



wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 12:19 AM UTC

PDB ID : 9R6C / pdb_00009r6c
EMDB ID : EMD-53610
Title : CPS secretion pathway Wza-Wzc (Conf 5)
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2025-05-11
Resolution : 6.70 Å(reported)

This is a wwPDB EM Validation Summary 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 : 2022.3.0, CSD as543be (2022)
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 : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

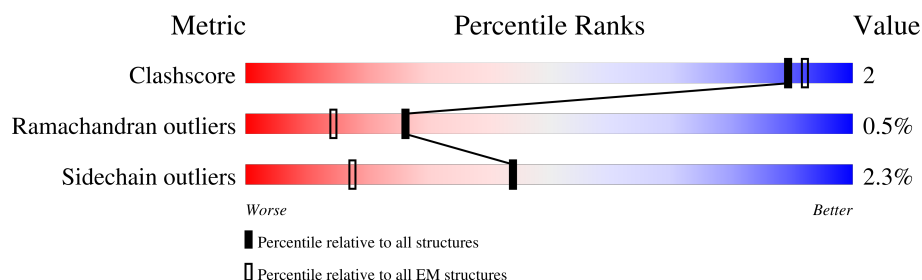
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.70 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	394	81% 10% 9%
1	B	394	84% 7% 9%
1	C	394	78% 12% 9%
1	D	394	85% 6% 9%
1	E	394	84% 7% 9%
1	F	394	82% 8% • 9%
1	G	394	83% 8% 9%
1	H	394	80% 10% • 9%
1	a	394	80% 9% • 9%

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Mol	Chain	Length	Quality of chain
1	b	394	 84% 7% • 9%
1	c	394	 81% 9% • 9%
1	d	394	 84% 7% 9%
1	e	394	 82% 9% 9%
1	f	394	 80% 11% • 9%
1	g	394	 80% 10% • 9%
1	h	394	 82% 7% • 9%
2	I	738	 70% 18% • 9%
2	J	738	 67% 21% • 9%
2	K	738	 80% 9% • 9%
2	L	738	 69% 20% • 9%
2	M	738	 72% 17% • 9%
2	N	738	 72% 17% • 9%
2	O	738	 72% 15% • 9%
2	P	738	 71% 18% •• 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 172976 atoms, of which 86752 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 Putative polysaccharide export protein Wza.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	B	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	C	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	D	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	E	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	F	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	G	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	H	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	a	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	b	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	c	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	d	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	e	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	f	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	g	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		
1	h	358	Total	C	H	N	O	S	0	0
			5548	1745	2765	486	539	13		

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	GLU	-	expression tag	UNP P0A930
A	381	ASN	-	expression tag	UNP P0A930
A	382	LEU	-	expression tag	UNP P0A930
A	383	TYR	-	expression tag	UNP P0A930
A	384	PHE	-	expression tag	UNP P0A930
A	385	GLN	-	expression tag	UNP P0A930
A	386	SER	-	expression tag	UNP P0A930
A	387	TRP	-	expression tag	UNP P0A930
A	388	SER	-	expression tag	UNP P0A930
A	389	HIS	-	expression tag	UNP P0A930
A	390	PRO	-	expression tag	UNP P0A930
A	391	GLN	-	expression tag	UNP P0A930
A	392	PHE	-	expression tag	UNP P0A930
A	393	GLU	-	expression tag	UNP P0A930
A	394	LYS	-	expression tag	UNP P0A930
B	380	GLU	-	expression tag	UNP P0A930
B	381	ASN	-	expression tag	UNP P0A930
B	382	LEU	-	expression tag	UNP P0A930
B	383	TYR	-	expression tag	UNP P0A930
B	384	PHE	-	expression tag	UNP P0A930
B	385	GLN	-	expression tag	UNP P0A930
B	386	SER	-	expression tag	UNP P0A930
B	387	TRP	-	expression tag	UNP P0A930
B	388	SER	-	expression tag	UNP P0A930
B	389	HIS	-	expression tag	UNP P0A930
B	390	PRO	-	expression tag	UNP P0A930
B	391	GLN	-	expression tag	UNP P0A930
B	392	PHE	-	expression tag	UNP P0A930
B	393	GLU	-	expression tag	UNP P0A930
B	394	LYS	-	expression tag	UNP P0A930
C	380	GLU	-	expression tag	UNP P0A930
C	381	ASN	-	expression tag	UNP P0A930
C	382	LEU	-	expression tag	UNP P0A930
C	383	TYR	-	expression tag	UNP P0A930
C	384	PHE	-	expression tag	UNP P0A930
C	385	GLN	-	expression tag	UNP P0A930
C	386	SER	-	expression tag	UNP P0A930
C	387	TRP	-	expression tag	UNP P0A930
C	388	SER	-	expression tag	UNP P0A930
C	389	HIS	-	expression tag	UNP P0A930
C	390	PRO	-	expression tag	UNP P0A930
C	391	GLN	-	expression tag	UNP P0A930
C	392	PHE	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
C	393	GLU	-	expression tag	UNP P0A930
C	394	LYS	-	expression tag	UNP P0A930
D	380	GLU	-	expression tag	UNP P0A930
D	381	ASN	-	expression tag	UNP P0A930
D	382	LEU	-	expression tag	UNP P0A930
D	383	TYR	-	expression tag	UNP P0A930
D	384	PHE	-	expression tag	UNP P0A930
D	385	GLN	-	expression tag	UNP P0A930
D	386	SER	-	expression tag	UNP P0A930
D	387	TRP	-	expression tag	UNP P0A930
D	388	SER	-	expression tag	UNP P0A930
D	389	HIS	-	expression tag	UNP P0A930
D	390	PRO	-	expression tag	UNP P0A930
D	391	GLN	-	expression tag	UNP P0A930
D	392	PHE	-	expression tag	UNP P0A930
D	393	GLU	-	expression tag	UNP P0A930
D	394	LYS	-	expression tag	UNP P0A930
E	380	GLU	-	expression tag	UNP P0A930
E	381	ASN	-	expression tag	UNP P0A930
E	382	LEU	-	expression tag	UNP P0A930
E	383	TYR	-	expression tag	UNP P0A930
E	384	PHE	-	expression tag	UNP P0A930
E	385	GLN	-	expression tag	UNP P0A930
E	386	SER	-	expression tag	UNP P0A930
E	387	TRP	-	expression tag	UNP P0A930
E	388	SER	-	expression tag	UNP P0A930
E	389	HIS	-	expression tag	UNP P0A930
E	390	PRO	-	expression tag	UNP P0A930
E	391	GLN	-	expression tag	UNP P0A930
E	392	PHE	-	expression tag	UNP P0A930
E	393	GLU	-	expression tag	UNP P0A930
E	394	LYS	-	expression tag	UNP P0A930
F	380	GLU	-	expression tag	UNP P0A930
F	381	ASN	-	expression tag	UNP P0A930
F	382	LEU	-	expression tag	UNP P0A930
F	383	TYR	-	expression tag	UNP P0A930
F	384	PHE	-	expression tag	UNP P0A930
F	385	GLN	-	expression tag	UNP P0A930
F	386	SER	-	expression tag	UNP P0A930
F	387	TRP	-	expression tag	UNP P0A930
F	388	SER	-	expression tag	UNP P0A930
F	389	HIS	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
F	390	PRO	-	expression tag	UNP P0A930
F	391	GLN	-	expression tag	UNP P0A930
F	392	PHE	-	expression tag	UNP P0A930
F	393	GLU	-	expression tag	UNP P0A930
F	394	LYS	-	expression tag	UNP P0A930
G	380	GLU	-	expression tag	UNP P0A930
G	381	ASN	-	expression tag	UNP P0A930
G	382	LEU	-	expression tag	UNP P0A930
G	383	TYR	-	expression tag	UNP P0A930
G	384	PHE	-	expression tag	UNP P0A930
G	385	GLN	-	expression tag	UNP P0A930
G	386	SER	-	expression tag	UNP P0A930
G	387	TRP	-	expression tag	UNP P0A930
G	388	SER	-	expression tag	UNP P0A930
G	389	HIS	-	expression tag	UNP P0A930
G	390	PRO	-	expression tag	UNP P0A930
G	391	GLN	-	expression tag	UNP P0A930
G	392	PHE	-	expression tag	UNP P0A930
G	393	GLU	-	expression tag	UNP P0A930
G	394	LYS	-	expression tag	UNP P0A930
H	380	GLU	-	expression tag	UNP P0A930
H	381	ASN	-	expression tag	UNP P0A930
H	382	LEU	-	expression tag	UNP P0A930
H	383	TYR	-	expression tag	UNP P0A930
H	384	PHE	-	expression tag	UNP P0A930
H	385	GLN	-	expression tag	UNP P0A930
H	386	SER	-	expression tag	UNP P0A930
H	387	TRP	-	expression tag	UNP P0A930
H	388	SER	-	expression tag	UNP P0A930
H	389	HIS	-	expression tag	UNP P0A930
H	390	PRO	-	expression tag	UNP P0A930
H	391	GLN	-	expression tag	UNP P0A930
H	392	PHE	-	expression tag	UNP P0A930
H	393	GLU	-	expression tag	UNP P0A930
H	394	LYS	-	expression tag	UNP P0A930
a	380	GLU	-	expression tag	UNP P0A930
a	381	ASN	-	expression tag	UNP P0A930
a	382	LEU	-	expression tag	UNP P0A930
a	383	TYR	-	expression tag	UNP P0A930
a	384	PHE	-	expression tag	UNP P0A930
a	385	GLN	-	expression tag	UNP P0A930
a	386	SER	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
a	387	TRP	-	expression tag	UNP P0A930
a	388	SER	-	expression tag	UNP P0A930
a	389	HIS	-	expression tag	UNP P0A930
a	390	PRO	-	expression tag	UNP P0A930
a	391	GLN	-	expression tag	UNP P0A930
a	392	PHE	-	expression tag	UNP P0A930
a	393	GLU	-	expression tag	UNP P0A930
a	394	LYS	-	expression tag	UNP P0A930
b	380	GLU	-	expression tag	UNP P0A930
b	381	ASN	-	expression tag	UNP P0A930
b	382	LEU	-	expression tag	UNP P0A930
b	383	TYR	-	expression tag	UNP P0A930
b	384	PHE	-	expression tag	UNP P0A930
b	385	GLN	-	expression tag	UNP P0A930
b	386	SER	-	expression tag	UNP P0A930
b	387	TRP	-	expression tag	UNP P0A930
b	388	SER	-	expression tag	UNP P0A930
b	389	HIS	-	expression tag	UNP P0A930
b	390	PRO	-	expression tag	UNP P0A930
b	391	GLN	-	expression tag	UNP P0A930
b	392	PHE	-	expression tag	UNP P0A930
b	393	GLU	-	expression tag	UNP P0A930
b	394	LYS	-	expression tag	UNP P0A930
c	380	GLU	-	expression tag	UNP P0A930
c	381	ASN	-	expression tag	UNP P0A930
c	382	LEU	-	expression tag	UNP P0A930
c	383	TYR	-	expression tag	UNP P0A930
c	384	PHE	-	expression tag	UNP P0A930
c	385	GLN	-	expression tag	UNP P0A930
c	386	SER	-	expression tag	UNP P0A930
c	387	TRP	-	expression tag	UNP P0A930
c	388	SER	-	expression tag	UNP P0A930
c	389	HIS	-	expression tag	UNP P0A930
c	390	PRO	-	expression tag	UNP P0A930
c	391	GLN	-	expression tag	UNP P0A930
c	392	PHE	-	expression tag	UNP P0A930
c	393	GLU	-	expression tag	UNP P0A930
c	394	LYS	-	expression tag	UNP P0A930
d	380	GLU	-	expression tag	UNP P0A930
d	381	ASN	-	expression tag	UNP P0A930
d	382	LEU	-	expression tag	UNP P0A930
d	383	TYR	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
d	384	PHE	-	expression tag	UNP P0A930
d	385	GLN	-	expression tag	UNP P0A930
d	386	SER	-	expression tag	UNP P0A930
d	387	TRP	-	expression tag	UNP P0A930
d	388	SER	-	expression tag	UNP P0A930
d	389	HIS	-	expression tag	UNP P0A930
d	390	PRO	-	expression tag	UNP P0A930
d	391	GLN	-	expression tag	UNP P0A930
d	392	PHE	-	expression tag	UNP P0A930
d	393	GLU	-	expression tag	UNP P0A930
d	394	LYS	-	expression tag	UNP P0A930
e	380	GLU	-	expression tag	UNP P0A930
e	381	ASN	-	expression tag	UNP P0A930
e	382	LEU	-	expression tag	UNP P0A930
e	383	TYR	-	expression tag	UNP P0A930
e	384	PHE	-	expression tag	UNP P0A930
e	385	GLN	-	expression tag	UNP P0A930
e	386	SER	-	expression tag	UNP P0A930
e	387	TRP	-	expression tag	UNP P0A930
e	388	SER	-	expression tag	UNP P0A930
e	389	HIS	-	expression tag	UNP P0A930
e	390	PRO	-	expression tag	UNP P0A930
e	391	GLN	-	expression tag	UNP P0A930
e	392	PHE	-	expression tag	UNP P0A930
e	393	GLU	-	expression tag	UNP P0A930
e	394	LYS	-	expression tag	UNP P0A930
f	380	GLU	-	expression tag	UNP P0A930
f	381	ASN	-	expression tag	UNP P0A930
f	382	LEU	-	expression tag	UNP P0A930
f	383	TYR	-	expression tag	UNP P0A930
f	384	PHE	-	expression tag	UNP P0A930
f	385	GLN	-	expression tag	UNP P0A930
f	386	SER	-	expression tag	UNP P0A930
f	387	TRP	-	expression tag	UNP P0A930
f	388	SER	-	expression tag	UNP P0A930
f	389	HIS	-	expression tag	UNP P0A930
f	390	PRO	-	expression tag	UNP P0A930
f	391	GLN	-	expression tag	UNP P0A930
f	392	PHE	-	expression tag	UNP P0A930
f	393	GLU	-	expression tag	UNP P0A930
f	394	LYS	-	expression tag	UNP P0A930
g	380	GLU	-	expression tag	UNP P0A930

