F	801	PTY	C31-C30-O4-C1
3	G	801	PTY	C31-C30-O4-C1
3	H	801	PTY	C31-C30-O4-C1
3	I	801	PTY	C31-C30-O4-C1

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Mol	Chain	Res	Type	Atoms
3	J	801	PTY	C31-C30-O4-C1
3	K	801	PTY	C31-C30-O4-C1
3	L	801	PTY	C31-C30-O4-C1
3	M	801	PTY	C31-C30-O4-C1
3	N	801	PTY	C31-C30-O4-C1
3	A	801	PTY	C11-C8-O7-C6
3	B	801	PTY	C11-C8-O7-C6
3	C	801	PTY	C11-C8-O7-C6
3	D	801	PTY	C11-C8-O7-C6
3	E	801	PTY	C11-C8-O7-C6
3	F	801	PTY	C11-C8-O7-C6
3	G	801	PTY	C11-C8-O7-C6
3	H	801	PTY	C11-C8-O7-C6
3	I	801	PTY	C11-C8-O7-C6
3	J	801	PTY	C11-C8-O7-C6
3	K	801	PTY	C11-C8-O7-C6
3	L	801	PTY	C11-C8-O7-C6
3	M	801	PTY	C11-C8-O7-C6
3	N	801	PTY	C11-C8-O7-C6
3	A	801	PTY	O10-C8-O7-C6
3	B	801	PTY	O10-C8-O7-C6
3	C	801	PTY	O10-C8-O7-C6
3	D	801	PTY	O10-C8-O7-C6
3	E	801	PTY	O10-C8-O7-C6
3	F	801	PTY	O10-C8-O7-C6
3	G	801	PTY	O10-C8-O7-C6
3	H	801	PTY	O10-C8-O7-C6
3	I	801	PTY	O10-C8-O7-C6
3	J	801	PTY	O10-C8-O7-C6
3	K	801	PTY	O10-C8-O7-C6
3	L	801	PTY	O10-C8-O7-C6
3	M	801	PTY	O10-C8-O7-C6
3	N	801	PTY	O10-C8-O7-C6
3	A	801	PTY	C30-C31-C32-C33
3	C	801	PTY	C30-C31-C32-C33
3	D	801	PTY	C30-C31-C32-C33
3	E	801	PTY	C30-C31-C32-C33
3	F	801	PTY	C30-C31-C32-C33
3	G	801	PTY	C30-C31-C32-C33
3	H	801	PTY	C30-C31-C32-C33
3	I	801	PTY	C30-C31-C32-C33
3	K	801	PTY	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
3	L	801	PTY	C30-C31-C32-C33
3	M	801	PTY	C30-C31-C32-C33
3	N	801	PTY	C30-C31-C32-C33
3	B	801	PTY	C30-C31-C32-C33
3	J	801	PTY	C30-C31-C32-C33
3	J	801	PTY	C21-C22-C23-C24
3	D	801	PTY	C21-C22-C23-C24
3	E	801	PTY	C21-C22-C23-C24
3	F	801	PTY	C21-C22-C23-C24
3	H	801	PTY	C21-C22-C23-C24
3	A	801	PTY	C21-C22-C23-C24
3	C	801	PTY	C21-C22-C23-C24
3	I	801	PTY	C21-C22-C23-C24
3	L	801	PTY	C21-C22-C23-C24
3	N	801	PTY	C21-C22-C23-C24
3	B	801	PTY	C21-C22-C23-C24
3	G	801	PTY	C21-C22-C23-C24
3	K	801	PTY	C21-C22-C23-C24
3	M	801	PTY	C21-C22-C23-C24
3	A	801	PTY	O4-C1-C6-C5
3	B	801	PTY	O4-C1-C6-C5
3	C	801	PTY	O4-C1-C6-C5
3	D	801	PTY	O4-C1-C6-C5
3	E	801	PTY	O4-C1-C6-C5
3	F	801	PTY	O4-C1-C6-C5
3	G	801	PTY	O4-C1-C6-C5
3	H	801	PTY	O4-C1-C6-C5
3	I	801	PTY	O4-C1-C6-C5
3	J	801	PTY	O4-C1-C6-C5
3	K	801	PTY	O4-C1-C6-C5
3	L	801	PTY	O4-C1-C6-C5
3	M	801	PTY	O4-C1-C6-C5
3	N	801	PTY	O4-C1-C6-C5
3	J	801	PTY	C41-C42-C43-C44
3	A	801	PTY	C41-C42-C43-C44
3	B	801	PTY	C41-C42-C43-C44
3	C	801	PTY	C41-C42-C43-C44
3	D	801	PTY	C41-C42-C43-C44
3	E	801	PTY	C41-C42-C43-C44
3	F	801	PTY	C41-C42-C43-C44
3	G	801	PTY	C41-C42-C43-C44
3	H	801	PTY	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
3	I	801	PTY	C41-C42-C43-C44
3	K	801	PTY	C41-C42-C43-C44
3	L	801	PTY	C41-C42-C43-C44
3	M	801	PTY	C41-C42-C43-C44
3	N	801	PTY	C41-C42-C43-C44
3	A	801	PTY	O4-C1-C6-O7
3	B	801	PTY	O4-C1-C6-O7
3	C	801	PTY	O4-C1-C6-O7
3	D	801	PTY	O4-C1-C6-O7
3	E	801	PTY	O4-C1-C6-O7
3	F	801	PTY	O4-C1-C6-O7
3	G	801	PTY	O4-C1-C6-O7
3	H	801	PTY	O4-C1-C6-O7
3	I	801	PTY	O4-C1-C6-O7
3	J	801	PTY	O4-C1-C6-O7
3	K	801	PTY	O4-C1-C6-O7
3	L	801	PTY	O4-C1-C6-O7
3	M	801	PTY	O4-C1-C6-O7
3	N	801	PTY	O4-C1-C6-O7
3	A	801	PTY	C5-O14-P1-O11
3	B	801	PTY	C5-O14-P1-O11
3	C	801	PTY	C5-O14-P1-O11
3	D	801	PTY	C5-O14-P1-O11
3	E	801	PTY	C5-O14-P1-O11
3	F	801	PTY	C5-O14-P1-O11
3	G	801	PTY	C5-O14-P1-O11
3	H	801	PTY	C5-O14-P1-O11
3	I	801	PTY	C5-O14-P1-O11
3	J	801	PTY	C5-O14-P1-O11
3	K	801	PTY	C5-O14-P1-O11
3	L	801	PTY	C5-O14-P1-O11
3	M	801	PTY	C5-O14-P1-O11
3	N	801	PTY	C5-O14-P1-O11
3	A	801	PTY	C31-C32-C33-C34
3	B	801	PTY	C31-C32-C33-C34
3	E	801	PTY	C31-C32-C33-C34
3	F	801	PTY	C31-C32-C33-C34
3	I	801	PTY	C31-C32-C33-C34
3	K	801	PTY	C31-C32-C33-C34
3	J	801	PTY	C31-C32-C33-C34
3	M	801	PTY	C31-C32-C33-C34
3	N	801	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	D	801	PTY	C31-C32-C33-C34
3	G	801	PTY	C31-C32-C33-C34
3	L	801	PTY	C31-C32-C33-C34
3	C	801	PTY	C31-C32-C33-C34
3	H	801	PTY	C31-C32-C33-C34
3	B	801	PTY	C25-C26-C27-C28
3	J	801	PTY	C25-C26-C27-C28
3	H	801	PTY	C25-C26-C27-C28
3	I	801	PTY	C25-C26-C27-C28
3	L	801	PTY	C25-C26-C27-C28
3	C	801	PTY	C25-C26-C27-C28
3	E	801	PTY	C25-C26-C27-C28
3	G	801	PTY	C25-C26-C27-C28
3	K	801	PTY	C25-C26-C27-C28
3	M	801	PTY	C25-C26-C27-C28
3	N	801	PTY	C25-C26-C27-C28
3	A	801	PTY	C25-C26-C27-C28
3	D	801	PTY	C25-C26-C27-C28
3	F	801	PTY	C25-C26-C27-C28
3	L	801	PTY	C3-O11-P1-O12
3	M	801	PTY	C3-O11-P1-O12

