



Full wwPDB EM Validation Report ⓘ

Jul 23, 2026 – 06:06 pm BST

PDB ID : 9R6A / pdb_00009r6a
EMDB ID : EMD-53608
Title : CPS secretion pathway Wza-Wzc (Conf 3)
Authors : Yuan, B.; Heinz, D.W.
Deposited on : 2025-05-11
Resolution : 6.30 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:

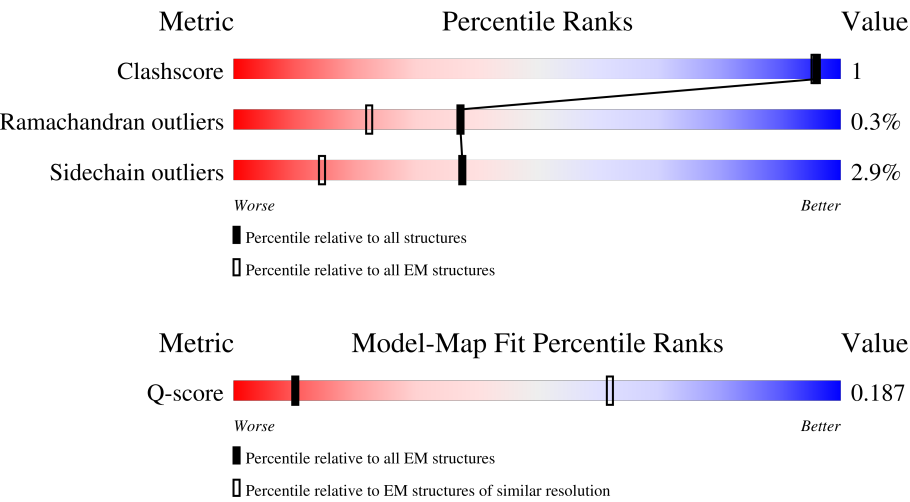
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 6.30 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.



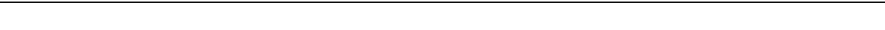
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	550 (5.80 - 6.80)

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	84%7%9%
1	B	394	81%10%9%
1	C	394	84%7%9%
1	D	394	85%6%9%

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Mol	Chain	Length	Quality of chain
1	E	394	 79%11%9%
1	F	394	 84%7%9%
1	G	394	 80%11%9%
1	H	394	 85%6%9%
2	I	738	 85%6%9%
2	J	738	 86%5%9%
2	K	738	 85%6%9%
2	L	738	 86%5%9%
2	M	738	 83%7%9%
2	N	738	 86%5%9%
2	O	738	 86%5%9%
2	P	738	 85%6%9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 129144 atoms, of which 64896 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 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	B	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	C	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	D	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	E	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	F	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	G	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0
1	H	358	Total 5548	C 1745	H 2765	N 486	O 539	S 13	0	0

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	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	J	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	K	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	L	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	M	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	N	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	O	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	20		
2	P	673	Total	C	H	N	O	S	0	0
			10556	3298	5335	898	1005	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
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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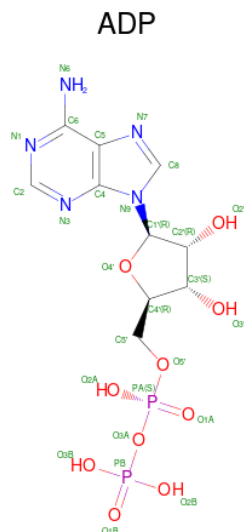
Chain	Residue	Modelled	Actual	Comment	Reference
M	728	PHE	-	expression tag	UNP P76387
M	729	GLN	-	expression tag	UNP P76387
M	730	GLY	-	expression tag	UNP P76387
M	731	TRP	-	expression tag	UNP P76387
M	732	SER	-	expression tag	UNP P76387
M	733	HIS	-	expression tag	UNP P76387
M	734	PRO	-	expression tag	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: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



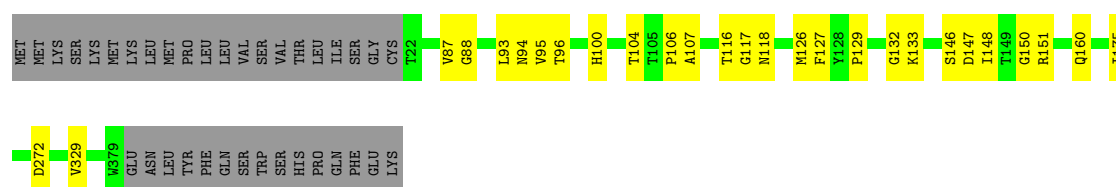
Mol	Chain	Residues	Atoms						AltConf
3	I	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	J	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	K	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	L	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	M	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	N	1	Total 39	C 10	H 12	N 5	O 10	P 2	0
3	O	1	Total 39	C 10	H 12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

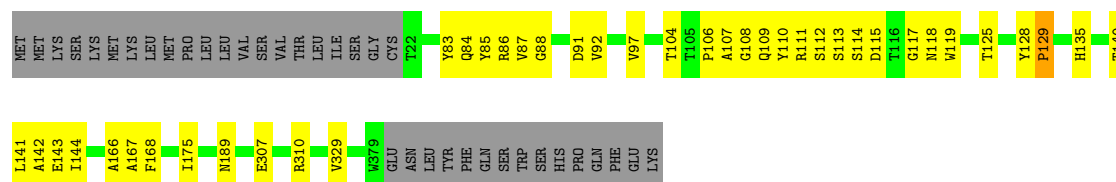
- Molecule 1: Putative polysaccharide export protein Wza

Chain A: 



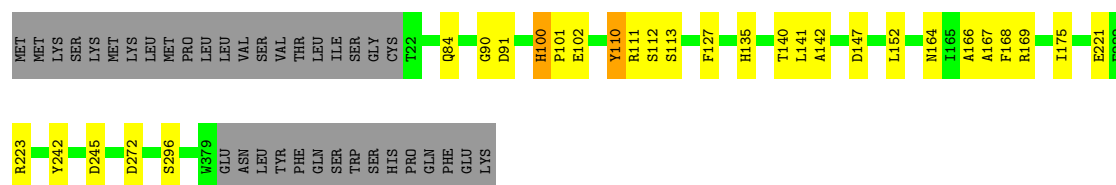
- Molecule 1: Putative polysaccharide export protein Wza

Chain B: 



- Molecule 1: Putative polysaccharide export protein Wza

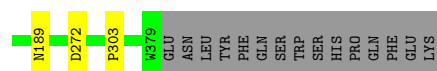
Chain C: 



- Molecule 1: Putative polysaccharide export protein Wza

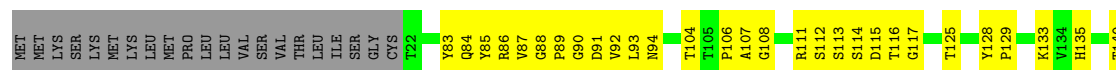
Chain D: 





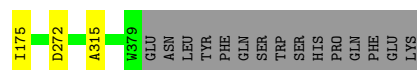
- Molecule 1: Putative polysaccharide export protein Wza

Chain E: 79% 11% 9%



- Molecule 1: Putative polysaccharide export protein Wza

Chain F: 84% 7% 9%



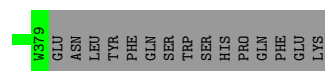
- Molecule 1: Putative polysaccharide export protein Wza

Chain G: 80% 11% 9%



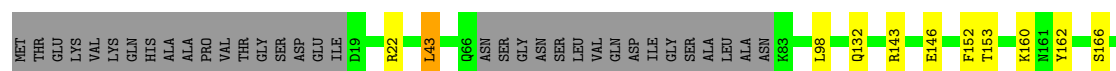
- Molecule 1: Putative polysaccharide export protein Wza

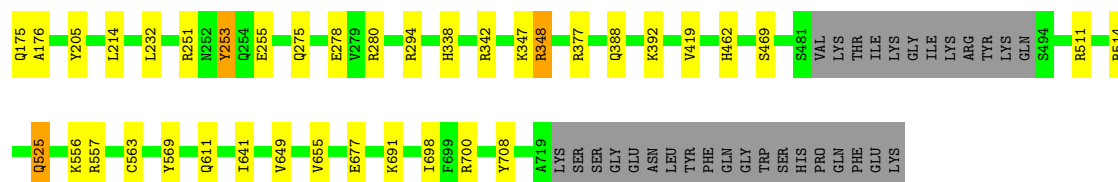
Chain H: 85% 6% 9%



- Molecule 2: Tyrosine-protein kinase wzc

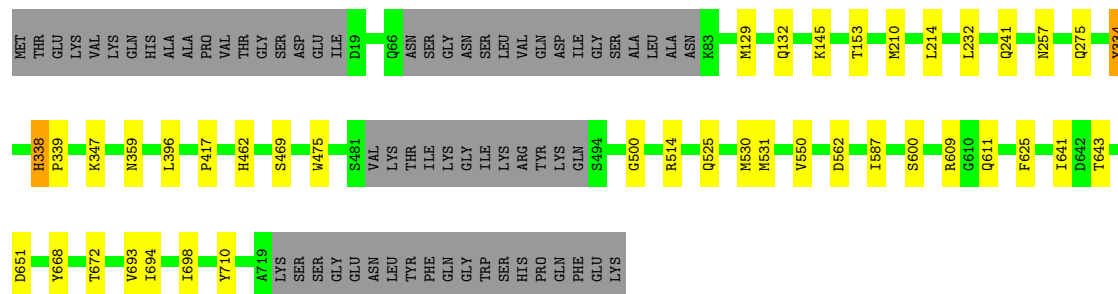
Chain I: 85% 6% 9%





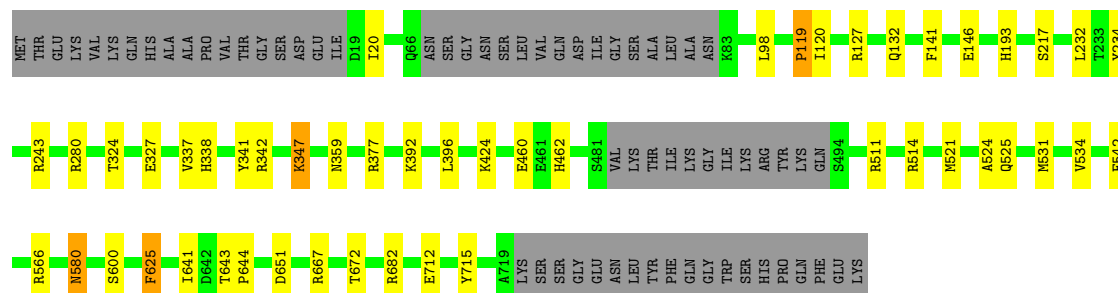
- Molecule 2: Tyrosine-protein kinase wzc

Chain J: 86% 5% 9%



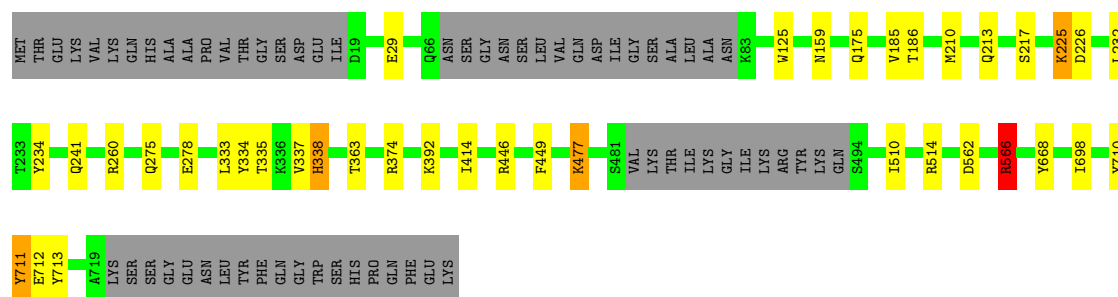
- Molecule 2: Tyrosine-protein kinase wzc

Chain K: 85% 6% 9%



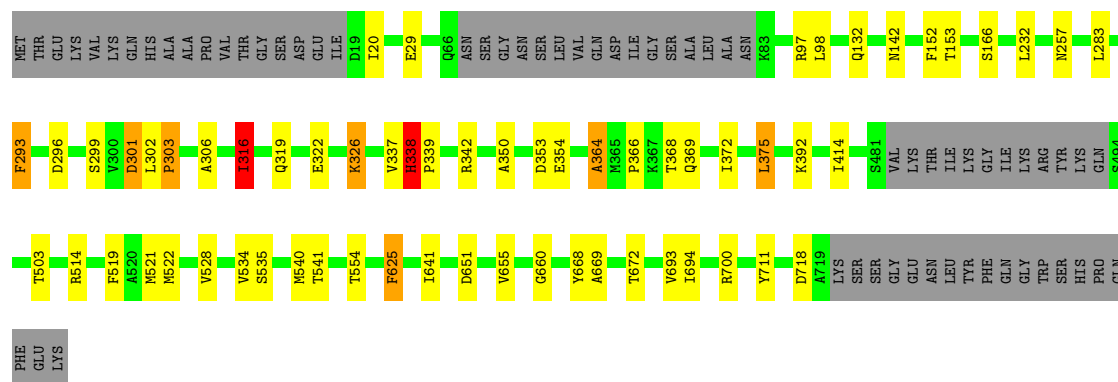
- Molecule 2: Tyrosine-protein kinase wzc