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Chain	Residue	Modelled	Actual	Comment	Reference
g	381	ASN	-	expression tag	UNP P0A930
g	382	LEU	-	expression tag	UNP P0A930
g	383	TYR	-	expression tag	UNP P0A930
g	384	PHE	-	expression tag	UNP P0A930
g	385	GLN	-	expression tag	UNP P0A930
g	386	SER	-	expression tag	UNP P0A930
g	387	TRP	-	expression tag	UNP P0A930
g	388	SER	-	expression tag	UNP P0A930
g	389	HIS	-	expression tag	UNP P0A930
g	390	PRO	-	expression tag	UNP P0A930
g	391	GLN	-	expression tag	UNP P0A930
g	392	PHE	-	expression tag	UNP P0A930
g	393	GLU	-	expression tag	UNP P0A930
g	394	LYS	-	expression tag	UNP P0A930
h	380	GLU	-	expression tag	UNP P0A930
h	381	ASN	-	expression tag	UNP P0A930
h	382	LEU	-	expression tag	UNP P0A930
h	383	TYR	-	expression tag	UNP P0A930
h	384	PHE	-	expression tag	UNP P0A930
h	385	GLN	-	expression tag	UNP P0A930
h	386	SER	-	expression tag	UNP P0A930
h	387	TRP	-	expression tag	UNP P0A930
h	388	SER	-	expression tag	UNP P0A930
h	389	HIS	-	expression tag	UNP P0A930
h	390	PRO	-	expression tag	UNP P0A930
h	391	GLN	-	expression tag	UNP P0A930
h	392	PHE	-	expression tag	UNP P0A930
h	393	GLU	-	expression tag	UNP P0A930
h	394	LYS	-	expression tag	UNP P0A930

- Molecule 2 is a protein called Tyrosine-protein kinase wzc.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	I	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	J	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	K	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	L	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	M	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		

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Mol	Chain	Residues	Atoms						AltConf	Trace
2	N	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	O	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	P	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	540	MET	LYS	engineered mutation	UNP P76387
I	721	SER	-	expression tag	UNP P76387
I	722	SER	-	expression tag	UNP P76387
I	723	GLY	-	expression tag	UNP P76387
I	724	GLU	-	expression tag	UNP P76387
I	725	ASN	-	expression tag	UNP P76387
I	726	LEU	-	expression tag	UNP P76387
I	727	TYR	-	expression tag	UNP P76387
I	728	PHE	-	expression tag	UNP P76387
I	729	GLN	-	expression tag	UNP P76387
I	730	GLY	-	expression tag	UNP P76387
I	731	TRP	-	expression tag	UNP P76387
I	732	SER	-	expression tag	UNP P76387
I	733	HIS	-	expression tag	UNP P76387
I	734	PRO	-	expression tag	UNP P76387
I	735	GLN	-	expression tag	UNP P76387
I	736	PHE	-	expression tag	UNP P76387
I	737	GLU	-	expression tag	UNP P76387
I	738	LYS	-	expression tag	UNP P76387
J	540	MET	LYS	engineered mutation	UNP P76387
J	721	SER	-	expression tag	UNP P76387
J	722	SER	-	expression tag	UNP P76387
J	723	GLY	-	expression tag	UNP P76387
J	724	GLU	-	expression tag	UNP P76387
J	725	ASN	-	expression tag	UNP P76387
J	726	LEU	-	expression tag	UNP P76387
J	727	TYR	-	expression tag	UNP P76387
J	728	PHE	-	expression tag	UNP P76387
J	729	GLN	-	expression tag	UNP P76387
J	730	GLY	-	expression tag	UNP P76387
J	731	TRP	-	expression tag	UNP P76387
J	732	SER	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
J	733	HIS	-	expression tag	UNP P76387
J	734	PRO	-	expression tag	UNP P76387
J	735	GLN	-	expression tag	UNP P76387
J	736	PHE	-	expression tag	UNP P76387
J	737	GLU	-	expression tag	UNP P76387
J	738	LYS	-	expression tag	UNP P76387
K	540	MET	LYS	engineered mutation	UNP P76387
K	721	SER	-	expression tag	UNP P76387
K	722	SER	-	expression tag	UNP P76387
K	723	GLY	-	expression tag	UNP P76387
K	724	GLU	-	expression tag	UNP P76387
K	725	ASN	-	expression tag	UNP P76387
K	726	LEU	-	expression tag	UNP P76387
K	727	TYR	-	expression tag	UNP P76387
K	728	PHE	-	expression tag	UNP P76387
K	729	GLN	-	expression tag	UNP P76387
K	730	GLY	-	expression tag	UNP P76387
K	731	TRP	-	expression tag	UNP P76387
K	732	SER	-	expression tag	UNP P76387
K	733	HIS	-	expression tag	UNP P76387
K	734	PRO	-	expression tag	UNP P76387
K	735	GLN	-	expression tag	UNP P76387
K	736	PHE	-	expression tag	UNP P76387
K	737	GLU	-	expression tag	UNP P76387
K	738	LYS	-	expression tag	UNP P76387
L	540	MET	LYS	engineered mutation	UNP P76387
L	721	SER	-	expression tag	UNP P76387
L	722	SER	-	expression tag	UNP P76387
L	723	GLY	-	expression tag	UNP P76387
L	724	GLU	-	expression tag	UNP P76387
L	725	ASN	-	expression tag	UNP P76387
L	726	LEU	-	expression tag	UNP P76387
L	727	TYR	-	expression tag	UNP P76387
L	728	PHE	-	expression tag	UNP P76387
L	729	GLN	-	expression tag	UNP P76387
L	730	GLY	-	expression tag	UNP P76387
L	731	TRP	-	expression tag	UNP P76387
L	732	SER	-	expression tag	UNP P76387
L	733	HIS	-	expression tag	UNP P76387
L	734	PRO	-	expression tag	UNP P76387
L	735	GLN	-	expression tag	UNP P76387
L	736	PHE	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
L	737	GLU	-	expression tag	UNP P76387
L	738	LYS	-	expression tag	UNP P76387
M	540	MET	LYS	engineered mutation	UNP P76387
M	721	SER	-	expression tag	UNP P76387
M	722	SER	-	expression tag	UNP P76387
M	723	GLY	-	expression tag	UNP P76387
M	724	GLU	-	expression tag	UNP P76387
M	725	ASN	-	expression tag	UNP P76387
M	726	LEU	-	expression tag	UNP P76387
M	727	TYR	-	expression tag	UNP P76387
M	728	PHE	-	expression tag	UNP P76387
M	729	GLN	-	expression tag	UNP P76387
M	730	GLY	-	expression tag	UNP P76387
M	731	TRP	-	expression tag	UNP P76387
M	732	SER	-	expression tag	UNP P76387
M	733	HIS	-	expression tag	UNP P76387
M	734	PRO	-	expression tag	UNP P76387
M	735	GLN	-	expression tag	UNP P76387
M	736	PHE	-	expression tag	UNP P76387
M	737	GLU	-	expression tag	UNP P76387
M	738	LYS	-	expression tag	UNP P76387
N	540	MET	LYS	engineered mutation	UNP P76387
N	721	SER	-	expression tag	UNP P76387
N	722	SER	-	expression tag	UNP P76387
N	723	GLY	-	expression tag	UNP P76387
N	724	GLU	-	expression tag	UNP P76387
N	725	ASN	-	expression tag	UNP P76387
N	726	LEU	-	expression tag	UNP P76387
N	727	TYR	-	expression tag	UNP P76387
N	728	PHE	-	expression tag	UNP P76387
N	729	GLN	-	expression tag	UNP P76387
N	730	GLY	-	expression tag	UNP P76387
N	731	TRP	-	expression tag	UNP P76387
N	732	SER	-	expression tag	UNP P76387
N	733	HIS	-	expression tag	UNP P76387
N	734	PRO	-	expression tag	UNP P76387
N	735	GLN	-	expression tag	UNP P76387
N	736	PHE	-	expression tag	UNP P76387
N	737	GLU	-	expression tag	UNP P76387
N	738	LYS	-	expression tag	UNP P76387
O	540	MET	LYS	engineered mutation	UNP P76387
O	721	SER	-	expression tag	UNP P76387

