



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 06:10 pm BST

PDB ID : 9R6B / pdb_00009r6b
EMDB ID : EMD-53609
Title : CPS secretion pathway Wza-Wzc (Conf 4)
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2025-05-11
Resolution : 4.60 Å (reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

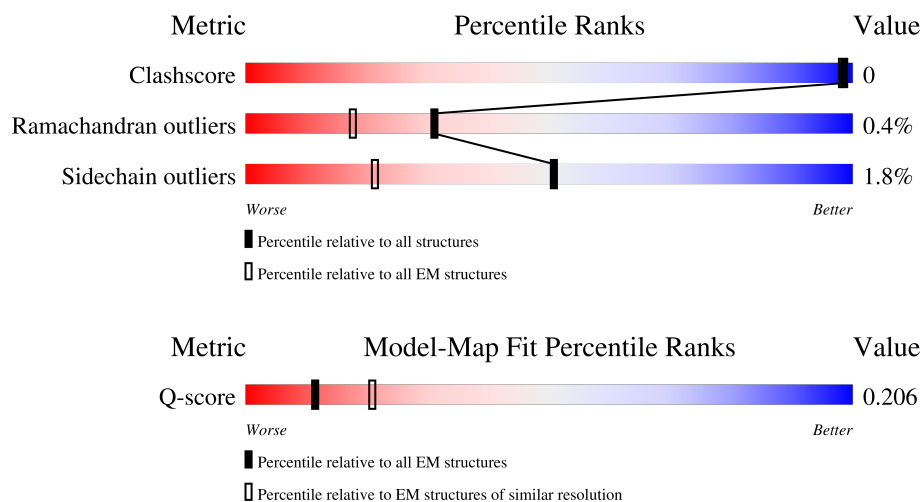
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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	2407 (4.10 - 5.10)

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	394	
1	B	394	
1	C	394	
1	D	394	

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Mol	Chain	Length	Quality of chain
1	E	394	 89% 9%
1	F	394	 88% 9%
1	G	394	 88% 9%
1	H	394	 90% 9%
2	I	738	 80% 18%
2	J	738	 80% 18%
2	K	738	 86% 9%
2	L	738	 88% 9%
2	M	738	 87% 9%
2	N	738	 87% 9%
2	O	738	 79% 18%
2	P	738	 80% 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 124704 atoms, of which 62652 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		

There are 120 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	608	Total	C	H	N	O	S	0	0
			9515	2978	4807	809	902	19		
2	J	608	Total	C	H	N	O	S	0	0
			9515	2978	4807	809	902	19		
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		
2	N	668	Total	C	H	N	O	S	0	0
			10487	3278	5302	892	995	20		
2	O	608	Total	C	H	N	O	S	0	0
			9515	2978	4807	809	902	19		
2	P	608	Total	C	H	N	O	S	0	0
			9515	2978	4807	809	902	19		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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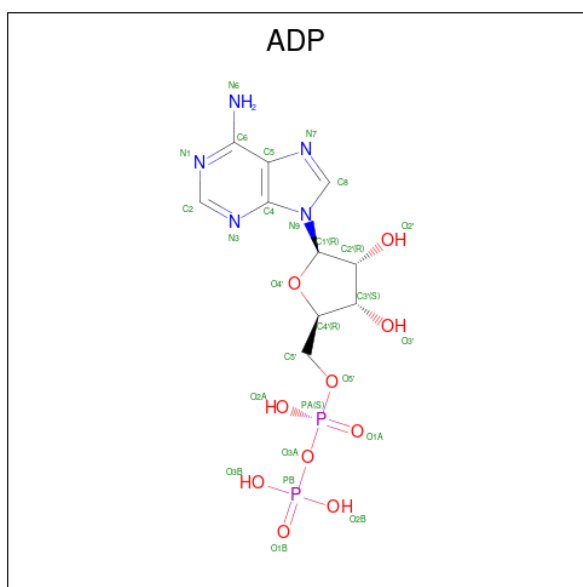
Chain	Residue	Modelled	Actual	Comment	Reference
M	728	PHE	-	expression tag	UNP P76387
M	729	GLN	-	expression tag	UNP P76387
M	730	GLY	-	expression tag	UNP P76387
M	731	TRP	-	expression tag	UNP P76387
M	732	SER	-	expression tag	UNP P76387
M	733	HIS	-	expression tag	UNP P76387
M	734	PRO	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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: C₁₀H₁₅N₅O₁₀P₂) (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 [i](#)

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

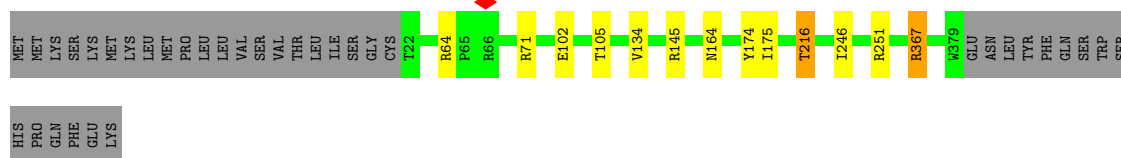
- Molecule 1: Putative polysaccharide export protein Wza

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

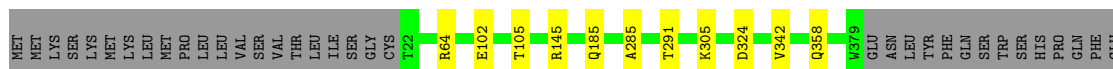
Chain E: 





- Molecule 1: Putative polysaccharide export protein Wza

Chain F: 88% 9%



LYS

- Molecule 1: Putative polysaccharide export protein Wza

Chain G: 88% 9%



GLN
PHE
GLU
LYS

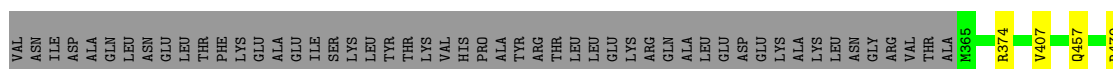
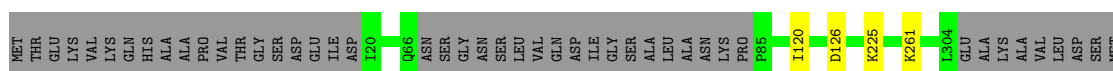
- Molecule 1: Putative polysaccharide export protein Wza

Chain H: 90% 9%



- Molecule 2: Tyrosine-protein kinase wzc

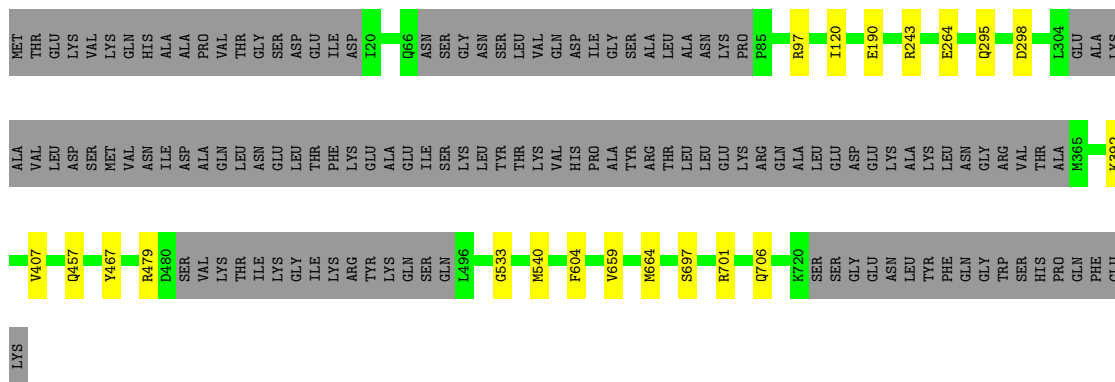
Chain I: 80% 18%



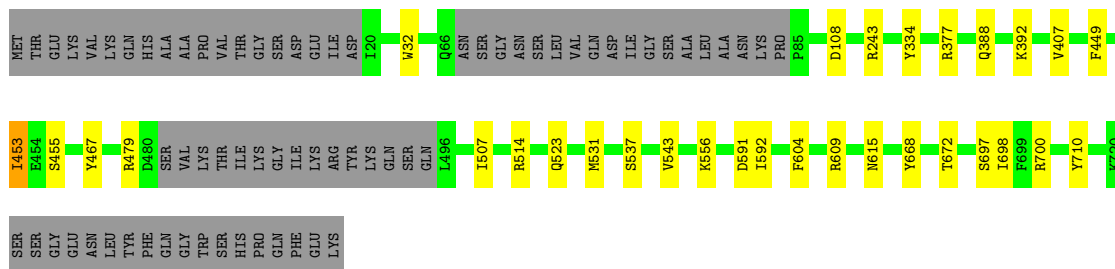
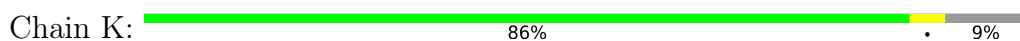
PHE
GLU
LYS

- Molecule 2: Tyrosine-protein kinase wzc

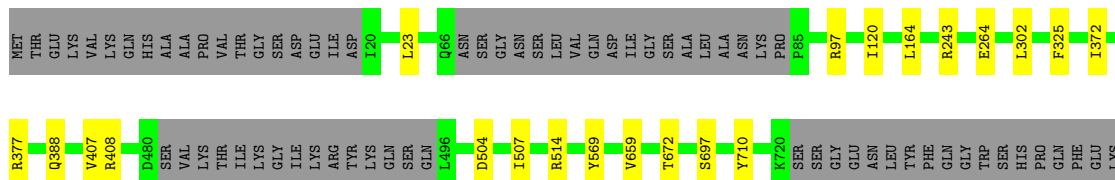
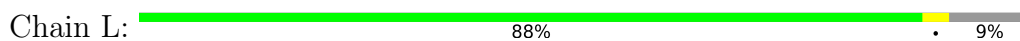
Chain J: 80% 18%



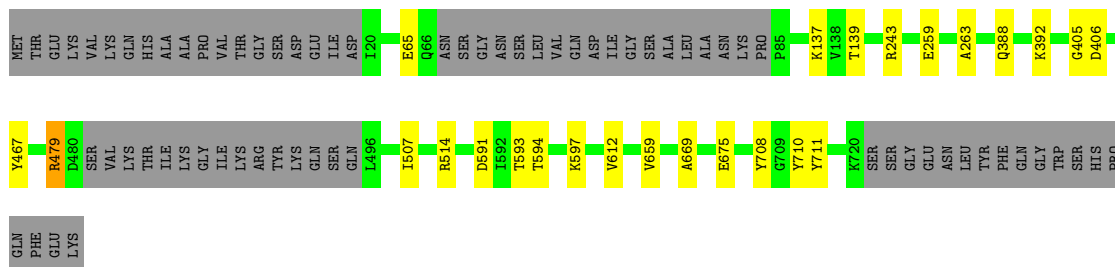
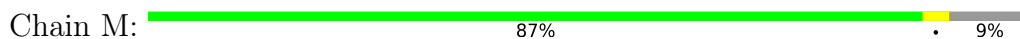
- Molecule 2: Tyrosine-protein kinase wzc



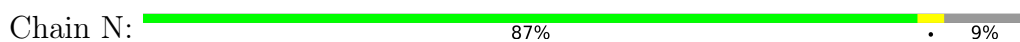
- Molecule 2: Tyrosine-protein kinase wzc



- Molecule 2: Tyrosine-protein kinase wzc



- 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	40245	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
Maximum map value	0.281	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	546.0, 546.0, 546.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.91, 0.91, 0.91	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	0.84	0/2836	1.35	5/3862 (0.1%)
1	B	0.83	0/2836	1.34	4/3862 (0.1%)
1	C	0.85	0/2836	1.32	1/3862 (0.0%)
1	D	0.83	0/2836	1.33	3/3862 (0.1%)
1	E	0.85	0/2836	1.35	4/3862 (0.1%)
1	F	0.86	0/2836	1.37	2/3862 (0.1%)
1	G	0.83	0/2836	1.33	3/3862 (0.1%)
1	H	0.85	0/2836	1.36	2/3862 (0.1%)
2	I	0.68	0/4777	1.19	5/6474 (0.1%)
2	J	0.69	0/4777	1.19	2/6474 (0.0%)
2	K	0.69	0/5260	1.21	7/7126 (0.1%)
2	L	0.69	0/5260	1.19	5/7126 (0.1%)
2	M	0.70	0/5260	1.21	2/7126 (0.0%)
2	N	0.71	0/5260	1.22	8/7126 (0.1%)
2	O	1.69	3/4777 (0.1%)	1.24	8/6474 (0.1%)
2	P	0.69	0/4777	1.19	3/6474 (0.0%)
All	All	0.86	3/62836 (0.0%)	1.26	64/85296 (0.1%)

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	B	0	1
1	C	0	1
2	I	0	3
2	J	0	2
2	K	0	2
2	L	0	3
2	M	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	N	0	3
2	O	0	4
2	P	0	3
All	All	0	27