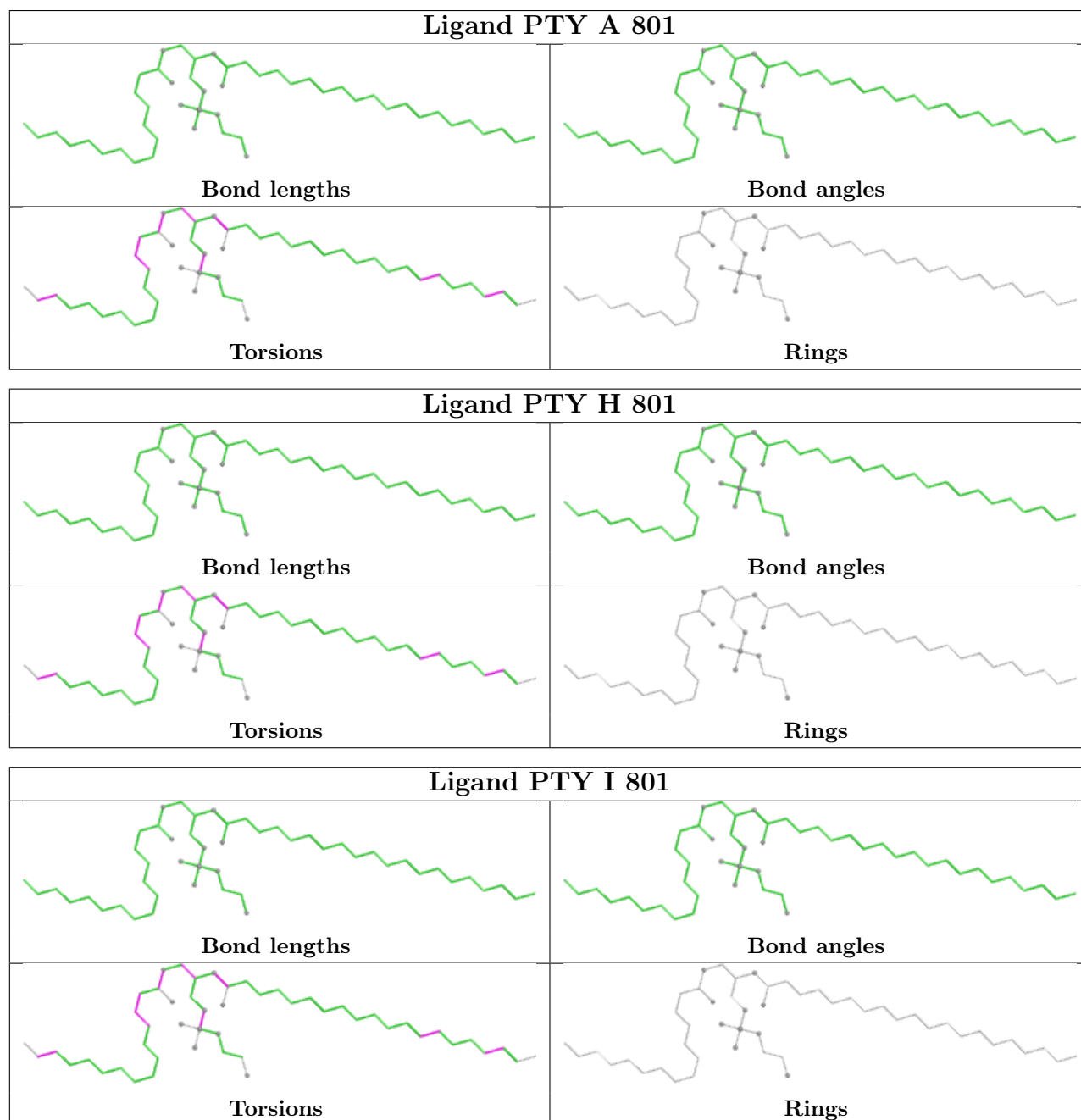
There are no ring outliers.

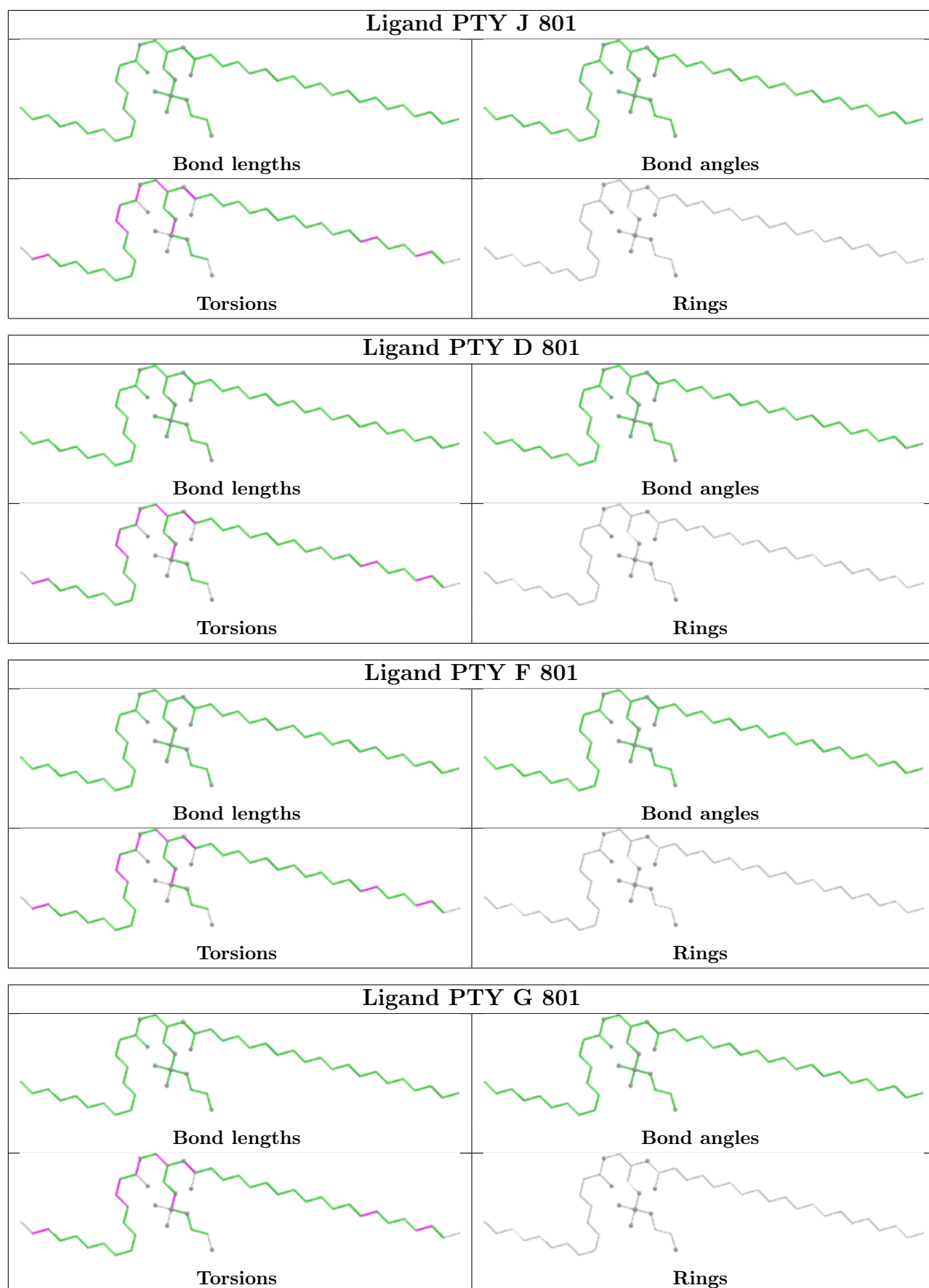
14 monomers are involved in 27 short contacts:

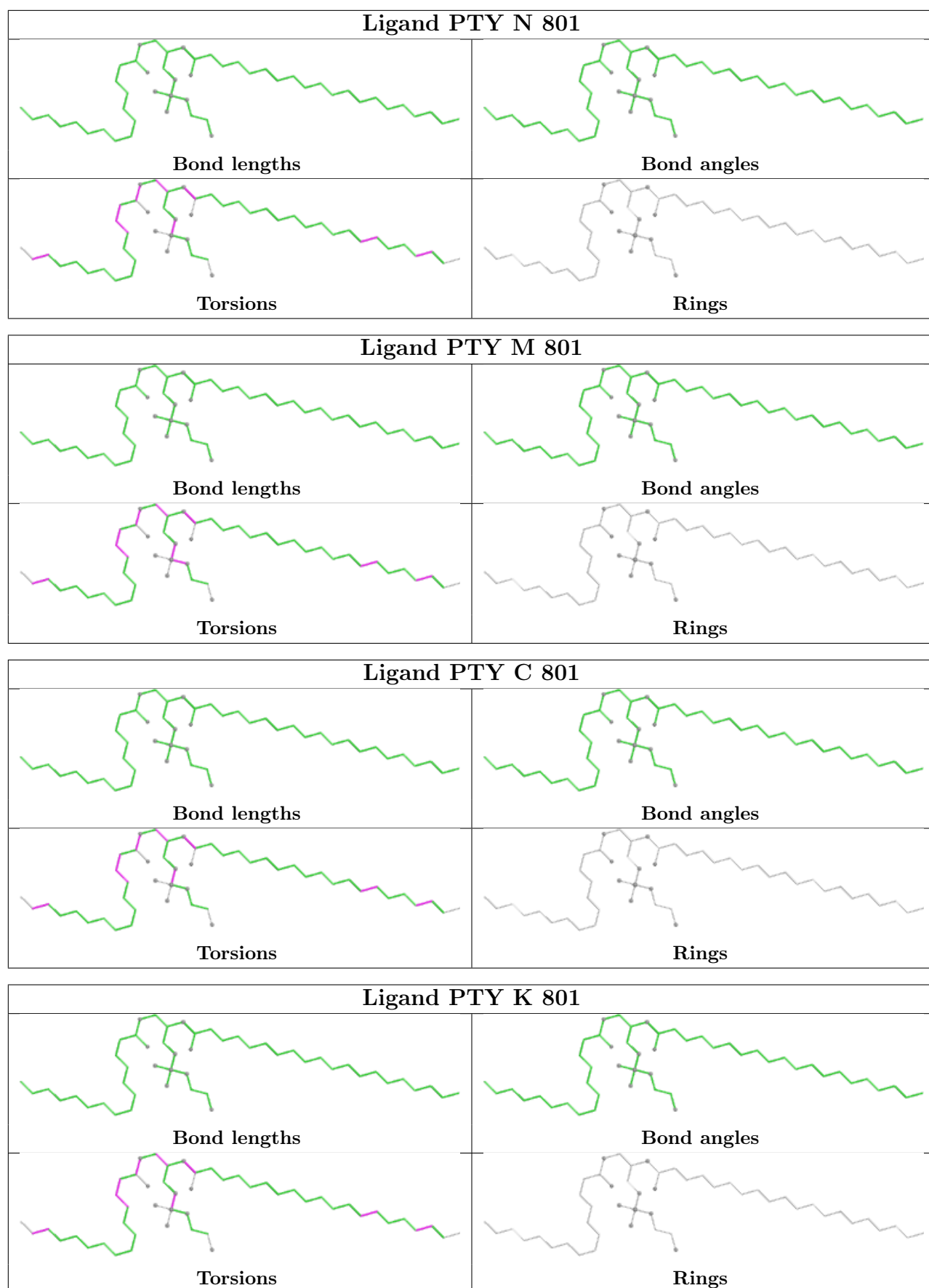
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	PTY	3	0
3	H	801	PTY	3	0
3	I	801	PTY	2	0
3	J	801	PTY	1	0
3	D	801	PTY	2	0
3	F	801	PTY	1	0
3	G	801	PTY	2	0
3	N	801	PTY	1	0
3	M	801	PTY	2	0
3	C	801	PTY	2	0
3	K	801	PTY	3	0
3	E	801	PTY	2	0
3	B	801	PTY	1	0
3	L	801	PTY	2	0

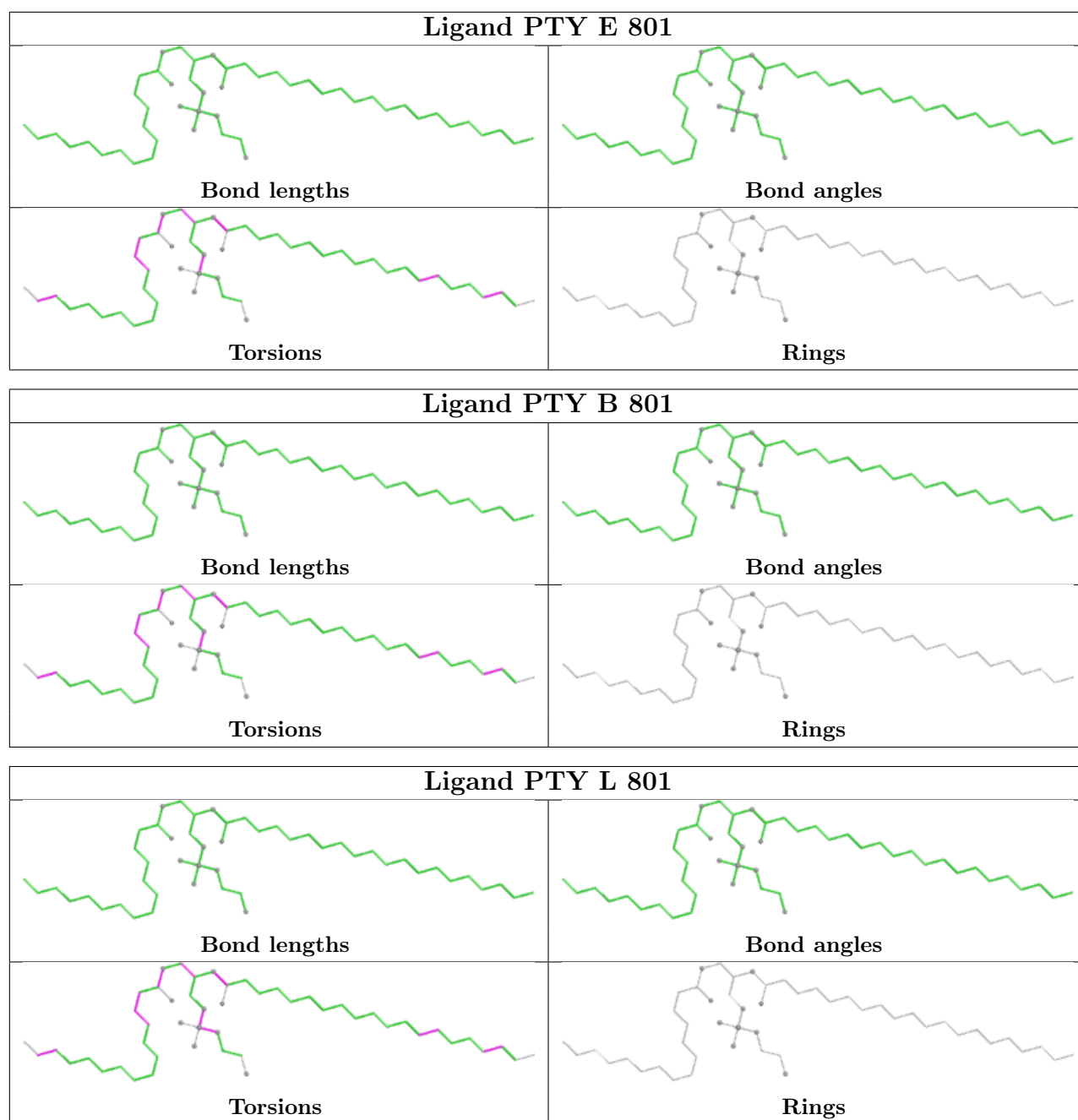
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

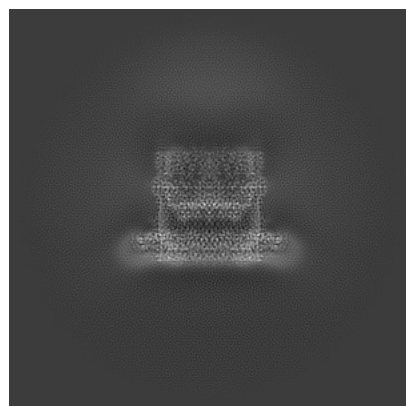
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66449. These allow visual inspection of the internal detail of the map and identification of artifacts.