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Chain	Residue	Modelled	Actual	Comment	Reference
O	722	SER	-	expression tag	UNP P76387
O	723	GLY	-	expression tag	UNP P76387
O	724	GLU	-	expression tag	UNP P76387
O	725	ASN	-	expression tag	UNP P76387
O	726	LEU	-	expression tag	UNP P76387
O	727	TYR	-	expression tag	UNP P76387
O	728	PHE	-	expression tag	UNP P76387
O	729	GLN	-	expression tag	UNP P76387
O	730	GLY	-	expression tag	UNP P76387
O	731	TRP	-	expression tag	UNP P76387
O	732	SER	-	expression tag	UNP P76387
O	733	HIS	-	expression tag	UNP P76387
O	734	PRO	-	expression tag	UNP P76387
O	735	GLN	-	expression tag	UNP P76387
O	736	PHE	-	expression tag	UNP P76387
O	737	GLU	-	expression tag	UNP P76387
O	738	LYS	-	expression tag	UNP P76387
P	540	MET	LYS	engineered mutation	UNP P76387
P	721	SER	-	expression tag	UNP P76387
P	722	SER	-	expression tag	UNP P76387
P	723	GLY	-	expression tag	UNP P76387
P	724	GLU	-	expression tag	UNP P76387
P	725	ASN	-	expression tag	UNP P76387
P	726	LEU	-	expression tag	UNP P76387
P	727	TYR	-	expression tag	UNP P76387
P	728	PHE	-	expression tag	UNP P76387
P	729	GLN	-	expression tag	UNP P76387
P	730	GLY	-	expression tag	UNP P76387
P	731	TRP	-	expression tag	UNP P76387
P	732	SER	-	expression tag	UNP P76387
P	733	HIS	-	expression tag	UNP P76387
P	734	PRO	-	expression tag	UNP P76387
P	735	GLN	-	expression tag	UNP P76387
P	736	PHE	-	expression tag	UNP P76387
P	737	GLU	-	expression tag	UNP P76387
P	738	LYS	-	expression tag	UNP P76387

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).




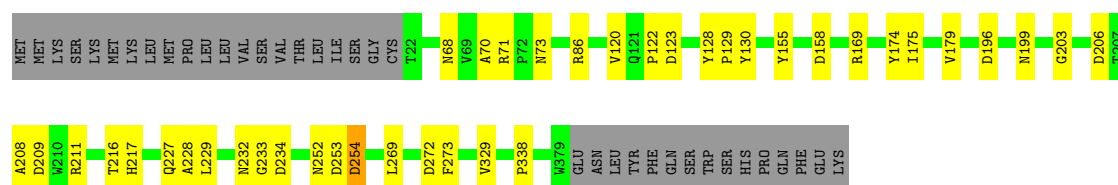
Mol	Chain	Residues	Atoms						AltConf
3	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	J	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	K	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	L	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	O	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	P	1	Total 39	C 10	H 12	N 5	O 10	P 2	0

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

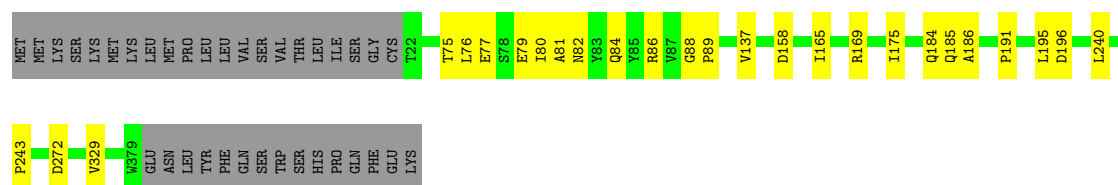
- Molecule 1: Putative polysaccharide export protein Wza

Chain A: 




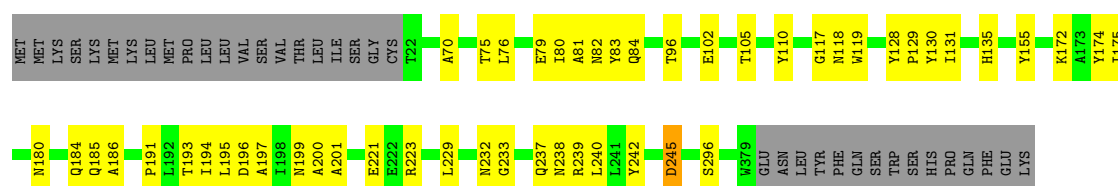
- Molecule 1: Putative polysaccharide export protein Wza

Chain B: 




- Molecule 1: Putative polysaccharide export protein Wza

Chain C: 




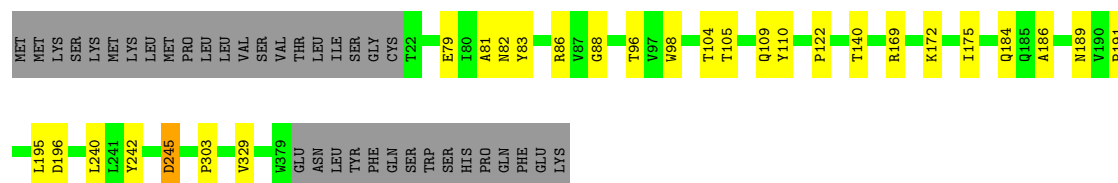
- Molecule 1: Putative polysaccharide export protein Wza

Chain D: 




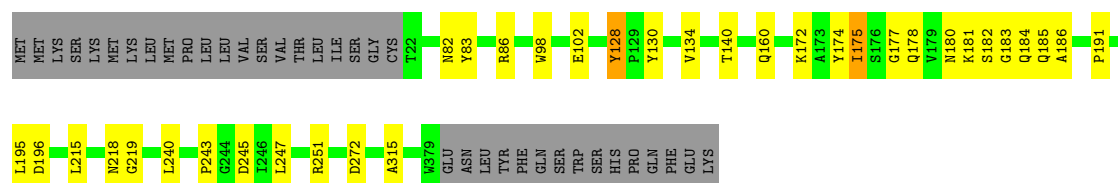
- Molecule 1: Putative polysaccharide export protein Wza

Chain E:  84% 7% 9%




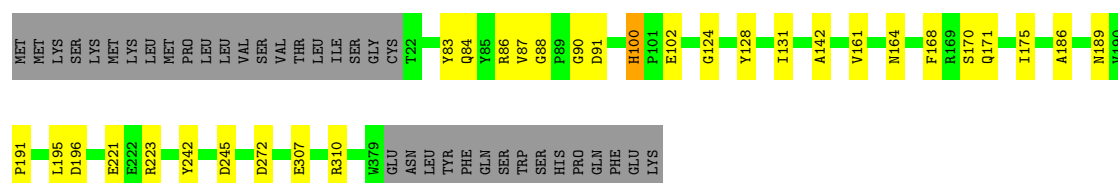
- Molecule 1: Putative polysaccharide export protein Wza