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	477	LYS	N-CA	105.84	2.82	1.46
2	O	477	LYS	CA-C	8.21	1.63	1.52
2	O	477	LYS	CA-CB	7.14	1.65	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	476	GLN	CA-C-N	12.62	145.66	121.54
2	O	476	GLN	C-N-CA	12.62	145.66	121.54
2	O	477	LYS	N-CA-CB	10.24	127.80	110.49
2	O	477	LYS	N-CA-C	8.65	129.23	110.80
2	O	477	LYS	CB-CA-C	-8.45	93.61	110.42
2	K	455	SER	N-CA-C	7.20	117.40	108.11
2	N	534	VAL	N-CA-C	7.00	117.61	110.82
2	N	143	ARG	N-CA-C	6.88	114.42	108.22
2	N	534	VAL	CB-CA-C	-6.83	103.10	112.04
2	I	374	ARG	NE-CZ-NH2	6.82	125.33	119.20
2	O	514	ARG	NE-CZ-NH2	6.31	124.88	119.20
2	L	514	ARG	NE-CZ-NH2	6.27	124.85	119.20
1	G	158	ASP	CA-CB-CG	6.20	118.80	112.60
1	E	158	ASP	CA-CB-CG	6.09	118.69	112.60
2	J	604	PHE	CA-CB-CG	6.04	119.84	113.80
1	G	316	ASN	CA-CB-CG	6.00	118.60	112.60
1	B	367	ARG	NE-CZ-NH2	5.98	124.58	119.20
2	M	514	ARG	NE-CZ-NH2	5.93	124.53	119.20
1	B	251	ARG	NE-CZ-NH2	5.80	124.42	119.20
2	N	666	ALA	N-CA-C	5.80	117.78	109.14
1	H	45	ASP	CA-CB-CG	5.71	118.31	112.60
2	I	514	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	F	145	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	D	68	ASN	CA-CB-CG	5.64	118.24	112.60
2	L	377	ARG	NE-CZ-NH2	5.61	124.25	119.20
2	K	514	ARG	NE-CZ-NH2	5.56	124.20	119.20
2	K	591	ASP	CA-CB-CG	-5.56	107.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	557	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	H	158	ASP	CA-CB-CG	5.53	118.13	112.60
1	C	321	ASP	CA-CB-CG	5.53	118.13	112.60
2	M	612	VAL	N-CA-C	5.53	114.03	107.73
2	K	377	ARG	NE-CZ-NH2	5.47	124.12	119.20
1	A	256	LYS	CA-C-N	5.47	129.67	122.51
1	A	256	LYS	C-N-CA	5.47	129.67	122.51
2	L	408	ARG	NE-CZ-NH2	5.43	124.09	119.20
2	K	609	ARG	NE-CZ-NH2	5.41	124.07	119.20
2	P	514	ARG	NE-CZ-NH2	5.36	124.03	119.20
2	I	518	HIS	CB-CG-CD2	-5.35	124.25	131.20
2	J	701	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	E	302	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	E	236	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	G	64	ARG	NE-CZ-NH2	5.29	123.96	119.20
2	K	700	ARG	NE-CZ-NH2	5.27	123.94	119.20
2	N	361	ARG	NE-CZ-NH2	5.23	123.91	119.20
2	P	604	PHE	CA-CB-CG	5.21	119.02	113.80
1	D	354	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	223	ARG	NE-CZ-NH2	5.20	123.88	119.20
2	I	604	PHE	CA-CB-CG	5.17	118.97	113.80
2	K	604	PHE	CA-CB-CG	5.14	118.94	113.80
2	L	504	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	251	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	A	212	ASN	N-CA-CB	-5.11	105.66	111.79
2	O	280	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	E	220	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	L	325	PHE	CA-CB-CG	5.09	118.89	113.80
2	N	374	ARG	NE-CZ-NH2	5.08	123.77	119.20
2	O	658	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	D	145	ARG	NE-CZ-NH2	5.05	123.75	119.20
2	N	604	PHE	CA-CB-CG	5.05	118.85	113.80
2	I	609	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	B	164	ASN	CA-CB-CG	5.04	117.64	112.60
1	F	64	ARG	NE-CZ-NH2	5.03	123.73	119.20
2	N	658	HIS	CB-CG-CD2	-5.02	124.67	131.20
1	B	64	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	145	ARG	Sidechain
1	C	367	ARG	Sidechain
2	I	657	ARG	Sidechain
2	I	708	TYR	Sidechain
2	I	710	TYR	Sidechain
2	J	243	ARG	Sidechain
2	J	97	ARG	Sidechain
2	K	243	ARG	Sidechain
2	K	710	TYR	Sidechain
2	L	243	ARG	Sidechain
2	L	710	TYR	Sidechain
2	L	97	ARG	Sidechain
2	M	243	ARG	Sidechain
2	M	479	ARG	Sidechain
2	M	708	TYR	Sidechain
2	M	710	TYR	Sidechain
2	M	711	TYR	Sidechain
2	N	243	ARG	Sidechain
2	N	708	TYR	Sidechain
2	N	97	ARG	Sidechain
2	O	243	ARG	Sidechain
2	O	251	ARG	Sidechain
2	O	609	ARG	Sidechain
2	O	708	TYR	Sidechain
2	P	243	ARG	Sidechain
2	P	710	TYR	Sidechain
2	P	97	ARG	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	0	0
1	B	2783	2765	2764	3	0
1	C	2783	2765	2764	0	0
1	D	2783	2765	2764	0	0
1	E	2783	2765	2764	0	0
1	F	2783	2765	2764	0	0
1	G	2783	2765	2764	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2783	2765	2764	0	0
2	I	4708	4807	4804	1	0
2	J	4708	4807	4804	2	0
2	K	5185	5302	5300	5	0
2	L	5185	5302	5300	2	0
2	M	5185	5302	5300	4	0
2	N	5185	5302	5300	0	0
2	O	4708	4807	4804	3	0
2	P	4708	4807	4804	1	0
3	I	27	12	12	0	0
3	J	27	12	12	0	0
3	K	27	12	12	0	0
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	62052	62652	62624	22	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 0.

All (22) 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:M:593:THR:HG23	2:M:594:THR:HG23	1.78	0.64
2:I:504:ASP:O	2:I:507:ILE:HG22	2.05	0.56
2:K:668:TYR:CD2	2:K:698:ILE:HA	2.45	0.52
2:L:507:ILE:H	2:L:507:ILE:HD12	1.74	0.51
2:K:507:ILE:HD12	2:K:507:ILE:H	1.76	0.51
2:P:507:ILE:H	2:P:507:ILE:HD12	1.75	0.51
2:M:507:ILE:H	2:M:507:ILE:HD12	1.79	0.48
2:K:531:MET:HE1	2:K:543:VAL:HG13	1.96	0.47
2:O:507:ILE:HD12	2:O:507:ILE:H	1.79	0.47
2:J:533:GLY:HA2	2:J:664:MET:SD	2.55	0.47
1:B:216:THR:HG21	1:G:233:GLY:HA2	1.98	0.45
2:M:259:GLU:O	2:M:263:ALA:HB2	2.17	0.44
1:B:216:THR:HG23	1:B:246:ILE:HB	2.00	0.44
2:K:531:MET:HE1	2:K:543:VAL:CG1	2.48	0.44
2:O:533:GLY:HA2	2:O:664:MET:SD	2.59	0.43
2:L:302:LEU:HD11	2:L:372:ILE:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:477:LYS:CA	2:O:477:LYS:N	2.82	0.42
2:M:591:ASP:CG	2:M:593:THR:HG22	2.45	0.42
1:G:128:TYR:CG	1:G:129:PRO:HD2	2.56	0.41
2:K:453:ILE:N	2:K:453:ILE:HD12	2.36	0.41
2:J:533:GLY:CA	2:J:664:MET:SD	3.09	0.41
1:B:174:TYR:C	1:B:175:ILE:HD12	2.46	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	356/394 (90%)	334 (94%)	22 (6%)	0	100	100
1	B	356/394 (90%)	336 (94%)	20 (6%)	0	100	100
1	C	356/394 (90%)	336 (94%)	19 (5%)	1 (0%)	36	71
1	D	356/394 (90%)	336 (94%)	19 (5%)	1 (0%)	36	71
1	E	356/394 (90%)	337 (95%)	18 (5%)	1 (0%)	36	71
1	F	356/394 (90%)	338 (95%)	16 (4%)	2 (1%)	21	58
1	G	356/394 (90%)	341 (96%)	15 (4%)	0	100	100
1	H	356/394 (90%)	334 (94%)	21 (6%)	1 (0%)	36	71
2	I	600/738 (81%)	580 (97%)	17 (3%)	3 (0%)	24	63
2	J	600/738 (81%)	570 (95%)	27 (4%)	3 (0%)	24	63
2	K	662/738 (90%)	632 (96%)	26 (4%)	4 (1%)	21	58
2	L	662/738 (90%)	633 (96%)	27 (4%)	2 (0%)	36	71
2	M	662/738 (90%)	636 (96%)	24 (4%)	2 (0%)	36	71
2	N	662/738 (90%)	632 (96%)	27 (4%)	3 (0%)	24	63
2	O	600/738 (81%)	566 (94%)	29 (5%)	5 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	600/738 (81%)	578 (96%)	19 (3%)	3 (0%)	24	63
All	All	7896/9056 (87%)	7519 (95%)	346 (4%)	31 (0%)	31	67

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	305	LYS
2	K	334	TYR
2	P	298	ASP
2	P	407	VAL
1	F	305	LYS
2	J	298	ASP
2	N	702	ALA
2	O	403	THR
2	O	669	ALA
2	K	537	SER
2	O	477	LYS
2	P	718	ASP
1	F	285	ALA
1	H	305	LYS
2	I	407	VAL
2	I	669	ALA
2	J	407	VAL
2	M	405	GLY
2	N	407	VAL
2	O	120	ILE
1	C	322	MET
2	M	669	ALA
2	N	120	ILE
2	O	407	VAL
2	I	120	ILE
2	L	120	ILE
1	D	159	PRO
2	K	407	VAL
2	L	407	VAL
2	J	120	ILE
2	K	615	ASN

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%)	300 (98%)	7 (2%)	44	63
1	B	307/342 (90%)	301 (98%)	6 (2%)	48	65
1	C	307/342 (90%)	303 (99%)	4 (1%)	61	72
1	D	307/342 (90%)	302 (98%)	5 (2%)	55	69
1	E	307/342 (90%)	303 (99%)	4 (1%)	61	72
1	F	307/342 (90%)	300 (98%)	7 (2%)	44	63
1	G	307/342 (90%)	300 (98%)	7 (2%)	44	63
1	H	307/342 (90%)	305 (99%)	2 (1%)	76	79
2	I	519/630 (82%)	510 (98%)	9 (2%)	53	67
2	J	519/630 (82%)	508 (98%)	11 (2%)	47	65
2	K	570/630 (90%)	557 (98%)	13 (2%)	44	63
2	L	570/630 (90%)	562 (99%)	8 (1%)	59	71
2	M	570/630 (90%)	559 (98%)	11 (2%)	50	66
2	N	570/630 (90%)	560 (98%)	10 (2%)	51	67
2	O	519/630 (82%)	509 (98%)	10 (2%)	50	66
2	P	519/630 (82%)	510 (98%)	9 (2%)	53	67
All	All	6812/7776 (88%)	6689 (98%)	123 (2%)	51	67

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLU
1	A	105	THR
1	A	185	GLN
1	A	236	ASN
1	A	240	LEU
1	A	329	VAL
1	A	379	TRP
1	B	71	ARG

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Mol	Chain	Res	Type
1	B	102	GLU
1	B	105	THR
1	B	134	VAL
1	B	216	THR
1	B	367	ARG
1	C	92	VAL
1	C	206	ASP
1	C	232	ASN
1	C	300	VAL
1	D	56	THR
1	D	213	VAL
1	D	221	GLU
1	D	286	GLU
1	D	367	ARG
1	E	92	VAL
1	E	184	GLN
1	E	214	VAL
1	E	256	LYS
1	F	102	GLU
1	F	105	THR
1	F	185	GLN
1	F	291	THR
1	F	324	ASP
1	F	342	VAL
1	F	358	GLN
1	G	102	GLU
1	G	214	VAL
1	G	291	THR
1	G	342	VAL
1	G	346	THR
1	G	360	LEU
1	G	367	ARG
1	H	105	THR
1	H	130	TYR
2	I	126	ASP
2	I	225	LYS
2	I	261	LYS
2	I	457	GLN
2	I	479	ARG
2	I	540	MET
2	I	620	LEU
2	I	657	ARG

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Mol	Chain	Res	Type
2	I	659	VAL
2	J	190	GLU
2	J	264	GLU
2	J	295	GLN
2	J	392	LYS
2	J	457	GLN
2	J	467	TYR
2	J	479	ARG
2	J	540	MET
2	J	659	VAL
2	J	697	SER
2	J	706	GLN
2	K	32	TRP
2	K	108	ASP
2	K	388	GLN
2	K	392	LYS
2	K	449	PHE
2	K	453	ILE
2	K	467	TYR
2	K	479	ARG
2	K	523	GLN
2	K	556	LYS
2	K	592	ILE
2	K	672	THR
2	K	697	SER
2	L	23	LEU
2	L	164	LEU
2	L	264	GLU
2	L	388	GLN
2	L	569	TYR
2	L	659	VAL
2	L	672	THR
2	L	697	SER
2	M	65	GLU
2	M	137	LYS
2	M	139	THR
2	M	388	GLN
2	M	392	LYS
2	M	406	ASP
2	M	467	TYR
2	M	479	ARG
2	M	597	LYS

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Mol	Chain	Res	Type
2	M	659	VAL
2	M	675	GLU
2	N	264	GLU
2	N	267	LYS
2	N	392	LYS
2	N	459	LEU
2	N	479	ARG
2	N	540	MET
2	N	563	CYS
2	N	565	MET
2	N	659	VAL
2	N	697	SER
2	O	137	LYS
2	O	145	LYS
2	O	160	LYS
2	O	175	GLN
2	O	457	GLN
2	O	474	GLU
2	O	477	LYS
2	O	606	LEU
2	O	697	SER
2	O	714	GLU
2	P	126	ASP
2	P	160	LYS
2	P	190	GLU
2	P	392	LYS
2	P	467	TYR
2	P	479	ARG
2	P	647	LEU
2	P	659	VAL
2	P	697	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	164	ASN
1	A	171	GLN
1	A	184	GLN
1	A	185	GLN
1	A	227	GLN
1	A	231	GLN