Chain L: 86% 5% 9%



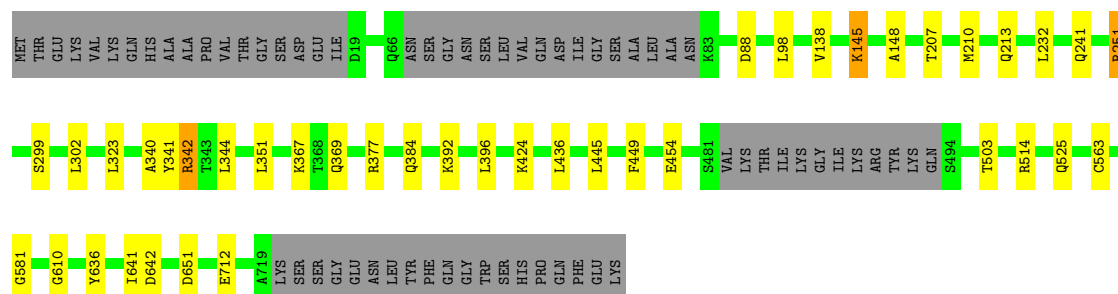
- Molecule 2: Tyrosine-protein kinase wzc

Chain M: 83% 7% 9%



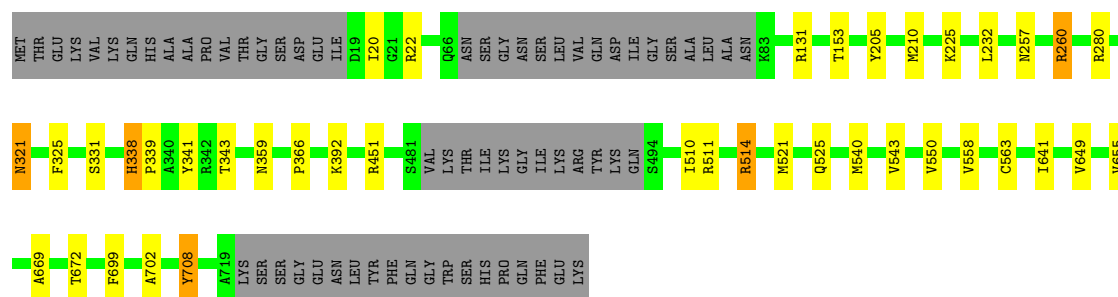
• Molecule 2: Tyrosine-protein kinase wzc

Chain N: 86% 5% 9%



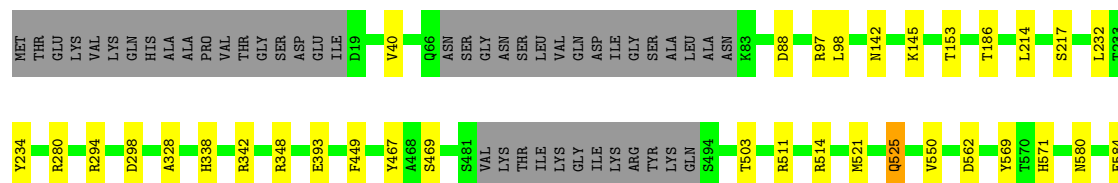
• Molecule 2: Tyrosine-protein kinase wzc

Chain O: 86% 5% 9%



• Molecule 2: Tyrosine-protein kinase wzc

Chain P: 85% 6% 9%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27501	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	0.208	Depositor
Minimum map value	-0.054	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	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	0.92	7/2836 (0.2%)	0.98	34/3862 (0.9%)
1	B	1.10	14/2836 (0.5%)	1.17	54/3862 (1.4%)
1	C	0.78	7/2836 (0.2%)	0.99	22/3862 (0.6%)
1	D	1.03	11/2836 (0.4%)	1.14	19/3862 (0.5%)
1	E	1.11	19/2836 (0.7%)	1.18	54/3862 (1.4%)
1	F	1.05	13/2836 (0.5%)	1.09	35/3862 (0.9%)
1	G	1.05	18/2836 (0.6%)	1.14	40/3862 (1.0%)
1	H	0.95	7/2836 (0.2%)	1.01	22/3862 (0.6%)
2	I	0.69	0/5297	1.31	9/7178 (0.1%)
2	J	0.69	0/5297	1.33	6/7178 (0.1%)
2	K	0.70	0/5297	1.31	11/7178 (0.2%)
2	L	0.69	0/5297	1.30	6/7178 (0.1%)
2	M	0.72	0/5297	1.37	9/7178 (0.1%)
2	N	0.71	0/5297	1.33	5/7178 (0.1%)
2	O	0.70	0/5297	1.33	7/7178 (0.1%)
2	P	0.69	0/5297	1.31	12/7178 (0.2%)
All	All	0.82	96/65064 (0.1%)	1.25	345/88320 (0.4%)

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	C	0	1
1	G	0	1
1	H	0	1
2	I	0	6
2	J	0	1
2	K	0	2
2	L	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	M	0	3
2	N	0	2
2	O	0	1
2	P	0	8
All	All	0	27

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	107	ALA	CA-CB	-8.19	1.42	1.53
1	B	107	ALA	CA-CB	-8.17	1.42	1.53
1	G	107	ALA	CA-CB	-8.08	1.42	1.53
1	A	107	ALA	CA-CB	-8.01	1.42	1.53
1	F	107	ALA	CA-CB	-8.00	1.42	1.53
1	G	86	ARG	CZ-NH2	-7.92	1.23	1.33
1	E	107	ALA	CA-CB	-7.90	1.42	1.53
1	B	111	ARG	CZ-NH2	-7.89	1.23	1.33
1	D	111	ARG	CZ-NH2	-7.86	1.23	1.33
1	H	151	ARG	CZ-NH2	-7.86	1.23	1.33
1	F	111	ARG	CZ-NH2	-7.86	1.23	1.33
1	E	111	ARG	CZ-NH2	-7.84	1.23	1.33
1	E	86	ARG	CZ-NH2	-7.83	1.23	1.33
1	F	151	ARG	CZ-NH2	-7.82	1.23	1.33
1	E	169	ARG	CZ-NH2	-7.81	1.23	1.33
1	C	169	ARG	CZ-NH2	-7.80	1.23	1.33
1	G	111	ARG	CZ-NH2	-7.79	1.23	1.33
1	D	86	ARG	CZ-NH2	-7.78	1.23	1.33
1	G	145	ARG	CZ-NH2	-7.78	1.23	1.33
1	B	86	ARG	CZ-NH2	-7.76	1.23	1.33
1	A	151	ARG	CZ-NH2	-7.75	1.23	1.33
1	F	111	ARG	CZ-NH1	-7.31	1.22	1.32
1	H	151	ARG	CZ-NH1	-7.30	1.22	1.32
1	E	111	ARG	CZ-NH1	-7.30	1.22	1.32
1	G	86	ARG	CZ-NH1	-7.29	1.22	1.32
1	D	111	ARG	CZ-NH1	-7.25	1.22	1.32
1	B	111	ARG	CZ-NH1	-7.24	1.22	1.32
1	E	169	ARG	CZ-NH1	-7.24	1.22	1.32
1	A	151	ARG	CZ-NH1	-7.24	1.22	1.32
1	E	86	ARG	CZ-NH1	-7.24	1.22	1.32
1	F	151	ARG	CZ-NH1	-7.24	1.22	1.32
1	B	86	ARG	CZ-NH1	-7.22	1.22	1.32
1	G	111	ARG	CZ-NH1	-7.21	1.22	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	142	ALA	CA-CB	-7.20	1.42	1.53
1	G	145	ARG	CZ-NH1	-7.20	1.22	1.32
1	D	86	ARG	CZ-NH1	-7.16	1.22	1.32
1	C	169	ARG	CZ-NH1	-7.15	1.22	1.32
1	B	142	ALA	CA-CB	-7.10	1.42	1.53
1	C	142	ALA	CA-CB	-7.08	1.42	1.53
1	E	142	ALA	CA-CB	-7.03	1.42	1.53
1	E	167	ALA	CA-CB	-6.94	1.41	1.53
1	D	81	ALA	CA-CB	-6.91	1.42	1.53
1	D	108	GLY	N-CA	-6.90	1.37	1.45
1	G	108	GLY	N-CA	-6.90	1.37	1.45
1	E	166	ALA	CA-CB	-6.77	1.42	1.53
1	C	166	ALA	CA-CB	-6.77	1.42	1.53
1	E	108	GLY	N-CA	-6.66	1.37	1.45
1	G	117	GLY	N-CA	-6.65	1.37	1.45
1	C	167	ALA	CA-CB	-6.64	1.42	1.53
1	B	167	ALA	CA-CB	-6.54	1.42	1.53
1	G	166	ALA	CA-CB	-6.39	1.42	1.53
1	D	189	ASN	C-N	-6.24	1.28	1.33
1	F	150	GLY	N-CA	-6.19	1.37	1.45
1	B	166	ALA	CA-CB	-6.18	1.42	1.53
1	A	150	GLY	N-CA	-6.18	1.37	1.45
1	H	150	GLY	N-CA	-6.13	1.38	1.45
1	H	153	ALA	CA-CB	-5.99	1.42	1.53
1	H	135	HIS	CE1-NE2	-5.92	1.26	1.32
1	G	86	ARG	CD-NE	-5.76	1.38	1.46
1	F	108	GLY	N-CA	-5.67	1.37	1.45
1	B	108	GLY	N-CA	-5.66	1.37	1.45
1	A	151	ARG	CD-NE	-5.66	1.38	1.46
1	D	86	ARG	CD-NE	-5.66	1.38	1.46
1	E	86	ARG	CD-NE	-5.63	1.38	1.46
1	H	151	ARG	CD-NE	-5.62	1.38	1.46
1	B	117	GLY	N-CA	-5.61	1.37	1.45
1	B	86	ARG	CD-NE	-5.58	1.38	1.46
1	E	117	GLY	N-CA	-5.49	1.37	1.45
1	F	151	ARG	CD-NE	-5.47	1.38	1.46
1	E	111	ARG	CD-NE	-5.45	1.38	1.46
1	E	169	ARG	CD-NE	-5.43	1.38	1.46
1	B	111	ARG	CD-NE	-5.40	1.38	1.46
1	D	111	ARG	CD-NE	-5.40	1.38	1.46
1	F	111	ARG	CD-NE	-5.40	1.38	1.46
1	G	111	ARG	CD-NE	-5.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	90	GLY	N-CA	-5.36	1.37	1.45
1	G	145	ARG	CD-NE	-5.35	1.38	1.46
1	A	132	GLY	N-CA	-5.32	1.37	1.45
1	H	135	HIS	CD2-NE2	-5.32	1.31	1.37
1	C	169	ARG	CD-NE	-5.30	1.38	1.46
1	F	132	GLY	N-CA	-5.25	1.37	1.45
1	B	88	GLY	N-CA	-5.21	1.37	1.44
1	E	89	PRO	CA-CB	-5.21	1.46	1.53
1	C	90	GLY	N-CA	-5.20	1.37	1.45
1	D	132	GLY	N-CA	-5.17	1.37	1.45
1	F	106	PRO	CA-CB	-5.16	1.46	1.53
1	B	106	PRO	CA-CB	-5.15	1.46	1.53
1	G	88	GLY	N-CA	-5.15	1.37	1.44
1	E	88	GLY	N-CA	-5.12	1.37	1.44
1	F	164	ASN	CA-CB	-5.11	1.47	1.53
1	G	89	PRO	CA-CB	-5.06	1.46	1.53
1	F	129	PRO	CA-CB	-5.06	1.46	1.53
1	A	129	PRO	CA-CB	-5.03	1.47	1.53
1	G	164	ASN	CA-CB	-5.03	1.47	1.53
1	G	171	GLN	CD-NE2	-5.02	1.22	1.33
1	E	164	ASN	CA-CB	-5.01	1.47	1.53