Chain F:  82% 8% 9%




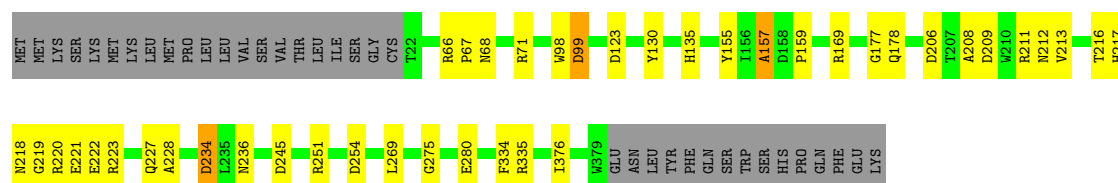
- Molecule 1: Putative polysaccharide export protein Wza

Chain G:  83% 8% 9%




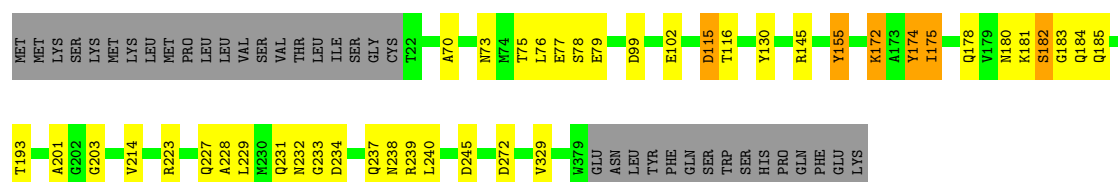
- Molecule 1: Putative polysaccharide export protein Wza

Chain H:  80% 10% 9%




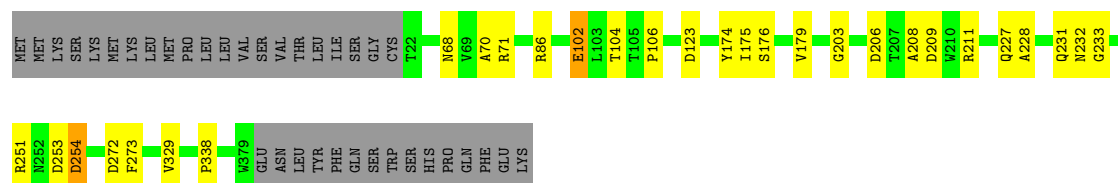
- Molecule 1: Putative polysaccharide export protein Wza

Chain a:  80% 9% 9%




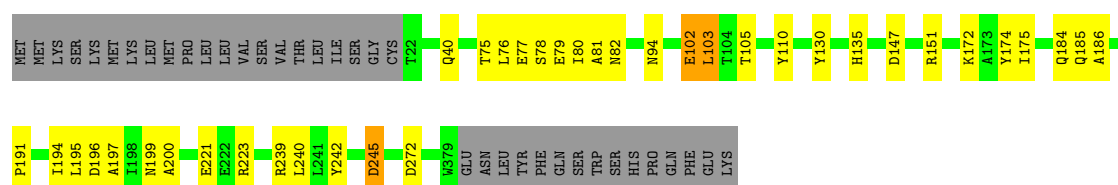
- Molecule 1: Putative polysaccharide export protein Wza

Chain b:  84% 7% 9%




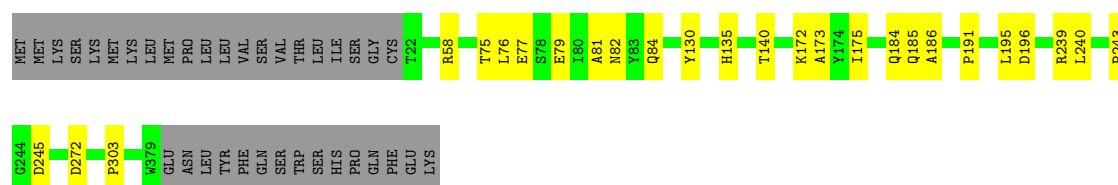
- Molecule 1: Putative polysaccharide export protein Wza

Chain c:  81% 9% 9%




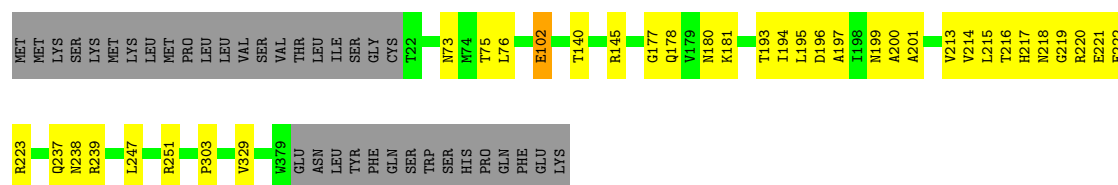
- Molecule 1: Putative polysaccharide export protein Wza

Chain d:  84% 7% 9%




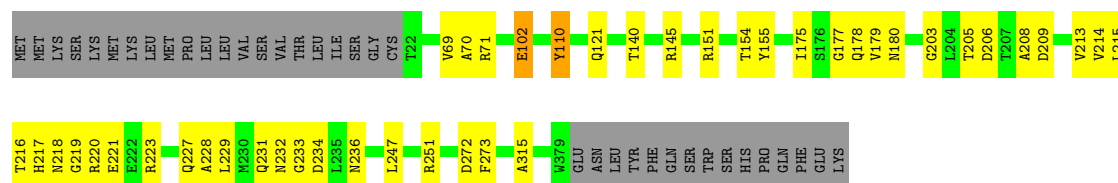
- Molecule 1: Putative polysaccharide export protein Wza

Chain e:  82% 9% 9%

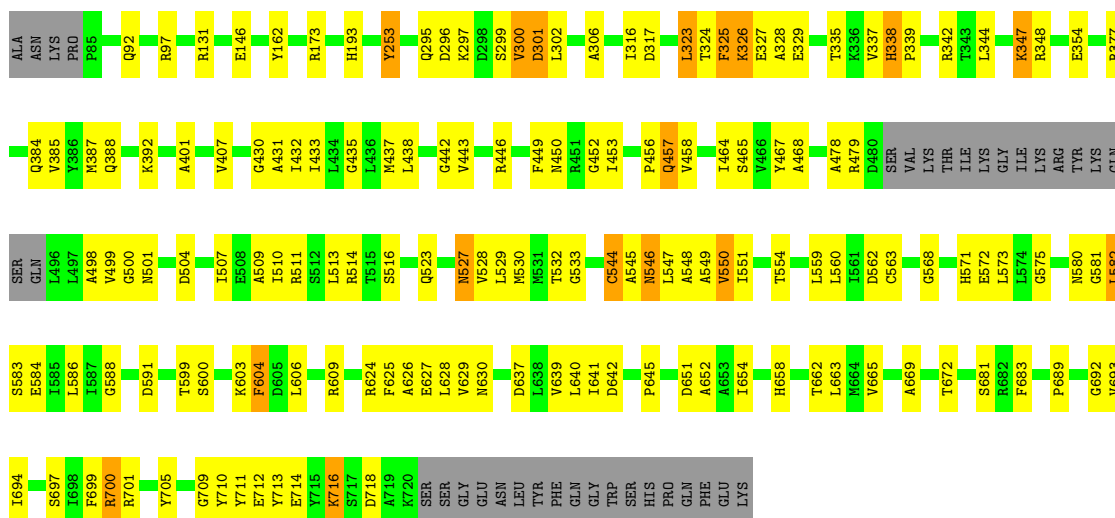


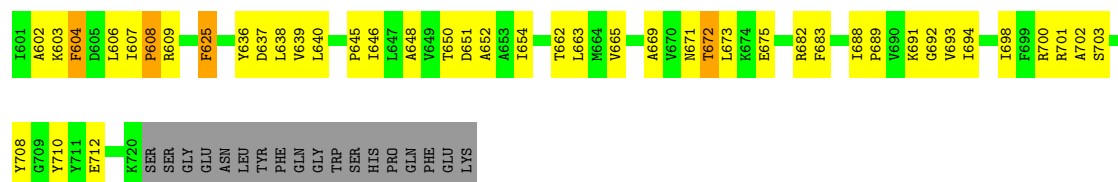
- Molecule 1: Putative polysaccharide export protein Wza

Chain f:  80% 11% 9%



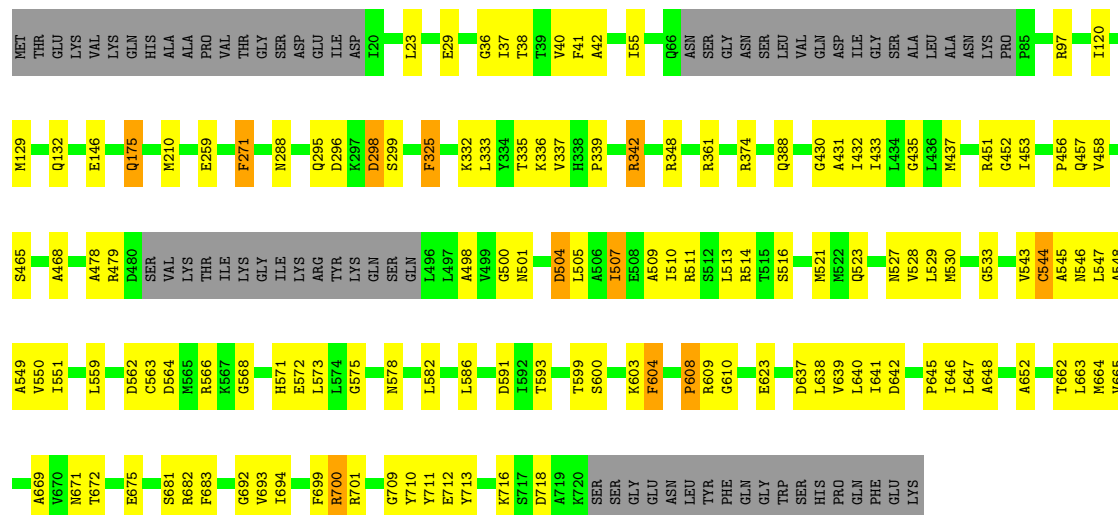
- [illegible]