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Mol	Chain	Res	Type
1	A	353	ASN
1	A	357	ASN
1	B	94	ASN
1	B	164	ASN
1	B	199	ASN
1	B	227	GLN
1	B	232	ASN
1	B	252	ASN
1	B	319	GLN
1	B	357	ASN
1	C	135	HIS
1	C	236	ASN
1	C	319	GLN
1	C	353	ASN
1	C	357	ASN
1	C	358	GLN
1	D	94	ASN
1	D	164	ASN
1	D	227	GLN
1	D	231	GLN
1	D	337	GLN
1	D	358	GLN
1	E	94	ASN
1	E	164	ASN
1	E	171	GLN
1	E	178	GLN
1	E	238	ASN
1	E	252	ASN
1	E	353	ASN
1	E	358	GLN
1	F	84	GLN
1	F	94	ASN
1	F	199	ASN
1	F	218	ASN
1	F	227	GLN
1	F	231	GLN
1	F	232	ASN
1	F	353	ASN
1	F	377	HIS
1	G	118	ASN
1	G	212	ASN
1	G	294	ASN

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Mol	Chain	Res	Type
1	G	353	ASN
1	G	358	GLN
1	H	68	ASN
1	H	94	ASN
1	H	180	ASN
1	H	232	ASN
1	H	319	GLN
1	H	337	GLN
1	H	353	ASN
2	I	175	GLN
2	I	275	GLN
2	I	288	ASN
2	I	370	GLN
2	I	457	GLN
2	I	525	GLN
2	J	175	GLN
2	J	178	GLN
2	J	193	HIS
2	J	275	GLN
2	J	384	GLN
2	J	457	GLN
2	J	476	GLN
2	K	63	GLN
2	K	193	HIS
2	K	321	ASN
2	K	384	GLN
2	K	391	ASN
2	K	476	GLN
2	K	526	ASN
2	K	555	ASN
2	K	589	GLN
2	K	615	ASN
2	L	161	ASN
2	L	175	GLN
2	L	193	HIS
2	L	213	GLN
2	L	257	ASN
2	L	319	GLN
2	L	321	ASN
2	L	553	GLN
2	M	155	ASN
2	M	161	ASN

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Mol	Chain	Res	Type
2	M	175	GLN
2	M	223	ASN
2	M	319	GLN
2	M	321	ASN
2	M	370	GLN
2	M	384	GLN
2	M	388	GLN
2	M	578	ASN
2	M	611	GLN
2	M	615	ASN
2	N	161	ASN
2	N	175	GLN
2	N	223	ASN
2	N	319	GLN
2	N	384	GLN
2	N	391	ASN
2	N	611	GLN
2	O	161	ASN
2	O	193	HIS
2	O	391	ASN
2	O	580	ASN
2	O	630	ASN
2	P	175	GLN
2	P	193	HIS
2	P	370	GLN

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

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	N	1000	-	27,29,29	1.07	0	42,45,45	1.32	6 (14%)
3	ADP	L	1000	-	27,29,29	0.95	1 (3%)	42,45,45	1.42	8 (19%)
3	ADP	K	1000	-	27,29,29	0.98	2 (7%)	42,45,45	1.28	7 (16%)
3	ADP	J	1000	-	27,29,29	0.96	1 (3%)	42,45,45	1.41	7 (16%)
3	ADP	O	1000	-	27,29,29	0.99	0	42,45,45	1.44	9 (21%)
3	ADP	I	1000	-	27,29,29	0.99	1 (3%)	42,45,45	1.39	9 (21%)
3	ADP	P	1000	-	27,29,29	1.00	1 (3%)	42,45,45	1.28	6 (14%)
3	ADP	M	1000	-	27,29,29	0.98	0	42,45,45	1.28	6 (14%)

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	N	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	L	1000	-	-	5/16/32/32	0/3/3/3
3	ADP	K	1000	-	-	8/16/32/32	0/3/3/3
3	ADP	J	1000	-	-	3/16/32/32	0/3/3/3
3	ADP	O	1000	-	-	2/16/32/32	0/3/3/3
3	ADP	I	1000	-	-	0/16/32/32	0/3/3/3
3	ADP	P	1000	-	-	0/16/32/32	0/3/3/3
3	ADP	M	1000	-	-	3/16/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1000	ADP	C5-C4	-2.24	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1000	ADP	C5-C4	-2.11	1.35	1.39
3	P	1000	ADP	C5-C4	-2.04	1.35	1.39
3	L	1000	ADP	C5-C4	-2.04	1.35	1.39
3	K	1000	ADP	C8-N7	2.02	1.35	1.31
3	K	1000	ADP	C5-C4	-2.01	1.35	1.39

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1000	ADP	PA-O3A-PB	-3.54	120.68	132.83
3	L	1000	ADP	PA-O3A-PB	-3.36	121.28	132.83
3	L	1000	ADP	C5-C4-N3	-3.29	122.46	126.75
3	J	1000	ADP	PA-O3A-PB	-3.28	121.56	132.83
3	O	1000	ADP	C5-C4-N3	-3.28	122.47	126.75
3	M	1000	ADP	C5-C4-N3	-3.18	122.61	126.75
3	P	1000	ADP	PA-O3A-PB	-3.11	122.14	132.83
3	O	1000	ADP	O2B-PB-O3A	3.08	114.97	104.64
3	J	1000	ADP	C5-C4-N3	-3.08	122.73	126.75
3	I	1000	ADP	PA-O3A-PB	-3.07	122.31	132.83
3	K	1000	ADP	C5-C4-N3	-3.06	122.76	126.75
3	N	1000	ADP	C5-C4-N3	-3.06	122.76	126.75
3	I	1000	ADP	C5-C4-N3	-3.02	122.81	126.75
3	L	1000	ADP	O3B-PB-O3A	2.94	114.49	104.64
3	P	1000	ADP	C5-C4-N3	-2.90	122.97	126.75
3	M	1000	ADP	PA-O3A-PB	-2.86	123.02	132.83
3	P	1000	ADP	C4-C5-N7	2.83	114.06	110.62
3	O	1000	ADP	C4-C5-N7	2.80	114.03	110.62
3	L	1000	ADP	C5-C6-N1	2.75	123.29	117.39
3	N	1000	ADP	C4-C5-N7	2.71	113.92	110.62
3	O	1000	ADP	PA-O3A-PB	-2.70	123.54	132.83
3	L	1000	ADP	N6-C6-N1	-2.69	112.45	118.35
3	J	1000	ADP	C5-C6-N1	2.69	123.17	117.39
3	I	1000	ADP	C4-C5-N7	2.67	113.87	110.62
3	K	1000	ADP	C5-C6-N1	2.67	123.12	117.39
3	O	1000	ADP	C5-C6-N1	2.66	123.11	117.39
3	I	1000	ADP	O3B-PB-O3A	2.64	113.48	104.64
3	P	1000	ADP	C5-C6-N1	2.64	123.05	117.39
3	I	1000	ADP	C5-C6-N1	2.62	123.01	117.39
3	M	1000	ADP	C5-C6-N1	2.56	122.89	117.39
3	K	1000	ADP	N6-C6-N1	-2.56	112.75	118.35
3	J	1000	ADP	C4-C5-N7	2.55	113.72	110.62
3	L	1000	ADP	C4-C5-N7	2.55	113.72	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	N	1000	ADP	C5-C6-N1	2.52	122.79	117.39
3	K	1000	ADP	C4-C5-N7	2.49	113.66	110.62
3	K	1000	ADP	PA-O3A-PB	-2.48	124.33	132.83
3	J	1000	ADP	N6-C6-N1	-2.47	112.94	118.35
3	K	1000	ADP	O3B-PB-O3A	2.45	112.87	104.64
3	M	1000	ADP	C4-C5-N7	2.43	113.58	110.62
3	I	1000	ADP	O2B-PB-O3A	2.37	112.60	104.64
3	I	1000	ADP	C2-N1-C6	-2.35	114.73	118.77
3	O	1000	ADP	C2-N1-C6	-2.33	114.77	118.77
3	N	1000	ADP	C2-N1-C6	-2.32	114.78	118.77
3	P	1000	ADP	C2-N1-C6	-2.30	114.81	118.77
3	M	1000	ADP	N6-C6-N1	-2.30	113.32	118.35
3	O	1000	ADP	N3-C4-N9	2.30	130.87	127.08
3	L	1000	ADP	C2-N1-C6	-2.29	114.83	118.77
3	J	1000	ADP	C2-N1-C6	-2.27	114.87	118.77
3	K	1000	ADP	C2-N1-C6	-2.26	114.88	118.77
3	O	1000	ADP	O4'-C1'-C2'	-2.24	101.76	106.64
3	J	1000	ADP	O2B-PB-O3A	2.21	112.06	104.64
3	P	1000	ADP	N3-C4-N9	2.20	130.70	127.08
3	M	1000	ADP	C2-N1-C6	-2.17	115.04	118.77
3	O	1000	ADP	N6-C6-N1	-2.17	113.61	118.35
3	N	1000	ADP	N3-C4-N9	2.10	130.55	127.08
3	I	1000	ADP	N3-C4-N9	2.06	130.48	127.08
3	L	1000	ADP	N3-C4-N9	2.01	130.40	127.08
3	I	1000	ADP	N6-C6-N1	-2.01	113.96	118.35

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	1000	ADP	C4'-C5'-O5'-PA
3	K	1000	ADP	O4'-C4'-C5'-O5'
3	K	1000	ADP	C3'-C4'-C5'-O5'
3	L	1000	ADP	PA-O3A-PB-O3B
3	L	1000	ADP	C5'-O5'-PA-O1A
3	N	1000	ADP	C2'-C1'-N9-C4
3	J	1000	ADP	C3'-C4'-C5'-O5'
3	L	1000	ADP	C2'-C1'-N9-C8
3	N	1000	ADP	C4'-C5'-O5'-PA
3	K	1000	ADP	PB-O3A-PA-O5'
3	J	1000	ADP	C2'-C1'-N9-C8
3	M	1000	ADP	PA-O3A-PB-O1B