All (345) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	HIS	CA-C-N	10.96	134.28	122.77
1	D	135	HIS	C-N-CA	10.96	134.28	122.77
1	D	189	ASN	CA-C-N	9.42	131.52	123.33
1	D	189	ASN	C-N-CA	9.42	131.52	123.33
2	M	338	HIS	CA-CB-CG	7.59	121.39	113.80
1	G	91	ASP	CA-CB-CG	7.08	119.68	112.60
1	H	162	ASP	CA-CB-CG	7.04	119.64	112.60
1	E	115	ASP	CA-CB-CG	7.04	119.64	112.60
1	E	91	ASP	CA-CB-CG	7.04	119.64	112.60
1	B	115	ASP	CA-CB-CG	7.02	119.62	112.60
1	E	162	ASP	CA-CB-CG	7.01	119.61	112.60
1	F	147	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	91	ASP	CA-CB-CG	6.99	119.59	112.60
1	B	91	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	147	ASP	CA-CB-CG	6.93	119.53	112.60
1	E	135	HIS	CA-C-N	6.91	134.40	121.97
1	E	135	HIS	C-N-CA	6.91	134.40	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	514	ARG	NE-CZ-NH2	6.81	125.33	119.20
2	P	562	ASP	CA-CB-CG	6.80	119.40	112.60
1	H	147	ASP	CA-CB-CG	6.77	119.37	112.60
1	B	118	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	118	ASN	CA-CB-CG	6.68	119.28	112.60
2	M	303	PRO	CA-N-CD	-6.62	102.73	112.00
1	D	91	ASP	CA-CB-CG	6.62	119.22	112.60
1	D	82	ASN	CA-CB-CG	6.61	119.21	112.60
1	B	168	PHE	CA-CB-CG	6.59	120.39	113.80
1	D	168	PHE	CA-CB-CG	6.57	120.36	113.80
1	F	127	PHE	CA-CB-CG	6.55	120.35	113.80
2	O	514	ARG	NE-CZ-NH2	6.53	125.07	119.20
2	P	449	PHE	CA-CB-CG	6.52	120.32	113.80
1	F	118	ASN	CA-CB-CG	6.52	119.12	112.60
2	L	566	ARG	NE-CZ-NH2	6.51	125.06	119.20
1	H	153	ALA	CA-C-N	6.50	128.88	120.44
1	H	153	ALA	C-N-CA	6.50	128.88	120.44
2	I	143	ARG	N-CA-C	6.48	114.05	108.22
1	A	127	PHE	CA-CB-CG	6.48	120.28	113.80
1	H	133	LYS	CA-C-N	6.47	131.21	123.19
1	H	133	LYS	C-N-CA	6.47	131.21	123.19
1	C	127	PHE	CA-CB-CG	6.42	120.22	113.80
1	A	94	ASN	CA-CB-CG	6.41	119.01	112.60
1	A	117	GLY	CA-C-N	6.40	131.28	122.77
1	A	117	GLY	C-N-CA	6.40	131.28	122.77
1	H	94	ASN	CA-C-N	6.38	131.41	123.12
1	H	94	ASN	C-N-CA	6.38	131.41	123.12
1	E	94	ASN	CA-CB-CG	6.36	118.96	112.60
1	G	94	ASN	CA-CB-CG	6.36	118.96	112.60
1	G	135	HIS	CA-C-N	6.34	133.38	121.97
1	G	135	HIS	C-N-CA	6.34	133.38	121.97
1	F	94	ASN	CA-CB-CG	6.29	118.89	112.60
1	A	133	LYS	CA-C-N	6.28	131.46	123.10
1	A	133	LYS	C-N-CA	6.28	131.46	123.10
2	M	301	ASP	CA-CB-CG	6.27	118.87	112.60
1	F	94	ASN	CA-C-N	6.25	131.41	123.10
1	F	94	ASN	C-N-CA	6.25	131.41	123.10
1	G	119	TRP	CA-C-N	6.23	130.28	122.43
1	G	119	TRP	C-N-CA	6.23	130.28	122.43
1	A	160	GLN	CA-C-N	6.23	131.30	123.14
1	A	160	GLN	C-N-CA	6.23	131.30	123.14
2	J	514	ARG	NE-CZ-NH2	6.21	124.78	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLY	CA-C-N	6.20	131.02	122.77
1	B	117	GLY	C-N-CA	6.20	131.02	122.77
2	N	514	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	E	189	ASN	CA-C-N	6.15	128.68	123.33
1	E	189	ASN	C-N-CA	6.15	128.68	123.33
1	A	94	ASN	CA-C-N	6.15	131.28	123.10
1	A	94	ASN	C-N-CA	6.15	131.28	123.10
1	F	117	GLY	CA-C-N	6.15	130.95	122.77
1	F	117	GLY	C-N-CA	6.15	130.95	122.77
1	H	160	GLN	CA-C-N	6.14	131.18	123.14
1	H	160	GLN	C-N-CA	6.14	131.18	123.14
1	G	91	ASP	CA-C-N	6.14	131.26	123.10
1	G	91	ASP	C-N-CA	6.14	131.26	123.10
2	K	342	ARG	NE-CZ-NH2	6.13	124.72	119.20
1	B	111	ARG	CD-NE-CZ	6.13	132.98	124.40
1	C	91	ASP	CA-C-N	6.13	131.16	123.14
1	C	91	ASP	C-N-CA	6.13	131.16	123.14
1	D	111	ARG	CD-NE-CZ	6.12	132.97	124.40
1	E	91	ASP	CA-C-N	6.11	131.22	123.10
1	E	91	ASP	C-N-CA	6.11	131.22	123.10
1	E	111	ARG	CD-NE-CZ	6.10	132.94	124.40
1	B	91	ASP	CA-C-N	6.10	131.21	123.10
1	B	91	ASP	C-N-CA	6.10	131.21	123.10
1	G	111	ARG	CD-NE-CZ	6.08	132.91	124.40
1	G	162	ASP	CA-C-N	6.05	131.43	122.71
1	G	162	ASP	C-N-CA	6.05	131.43	122.71
1	F	93	LEU	CA-C-N	6.04	131.51	123.05
1	F	93	LEU	C-N-CA	6.04	131.51	123.05
2	I	514	ARG	NE-CZ-NH2	6.03	124.63	119.20
1	E	169	ARG	CD-NE-CZ	6.03	132.84	124.40
1	F	111	ARG	CD-NE-CZ	6.03	132.84	124.40
1	C	169	ARG	CD-NE-CZ	6.02	132.83	124.40
2	O	22	ARG	NE-CZ-NH2	6.02	124.62	119.20
1	B	135	HIS	CA-C-N	6.02	132.80	121.97
1	B	135	HIS	C-N-CA	6.02	132.80	121.97
1	F	95	VAL	CA-C-N	6.01	131.30	123.00
1	F	95	VAL	C-N-CA	6.01	131.30	123.00
1	G	145	ARG	CD-NE-CZ	6.01	132.82	124.40
1	B	112	SER	CA-C-N	6.01	128.25	120.44
1	B	112	SER	C-N-CA	6.01	128.25	120.44
1	A	104	THR	CA-C-N	5.99	130.53	123.16
1	A	104	THR	C-N-CA	5.99	130.53	123.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	104	THR	CA-C-N	5.97	130.50	123.16
1	E	104	THR	C-N-CA	5.97	130.50	123.16
1	F	104	THR	CA-C-N	5.96	130.49	123.16
1	F	104	THR	C-N-CA	5.96	130.49	123.16
1	C	140	THR	CA-C-N	5.96	128.26	120.28
1	C	140	THR	C-N-CA	5.96	128.26	120.28
1	B	104	THR	CA-C-N	5.96	130.49	123.16
1	B	104	THR	C-N-CA	5.96	130.49	123.16
1	E	93	LEU	CA-C-N	5.96	131.39	123.05
1	E	93	LEU	C-N-CA	5.96	131.39	123.05
1	A	95	VAL	CA-C-N	5.94	131.37	123.05
1	A	95	VAL	C-N-CA	5.94	131.37	123.05
1	A	93	LEU	CA-C-N	5.94	131.38	123.00
1	A	93	LEU	C-N-CA	5.94	131.38	123.00
1	H	104	THR	CA-C-N	5.93	130.45	123.16
1	H	104	THR	C-N-CA	5.93	130.45	123.16
1	C	168	PHE	CA-CB-CG	5.93	119.73	113.80
1	A	96	THR	CA-C-N	5.92	131.16	123.11
1	A	96	THR	C-N-CA	5.92	131.16	123.11
1	G	93	LEU	CA-C-N	5.92	131.33	123.05
1	G	93	LEU	C-N-CA	5.92	131.33	123.05
1	F	151	ARG	CD-NE-CZ	5.89	132.65	124.40
2	K	514	ARG	NE-CZ-NH2	5.88	124.50	119.20
1	H	95	VAL	CA-C-N	5.88	131.28	123.05
1	H	95	VAL	C-N-CA	5.88	131.28	123.05
2	L	566	ARG	CD-NE-CZ	5.87	132.61	124.40
2	P	571	HIS	CB-CG-CD2	-5.82	123.64	131.20
2	O	260	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	H	96	THR	CA-C-N	5.80	131.00	123.11
1	H	96	THR	C-N-CA	5.80	131.00	123.11
2	N	340	ALA	N-CA-C	5.80	118.55	111.82
2	L	514	ARG	NE-CZ-NH2	5.80	124.42	119.20
1	D	186	ALA	CA-C-N	5.79	129.73	122.43
1	D	186	ALA	C-N-CA	5.79	129.73	122.43
2	K	566	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	L	374	ARG	NE-CZ-NH2	5.78	124.40	119.20
1	F	130	TYR	CA-C-N	5.76	128.53	122.14
1	F	130	TYR	C-N-CA	5.76	128.53	122.14
2	M	296	ASP	N-CA-C	5.71	117.96	111.11
2	L	260	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	G	112	SER	CA-C-N	5.69	127.84	120.44
1	G	112	SER	C-N-CA	5.69	127.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	111	ARG	CA-C-N	5.65	133.18	121.32
1	C	111	ARG	C-N-CA	5.65	133.18	121.32
1	D	85	TYR	CA-C-N	5.62	130.70	122.77
1	D	85	TYR	C-N-CA	5.62	130.70	122.77
1	C	112	SER	CA-C-N	5.61	127.79	120.28
1	C	112	SER	C-N-CA	5.61	127.79	120.28
1	F	126	MET	CA-C-N	5.59	130.07	122.19
1	F	126	MET	C-N-CA	5.59	130.07	122.19
1	G	142	ALA	CA-C-N	5.59	128.04	120.44
1	G	142	ALA	C-N-CA	5.59	128.04	120.44
1	G	104	THR	CA-C-N	5.59	130.03	123.16
1	G	104	THR	C-N-CA	5.59	130.03	123.16
1	B	86	ARG	CB-CG-CD	5.58	124.14	111.30
1	G	87	VAL	CA-C-N	5.58	130.63	121.87
1	G	87	VAL	C-N-CA	5.58	130.63	121.87
1	C	135	HIS	CA-CB-CG	-5.56	108.24	113.80
1	B	114	SER	CA-C-N	5.55	128.17	120.29
1	B	114	SER	C-N-CA	5.55	128.17	120.29
1	E	142	ALA	CA-C-N	5.55	127.99	120.44
1	E	142	ALA	C-N-CA	5.55	127.99	120.44
1	G	86	ARG	CB-CG-CD	5.55	124.06	111.30
1	E	90	GLY	N-CA-C	5.54	121.34	114.37
1	B	87	VAL	CA-C-N	5.51	130.52	121.87
1	B	87	VAL	C-N-CA	5.51	130.52	121.87
1	D	86	ARG	CB-CG-CD	5.51	123.97	111.30
1	B	142	ALA	CA-C-N	5.51	127.93	120.44
1	B	142	ALA	C-N-CA	5.51	127.93	120.44
1	E	87	VAL	CA-C-N	5.50	130.51	121.87
1	E	87	VAL	C-N-CA	5.50	130.51	121.87
1	B	84	GLN	CA-C-N	5.50	130.31	122.72
1	B	84	GLN	C-N-CA	5.50	130.31	122.72
2	O	131	ARG	NE-CZ-NH2	5.47	124.12	119.20
2	P	625	PHE	CA-CB-CG	5.47	119.27	113.80
1	C	164	ASN	CA-C-N	5.46	129.89	122.90
1	C	164	ASN	C-N-CA	5.46	129.89	122.90
1	E	86	ARG	CB-CG-CD	5.46	123.85	111.30
2	O	321	ASN	CA-CB-CG	5.46	118.06	112.60
1	B	85	TYR	CA-C-N	5.45	130.68	123.00
1	B	85	TYR	C-N-CA	5.45	130.68	123.00
2	N	299	SER	N-CA-C	5.44	117.53	108.99
2	P	294	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	E	114	SER	CA-C-N	5.43	128.00	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	SER	C-N-CA	5.43	128.00	120.29
1	B	167	ALA	CA-C-N	5.43	130.39	122.41
1	B	167	ALA	C-N-CA	5.43	130.39	122.41
1	G	86	ARG	CA-C-N	5.43	127.89	120.35
1	G	86	ARG	C-N-CA	5.43	127.89	120.35
2	K	682	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	E	112	SER	CA-C-N	5.42	127.54	120.28
1	E	112	SER	C-N-CA	5.42	127.54	120.28
1	E	85	TYR	CA-C-N	5.41	130.40	122.77
1	E	85	TYR	C-N-CA	5.41	130.40	122.77
2	K	243	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	E	164	ASN	CA-C-N	5.39	130.12	123.12
1	E	164	ASN	C-N-CA	5.39	130.12	123.12
1	D	119	TRP	CA-C-N	5.38	129.78	122.90
1	D	119	TRP	C-N-CA	5.38	129.78	122.90
2	K	511	ARG	NE-CZ-NH2	5.36	124.02	119.20
2	M	338	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	D	167	ALA	CA-C-N	5.34	130.27	122.41
1	D	167	ALA	C-N-CA	5.34	130.27	122.41
1	B	83	TYR	CA-C-N	5.34	131.30	122.33
1	B	83	TYR	C-N-CA	5.34	131.30	122.33
1	C	113	SER	CA-C-N	5.33	127.42	120.28
1	C	113	SER	C-N-CA	5.33	127.42	120.28
2	J	562	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	100	HIS	CA-CB-CG	-5.33	108.47	113.80
1	F	148	ILE	N-CA-CB	5.33	116.78	110.55
1	F	146	SER	CA-C-N	5.32	127.36	120.44
1	F	146	SER	C-N-CA	5.32	127.36	120.44
1	B	143	GLU	CA-C-N	5.32	127.26	120.56
1	B	143	GLU	C-N-CA	5.32	127.26	120.56
1	D	83	TYR	N-CA-CB	5.32	117.72	109.48
2	N	449	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	113	SER	CA-C-N	5.31	127.93	120.28
1	B	113	SER	C-N-CA	5.31	127.93	120.28
1	E	143	GLU	CA-C-N	5.31	127.25	120.56
1	E	143	GLU	C-N-CA	5.31	127.25	120.56
1	A	146	SER	CA-C-N	5.30	127.33	120.44
1	A	146	SER	C-N-CA	5.30	127.33	120.44
1	G	164	ASN	CA-C-N	5.29	130.00	123.12
1	G	164	ASN	C-N-CA	5.29	130.00	123.12
2	K	377	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	G	143	GLU	CA-C-N	5.29	127.23	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	143	GLU	C-N-CA	5.29	127.23	120.56
2	I	347	LYS	CA-C-N	5.29	127.31	120.44
2	I	347	LYS	C-N-CA	5.29	127.31	120.44
1	F	162	ASP	CA-C-N	5.29	130.34	122.99
1	F	162	ASP	C-N-CA	5.29	130.34	122.99
2	O	511	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	E	162	ASP	CA-C-N	5.28	130.28	122.94
1	E	162	ASP	C-N-CA	5.28	130.28	122.94
1	A	148	ILE	N-CA-CB	5.28	116.72	110.55
2	P	683	PHE	CA-C-N	5.27	127.34	120.28
2	P	683	PHE	C-N-CA	5.27	127.34	120.28
2	K	132	GLN	N-CA-CB	-5.25	102.97	110.80
2	I	511	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	B	106	PRO	CA-C-N	5.23	130.87	122.86
1	B	106	PRO	C-N-CA	5.23	130.87	122.86
1	A	126	MET	CA-C-N	5.23	129.94	122.72
1	A	126	MET	C-N-CA	5.23	129.94	122.72
1	G	84	GLN	CA-C-N	5.22	129.81	122.09
1	G	84	GLN	C-N-CA	5.22	129.81	122.09
1	B	141	LEU	CA-C-N	5.22	127.27	120.28
1	B	141	LEU	C-N-CA	5.22	127.27	120.28
1	E	92	VAL	CA-C-N	5.21	130.41	122.65
1	E	92	VAL	C-N-CA	5.21	130.41	122.65
1	B	92	VAL	CA-C-N	5.21	130.41	122.65
1	B	92	VAL	C-N-CA	5.21	130.41	122.65
2	O	451	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	B	125	THR	CA-C-N	5.20	130.75	122.74
1	B	125	THR	C-N-CA	5.20	130.75	122.74
2	M	364	ALA	CA-C-O	5.19	126.10	120.55
1	E	84	GLN	CA-C-N	5.18	129.76	122.09
1	E	84	GLN	C-N-CA	5.18	129.76	122.09
1	G	92	VAL	CA-C-N	5.18	130.37	122.65
1	G	92	VAL	C-N-CA	5.18	130.37	122.65
1	H	151	ARG	CA-C-N	5.18	127.65	120.29
1	H	151	ARG	C-N-CA	5.18	127.65	120.29
1	E	106	PRO	CA-C-N	5.18	130.90	122.67
1	E	106	PRO	C-N-CA	5.18	130.90	122.67
1	G	170	SER	CA-C-N	5.18	130.29	122.99
1	G	170	SER	C-N-CA	5.18	130.29	122.99
1	A	132	GLY	CA-C-N	5.18	128.90	121.50
1	A	132	GLY	C-N-CA	5.18	128.90	121.50
2	N	341	TYR	N-CA-C	5.17	117.59	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	TRP	CA-C-N	5.17	129.70	122.93
1	B	119	TRP	C-N-CA	5.17	129.70	122.93
1	F	106	PRO	CA-C-N	5.17	130.79	122.83
1	F	106	PRO	C-N-CA	5.17	130.79	122.83
2	I	649	VAL	N-CA-C	5.16	115.40	108.17
1	F	108	GLY	CA-C-N	5.16	130.49	122.49
1	F	108	GLY	C-N-CA	5.16	130.49	122.49
2	K	127	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	M	316	ILE	CA-CB-CG1	5.15	119.16	110.40
1	G	145	ARG	N-CA-CB	5.15	117.47	110.01
1	E	113	SER	CA-C-N	5.14	127.17	120.28
1	E	113	SER	C-N-CA	5.14	127.17	120.28
1	A	147	ASP	CA-C-N	5.12	127.01	120.56
1	A	147	ASP	C-N-CA	5.12	127.01	120.56
2	P	88	ASP	CA-CB-CG	5.12	117.72	112.60
1	F	110	TYR	CA-C-N	5.11	127.97	120.71
1	F	110	TYR	C-N-CA	5.11	127.97	120.71
2	K	667	ARG	NE-CZ-NH2	5.11	123.80	119.20
1	A	106	PRO	CA-C-N	5.10	130.78	122.67
1	A	106	PRO	C-N-CA	5.10	130.78	122.67
1	F	147	ASP	CA-C-N	5.09	126.97	120.56
1	F	147	ASP	C-N-CA	5.09	126.97	120.56
1	C	147	ASP	CA-CB-CG	5.09	117.69	112.60
2	I	22	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	140	THR	CA-C-N	5.09	127.10	120.28
1	B	140	THR	C-N-CA	5.09	127.10	120.28
1	H	161	VAL	CA-C-N	5.08	130.55	122.62
1	H	161	VAL	C-N-CA	5.08	130.55	122.62
1	G	106	PRO	CA-C-N	5.08	130.63	122.86
1	G	106	PRO	C-N-CA	5.08	130.63	122.86
1	E	170	SER	CA-C-N	5.08	130.15	122.99
1	E	170	SER	C-N-CA	5.08	130.15	122.99
1	G	83	TYR	CA-C-N	5.08	130.87	121.94
1	G	83	TYR	C-N-CA	5.08	130.87	121.94
2	J	462	HIS	CB-CG-CD2	-5.08	124.60	131.20
1	E	140	THR	CA-C-N	5.06	127.07	120.28
1	E	140	THR	C-N-CA	5.06	127.07	120.28
1	E	169	ARG	CG-CD-NE	5.05	123.12	112.00
1	B	189	ASN	CA-C-N	5.05	131.54	123.46
1	B	189	ASN	C-N-CA	5.05	131.54	123.46
2	J	643	THR	CA-C-N	5.05	123.34	119.66
2	J	643	THR	C-N-CA	5.05	123.34	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	ARG	CB-CG-CD	5.04	122.90	111.30
2	M	342	ARG	N-CA-C	5.04	116.58	111.14
1	A	150	GLY	CA-C-N	5.04	127.29	120.44
1	A	150	GLY	C-N-CA	5.04	127.29	120.44
2	P	511	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	D	111	ARG	CB-CG-CD	5.04	122.88	111.30
1	F	140	THR	CA-C-N	5.04	127.03	120.28
1	F	140	THR	C-N-CA	5.04	127.03	120.28
1	H	150	GLY	CA-C-N	5.04	126.98	120.44
1	H	150	GLY	C-N-CA	5.04	126.98	120.44
2	I	462	HIS	CB-CG-CD2	-5.03	124.66	131.20
1	E	125	THR	CA-C-N	5.03	130.48	122.74
1	E	125	THR	C-N-CA	5.03	130.48	122.74
2	L	562	ASP	CA-CB-CG	5.03	117.62	112.60
1	B	110	TYR	CA-C-N	5.02	128.33	120.75
1	B	110	TYR	C-N-CA	5.02	128.33	120.75
1	B	118	ASN	CA-C-N	5.02	128.82	120.94
1	B	118	ASN	C-N-CA	5.02	128.82	120.94
1	E	168	PHE	CA-C-N	5.02	130.11	122.23
1	E	168	PHE	C-N-CA	5.02	130.11	122.23
1	B	144	ILE	N-CA-CB	5.02	116.42	110.55
1	C	168	PHE	CA-C-N	5.01	130.10	122.23
1	C	168	PHE	C-N-CA	5.01	130.10	122.23
2	J	609	ARG	NE-CZ-NH2	5.01	123.71	119.20
2	K	580	ASN	CA-CB-CG	5.01	117.61	112.60
1	E	83	TYR	CA-C-N	5.01	130.75	121.94
1	E	83	TYR	C-N-CA	5.01	130.75	121.94
1	E	144	ILE	N-CA-CB	5.01	116.41	110.55
1	C	141	LEU	CA-C-N	5.00	126.99	120.28
1	C	141	LEU	C-N-CA	5.00	126.99	120.28
2	I	348	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	M	514	ARG	NE-CZ-NH2	5.00	123.70	119.20
2	P	569	TYR	CA-C-N	5.00	127.23	120.38
2	P	569	TYR	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	110	TYR	Sidechain
1	G	130	TYR	Sidechain
1	H	130	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	I	205	TYR	Sidechain
2	I	253	TYR	Sidechain
2	I	280	ARG	Sidechain
2	I	294	ARG	Sidechain
2	I	377	ARG	Sidechain
2	I	708	TYR	Sidechain
2	J	710	TYR	Sidechain
2	K	280	ARG	Sidechain
2	K	715	TYR	Sidechain
2	L	334	TYR	Sidechain
2	M	668	TYR	Sidechain
2	M	711	TYR	Sidechain
2	M	97	ARG	Sidechain
2	N	251	ARG	Sidechain
2	N	636	TYR	Sidechain
2	O	280	ARG	Sidechain
2	P	280	ARG	Sidechain
2	P	348	ARG	Sidechain
2	P	467	TYR	Sidechain
2	P	636	TYR	Sidechain
2	P	668	TYR	Sidechain
2	P	705	TYR	Sidechain
2	P	711	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	6	0
1	B	2783	2765	2764	4	0
1	C	2783	2765	2764	5	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	9	0
1	H	2783	2765	2764	6	0
2	I	5221	5335	5328	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	5221	5335	5328	7	0
2	K	5221	5335	5328	9	0
2	L	5221	5335	5328	8	0
2	M	5221	5335	5328	18	0
2	N	5221	5335	5328	11	0
2	O	5221	5335	5328	10	0
2	P	5221	5335	5328	6	0
3	I	27	12	12	0	0
3	J	27	12	12	0	0
3	K	27	12	12	1	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	64248	64896	64832	118	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 1.