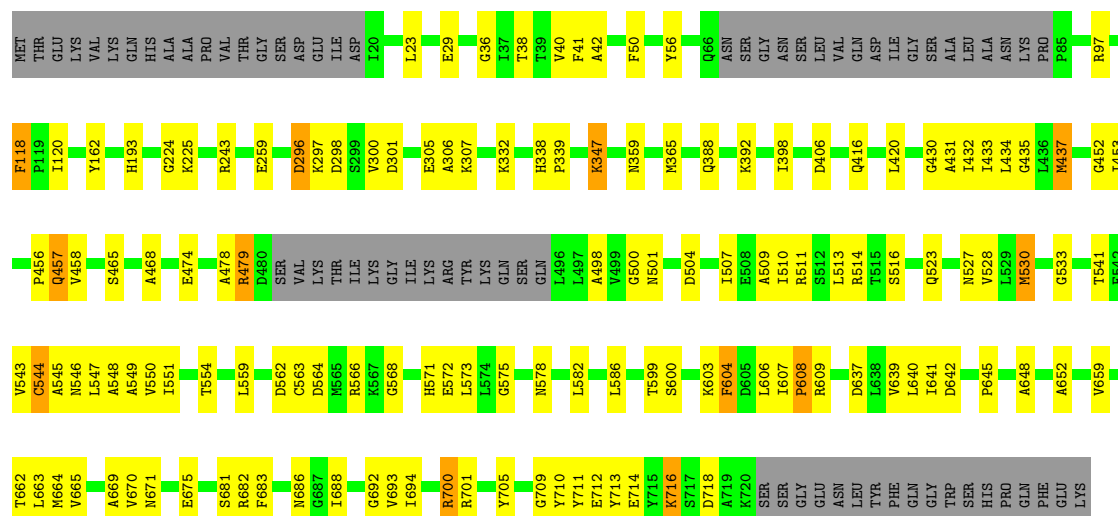
• Molecule 2: Tyrosine-protein kinase wzc

Chain M: 72% 17% 9%



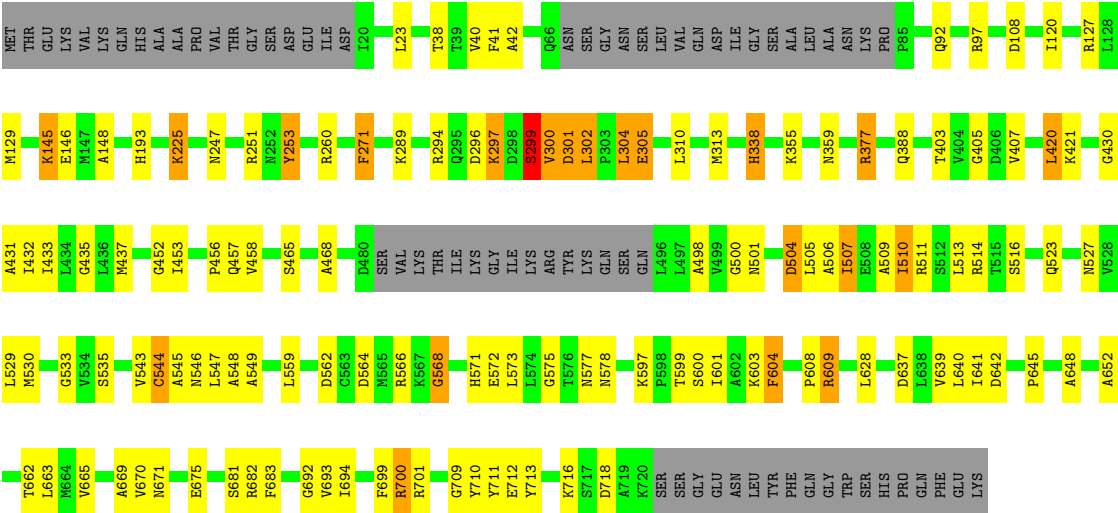
• Molecule 2: Tyrosine-protein kinase wzc

Chain N: 72% 17% 9%

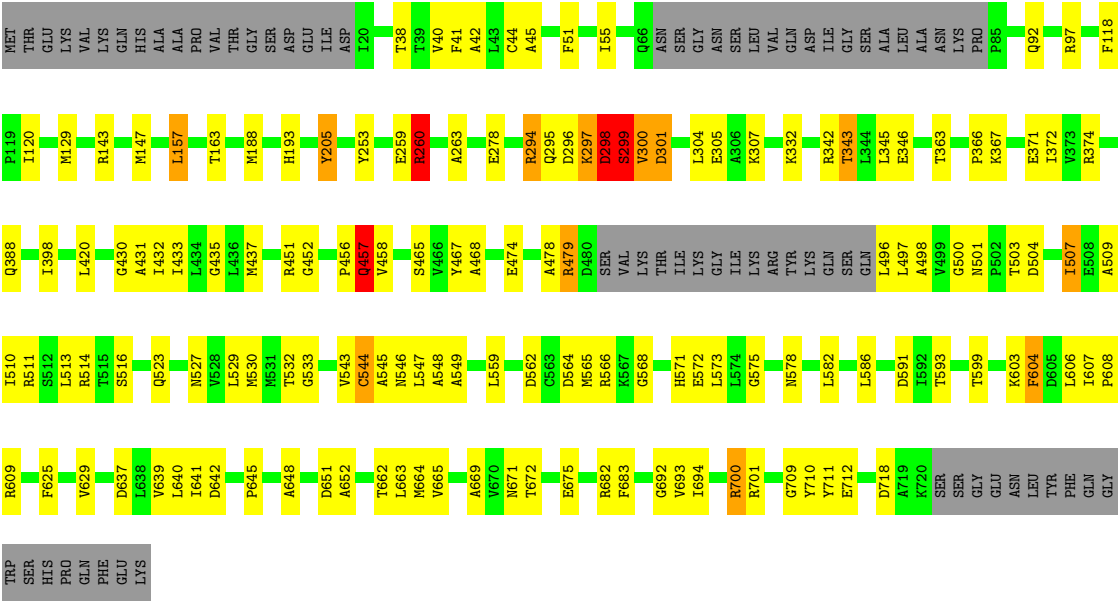


• Molecule 2: Tyrosine-protein kinase wzc

Chain O: 72% 15% 9%



● Molecule 2: Tyrosine-protein kinase wzc



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	59128	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	1.12	12/2836 (0.4%)	1.36	27/3862 (0.7%)
1	B	0.98	9/2836 (0.3%)	1.14	23/3862 (0.6%)
1	C	1.09	10/2836 (0.4%)	1.26	40/3862 (1.0%)
1	D	0.85	5/2836 (0.2%)	1.07	18/3862 (0.5%)
1	E	0.88	6/2836 (0.2%)	1.10	26/3862 (0.7%)
1	F	1.06	13/2836 (0.5%)	1.22	35/3862 (0.9%)
1	G	0.93	11/2836 (0.4%)	1.09	22/3862 (0.6%)
1	H	1.26	25/2836 (0.9%)	1.40	48/3862 (1.2%)
1	a	1.21	12/2836 (0.4%)	1.36	46/3862 (1.2%)
1	b	1.04	16/2836 (0.6%)	1.26	25/3862 (0.6%)
1	c	0.91	7/2836 (0.2%)	1.13	36/3862 (0.9%)
1	d	0.87	5/2836 (0.2%)	1.08	26/3862 (0.7%)
1	e	1.23	24/2836 (0.8%)	1.34	52/3862 (1.3%)
1	f	1.19	21/2836 (0.7%)	1.34	45/3862 (1.2%)
1	g	1.14	21/2836 (0.7%)	1.34	40/3862 (1.0%)
1	h	0.88	6/2836 (0.2%)	1.12	30/3862 (0.8%)
2	I	1.42	47/5260 (0.9%)	1.65	146/7126 (2.0%)
2	J	1.59	52/5260 (1.0%)	1.83	194/7126 (2.7%)
2	K	0.71	0/5260	1.28	16/7126 (0.2%)
2	L	1.57	54/5260 (1.0%)	1.77	167/7126 (2.3%)
2	M	1.40	46/5260 (0.9%)	1.62	139/7126 (2.0%)
2	N	1.41	44/5260 (0.8%)	1.62	143/7126 (2.0%)
2	O	1.39	43/5260 (0.8%)	1.62	131/7126 (1.8%)
2	P	1.42	46/5260 (0.9%)	1.63	135/7126 (1.9%)
All	All	1.22	535/87456 (0.6%)	1.44	1610/118800 (1.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	a	0	1
1	b	0	1
1	c	0	1
1	f	0	2
1	g	0	2
1	h	0	3
2	I	0	6
2	J	0	4
2	K	0	10
2	L	0	6
2	M	0	4
2	N	0	5
2	O	0	2
2	P	0	7
All	All	0	64

The worst 5 of 535 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	571	HIS	CE1-NE2	-8.87	1.23	1.32
1	f	217	HIS	ND1-CE1	-8.86	1.23	1.32
2	M	571	HIS	CE1-NE2	-8.83	1.23	1.32
1	g	217	HIS	ND1-CE1	-8.81	1.23	1.32
2	P	571	HIS	CE1-NE2	-8.79	1.23	1.32

The worst 5 of 1610 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	317	ASP	CA-CB-CG	10.40	123.00	112.60
1	G	189	ASN	CA-C-N	9.48	131.58	123.33
1	G	189	ASN	C-N-CA	9.48	131.58	123.33
2	L	608	PRO	CA-N-CD	-9.45	98.77	112.00
1	D	189	ASN	CA-C-N	9.44	131.54	123.33

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TYR	Sidechain
1	A	169	ARG	Sidechain
1	A	86	ARG	Sidechain
1	B	169	ARG	Peptide
1	C	155	TYR	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2783	2765	2764	4	0
1	B	2783	2765	2764	3	0
1	C	2783	2765	2764	7	0
1	D	2783	2765	2764	5	0
1	E	2783	2765	2764	6	0
1	F	2783	2765	2764	3	0
1	G	2783	2765	2764	21	0
1	H	2783	2765	2764	2	0
1	a	2783	2765	2764	5	0
1	b	2783	2765	2764	4	0
1	c	2783	2765	2762	13	0
1	d	2783	2765	2764	12	0
1	e	2783	2765	2764	3	0
1	f	2783	2765	2764	4	0
1	g	2783	2765	2764	6	0
1	h	2783	2765	2764	7	0
2	I	5185	5302	5300	39	0
2	J	5185	5302	5300	40	0
2	K	5185	5302	5300	29	0
2	L	5185	5302	5300	23	0
2	M	5185	5302	5300	26	0
2	N	5185	5302	5300	26	0
2	O	5185	5302	5300	33	0
2	P	5185	5302	5300	33	0
3	I	27	12	12	0	0
3	J	27	12	12	0	0
3	K	27	12	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	27	12	12	0	0
3	M	27	12	12	0	0
3	N	27	12	12	0	0
3	O	27	12	12	0	0
3	P	27	12	12	0	0
All	All	86224	86752	86718	304	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 2.