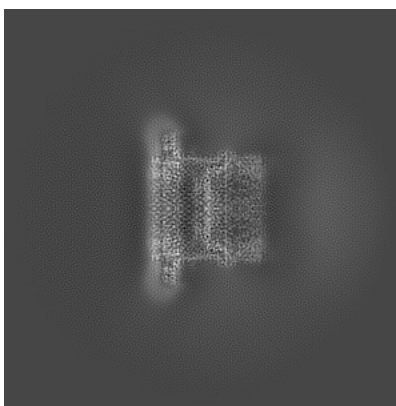
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

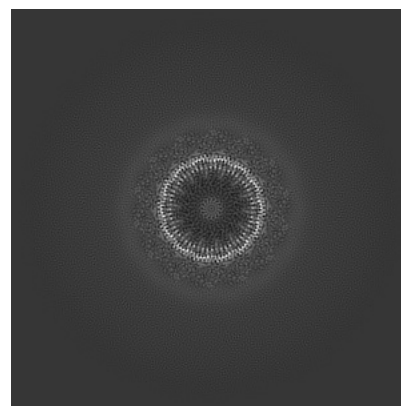
6.1.1 Primary map



X

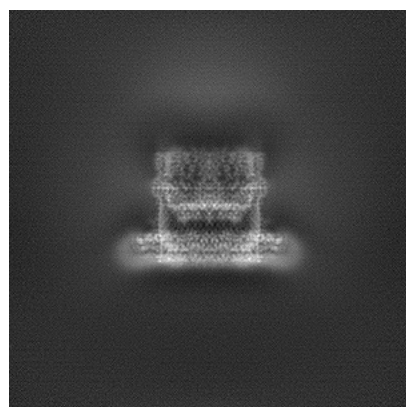


Y

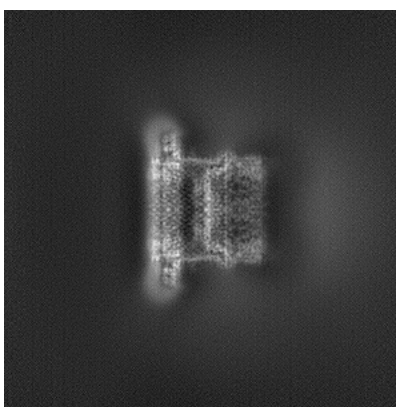


Z

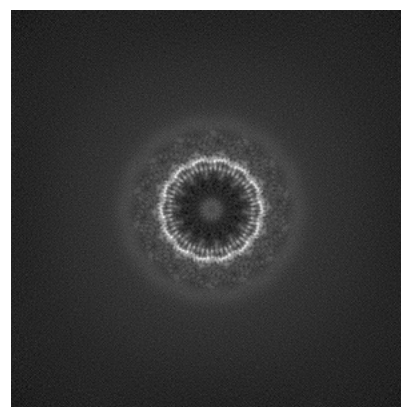
6.1.2 Raw map



X



Y

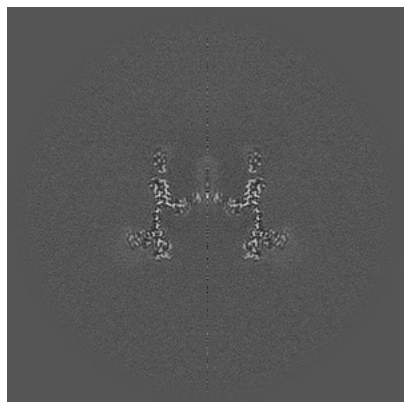


Z

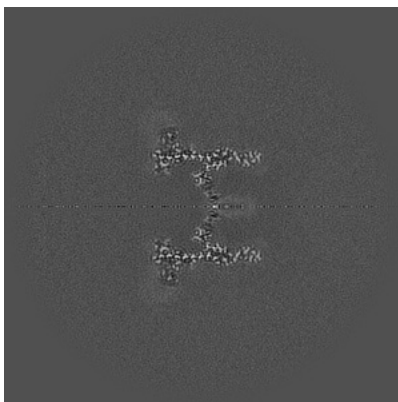
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

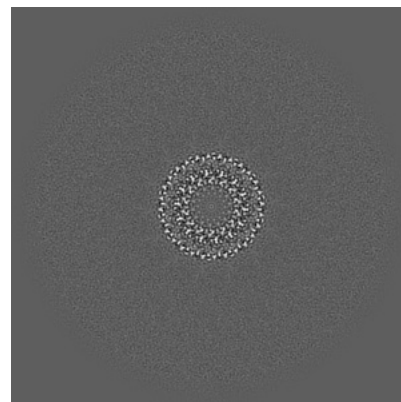
6.2.1 Primary map



X Index: 255

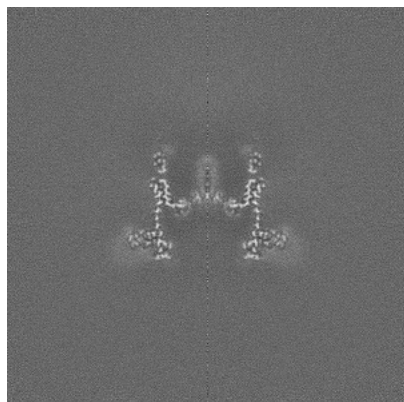


Y Index: 255

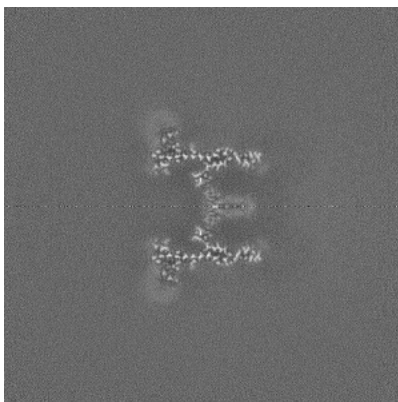


Z Index: 255

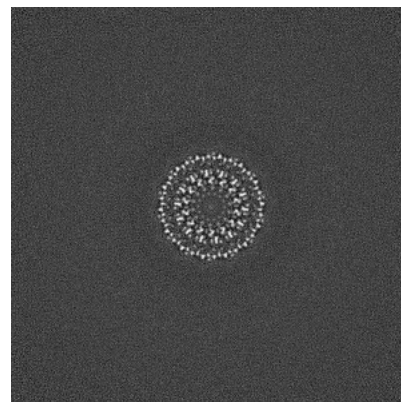
6.2.2 Raw map



X Index: 255



Y Index: 255

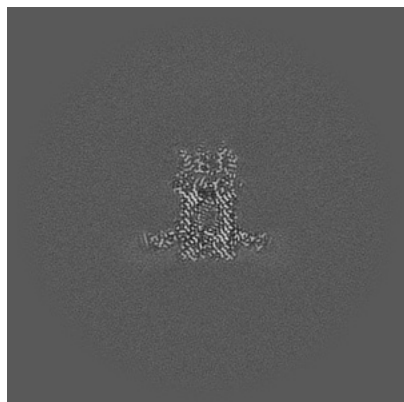


Z Index: 255

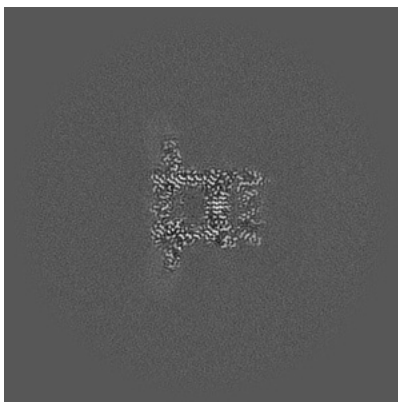
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