All (118) 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:E:116:THR:HG22	1:E:116:THR:O	1.96	0.64
2:M:375:LEU:C	2:M:375:LEU:HD13	2.28	0.58
1:A:116:THR:HG22	1:A:116:THR:O	2.06	0.54
1:C:242:TYR:N	1:C:245:ASP:OD2	2.39	0.53
1:G:102:GLU:H	1:G:102:GLU:CD	2.17	0.52
2:K:20:ILE:HD12	2:K:20:ILE:H	1.74	0.52
1:G:242:TYR:N	1:G:245:ASP:OD2	2.39	0.51
1:A:272:ASP:OD2	1:A:272:ASP:N	2.42	0.50
2:N:342:ARG:H	2:N:342:ARG:CD	2.23	0.50
2:K:542:PHE:CD2	3:K:1000:ADP:C8	2.99	0.50
2:M:534:VAL:HG13	2:M:535:SER:H	1.75	0.50
2:M:316:ILE:HG21	2:M:350:ALA:HB2	1.94	0.50
2:K:324:THR:HA	2:K:347:LYS:HE3	1.93	0.50
1:A:329:VAL:HG21	1:F:315:ALA:HB2	1.94	0.50
1:E:242:TYR:N	1:E:245:ASP:OD2	2.38	0.50
2:M:326:LYS:HE2	2:M:338:HIS:ND1	2.27	0.50
2:M:20:ILE:H	2:M:20:ILE:HD12	1.77	0.49
2:O:510:ILE:HG22	2:O:550:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:364:ALA:C	2:M:366:PRO:HD2	2.38	0.49
1:D:116:THR:HG22	1:D:116:THR:O	2.13	0.48
1:C:221:GLU:OE2	1:C:223:ARG:NH1	2.46	0.48
2:M:152:PHE:CE2	2:M:166:SER:HB3	2.48	0.48
2:N:563:CYS:SG	2:N:641:ILE:HG23	2.54	0.48
2:I:469:SER:C	2:I:698:ILE:HD12	2.38	0.48
2:I:525:GLN:CD	2:I:525:GLN:H	2.23	0.47
2:M:302:LEU:O	2:M:306:ALA:HB3	2.15	0.47
2:N:581:GLY:HA3	2:N:610:GLY:HA3	1.97	0.47
2:O:563:CYS:SG	2:O:641:ILE:HG23	2.55	0.47
1:C:100:HIS:N	1:C:101:PRO:CD	2.78	0.46
1:G:221:GLU:OE2	1:G:223:ARG:NH1	2.48	0.46
1:D:272:ASP:OD2	1:D:272:ASP:N	2.41	0.46
1:H:154:THR:HB	1:H:155:TYR:CD2	2.51	0.46
2:L:566:ARG:HH21	2:L:566:ARG:CG	2.29	0.46
1:H:175:ILE:N	1:H:175:ILE:HD12	2.30	0.46
2:M:519:PHE:HA	2:M:522:MET:HE3	1.98	0.46
2:N:145:LYS:HA	2:N:148:ALA:HB3	1.97	0.46
1:H:272:ASP:OD2	1:H:272:ASP:N	2.43	0.45
1:F:175:ILE:HD12	1:F:175:ILE:N	2.31	0.45
1:F:272:ASP:OD2	1:F:272:ASP:N	2.44	0.45
2:P:701:ARG:HD2	2:P:701:ARG:H	1.81	0.45
1:C:272:ASP:OD2	1:C:272:ASP:N	2.47	0.45
2:J:469:SER:C	2:J:698:ILE:HD13	2.42	0.45
2:O:702:ALA:HB1	2:O:708:TYR:H	1.80	0.45
1:D:175:ILE:N	1:D:175:ILE:HD12	2.31	0.45
1:B:128:TYR:CG	1:B:129:PRO:HD2	2.52	0.45
2:J:334:TYR:C	2:J:334:TYR:CD1	2.95	0.45
2:M:98:LEU:C	2:M:98:LEU:HD23	2.42	0.45
2:M:338:HIS:CG	2:M:339:PRO:HD3	2.52	0.45
2:N:351:LEU:HA	2:O:325:PHE:CZ	2.52	0.44
1:E:175:ILE:HD12	1:E:175:ILE:N	2.31	0.44
2:K:146:GLU:H	2:K:146:GLU:CD	2.26	0.44
2:P:525:GLN:H	2:P:525:GLN:CD	2.25	0.44
2:M:528:VAL:HG13	2:M:660:GLY:H	1.83	0.44
2:J:530:MET:HG2	2:J:531:MET:H	1.82	0.44
2:I:253:TYR:CD2	2:I:253:TYR:C	2.95	0.44
2:N:342:ARG:H	2:N:342:ARG:HD2	1.82	0.44
1:A:87:VAL:HG12	1:A:88:GLY:N	2.33	0.44
1:E:128:TYR:CG	1:E:129:PRO:HD2	2.52	0.44
1:B:175:ILE:HD12	1:B:175:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:299:SER:O	2:M:303:PRO:HD2	2.18	0.43
2:N:98:LEU:C	2:N:98:LEU:HD23	2.43	0.43
2:I:152:PHE:CE2	2:I:166:SER:HB3	2.53	0.43
2:K:98:LEU:C	2:K:98:LEU:HD23	2.43	0.43
1:C:175:ILE:HD12	1:C:175:ILE:N	2.33	0.43
2:K:217:SER:HB2	2:K:234:TYR:CE1	2.53	0.43
1:A:175:ILE:HD12	1:A:175:ILE:N	2.34	0.43
1:G:272:ASP:OD2	1:G:272:ASP:N	2.43	0.43
2:L:217:SER:HB2	2:L:234:TYR:CZ	2.54	0.43
2:N:436:LEU:C	2:N:436:LEU:HD23	2.44	0.43
2:O:343:THR:HA	2:P:328:ALA:HB1	2.00	0.43
2:K:625:PHE:CD1	2:K:625:PHE:C	2.96	0.43
1:G:175:ILE:HD12	1:G:175:ILE:N	2.33	0.43
2:L:210:MET:HE2	2:L:210:MET:N	2.34	0.43
1:G:121:GLN:CD	1:G:122:PRO:HD2	2.44	0.43
1:H:107:ALA:HB3	1:H:116:THR:HG23	1.99	0.43
1:B:329:VAL:HG23	1:E:303:PRO:HG3	2.00	0.43
2:L:477:LYS:HE3	2:L:477:LYS:HA	1.99	0.43
2:N:210:MET:N	2:N:210:MET:HE2	2.34	0.43
2:P:469:SER:C	2:P:698:ILE:HD12	2.44	0.43
1:G:102:GLU:CD	1:G:102:GLU:N	2.76	0.42
2:P:217:SER:HB2	2:P:234:TYR:CZ	2.53	0.42
1:H:130:TYR:HB3	1:H:155:TYR:CD2	2.54	0.42
2:K:521:MET:HA	2:K:524:ALA:HB3	2.02	0.42
2:M:372:ILE:HD12	2:M:375:LEU:HD12	2.02	0.42
2:L:446:ARG:HA	2:L:449:PHE:CD2	2.54	0.42
2:O:205:TYR:HB3	2:O:210:MET:HE3	2.01	0.42
2:O:210:MET:HE2	2:O:210:MET:N	2.34	0.42
2:O:514:ARG:NH2	2:O:550:VAL:HG22	2.34	0.42
1:D:303:PRO:HG3	1:E:329:VAL:HG23	2.01	0.42
2:M:693:VAL:HG12	2:M:694:ILE:N	2.34	0.42
2:P:98:LEU:C	2:P:98:LEU:HD23	2.45	0.42
2:K:643:THR:HB	2:K:644:PRO:CD	2.50	0.42
2:M:693:VAL:HG12	2:M:694:ILE:H	1.84	0.42
2:N:302:LEU:HD12	2:N:302:LEU:H	1.84	0.42
2:I:146:GLU:H	2:I:146:GLU:CD	2.28	0.41
2:I:563:CYS:SG	2:I:641:ILE:HG23	2.59	0.41
2:L:225:LYS:HE2	2:L:226:ASP:H	1.84	0.41
2:I:162:TYR:CE2	2:I:175:GLN:C	2.98	0.41
1:B:307:GLU:OE1	1:B:310:ARG:NH1	2.49	0.41
2:I:98:LEU:C	2:I:98:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:668:TYR:CG	2:J:698:ILE:HA	2.55	0.41
2:M:625:PHE:CD1	2:M:625:PHE:C	2.96	0.41
2:J:693:VAL:HG12	2:J:694:ILE:N	2.36	0.41
2:N:445:LEU:HD22	2:N:445:LEU:H	1.86	0.41
2:O:205:TYR:CD2	2:O:210:MET:SD	3.14	0.41
2:J:338:HIS:HB3	2:J:339:PRO:CD	2.49	0.41
1:D:102:GLU:H	1:D:102:GLU:CD	2.28	0.41
2:I:160:LYS:HE2	2:I:176:ALA:O	2.21	0.41
2:M:369:GLN:HA	2:M:372:ILE:HG22	2.02	0.41
1:H:376:ILE:HG22	1:H:376:ILE:O	2.20	0.40
2:I:43:LEU:HD23	2:I:43:LEU:C	2.46	0.40
2:L:668:TYR:CD2	2:L:698:ILE:HA	2.57	0.40
2:O:338:HIS:CG	2:O:339:PRO:HD2	2.56	0.40
1:G:307:GLU:OE2	1:G:310:ARG:NH1	2.52	0.40
2:J:475:TRP:CZ2	2:J:500:GLY:HA3	2.56	0.40
1:A:116:THR:O	1:A:116:THR:CG2	2.70	0.40
1:G:359:LEU:O	1:G:362:THR:HG22	2.22	0.40
2:L:710:TYR:C	2:L:711:TYR:CG	2.99	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%)	344 (97%)	12 (3%)	0	100	100
1	B	356/394 (90%)	340 (96%)	15 (4%)	1 (0%)	36	72
1	C	356/394 (90%)	341 (96%)	14 (4%)	1 (0%)	36	72
1	D	356/394 (90%)	342 (96%)	14 (4%)	0	100	100
1	E	356/394 (90%)	344 (97%)	12 (3%)	0	100	100
1	F	356/394 (90%)	346 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	356/394 (90%)	341 (96%)	14 (4%)	1 (0%)	36	72
1	H	356/394 (90%)	339 (95%)	17 (5%)	0	100	100
2	I	667/738 (90%)	618 (93%)	47 (7%)	2 (0%)	36	72
2	J	667/738 (90%)	628 (94%)	37 (6%)	2 (0%)	36	72
2	K	667/738 (90%)	622 (93%)	40 (6%)	5 (1%)	18	56
2	L	667/738 (90%)	628 (94%)	35 (5%)	4 (1%)	21	59
2	M	667/738 (90%)	615 (92%)	49 (7%)	3 (0%)	30	67
2	N	667/738 (90%)	622 (93%)	44 (7%)	1 (0%)	48	83
2	O	667/738 (90%)	625 (94%)	37 (6%)	5 (1%)	18	56
2	P	667/738 (90%)	626 (94%)	38 (6%)	3 (0%)	30	67
All	All	8184/9056 (90%)	7721 (94%)	435 (5%)	28 (0%)	37	72