The worst 5 of 304 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:ARG:HD3	1:d:58:ARG:NH1	1.46	1.30
1:G:310:ARG:CD	1:d:58:ARG:NH1	2.01	1.23
1:G:310:ARG:CD	1:d:58:ARG:HH12	1.60	1.13
1:G:310:ARG:NE	1:d:58:ARG:NH1	1.97	1.12
1:G:310:ARG:HB3	1:c:40:GLN:OE1	1.52	1.08

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	356/394 (90%)	333 (94%)	20 (6%)	3 (1%)	16	54
1	B	356/394 (90%)	337 (95%)	18 (5%)	1 (0%)	36	72
1	C	356/394 (90%)	342 (96%)	11 (3%)	3 (1%)	16	54
1	D	356/394 (90%)	339 (95%)	17 (5%)	0	100	100
1	E	356/394 (90%)	338 (95%)	16 (4%)	2 (1%)	21	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	356/394 (90%)	345 (97%)	11 (3%)	0	100	100
1	G	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	H	356/394 (90%)	338 (95%)	13 (4%)	5 (1%)	9	40
1	a	356/394 (90%)	339 (95%)	17 (5%)	0	100	100
1	b	356/394 (90%)	338 (95%)	18 (5%)	0	100	100
1	c	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	d	356/394 (90%)	345 (97%)	10 (3%)	1 (0%)	36	72
1	e	356/394 (90%)	340 (96%)	16 (4%)	0	100	100
1	f	356/394 (90%)	337 (95%)	18 (5%)	1 (0%)	36	72
1	g	356/394 (90%)	337 (95%)	19 (5%)	0	100	100
1	h	356/394 (90%)	341 (96%)	14 (4%)	1 (0%)	36	72
2	I	662/738 (90%)	637 (96%)	20 (3%)	5 (1%)	16	54
2	J	662/738 (90%)	630 (95%)	24 (4%)	8 (1%)	10	44
2	K	662/738 (90%)	622 (94%)	34 (5%)	6 (1%)	14	51
2	L	662/738 (90%)	636 (96%)	24 (4%)	2 (0%)	36	72
2	M	662/738 (90%)	636 (96%)	21 (3%)	5 (1%)	16	54
2	N	662/738 (90%)	637 (96%)	20 (3%)	5 (1%)	16	54
2	O	662/738 (90%)	640 (97%)	16 (2%)	6 (1%)	14	51
2	P	662/738 (90%)	633 (96%)	25 (4%)	4 (1%)	21	59
All	All	10992/12208 (90%)	10510 (96%)	422 (4%)	60 (0%)	26	63

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	300	VAL
2	J	301	ASP
2	J	326	LYS
2	J	327	GLU
2	J	328	ALA

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	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	B	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	C	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	D	307/342 (90%)	304 (99%)	3 (1%)	68	78
1	E	307/342 (90%)	306 (100%)	1 (0%)	86	86
1	F	307/342 (90%)	299 (97%)	8 (3%)	40	62
1	G	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	H	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	a	307/342 (90%)	298 (97%)	9 (3%)	37	58
1	b	307/342 (90%)	304 (99%)	3 (1%)	68	78
1	c	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	d	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	e	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	f	307/342 (90%)	302 (98%)	5 (2%)	55	70
1	g	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	h	307/342 (90%)	302 (98%)	5 (2%)	55	70
2	I	570/630 (90%)	549 (96%)	21 (4%)	30	51
2	J	570/630 (90%)	554 (97%)	16 (3%)	38	60
2	K	570/630 (90%)	540 (95%)	30 (5%)	20	41
2	L	570/630 (90%)	548 (96%)	22 (4%)	28	49
2	M	570/630 (90%)	558 (98%)	12 (2%)	47	65
2	N	570/630 (90%)	554 (97%)	16 (3%)	38	60
2	O	570/630 (90%)	553 (97%)	17 (3%)	36	57
2	P	570/630 (90%)	545 (96%)	25 (4%)	25	47
All	All	9472/10512 (90%)	9251 (98%)	221 (2%)	44	64

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	547	LEU
2	N	544	CYS
1	h	172	LYS

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Mol	Chain	Res	Type
1	c	94	ASN
2	M	132	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
2	O	384	GLN
1	c	121	GLN
2	O	476	GLN
2	P	580	ASN
1	d	164	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	ADP	I	1000	-	28,29,29	0.97	0	43,45,45	1.26	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	P	1000	-	28,29,29	0.96	0	43,45,45	1.25	7 (16%)
3	ADP	O	1000	-	28,29,29	0.97	1 (3%)	43,45,45	1.31	6 (13%)
3	ADP	N	1000	-	28,29,29	1.01	1 (3%)	43,45,45	1.29	5 (11%)
3	ADP	J	1000	-	28,29,29	1.05	0	43,45,45	1.37	6 (13%)
3	ADP	M	1000	-	28,29,29	1.00	1 (3%)	43,45,45	1.17	4 (9%)
3	ADP	L	1000	-	28,29,29	0.99	1 (3%)	43,45,45	1.09	5 (11%)
3	ADP	K	1000	-	28,29,29	1.01	1 (3%)	43,45,45	1.29	6 (13%)

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	ADP	I	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	P	1000	-	-	1/16/32/32	0/3/3/3
3	ADP	O	1000	-	-	2/16/32/32	0/3/3/3
3	ADP	N	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	J	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	M	1000	-	-	8/16/32/32	0/3/3/3
3	ADP	L	1000	-	-	0/16/32/32	0/3/3/3
3	ADP	K	1000	-	-	2/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1000	ADP	C8-N7	2.11	1.35	1.31
3	O	1000	ADP	C8-N7	2.09	1.35	1.31
3	K	1000	ADP	C8-N7	2.02	1.35	1.31
3	N	1000	ADP	C8-N7	2.01	1.35	1.31
3	L	1000	ADP	C8-N7	2.00	1.35	1.31

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1000	ADP	O2A-PA-O3A	3.84	117.66	107.27
3	O	1000	ADP	O2A-PA-O3A	3.50	116.73	107.27
3	K	1000	ADP	O2A-PA-O3A	3.12	115.72	107.27
3	J	1000	ADP	C5-C4-N3	-3.12	122.42	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	P	1000	ADP	C5-C4-N3	-2.96	122.63	126.72

There are no chirality outliers.