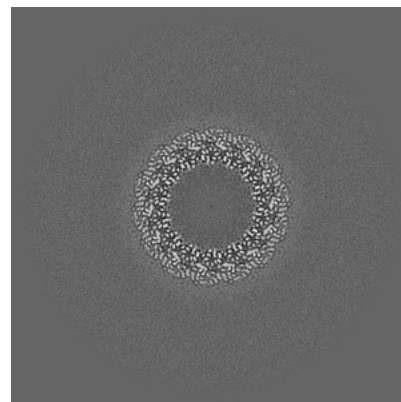
6.3.1 Primary map



X Index: 196

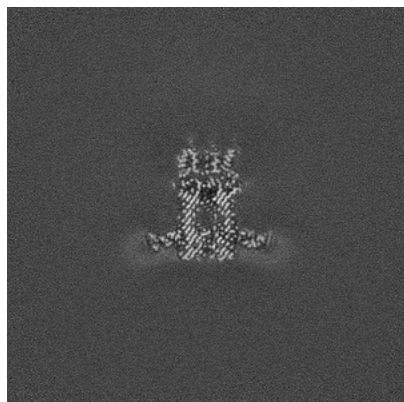


Y Index: 308

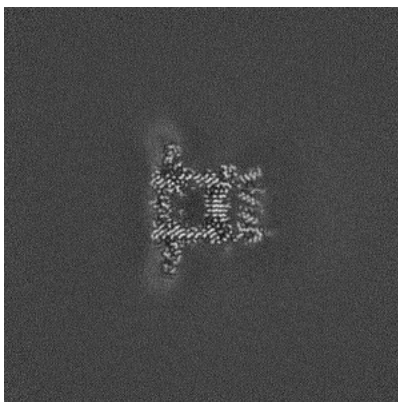


Z Index: 216

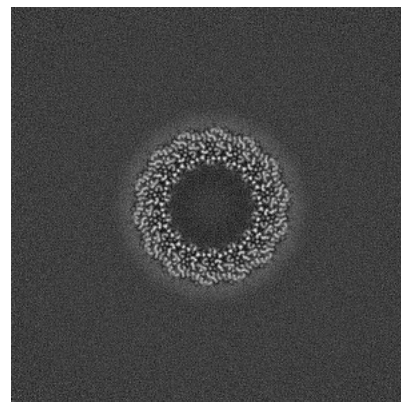
6.3.2 Raw map



X Index: 314



Y Index: 202

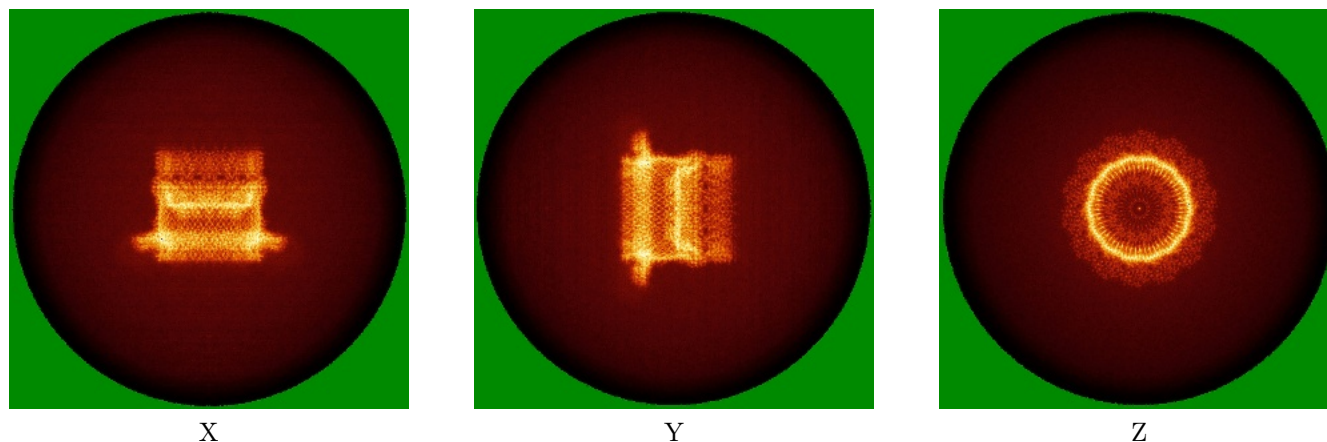


Z Index: 217

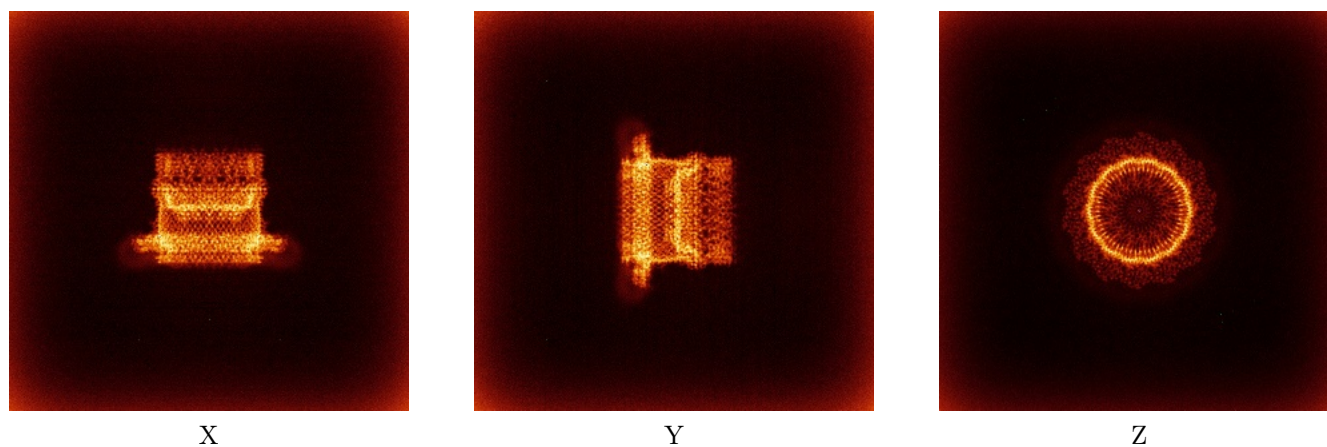
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



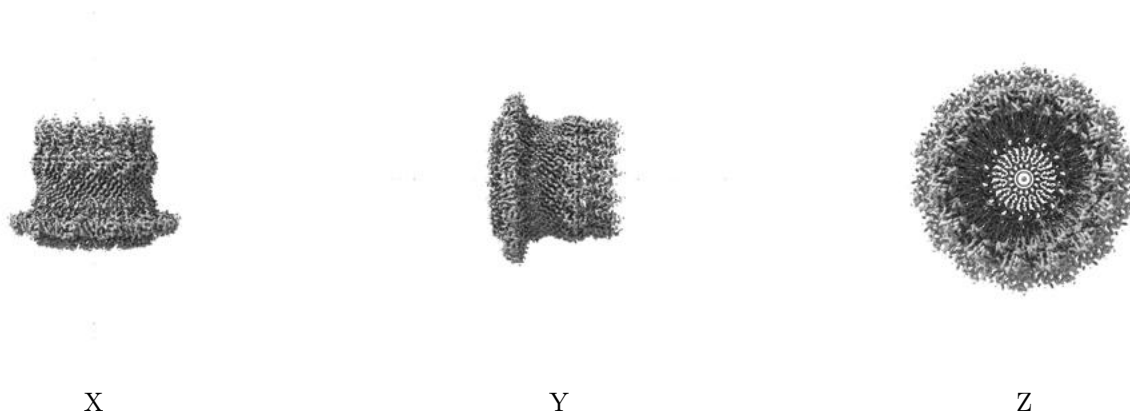
6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

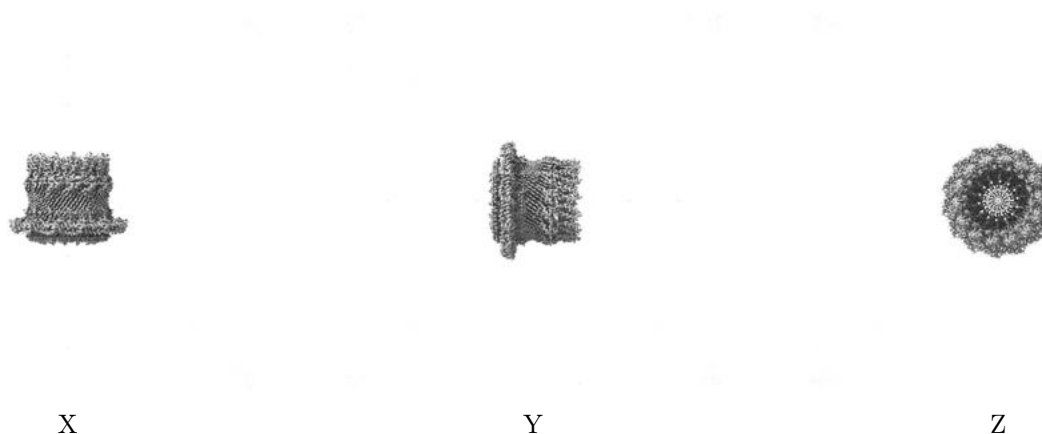
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 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.

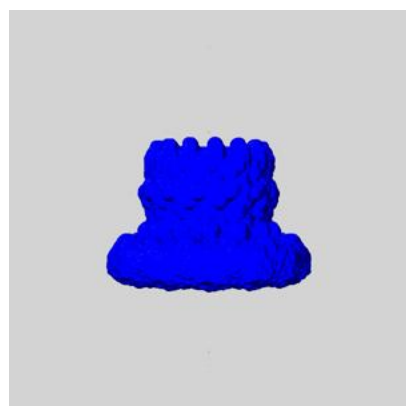
6.6 Mask visualisation [i](#)

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

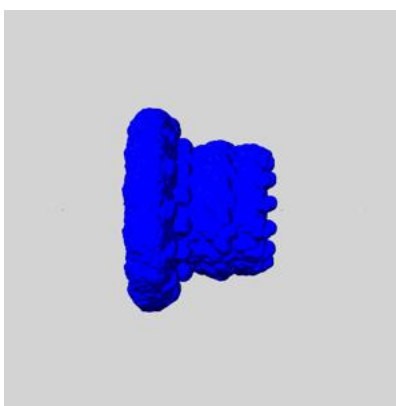
A mask typically either:

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

6.6.1 emd_66449_msk_1.map [i](#)