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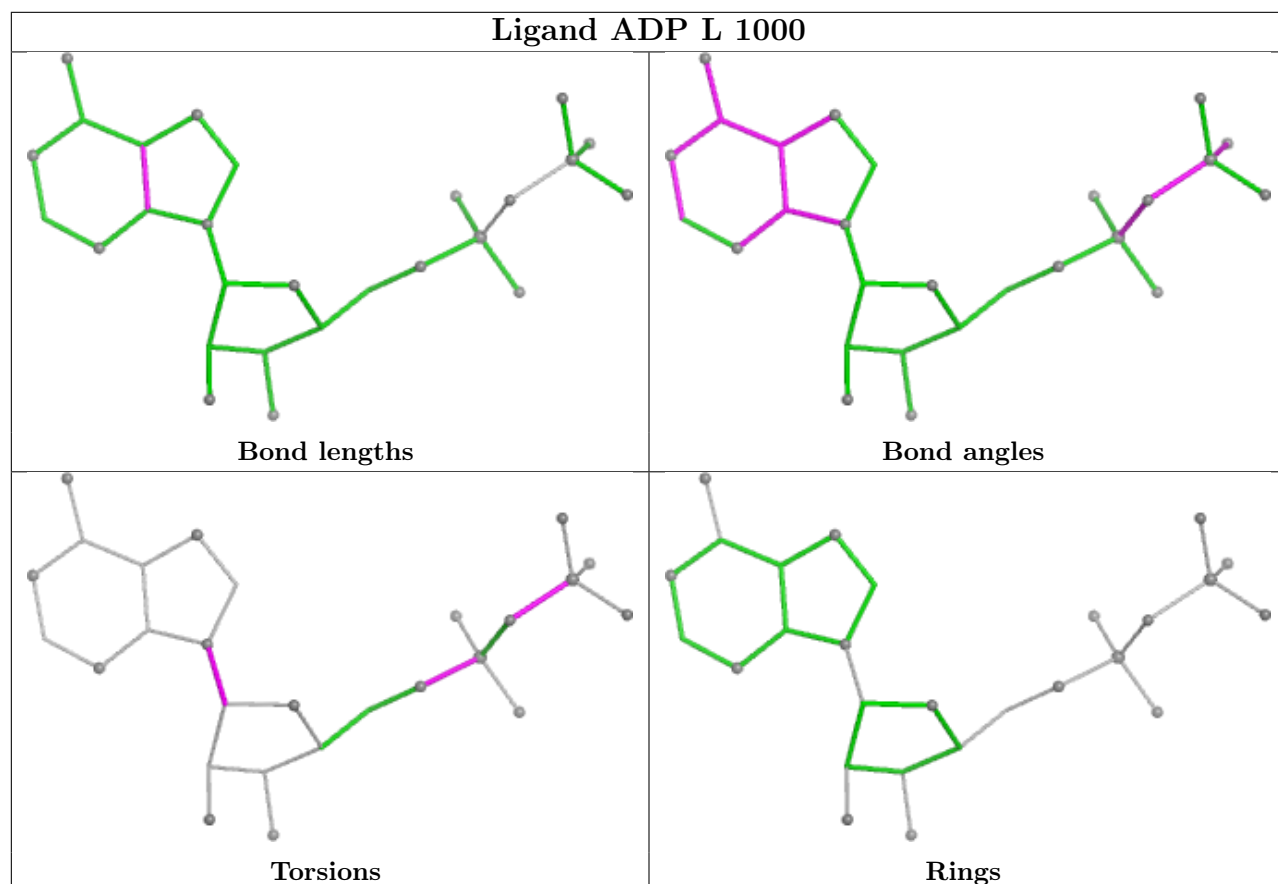
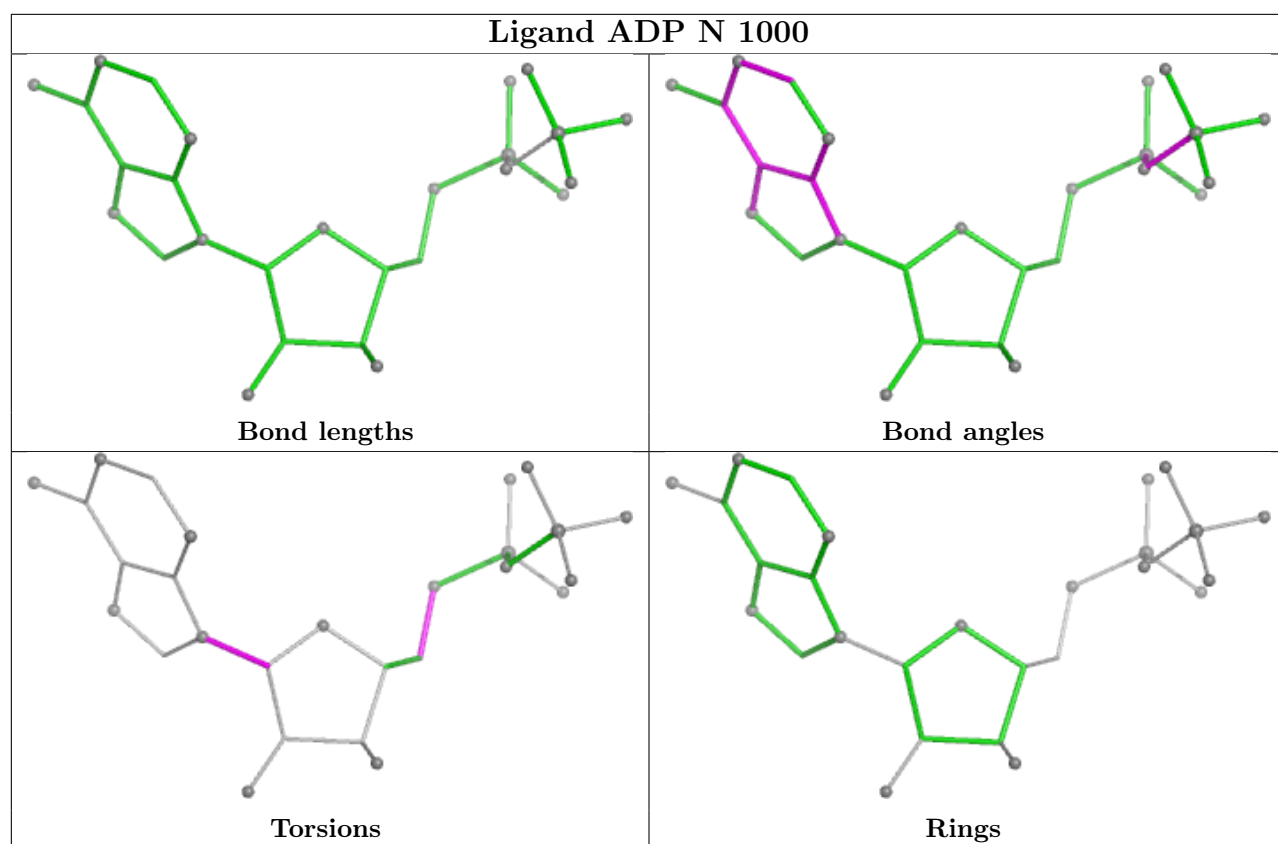
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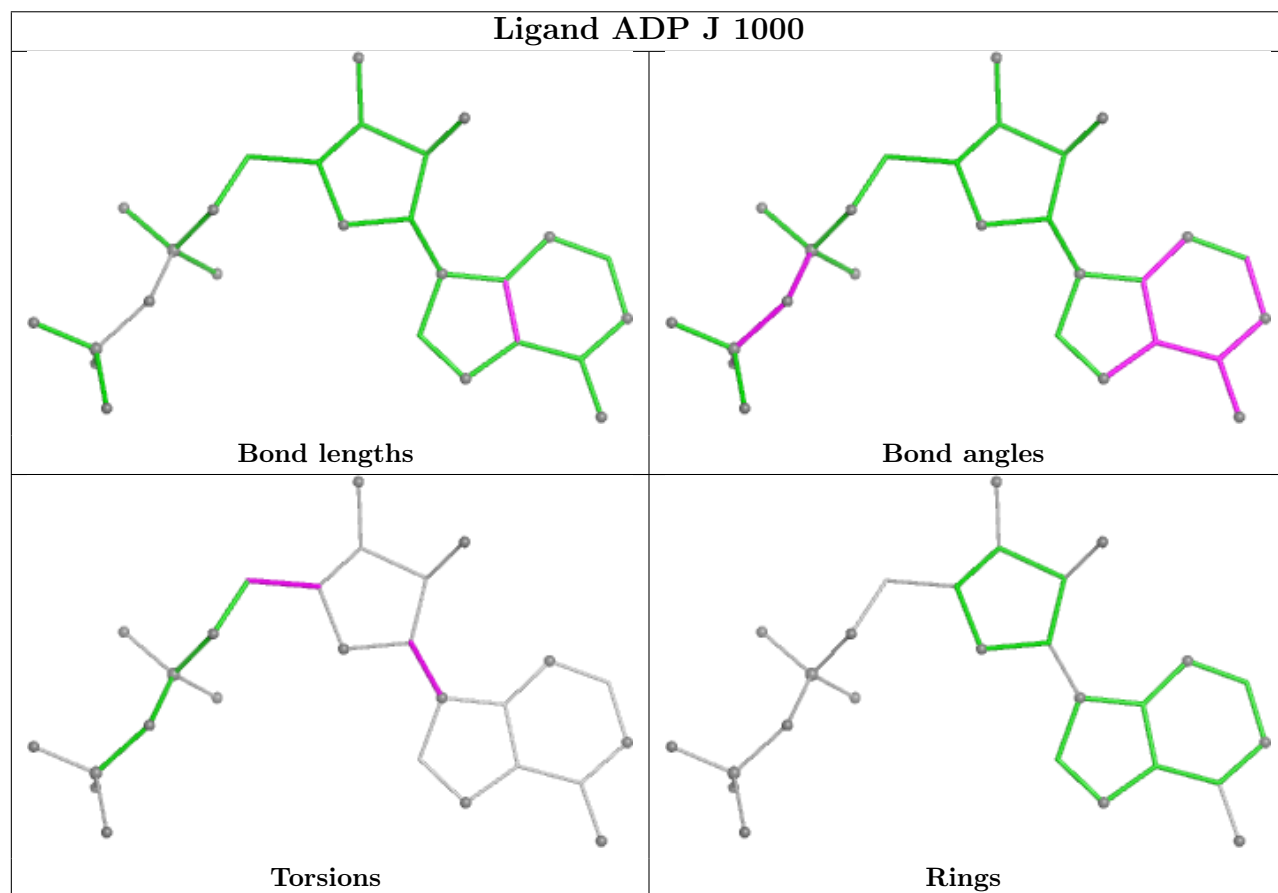
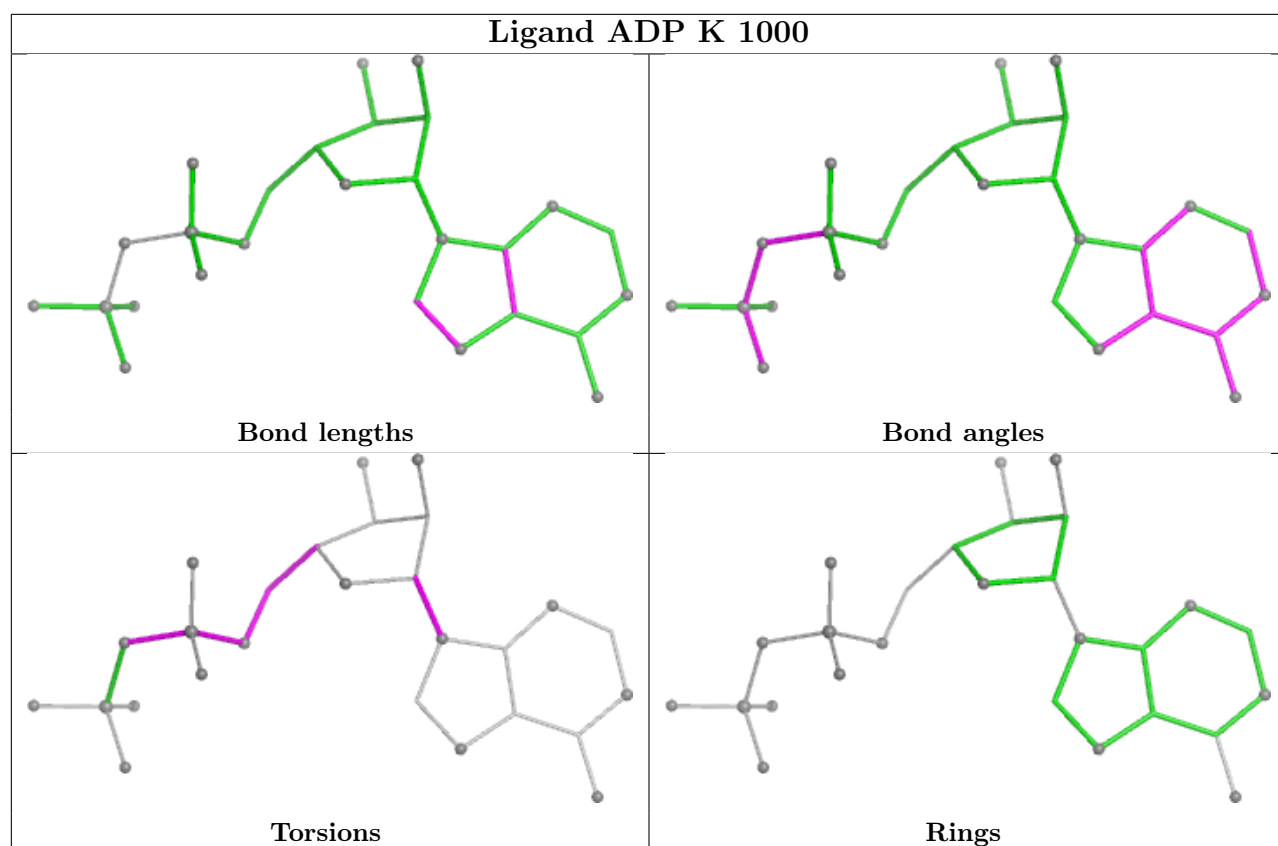
Mol	Chain	Res	Type	Atoms
3	K	1000	ADP	C5'-O5'-PA-O3A
3	K	1000	ADP	C2'-C1'-N9-C8
3	N	1000	ADP	C2'-C1'-N9-C8
3	K	1000	ADP	C5'-O5'-PA-O1A
3	L	1000	ADP	PA-O3A-PB-O1B
3	O	1000	ADP	PB-O3A-PA-O2A
3	O	1000	ADP	PB-O3A-PA-O1A
3	N	1000	ADP	O4'-C1'-N9-C8
3	M	1000	ADP	PA-O3A-PB-O2B
3	M	1000	ADP	PA-O3A-PB-O3B
3	L	1000	ADP	C5'-O5'-PA-O3A
3	K	1000	ADP	C5'-O5'-PA-O2A
3	J	1000	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

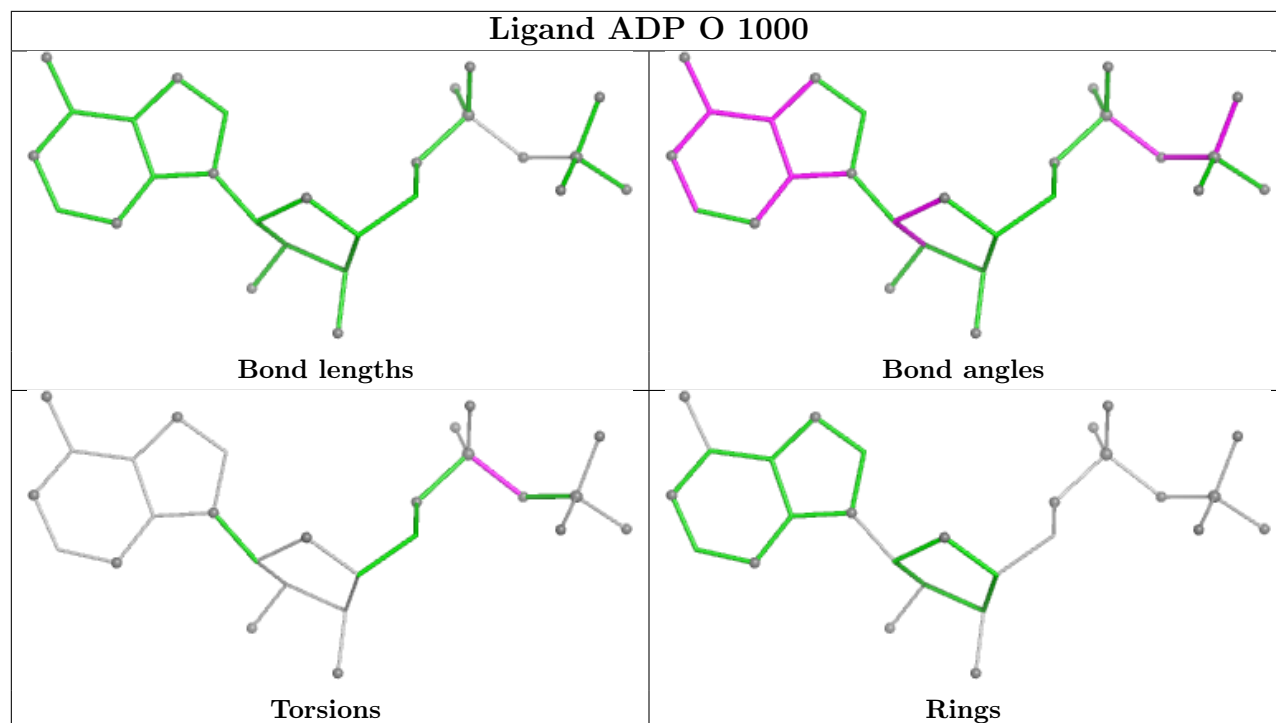
No monomer is involved in short contacts.