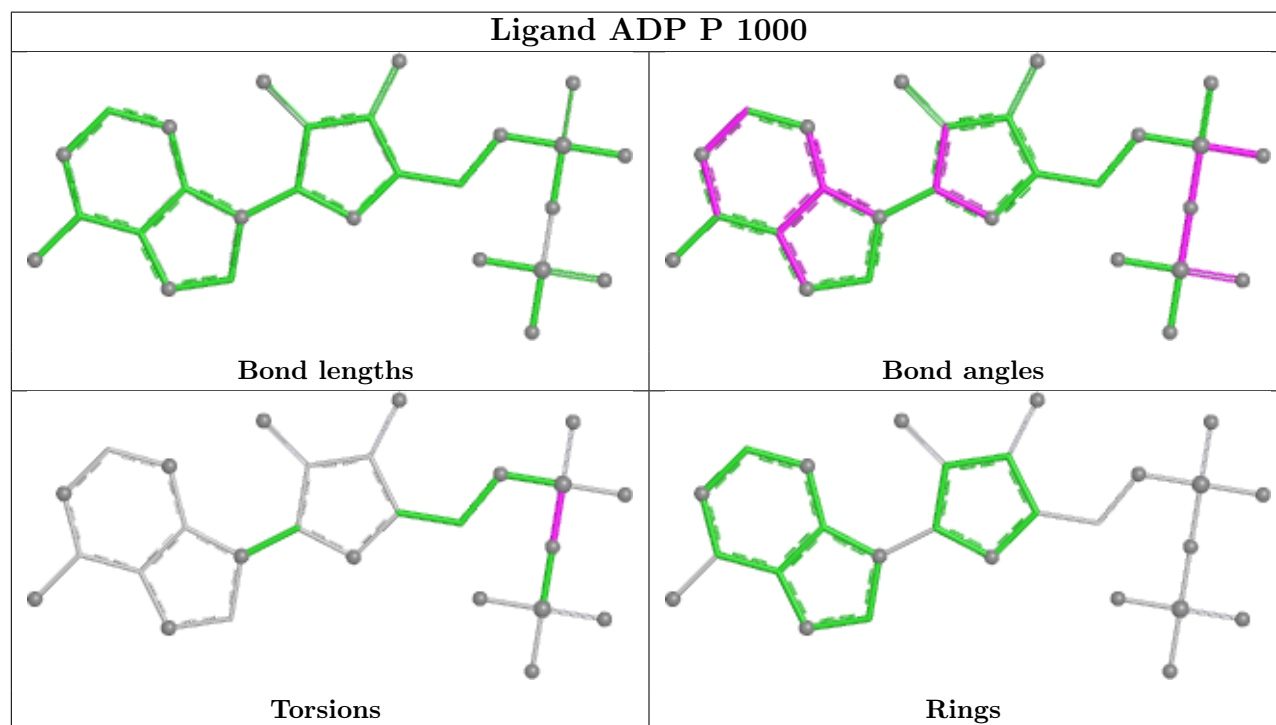
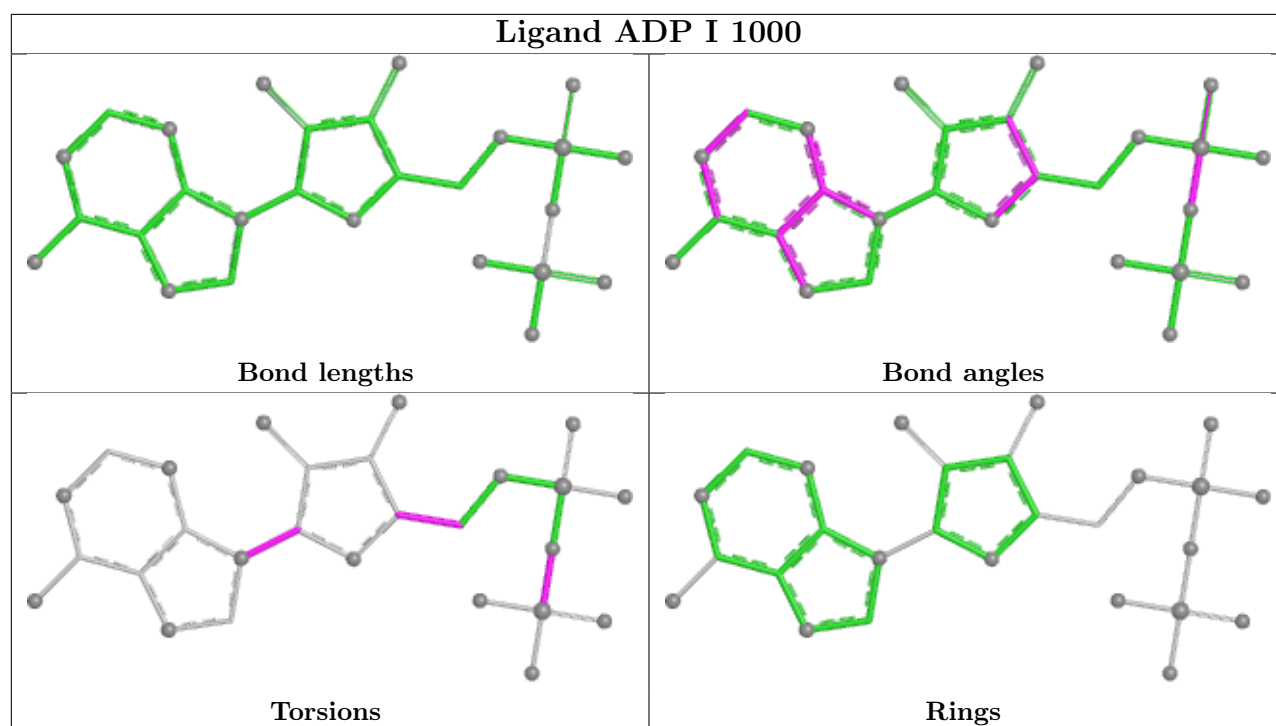
5 of 25 torsion outliers are listed below:

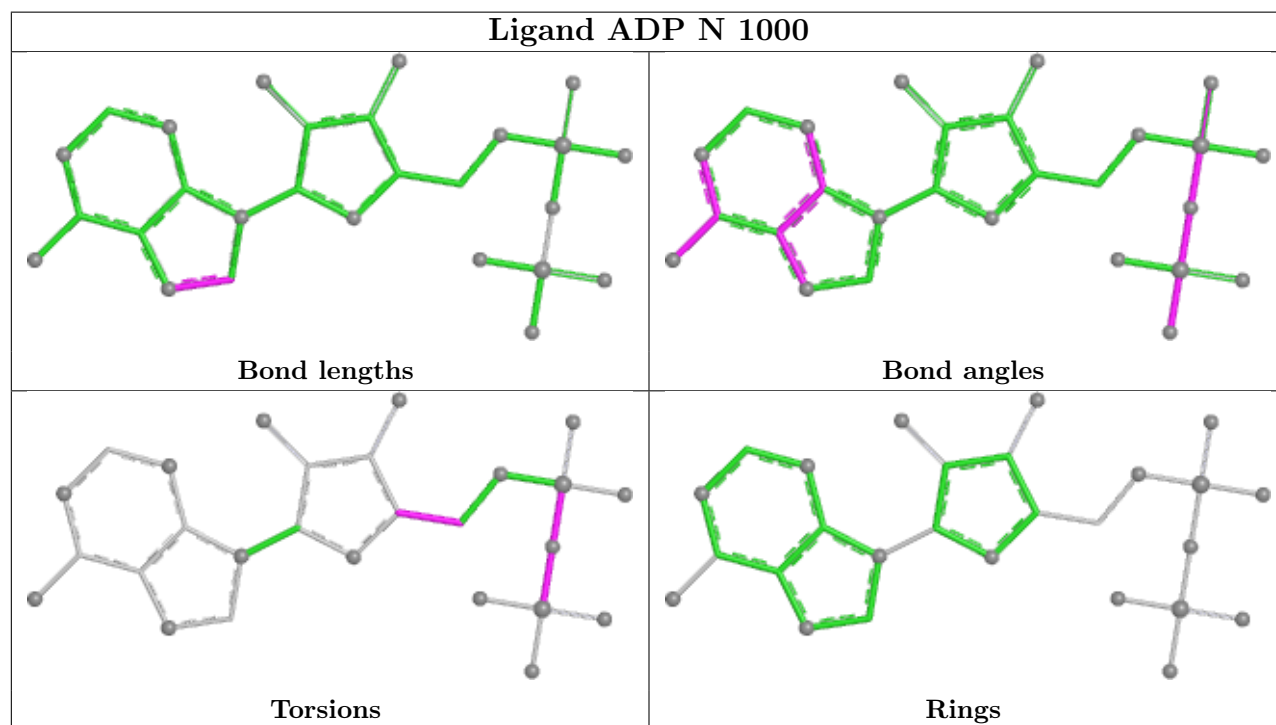
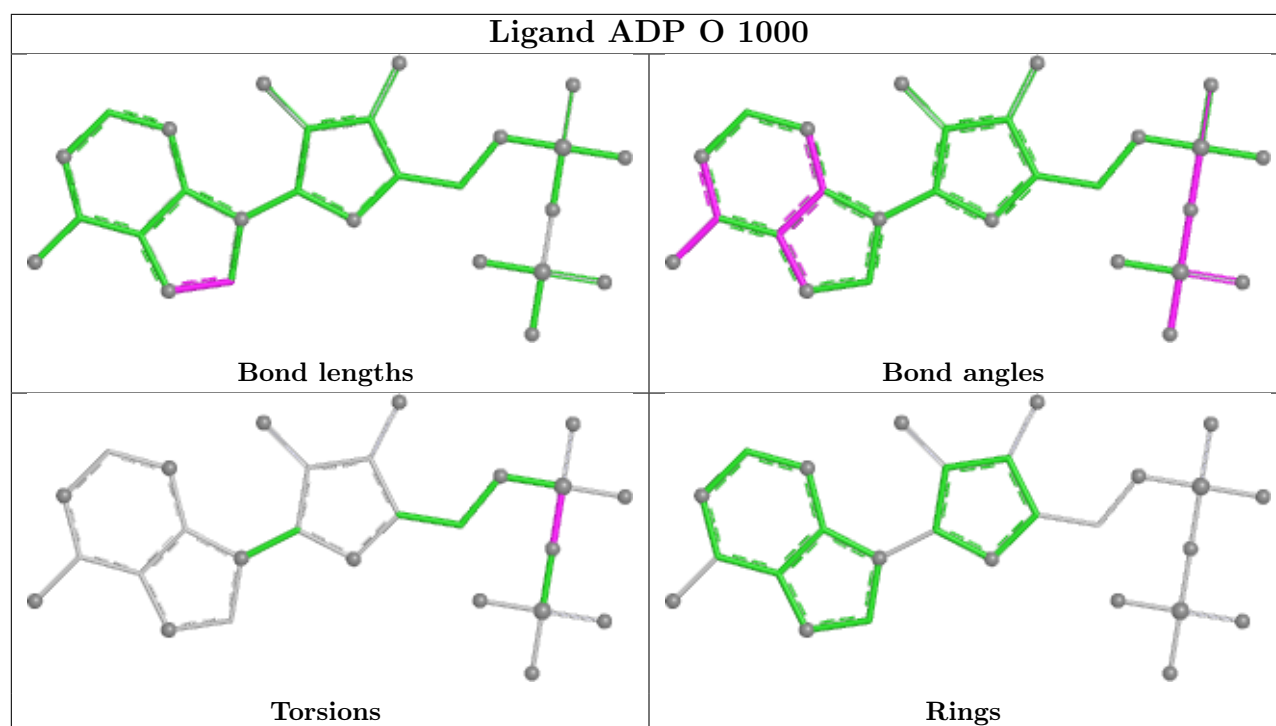
Mol	Chain	Res	Type	Atoms
3	J	1000	ADP	PA-O3A-PB-O3B
3	M	1000	ADP	PA-O3A-PB-O2B
3	M	1000	ADP	PA-O3A-PB-O3B
3	M	1000	ADP	C5'-O5'-PA-O1A
3	M	1000	ADP	C5'-O5'-PA-O2A