X



Y

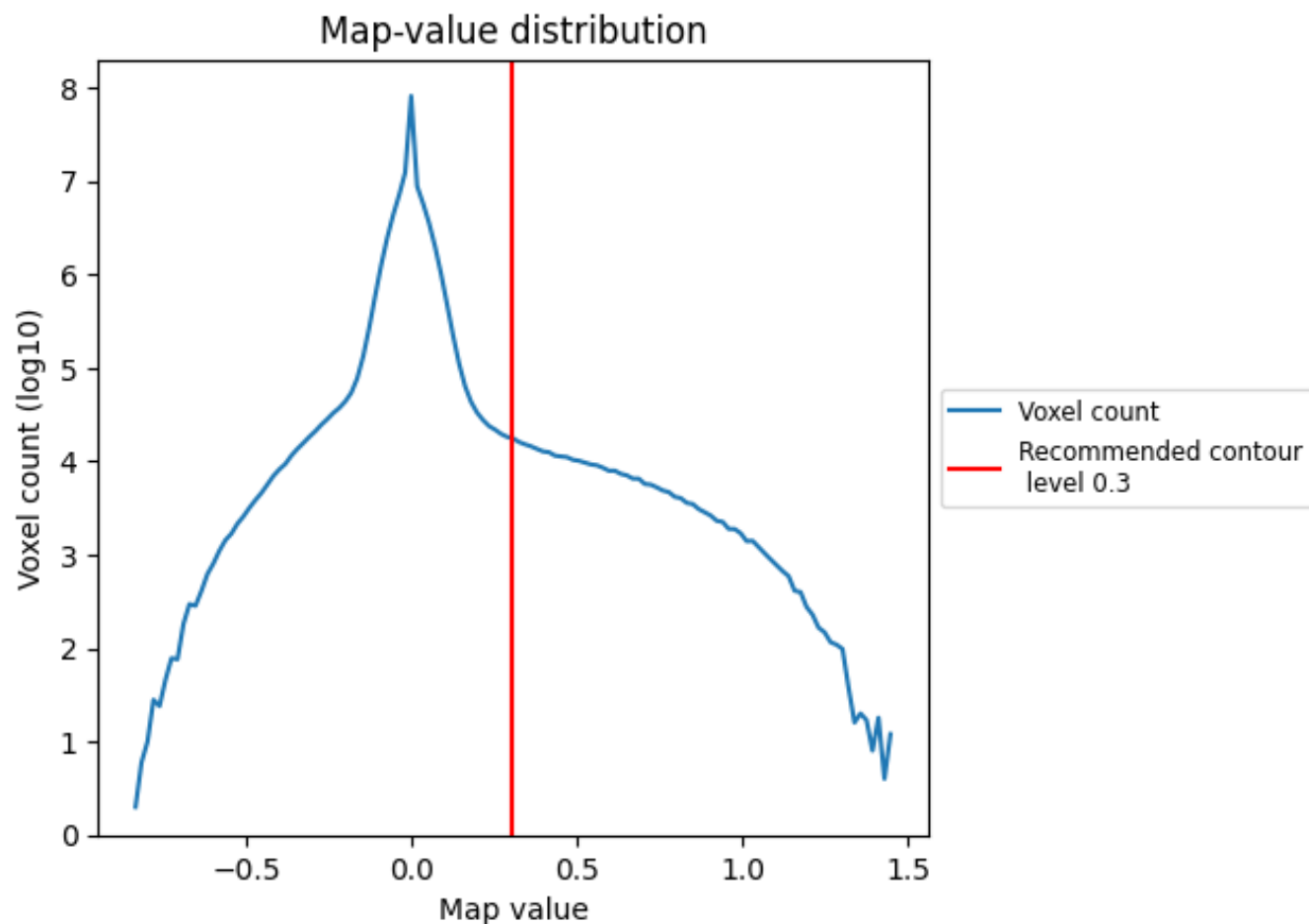


Z

7 Map analysis [i](#)

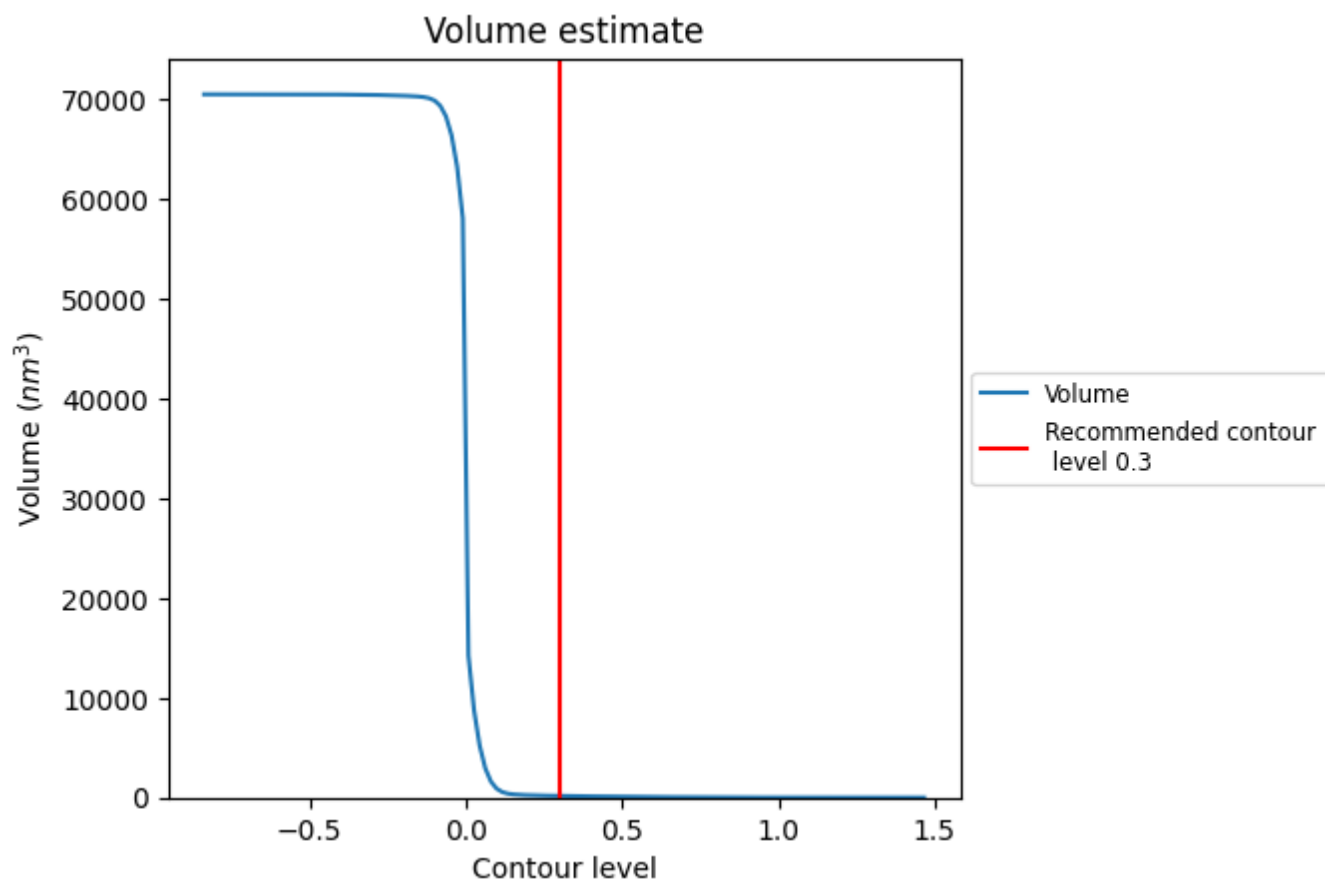
This section contains the results of statistical analysis of the map.

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.