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.

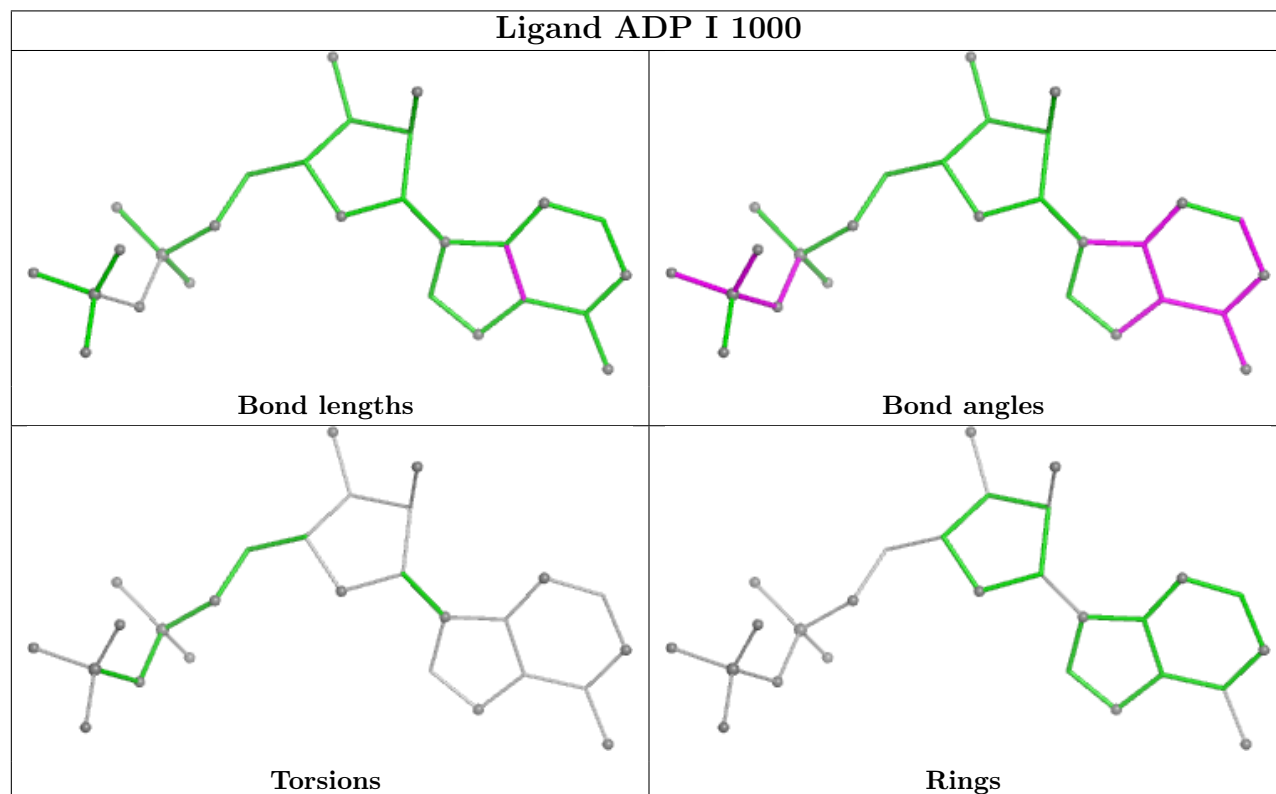


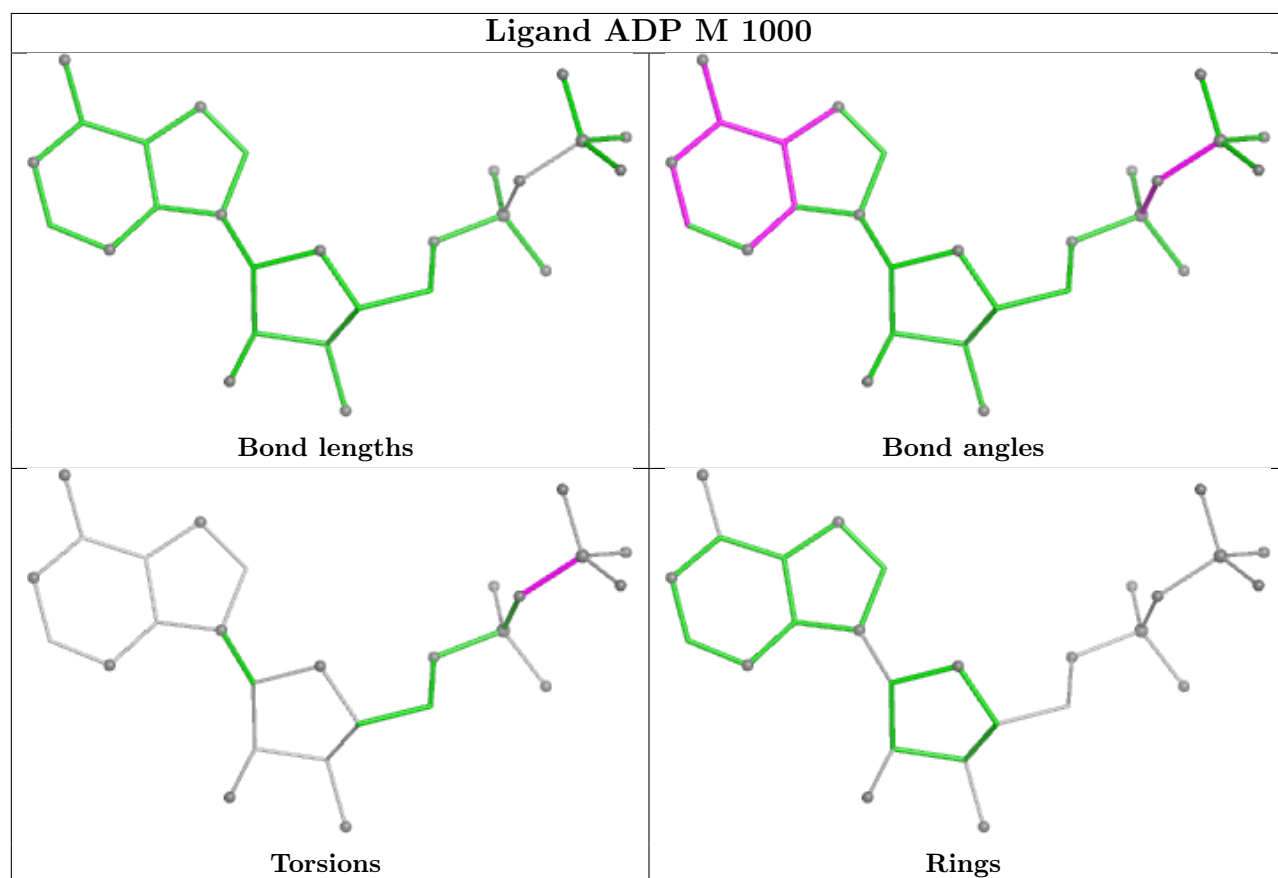
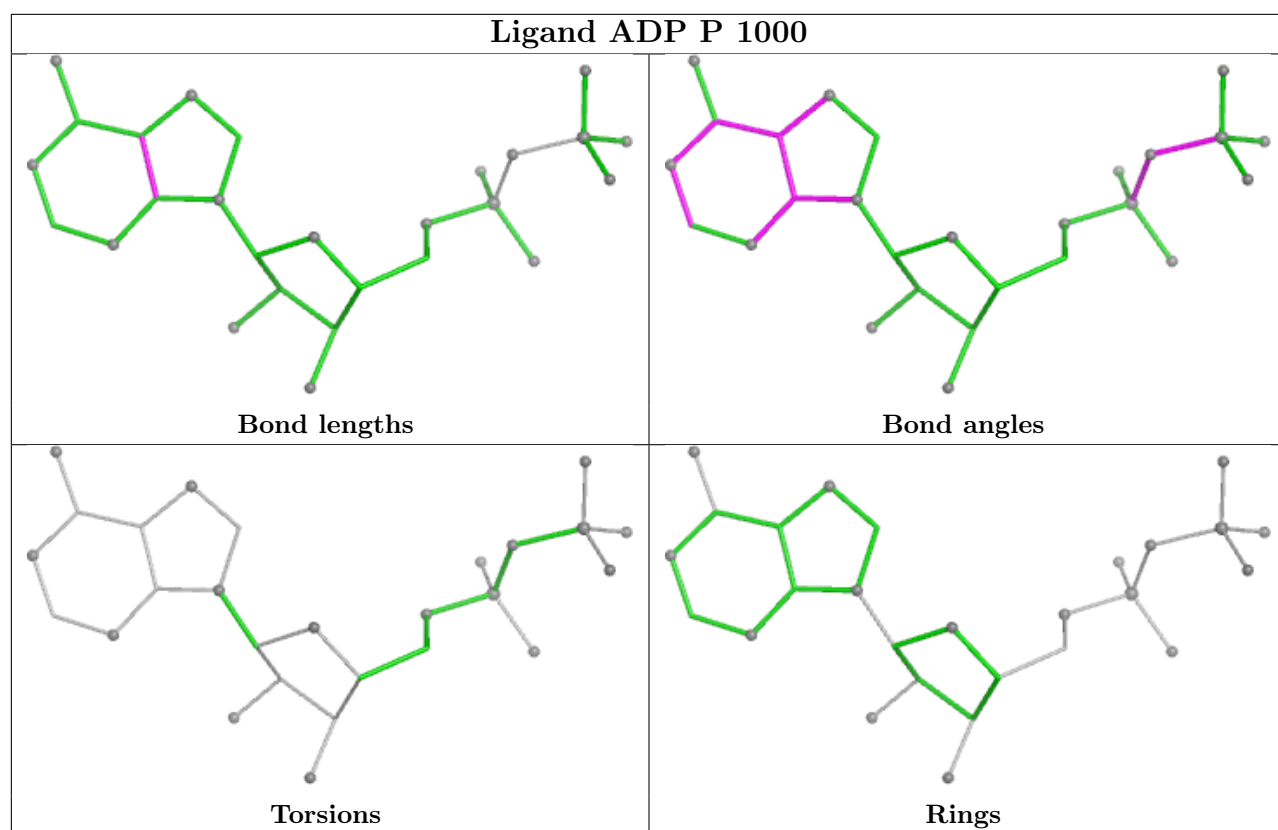


Ligand ADP O 1000



Ligand ADP I 1000





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.

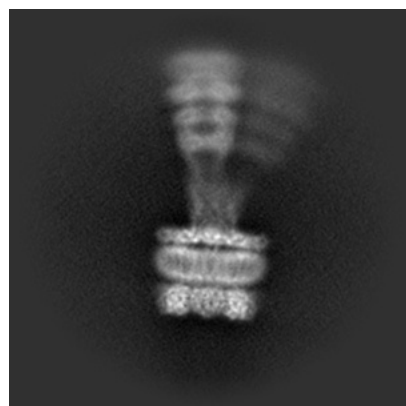
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53609. These allow visual inspection of the internal detail of the map and identification of artifacts.