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	158	ASP
2	I	338	HIS
2	M	293	PHE
2	K	119	PRO
2	K	120	ILE
2	M	669	ALA
2	I	700	ARG
2	K	338	HIS
2	L	335	THR
2	M	700	ARG
2	O	699	PHE
2	P	338	HIS
2	P	702	ALA
2	J	600	SER
2	L	333	LEU
2	L	338	HIS
2	O	20	ILE
2	O	669	ALA
2	N	424	LYS
2	O	331	SER
2	K	424	LYS
2	K	600	SER
2	L	159	ASN

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Mol	Chain	Res	Type
2	P	669	ALA
2	O	543	VAL
1	C	100	HIS
2	J	417	PRO
1	B	129	PRO

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%)	307 (100%)	0	100	100
1	B	307/342 (90%)	305 (99%)	2 (1%)	76	81
1	C	307/342 (90%)	302 (98%)	5 (2%)	55	70
1	D	307/342 (90%)	301 (98%)	6 (2%)	48	66
1	E	307/342 (90%)	306 (100%)	1 (0%)	86	85
1	F	307/342 (90%)	307 (100%)	0	100	100
1	G	307/342 (90%)	303 (99%)	4 (1%)	61	74
1	H	307/342 (90%)	305 (99%)	2 (1%)	76	81
2	I	575/630 (91%)	553 (96%)	22 (4%)	29	50
2	J	575/630 (91%)	552 (96%)	23 (4%)	28	49
2	K	575/630 (91%)	553 (96%)	22 (4%)	29	50
2	L	575/630 (91%)	553 (96%)	22 (4%)	29	50
2	M	575/630 (91%)	543 (94%)	32 (6%)	19	40
2	N	575/630 (91%)	552 (96%)	23 (4%)	28	49
2	O	575/630 (91%)	556 (97%)	19 (3%)	33	55
2	P	575/630 (91%)	552 (96%)	23 (4%)	28	49
All	All	7056/7776 (91%)	6850 (97%)	206 (3%)	38	58

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	97	VAL
1	B	109	GLN
1	C	84	GLN
1	C	102	GLU
1	C	110	TYR
1	C	152	LEU
1	C	296	SER
1	D	98	TRP
1	D	102	GLU
1	D	116	THR
1	D	130	TYR
1	D	133	LYS
1	D	155	TYR
1	E	133	LYS
1	G	97	VAL
1	G	102	GLU
1	G	155	TYR
1	G	158	ASP
1	H	109	GLN
1	H	156	ILE
2	I	43	LEU
2	I	132	GLN
2	I	153	THR
2	I	214	LEU
2	I	232	LEU
2	I	251	ARG
2	I	255	GLU
2	I	275	GLN
2	I	278	GLU
2	I	342	ARG
2	I	348	ARG
2	I	388	GLN
2	I	392	LYS
2	I	419	VAL
2	I	525	GLN
2	I	556	LYS
2	I	557	ARG
2	I	569	TYR
2	I	611	GLN
2	I	655	VAL
2	I	677	GLU
2	I	691	LYS
2	J	129	MET

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Mol	Chain	Res	Type
2	J	132	GLN
2	J	145	LYS
2	J	153	THR
2	J	210	MET
2	J	214	LEU
2	J	232	LEU
2	J	241	GLN
2	J	257	ASN
2	J	275	GLN
2	J	334	TYR
2	J	338	HIS
2	J	347	LYS
2	J	359	ASN
2	J	396	LEU
2	J	525	GLN
2	J	550	VAL
2	J	587	ILE
2	J	611	GLN
2	J	625	PHE
2	J	641	ILE
2	J	651	ASP
2	J	672	THR
2	K	119	PRO
2	K	141	PHE
2	K	193	HIS
2	K	232	LEU
2	K	327	GLU
2	K	337	VAL
2	K	341	TYR
2	K	347	LYS
2	K	359	ASN
2	K	392	LYS
2	K	396	LEU
2	K	460	GLU
2	K	462	HIS
2	K	525	GLN
2	K	531	MET
2	K	534	VAL
2	K	580	ASN
2	K	625	PHE
2	K	641	ILE
2	K	651	ASP

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Mol	Chain	Res	Type
2	K	672	THR
2	K	712	GLU
2	L	29	GLU
2	L	125	TRP
2	L	175	GLN
2	L	185	VAL
2	L	186	THR
2	L	213	GLN
2	L	225	LYS
2	L	232	LEU
2	L	241	GLN
2	L	275	GLN
2	L	278	GLU
2	L	337	VAL
2	L	338	HIS
2	L	363	THR
2	L	392	LYS
2	L	414	ILE
2	L	477	LYS
2	L	510	ILE
2	L	566	ARG
2	L	711	TYR
2	L	712	GLU
2	L	713	TYR
2	M	29	GLU
2	M	132	GLN
2	M	142	ASN
2	M	153	THR
2	M	232	LEU
2	M	257	ASN
2	M	283	LEU
2	M	293	PHE
2	M	301	ASP
2	M	316	ILE
2	M	319	GLN
2	M	322	GLU
2	M	326	LYS
2	M	337	VAL
2	M	338	HIS
2	M	353	ASP
2	M	354	GLU
2	M	368	THR

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Mol	Chain	Res	Type
2	M	375	LEU
2	M	392	LYS
2	M	414	ILE
2	M	503	THR
2	M	521	MET
2	M	540	MET
2	M	541	THR
2	M	554	THR
2	M	625	PHE
2	M	641	ILE
2	M	651	ASP
2	M	655	VAL
2	M	672	THR
2	M	718	ASP
2	N	88	ASP
2	N	138	VAL
2	N	145	LYS
2	N	207	THR
2	N	213	GLN
2	N	232	LEU
2	N	241	GLN
2	N	251	ARG
2	N	323	LEU
2	N	342	ARG
2	N	344	LEU
2	N	367	LYS
2	N	369	GLN
2	N	377	ARG
2	N	384	GLN
2	N	392	LYS
2	N	396	LEU
2	N	454	GLU
2	N	503	THR
2	N	525	GLN
2	N	642	ASP
2	N	651	ASP
2	N	712	GLU
2	O	153	THR
2	O	225	LYS
2	O	232	LEU
2	O	257	ASN
2	O	260	ARG