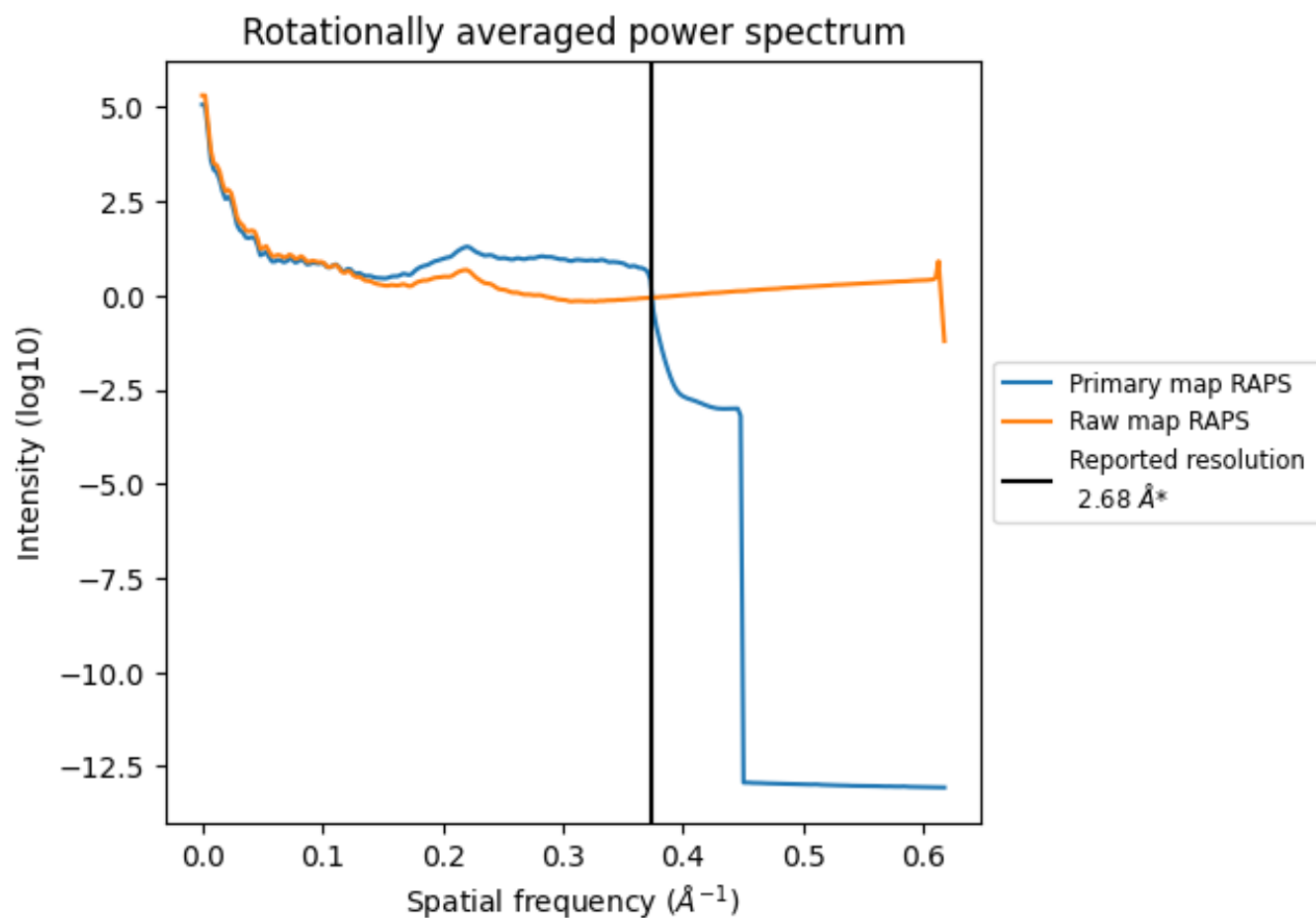
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 166 nm³; this corresponds to an approximate mass of 150 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 ⓘ

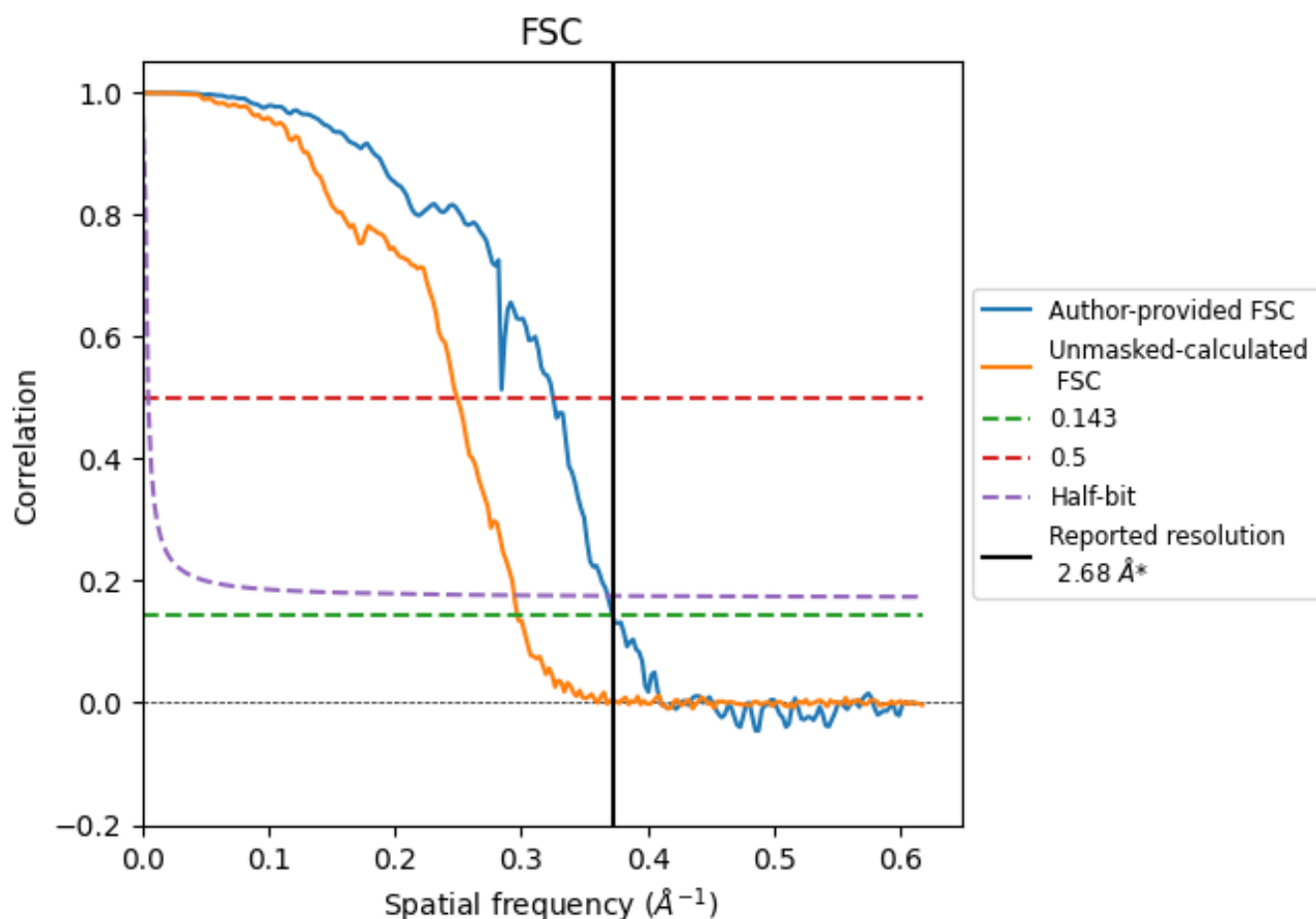


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 0.373 \AA^{-1}

8.2 Resolution estimates [i](#)

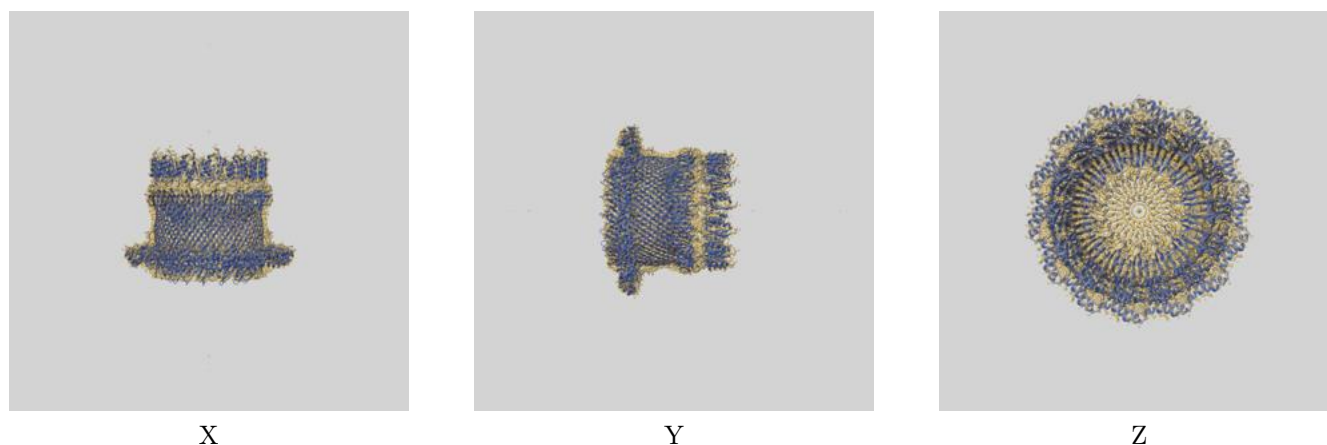
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.68	3.08	2.71
Unmasked-calculated*	3.37	4.01	3.40