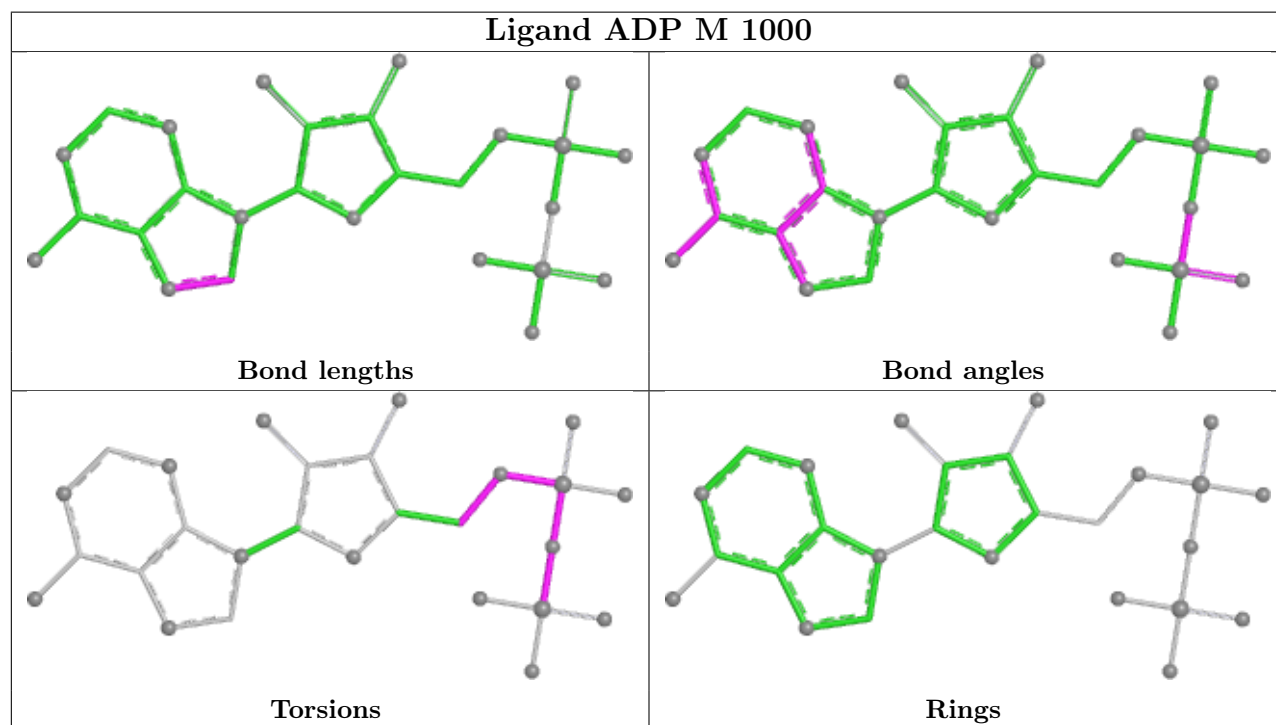
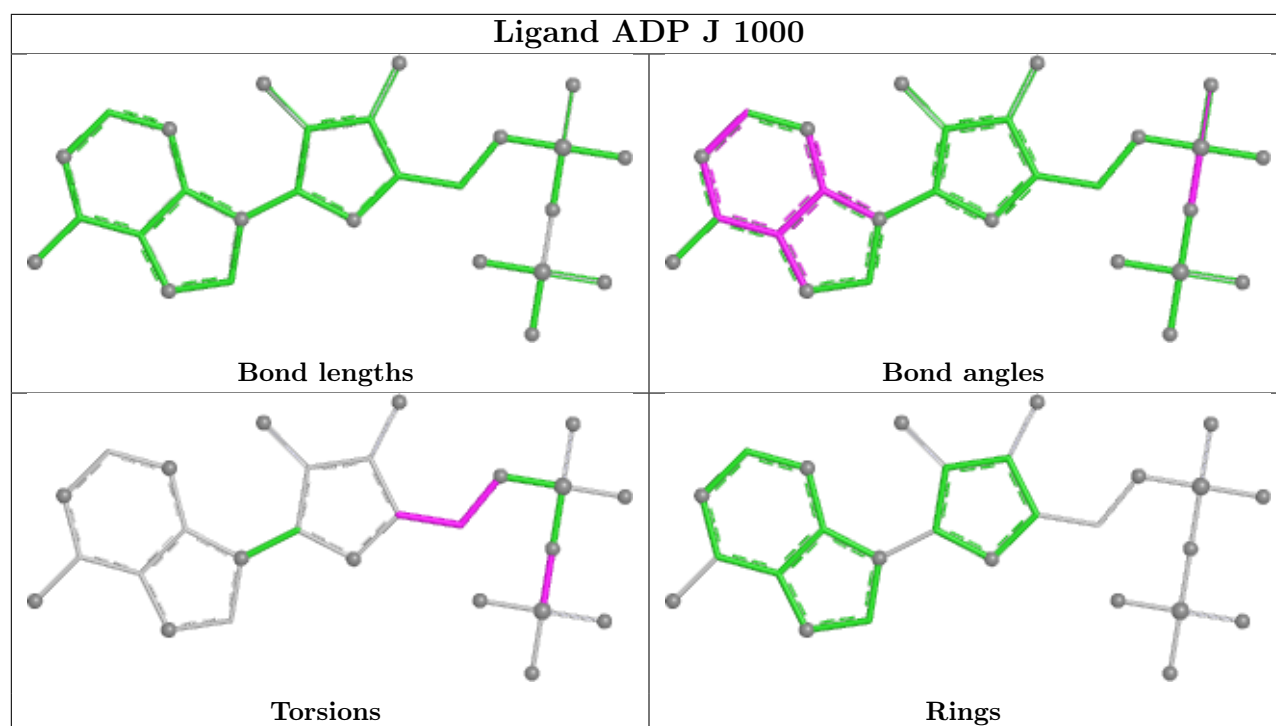
There are no ring outliers.

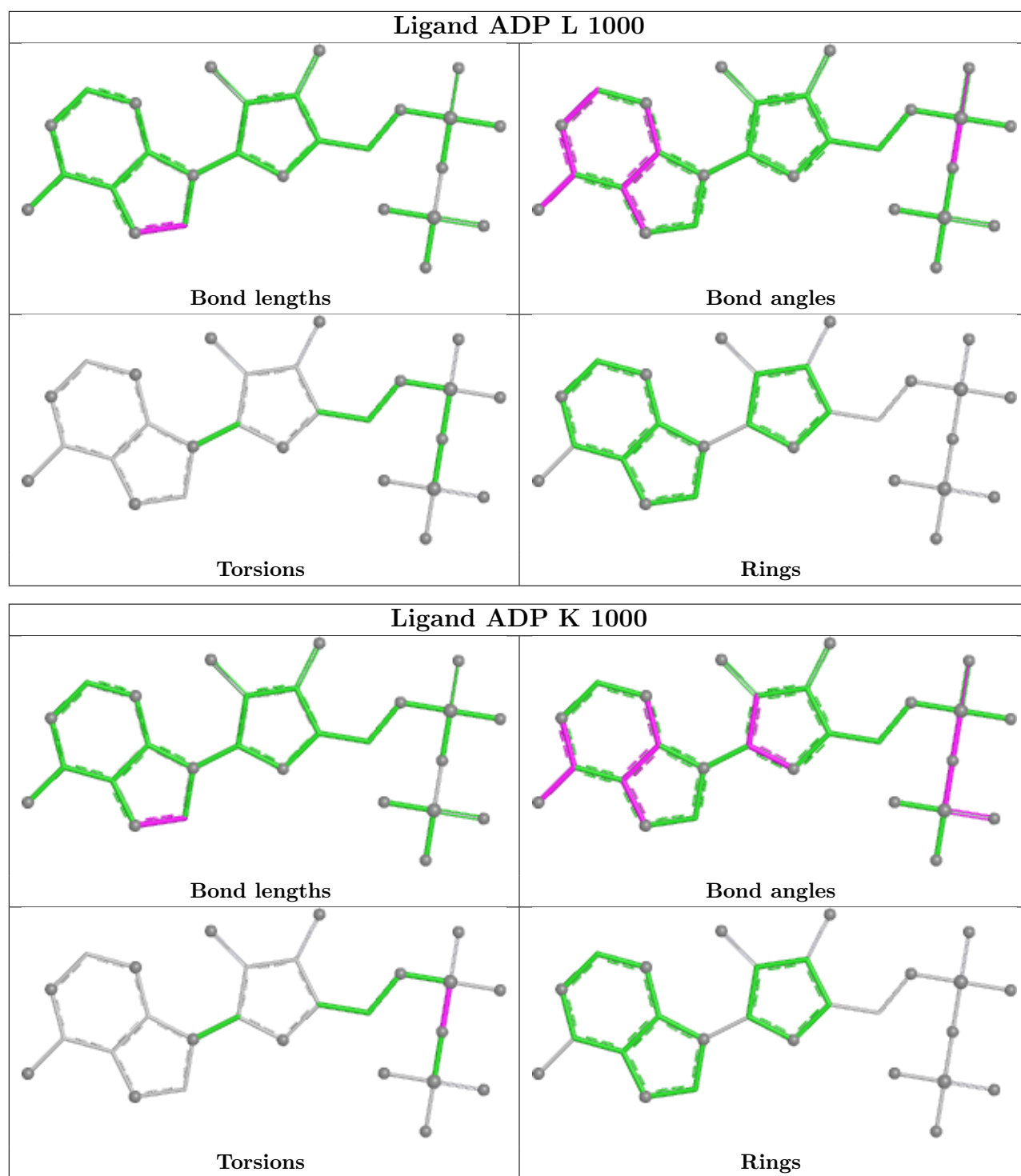
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-53610. 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

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.