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Mol	Chain	Res	Type
2	O	321	ASN
2	O	338	HIS
2	O	341	TYR
2	O	359	ASN
2	O	366	PRO
2	O	392	LYS
2	O	521	MET
2	O	525	GLN
2	O	540	MET
2	O	558	VAL
2	O	649	VAL
2	O	655	VAL
2	O	672	THR
2	O	708	TYR
2	P	40	VAL
2	P	142	ASN
2	P	145	LYS
2	P	153	THR
2	P	186	THR
2	P	214	LEU
2	P	232	LEU
2	P	298	ASP
2	P	342	ARG
2	P	393	GLU
2	P	503	THR
2	P	521	MET
2	P	525	GLN
2	P	550	VAL
2	P	580	ASN
2	P	584	GLU
2	P	601	ILE
2	P	625	PHE
2	P	651	ASP
2	P	655	VAL
2	P	672	THR
2	P	701	ARG
2	P	712	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	GLN

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Mol	Chain	Res	Type
1	B	94	ASN
1	B	171	GLN
1	B	353	ASN
1	C	94	ASN
1	D	109	GLN
1	D	164	ASN
1	D	184	GLN
1	E	236	ASN
1	F	171	GLN
1	F	236	ASN
1	G	68	ASN
1	G	232	ASN
2	I	142	ASN
2	I	155	ASN
2	I	193	HIS
2	I	274	GLN
2	I	288	ASN
2	I	291	ASN
2	I	321	ASN
2	I	349	GLN
2	I	383	GLN
2	I	553	GLN
2	I	658	HIS
2	I	686	ASN
2	J	133	ASN
2	J	193	HIS
2	J	291	ASN
2	J	370	GLN
2	J	394	GLN
2	J	476	GLN
2	J	495	GLN
2	K	63	GLN
2	K	132	GLN
2	K	319	GLN
2	K	321	ASN
2	K	359	ASN
2	K	388	GLN
2	K	457	GLN
2	L	175	GLN
2	L	321	ASN
2	L	383	GLN
2	L	384	GLN

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Mol	Chain	Res	Type
2	L	388	GLN
2	L	476	GLN
2	M	133	ASN
2	M	142	ASN
2	M	257	ASN
2	M	526	ASN
2	M	706	GLN
2	N	155	ASN
2	N	193	HIS
2	N	212	ASN
2	N	254	GLN
2	N	383	GLN
2	N	391	ASN
2	N	476	GLN
2	N	546	ASN
2	N	615	ASN
2	O	175	GLN
2	O	178	GLN
2	O	223	ASN
2	O	275	GLN
2	O	319	GLN
2	O	359	ASN
2	O	384	GLN
2	O	388	GLN
2	P	178	GLN
2	P	241	GLN
2	P	257	ASN
2	P	319	GLN
2	P	321	ASN
2	P	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	P	1000	-	27,29,29	0.95	1 (3%)	42,45,45	1.18	5 (11%)
3	ADP	K	1000	-	27,29,29	0.94	1 (3%)	42,45,45	1.37	5 (11%)
3	ADP	O	1000	-	27,29,29	0.94	0	42,45,45	1.39	8 (19%)
3	ADP	L	1000	-	27,29,29	0.91	0	42,45,45	1.20	5 (11%)
3	ADP	N	1000	-	27,29,29	0.97	1 (3%)	42,45,45	1.31	6 (14%)
3	ADP	M	1000	-	27,29,29	0.94	0	42,45,45	1.28	8 (19%)
3	ADP	I	1000	-	27,29,29	0.93	0	42,45,45	1.31	8 (19%)
3	ADP	J	1000	-	27,29,29	0.91	0	42,45,45	1.24	7 (16%)

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	P	1000	-	-	1/16/32/32	0/3/3/3
3	ADP	K	1000	-	-	6/16/32/32	0/3/3/3
3	ADP	O	1000	-	-	4/16/32/32	0/3/3/3
3	ADP	L	1000	-	-	3/16/32/32	0/3/3/3
3	ADP	N	1000	-	-	5/16/32/32	0/3/3/3
3	ADP	M	1000	-	-	1/16/32/32	0/3/3/3
3	ADP	I	1000	-	-	3/16/32/32	0/3/3/3
3	ADP	J	1000	-	-	3/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1000	ADP	C8-N7	2.29	1.35	1.31
3	P	1000	ADP	C8-N7	2.22	1.35	1.31
3	N	1000	ADP	C8-N7	2.11	1.35	1.31

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1000	ADP	PA-O3A-PB	-3.82	119.72	132.83
3	L	1000	ADP	PA-O3A-PB	-3.58	120.54	132.83
3	N	1000	ADP	PA-O3A-PB	-3.45	121.00	132.83
3	I	1000	ADP	PA-O3A-PB	-3.43	121.07	132.83
3	K	1000	ADP	O2B-PB-O3A	3.41	116.06	104.64
3	P	1000	ADP	PA-O3A-PB	-3.33	121.41	132.83
3	N	1000	ADP	C5-C4-N3	-3.23	122.54	126.75
3	O	1000	ADP	C5-C4-N3	-3.10	122.71	126.75
3	I	1000	ADP	O2B-PB-O3A	3.04	114.83	104.64
3	J	1000	ADP	C5-C4-N3	-3.00	122.84	126.75
3	O	1000	ADP	PA-O3A-PB	-3.00	122.54	132.83
3	I	1000	ADP	C5-C4-N3	-2.98	122.86	126.75
3	M	1000	ADP	C5-C4-N3	-2.92	122.95	126.75
3	O	1000	ADP	C4-C5-N7	2.89	114.14	110.62
3	K	1000	ADP	C5-C4-N3	-2.82	123.07	126.75
3	I	1000	ADP	C5-C6-N1	2.70	123.18	117.39
3	M	1000	ADP	O2B-PB-O3A	2.67	113.61	104.64
3	N	1000	ADP	C5-C6-N1	2.62	123.01	117.39
3	M	1000	ADP	C4-C5-N7	2.61	113.79	110.62
3	N	1000	ADP	N6-C6-N1	-2.60	112.65	118.35
3	I	1000	ADP	N6-C6-N1	-2.53	112.81	118.35
3	K	1000	ADP	C4-C5-N7	2.53	113.69	110.62
3	M	1000	ADP	C5-C6-N1	2.51	122.78	117.39
3	O	1000	ADP	C5-C6-N1	2.51	122.78	117.39
3	P	1000	ADP	N6-C6-N1	-2.50	112.87	118.35
3	P	1000	ADP	C5-C4-N3	-2.50	123.49	126.75
3	K	1000	ADP	C5-C6-N1	2.48	122.72	117.39
3	L	1000	ADP	C5-C6-N1	2.47	122.69	117.39
3	L	1000	ADP	C5-C4-N3	-2.45	123.55	126.75
3	M	1000	ADP	PA-O3A-PB	-2.45	124.41	132.83
3	J	1000	ADP	C5-C6-N1	2.45	122.65	117.39
3	P	1000	ADP	C5-C6-N1	2.43	122.60	117.39
3	L	1000	ADP	C4-C5-N7	2.42	113.57	110.62
3	O	1000	ADP	N6-C6-N1	-2.42	113.05	118.35
3	O	1000	ADP	C2'-C1'-N9	2.38	119.32	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1000	ADP	N6-C6-N1	-2.37	113.17	118.35
3	I	1000	ADP	C2-N1-C6	-2.34	114.76	118.77
3	P	1000	ADP	C4-C5-N7	2.32	113.44	110.62
3	N	1000	ADP	C2-N1-C6	-2.30	114.83	118.77
3	I	1000	ADP	C4-C5-N7	2.29	113.41	110.62
3	J	1000	ADP	C4-C5-N7	2.23	113.33	110.62
3	O	1000	ADP	N3-C4-N9	2.22	130.74	127.08
3	J	1000	ADP	C2-N1-C6	-2.20	114.98	118.77
3	M	1000	ADP	N3-C4-N9	2.17	130.66	127.08
3	L	1000	ADP	N6-C6-N1	-2.17	113.61	118.35
3	K	1000	ADP	N6-C6-N1	-2.13	113.68	118.35
3	J	1000	ADP	N3-C4-N9	2.13	130.59	127.08
3	O	1000	ADP	C2-N1-C6	-2.11	115.14	118.77
3	N	1000	ADP	N3-C4-N9	2.07	130.50	127.08
3	J	1000	ADP	N6-C6-N1	-2.03	113.90	118.35
3	M	1000	ADP	C2-N1-C6	-2.03	115.28	118.77
3	I	1000	ADP	N3-C4-N9	2.01	130.39	127.08

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

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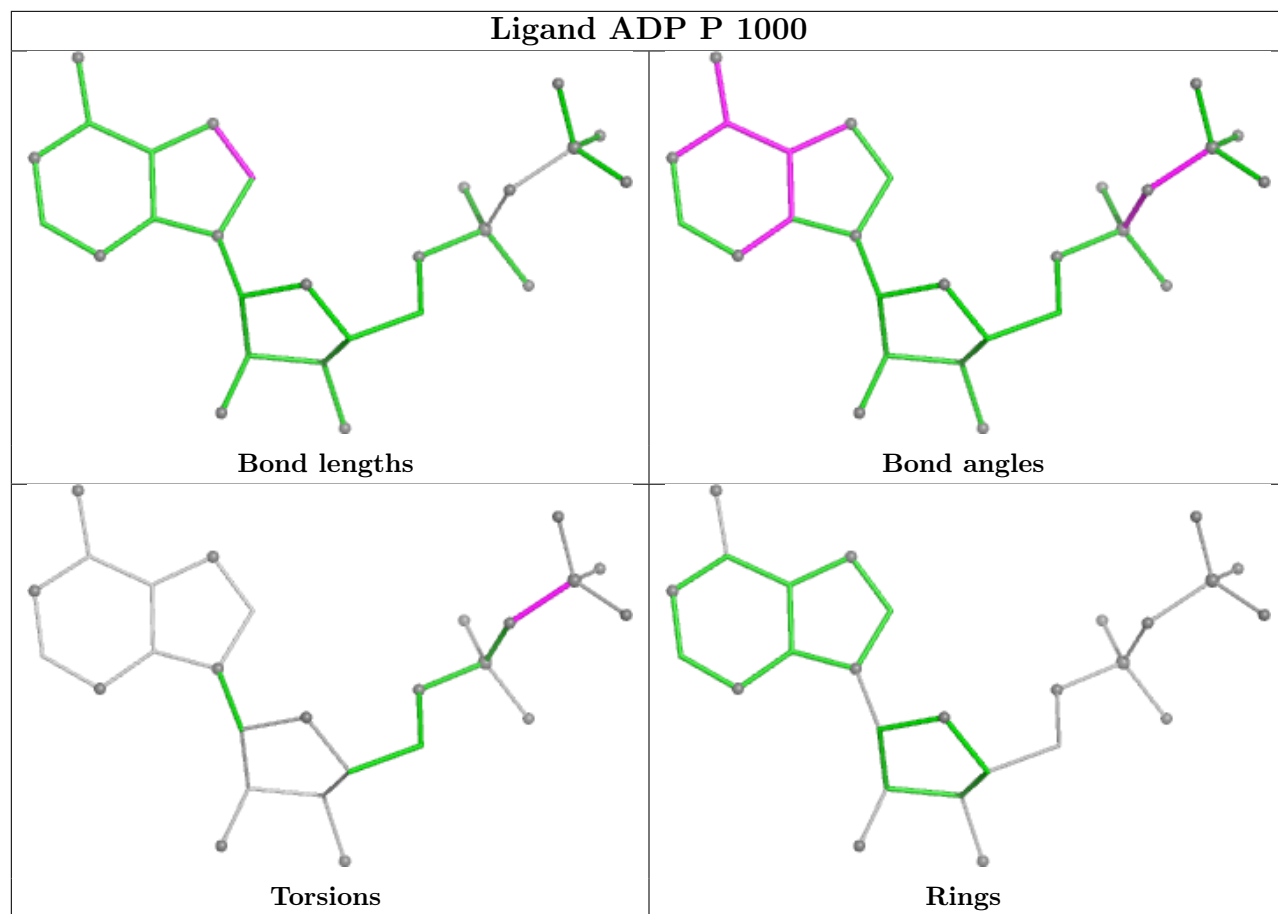
Mol	Chain	Res	Type	Atoms
3	N	1000	ADP	C5'-O5'-PA-O1A
3	O	1000	ADP	PB-O3A-PA-O1A
3	O	1000	ADP	PB-O3A-PA-O2A
3	I	1000	ADP	PA-O3A-PB-O1B
3	N	1000	ADP	C3'-C4'-C5'-O5'
3	K	1000	ADP	PA-O3A-PB-O1B