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.37 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

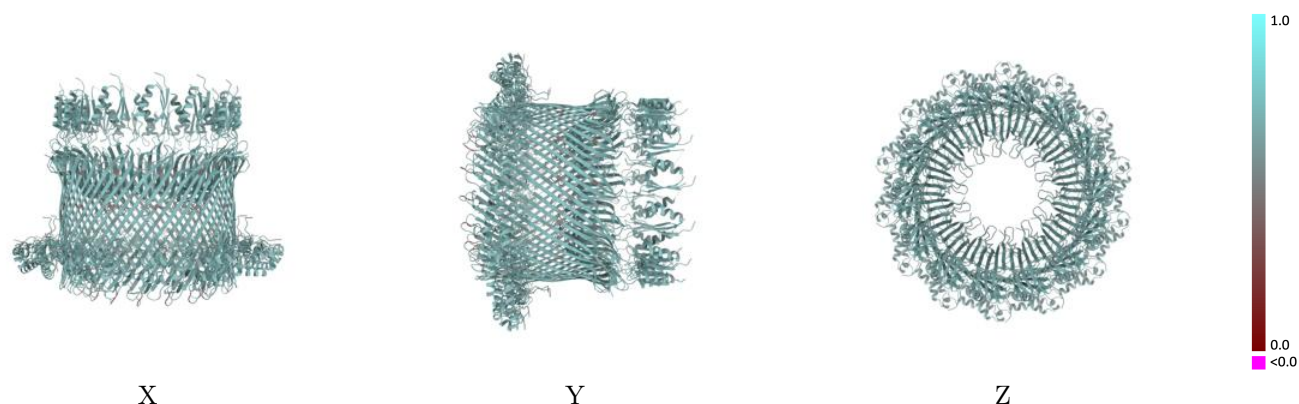
This section contains information regarding the fit between EMDB map EMD-66449 and PDB model 9X0Y. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



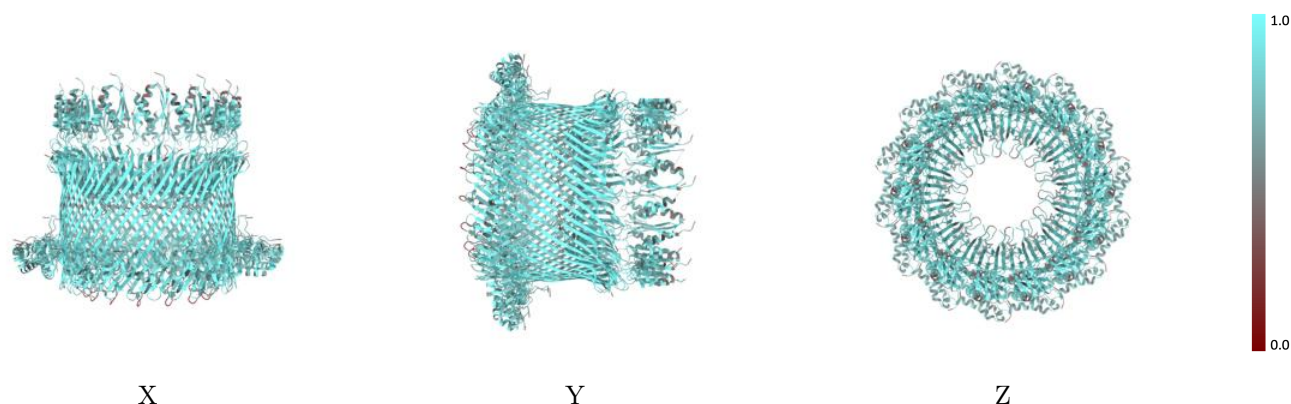
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



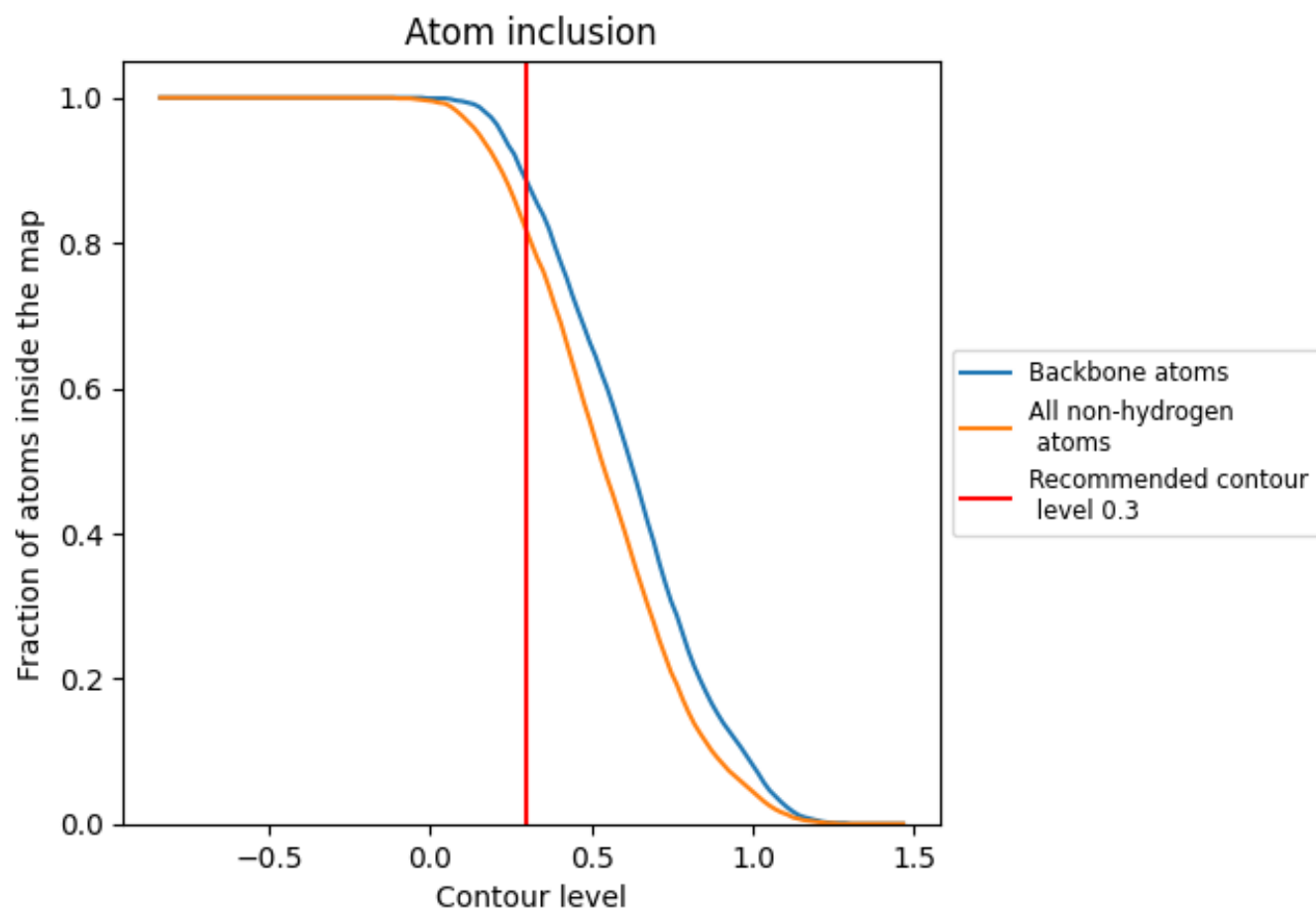
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).



























































9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 82% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8150	 0.6360
A	 0.8250	 0.6370
B	 0.8290	 0.6370
C	 0.8330	 0.6380
D	 0.8320	 0.6380
E	 0.8300	 0.6390
F	 0.8250	 0.6380
G	 0.8260	 0.6380
H	 0.8260	 0.6380
I	 0.8290	 0.6380
J	 0.8310	 0.6380
K	 0.8320	 0.6380
L	 0.8290	 0.6380
M	 0.8230	 0.6380
N	 0.8250	 0.6370
O	 0.7610	 0.6240
P	 0.7510	 0.6280
Q	 0.7480	 0.6230
R	 0.7550	 0.6270
S	 0.7590	 0.6250
T	 0.7570	 0.6280
U	 0.7510	 0.6270
V	 0.7590	 0.6220
W	 0.7460	 0.6280
X	 0.7510	 0.6270
Y	 0.7610	 0.6280
Z	 0.7570	 0.6280
a	 0.7670	 0.6260
b	 0.7550	 0.6270