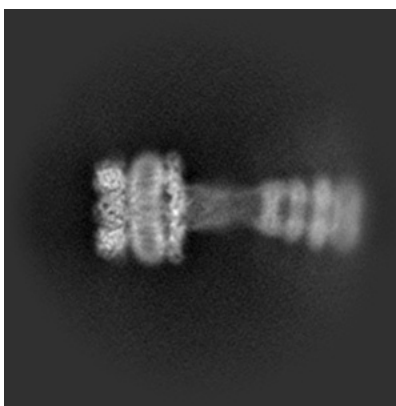
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

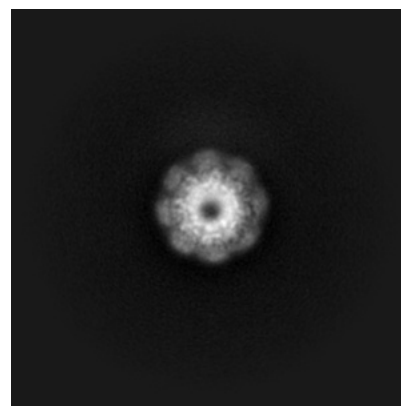
6.1.1 Primary map



X

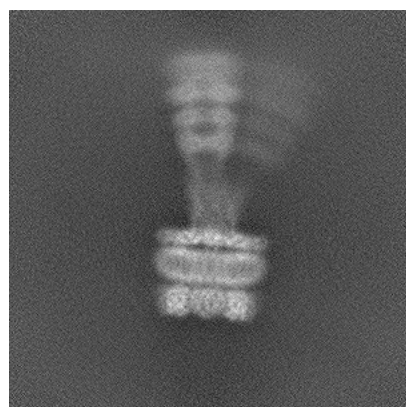


Y

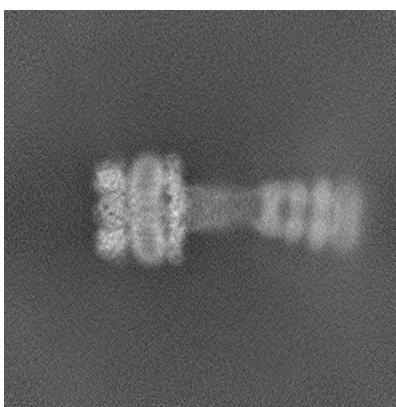


Z

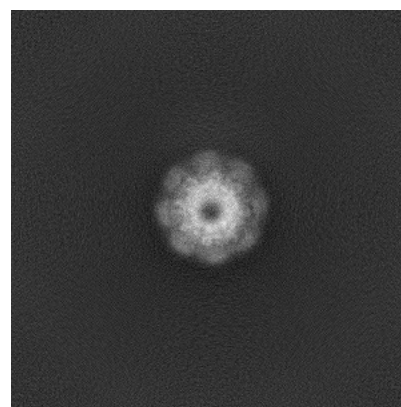
6.1.2 Raw map



X



Y

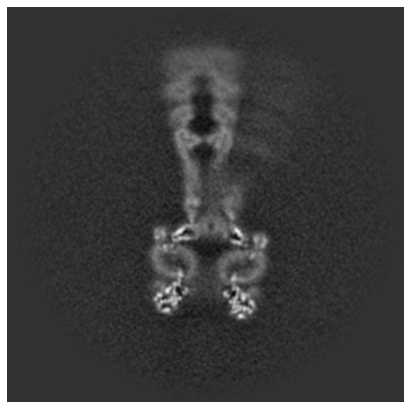


Z

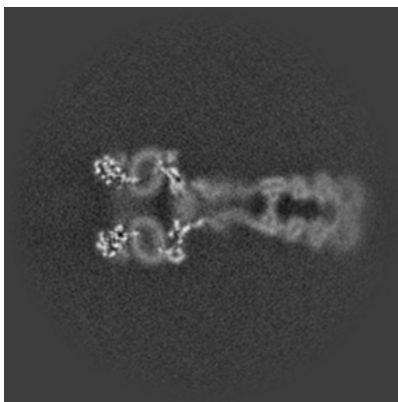
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

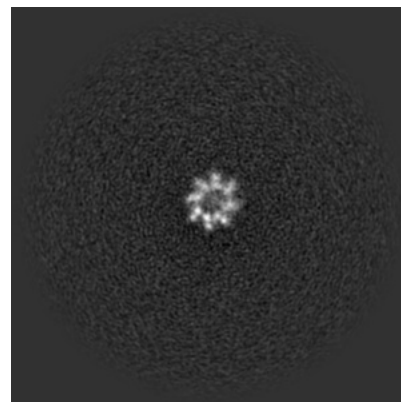
6.2.1 Primary map



X Index: 300

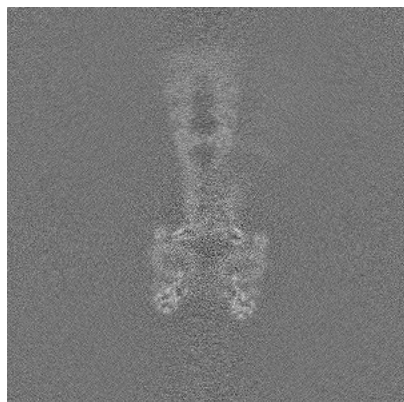


Y Index: 300

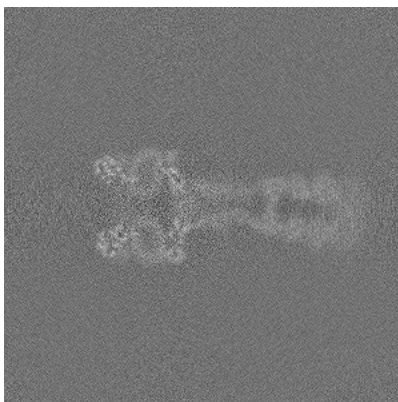


Z Index: 300

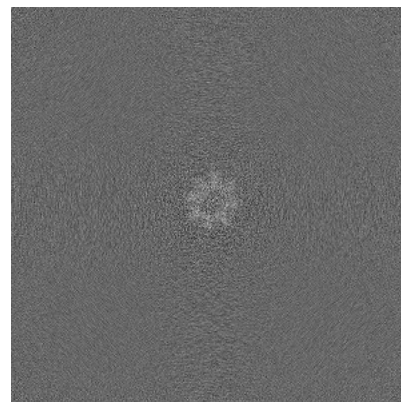
6.2.2 Raw map



X Index: 300



Y Index: 300

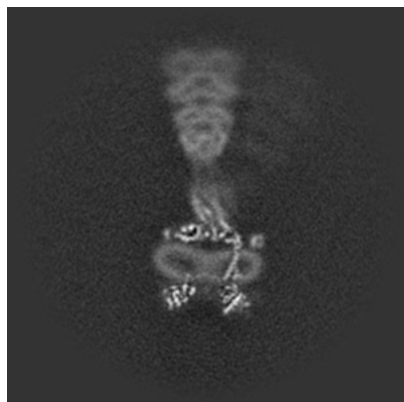


Z Index: 300

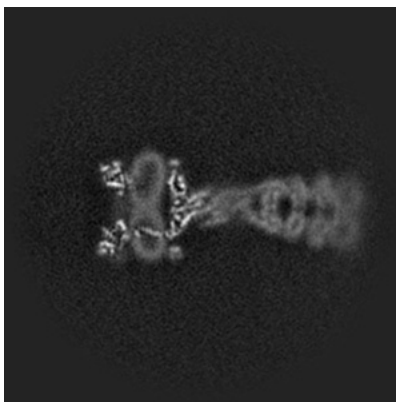
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

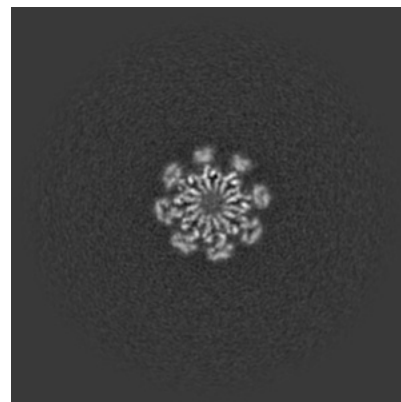
6.3.1 Primary map



X Index: 275

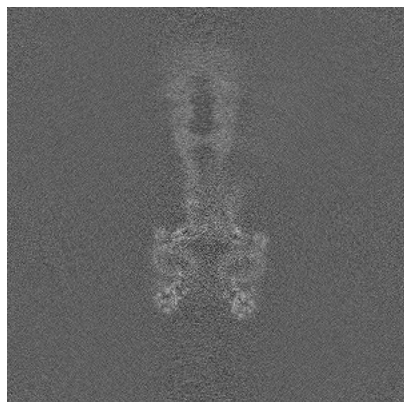


Y Index: 278

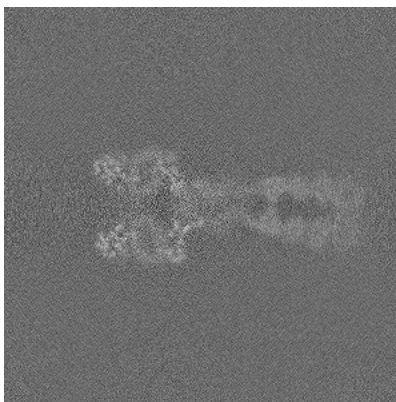


Z Index: 257

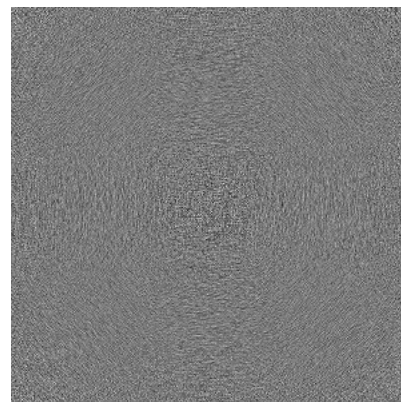
6.3.2 Raw map



X Index: 299



Y Index: 299

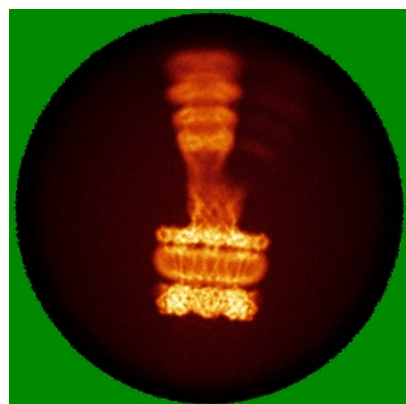


Z Index: 0

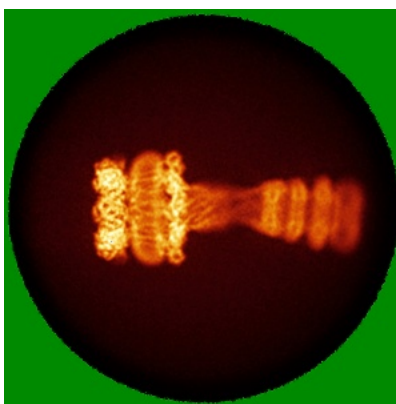
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

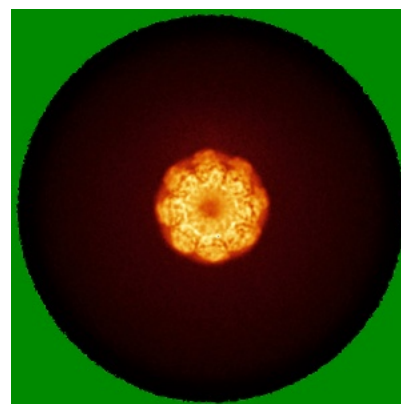
6.4.1 Primary map



X

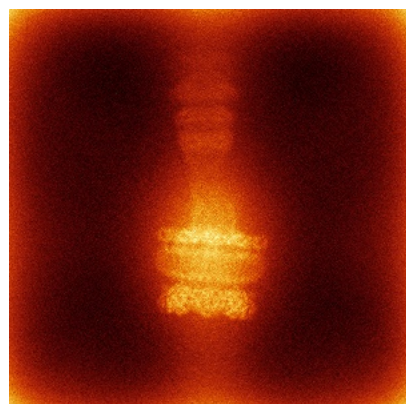


Y

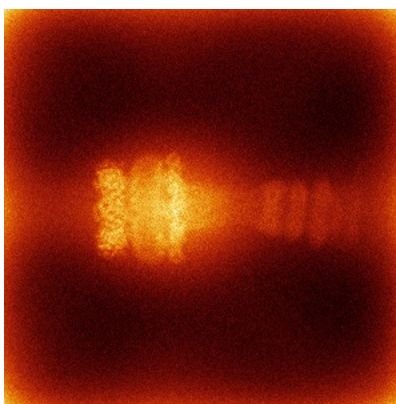


Z

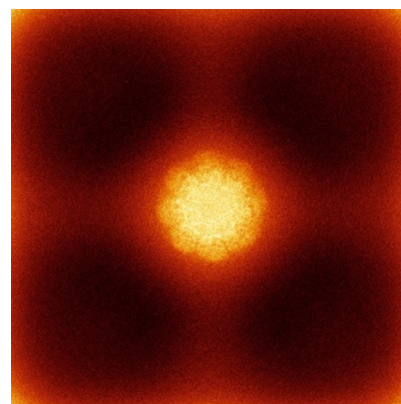
6.4.2 Raw map



X



Y

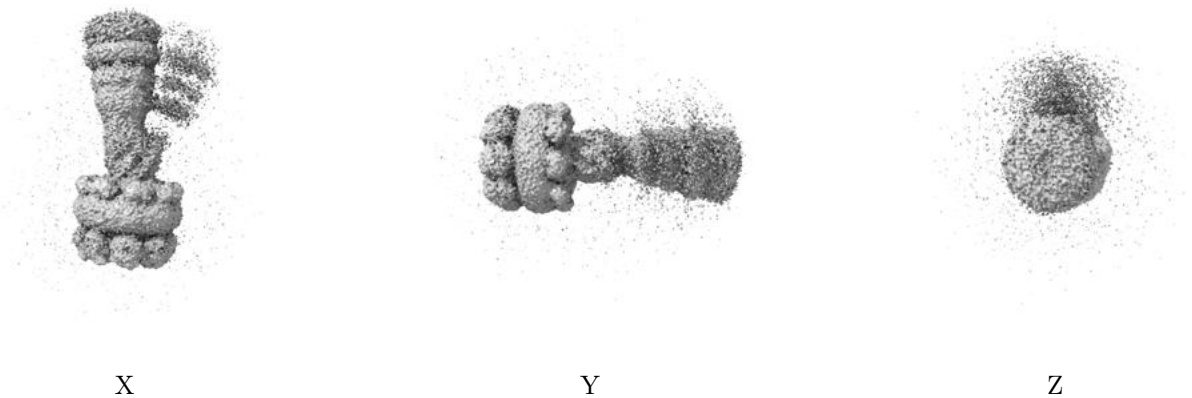


Z

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.