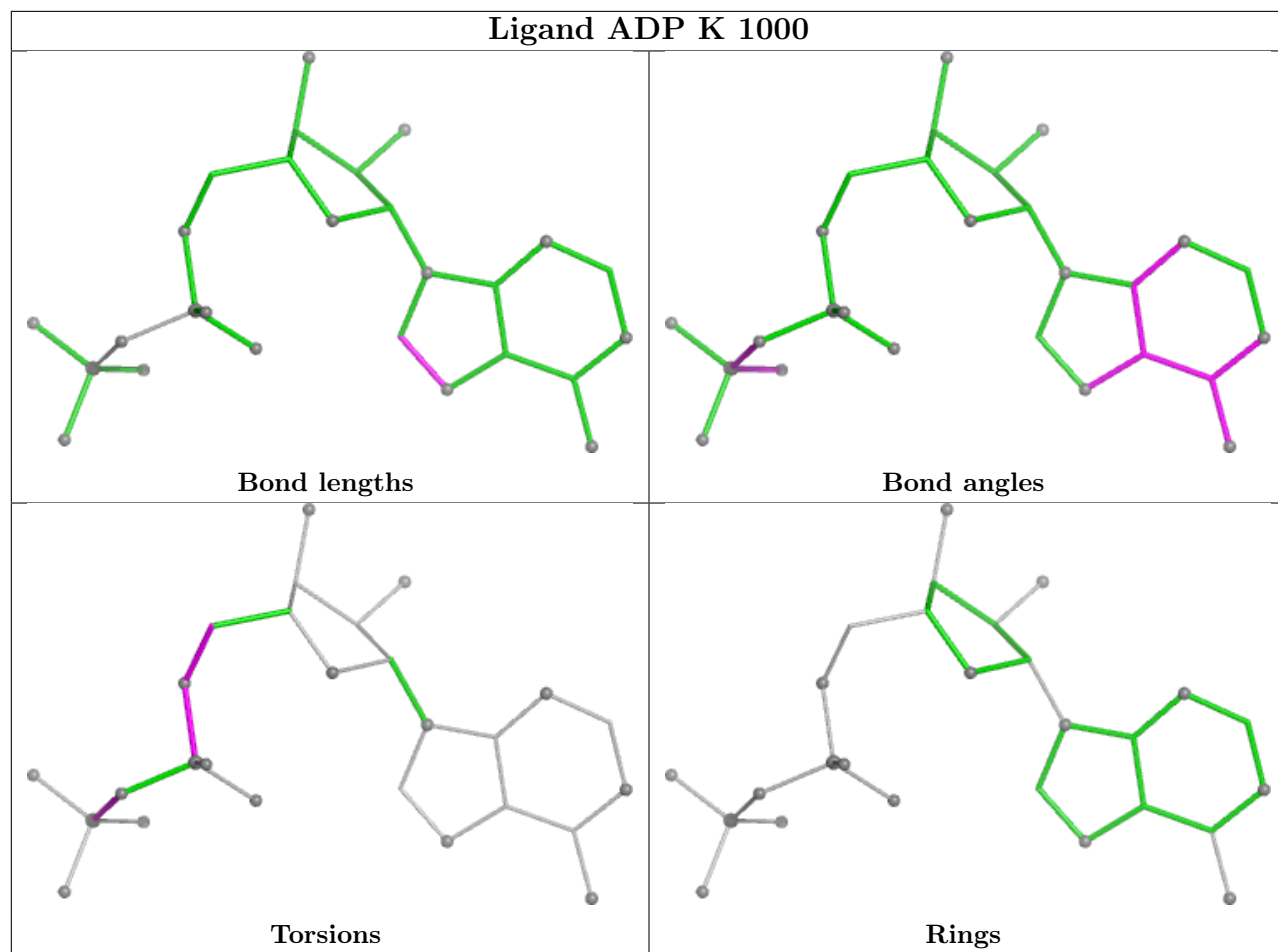
There are no ring outliers.

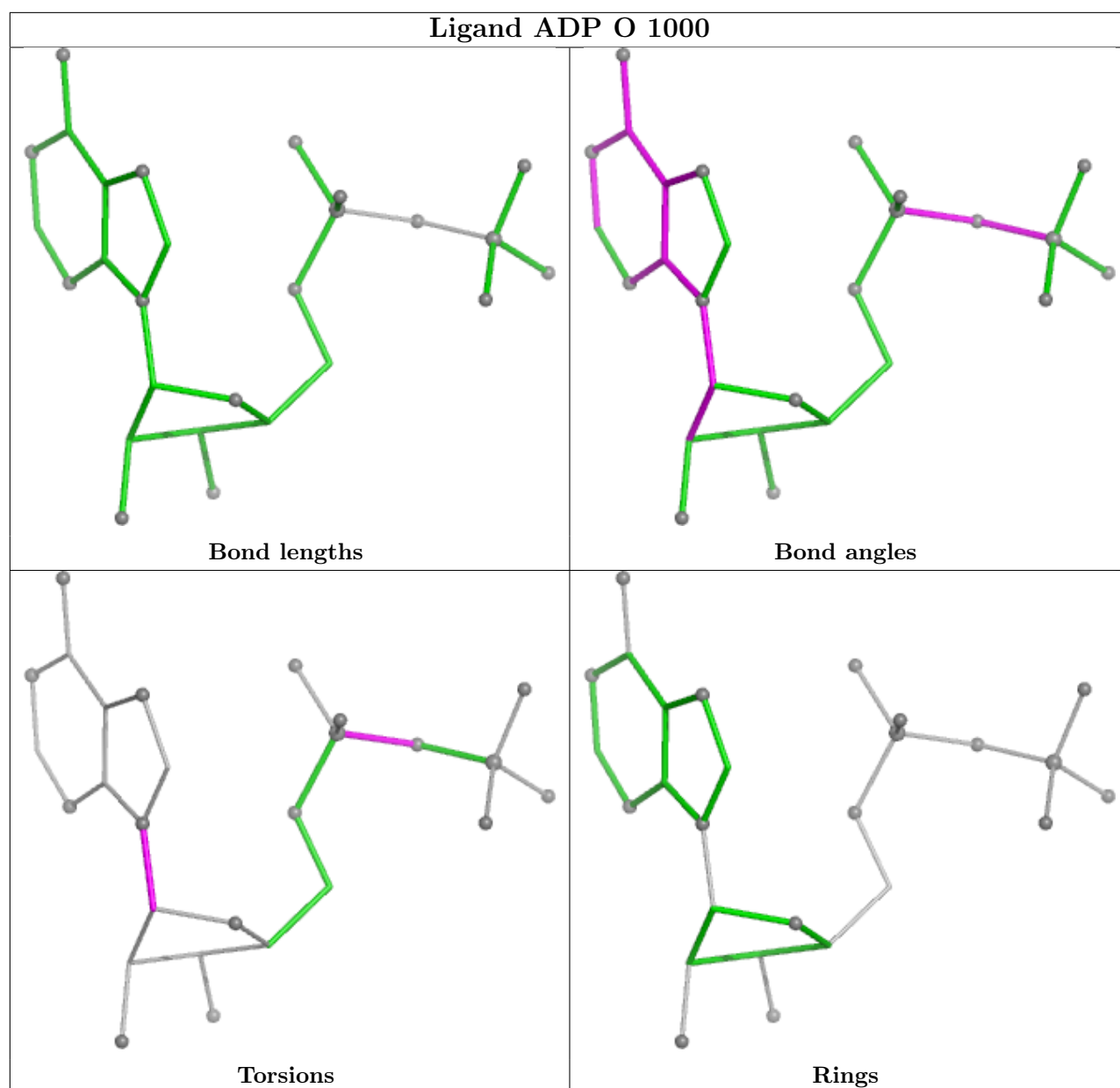
1 monomer is involved in 1 short contact:

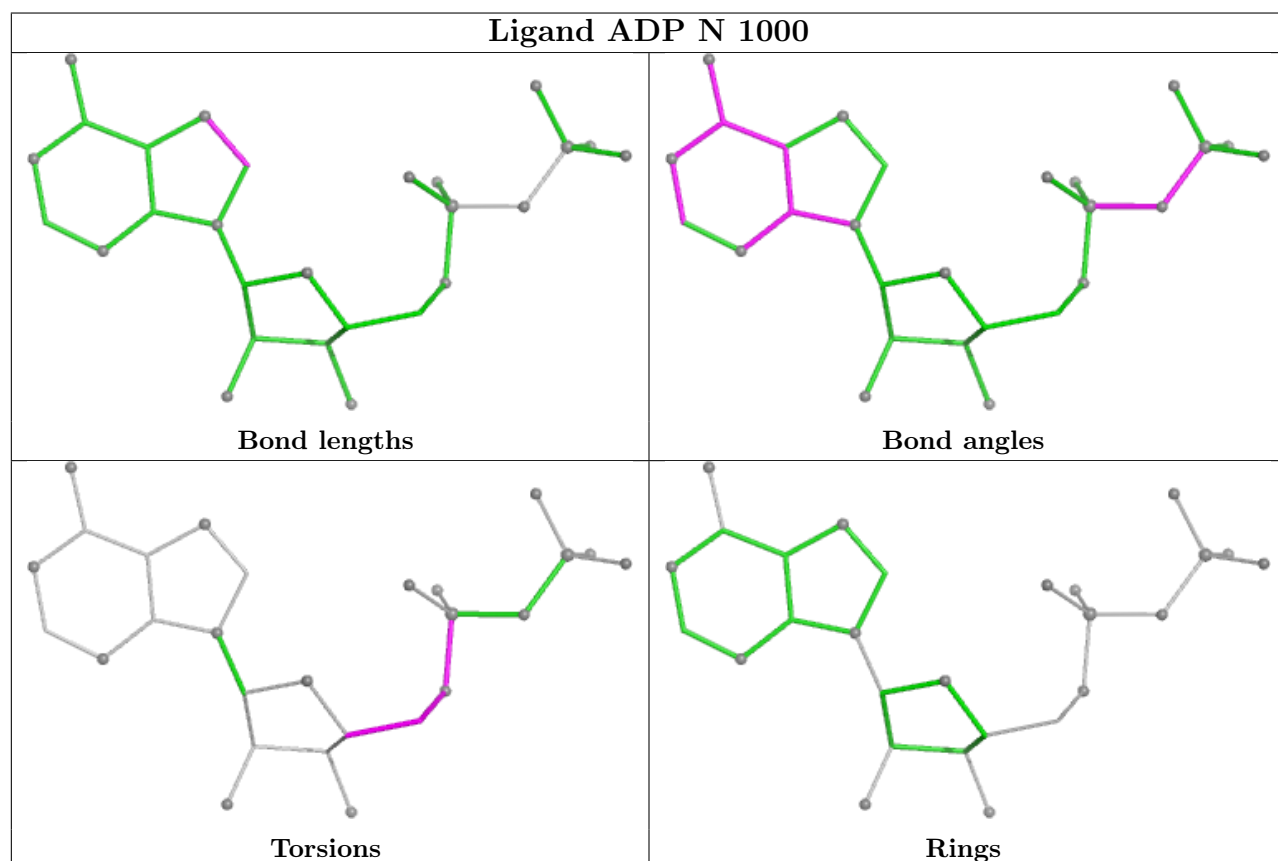
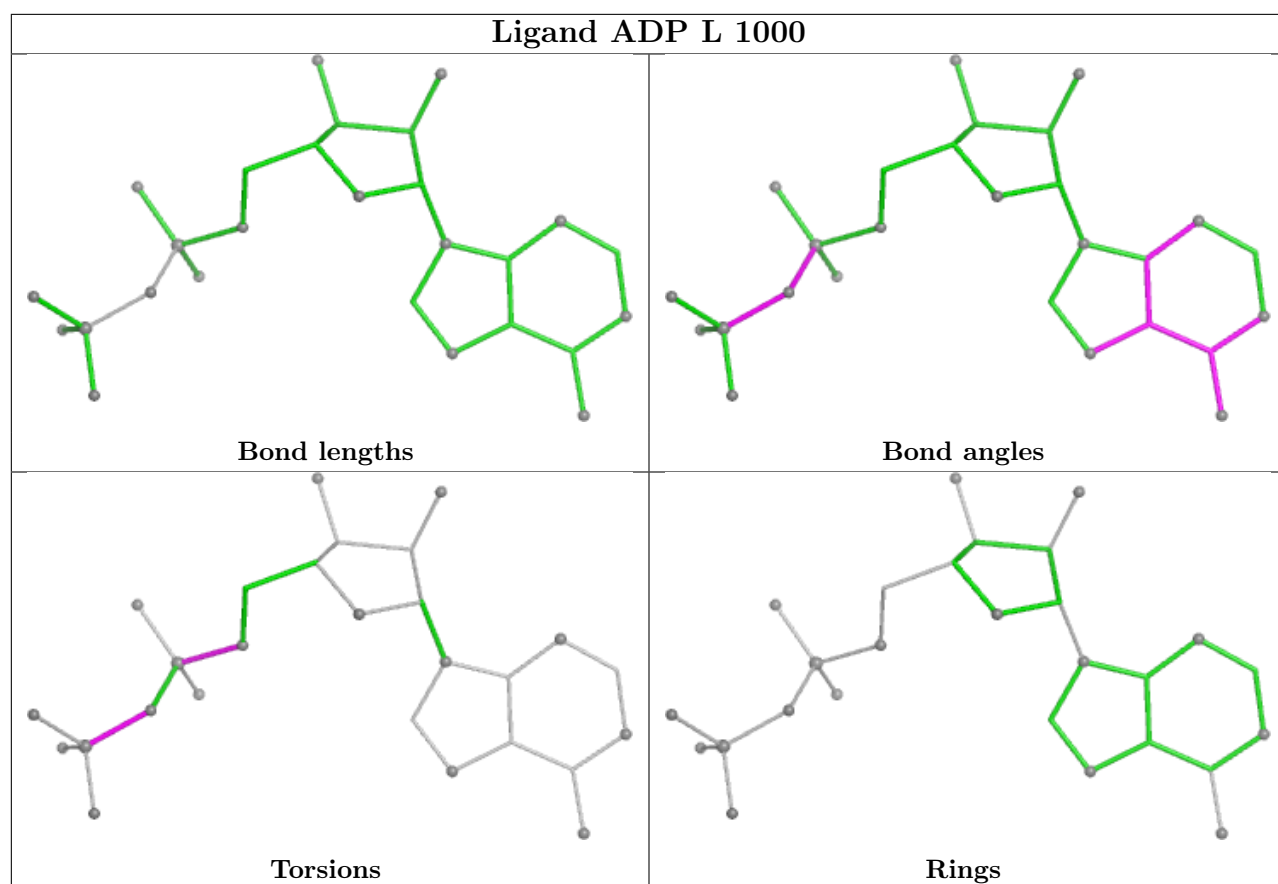
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	1000	ADP	1	0