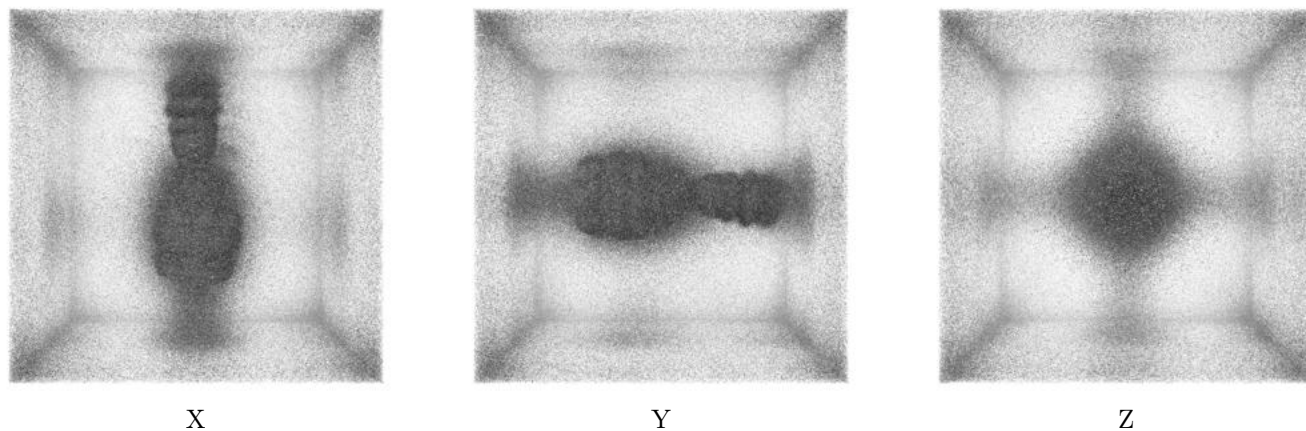
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

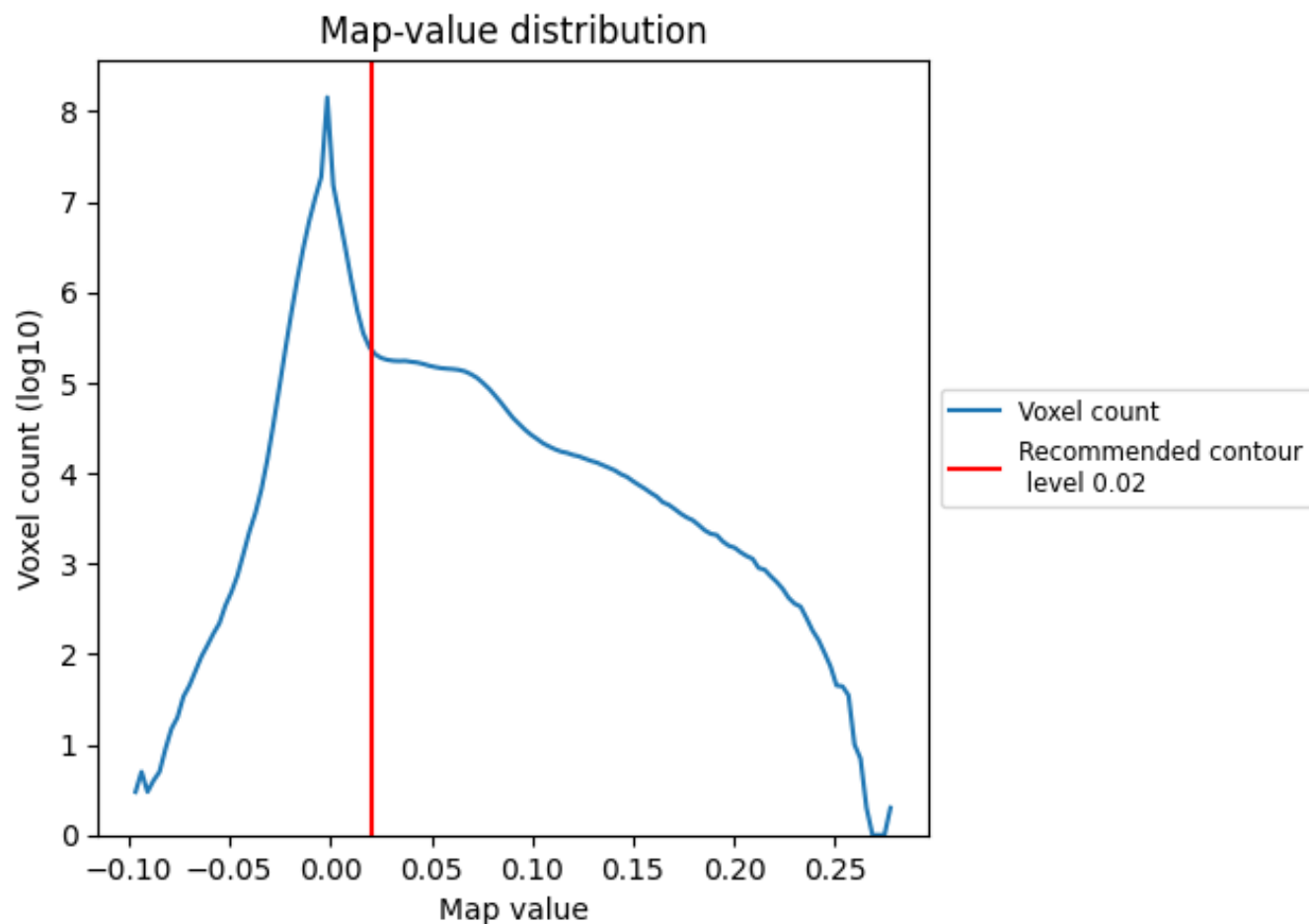
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

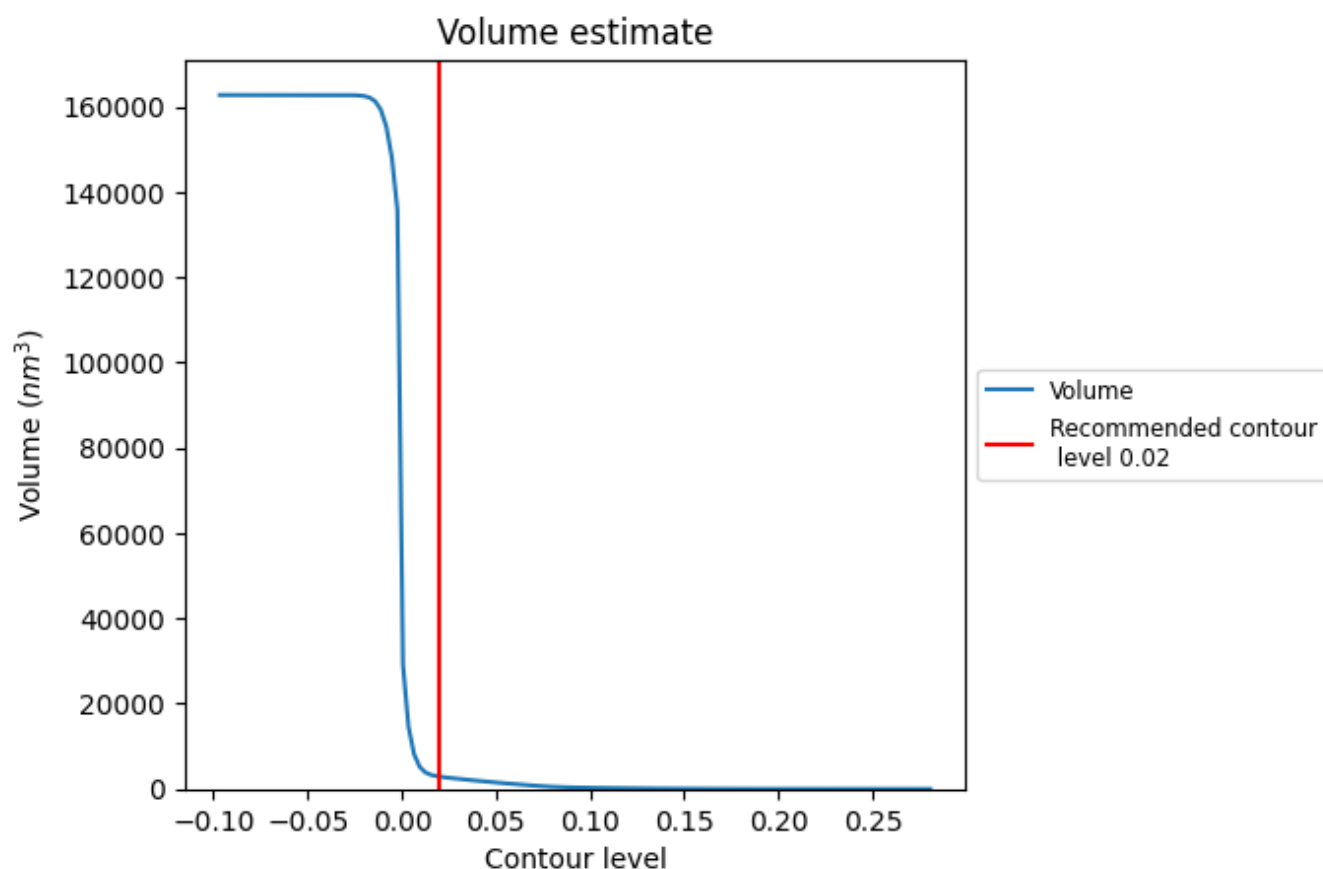
This section contains the results of statistical analysis of the map.

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.

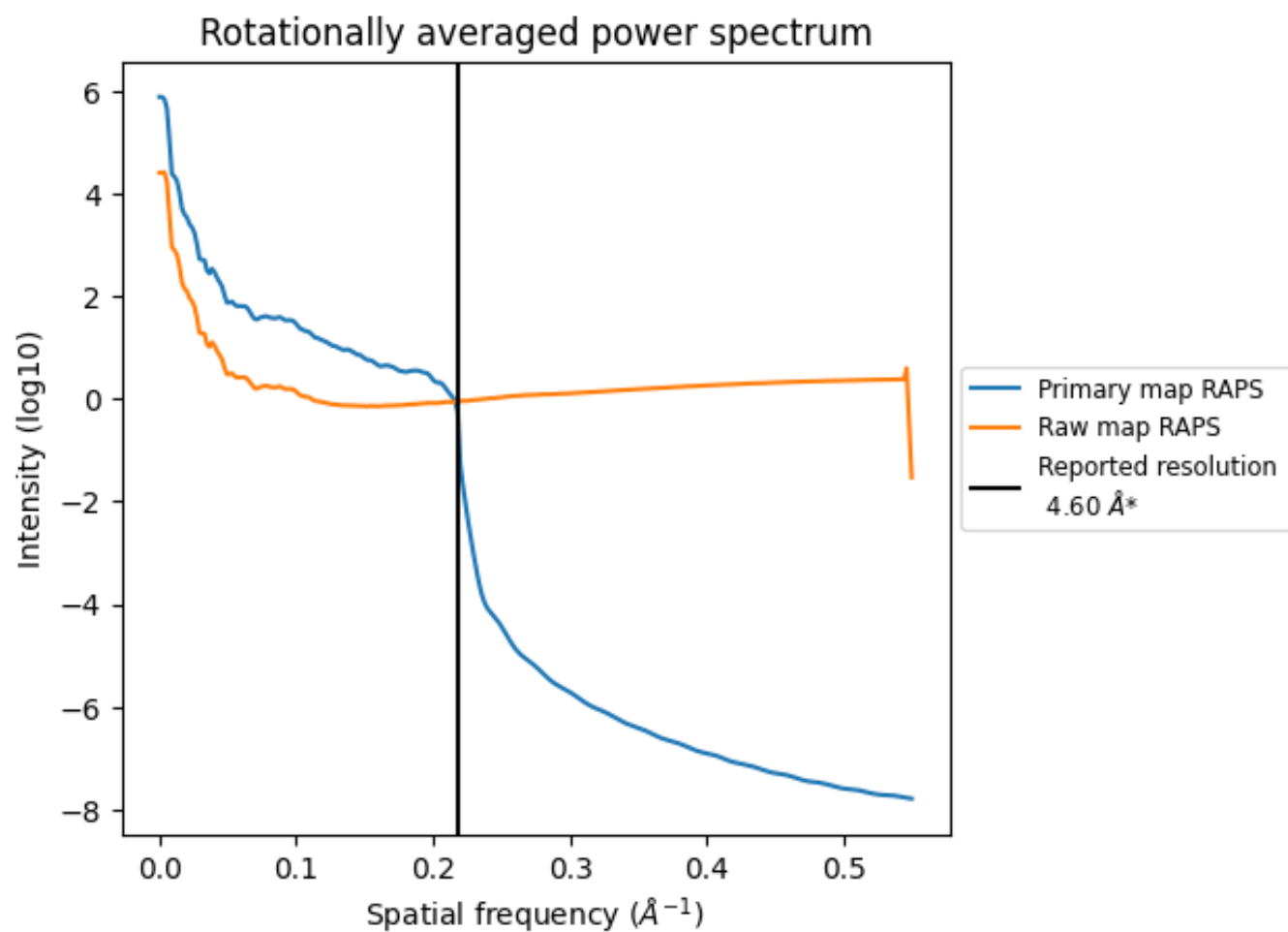
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2896 nm^3 ; this corresponds to an approximate mass of 2616 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 ⓘ

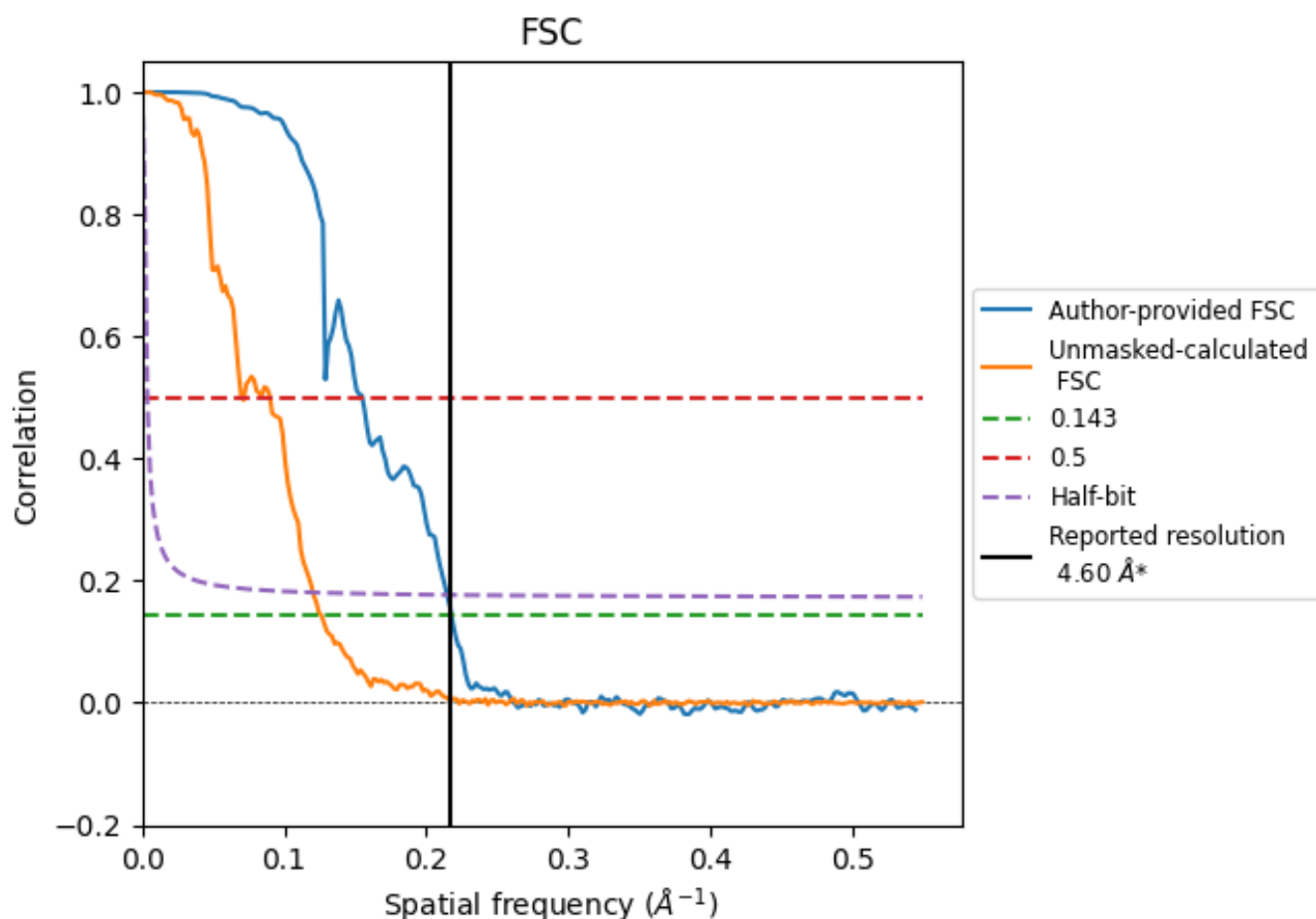


*Reported resolution corresponds to spatial frequency of 0.217 $\text{\AA}^{-1}$

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 0.217 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

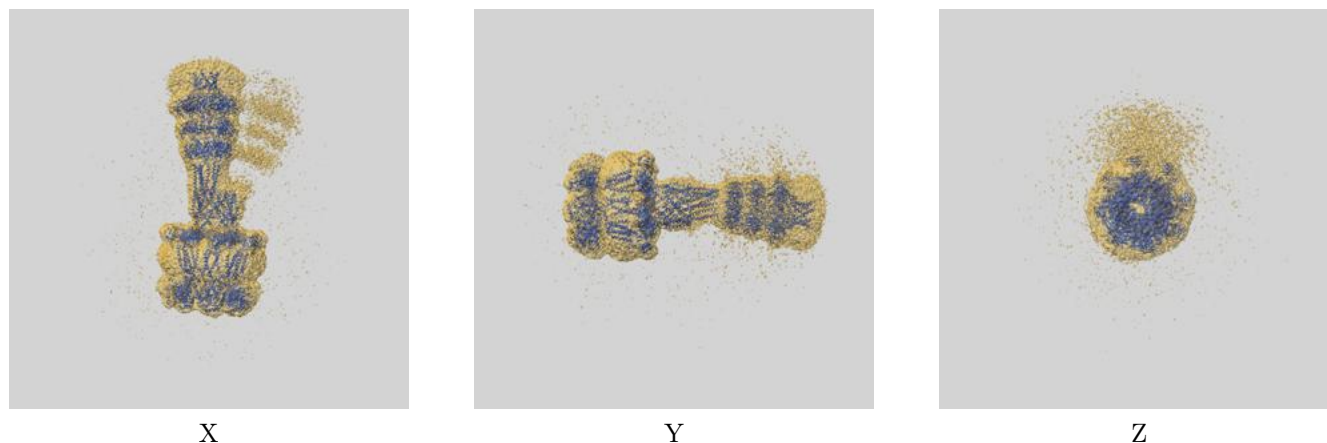
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.59	6.45	4.66
Unmasked-calculated*	7.93	14.20	8.31

*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 7.93 differs from the reported value 4.6 by more than 10 %

9 Map-model fit [i](#)

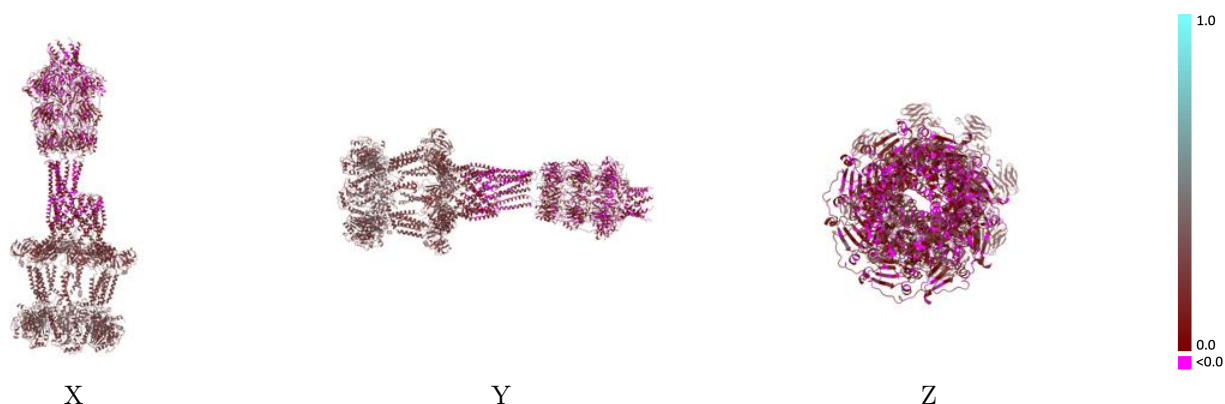
This section contains information regarding the fit between EMDB map EMD-53609 and PDB model 9R6B. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



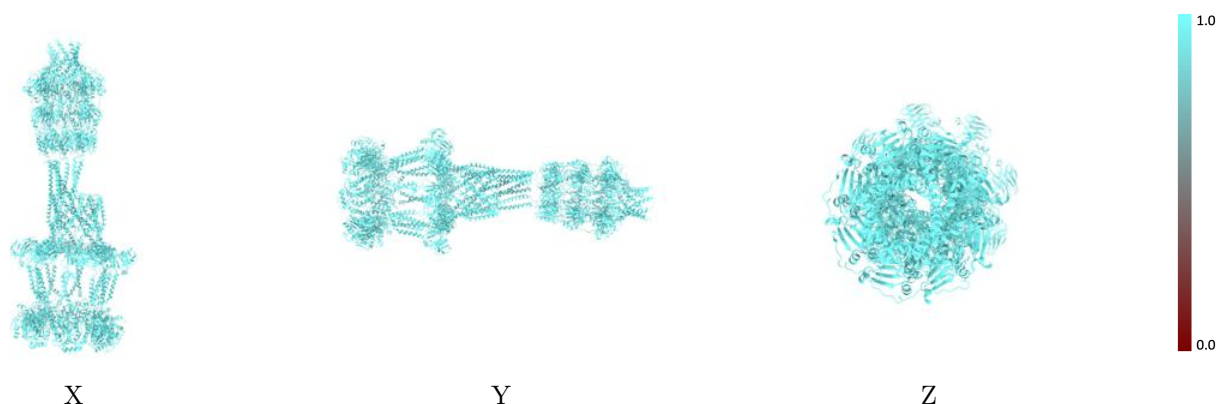
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



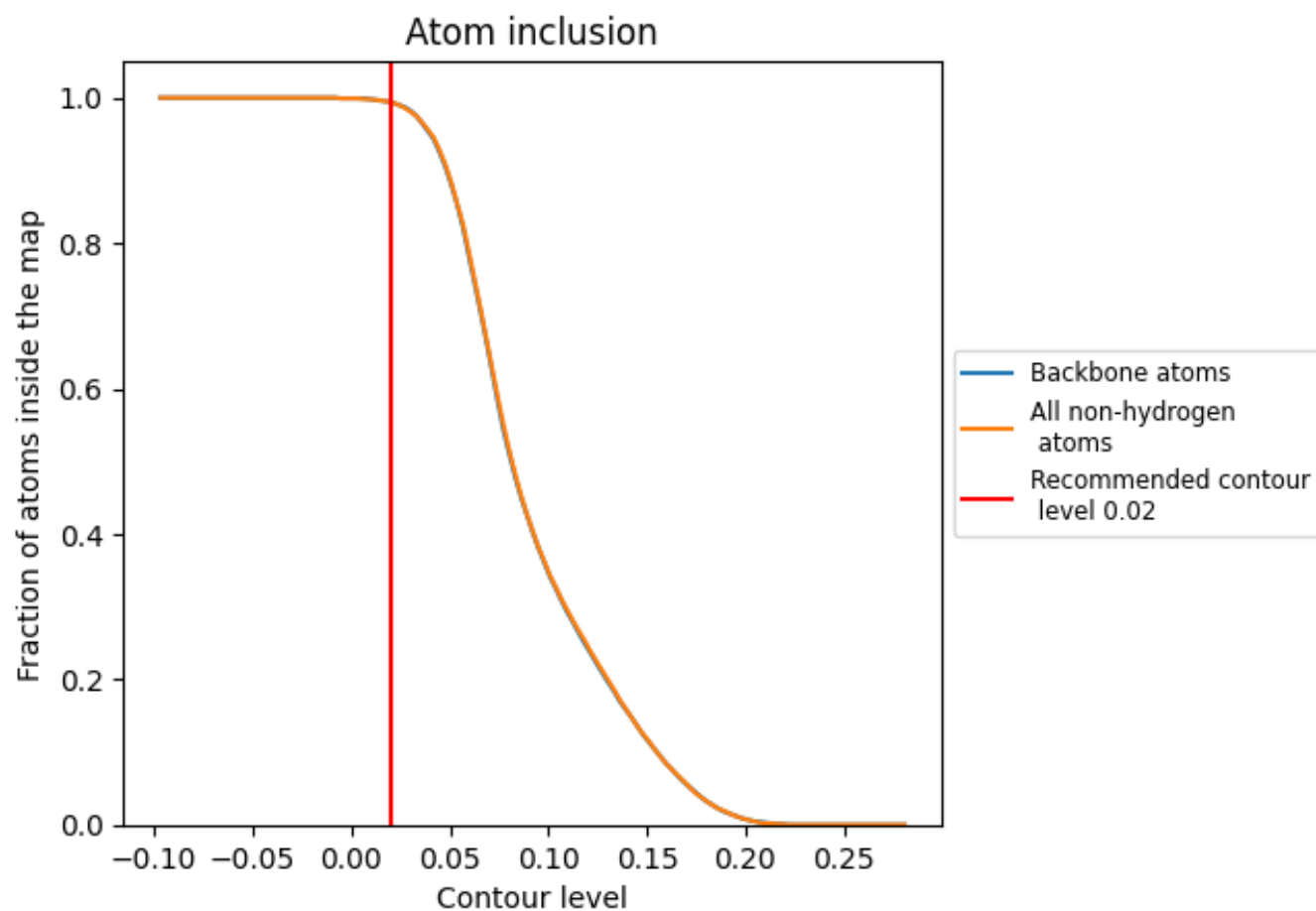
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9940	 0.2060
A	 0.9990	 0.1170
B	 0.9930	 0.1190
C	 1.0000	 0.1300
D	 0.9960	 0.1380
E	 0.9970	 0.1340
F	 1.0000	 0.1200
G	 0.9990	 0.1210
H	 1.0000	 0.1180
I	 0.9930	 0.2630
J	 0.9910	 0.2600
K	 0.9920	 0.2460
L	 0.9900	 0.2490
M	 0.9910	 0.2430
N	 0.9920	 0.2400
O	 0.9910	 0.2570
P	 0.9910	 0.2580