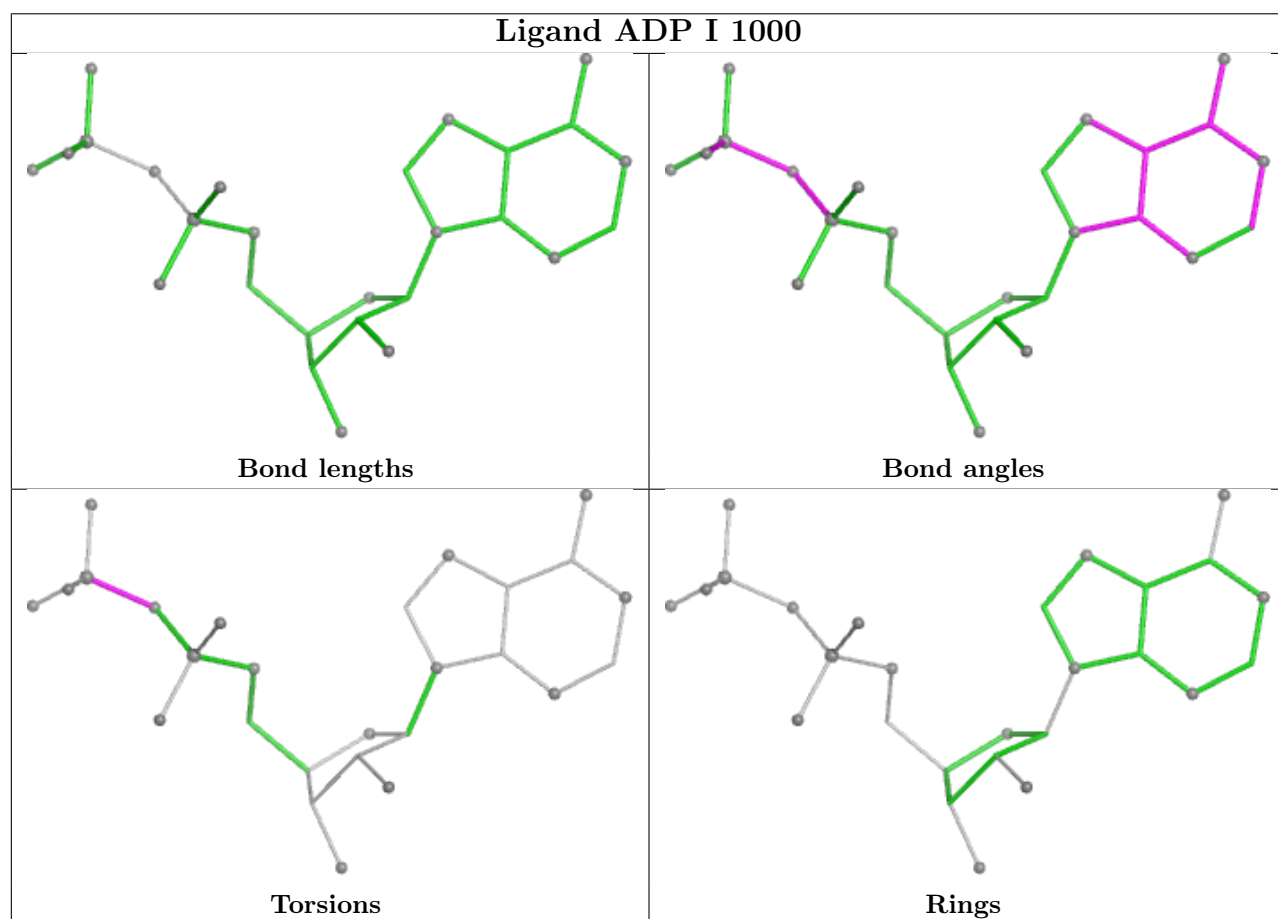
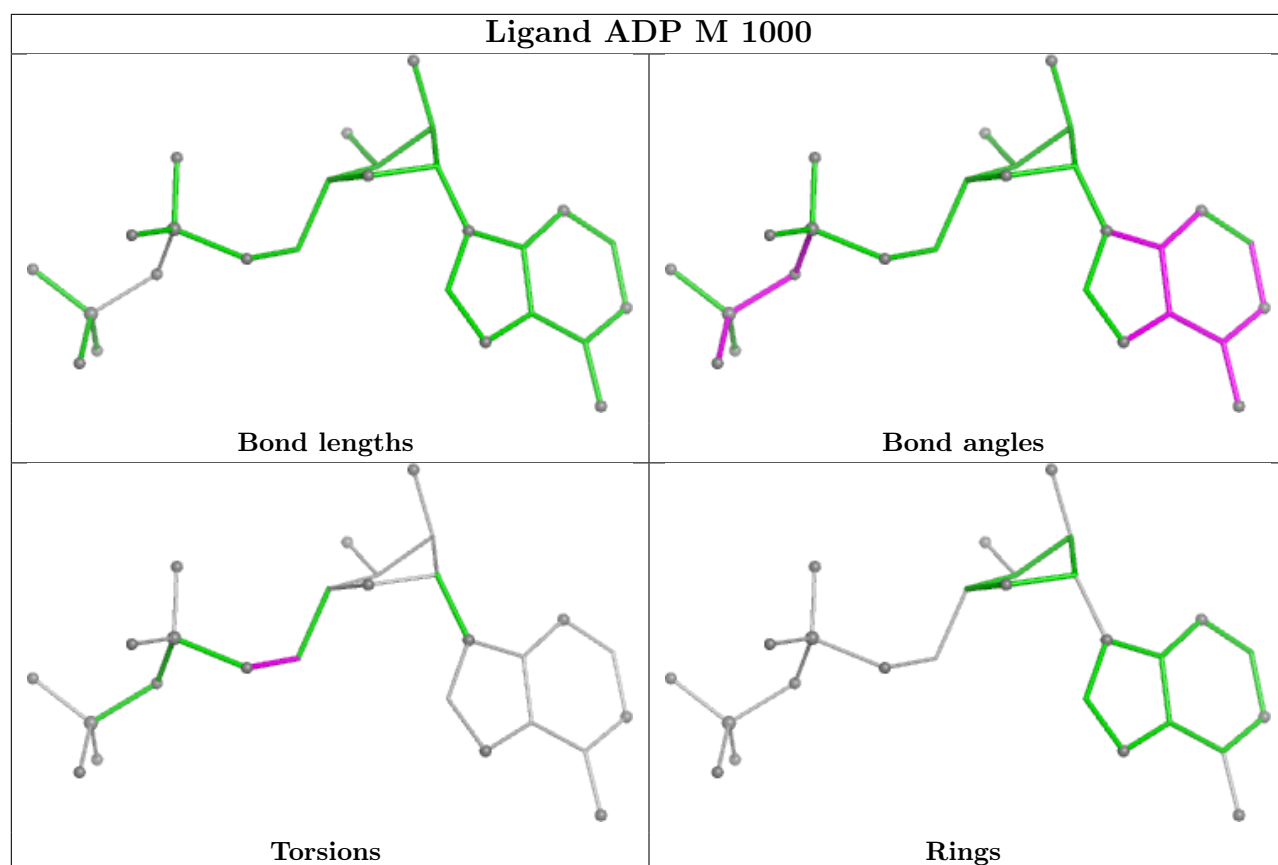
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

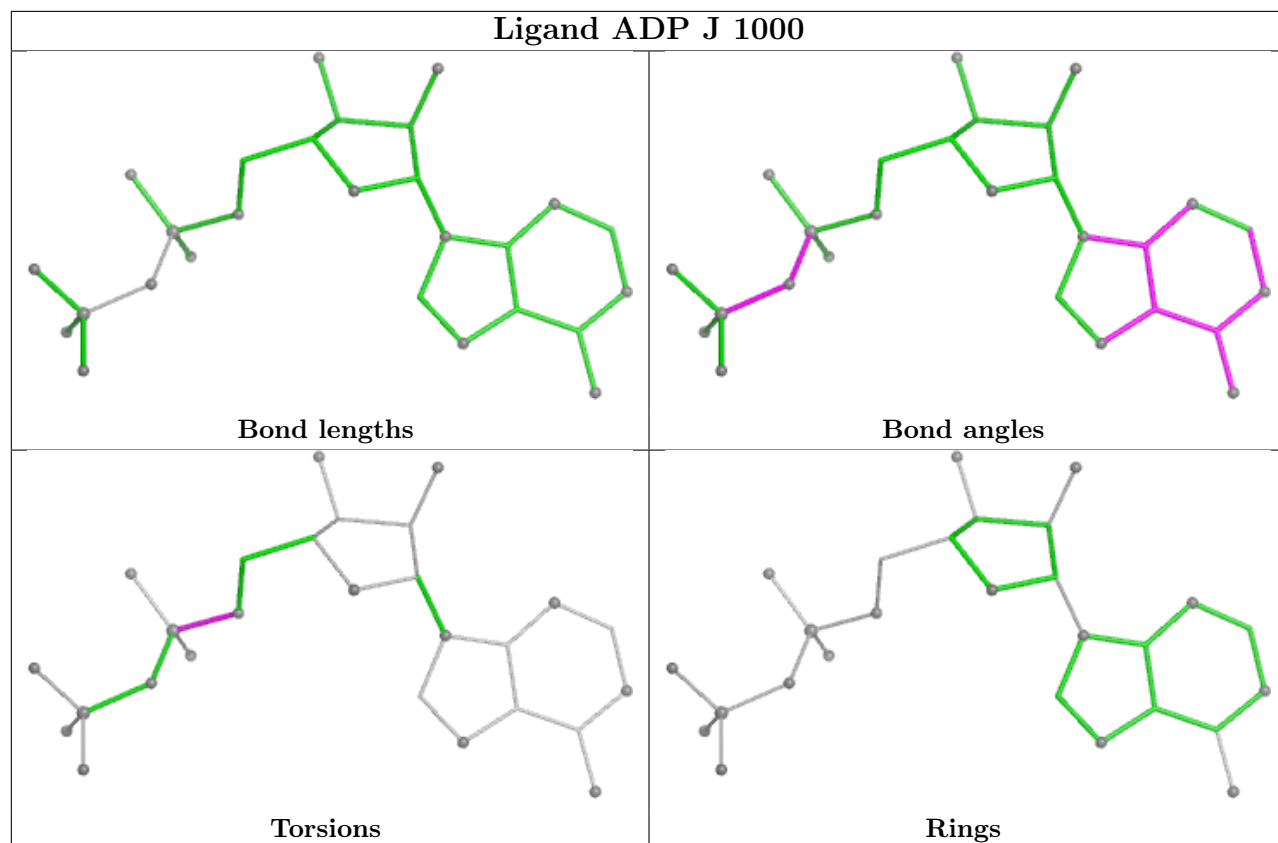












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53608. These allow visual inspection of the internal detail of the map and identification of artifacts.

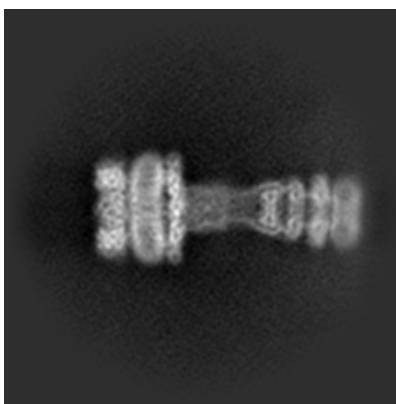
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

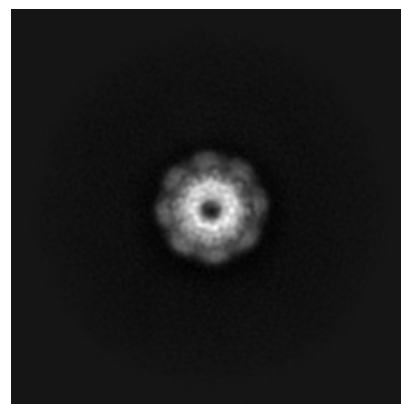
6.1.1 Primary map



X

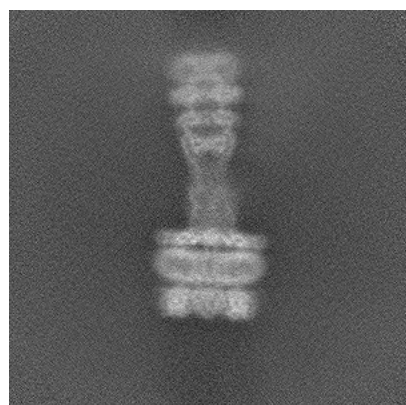


Y

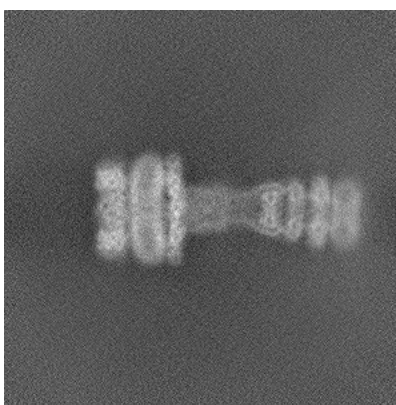


Z

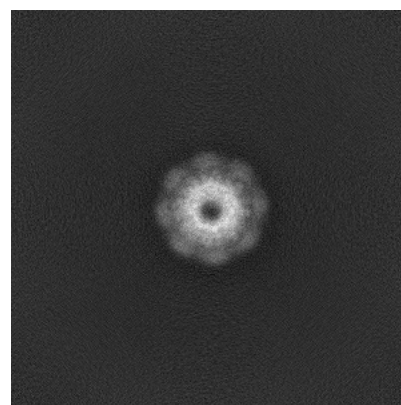
6.1.2 Raw map



X



Y

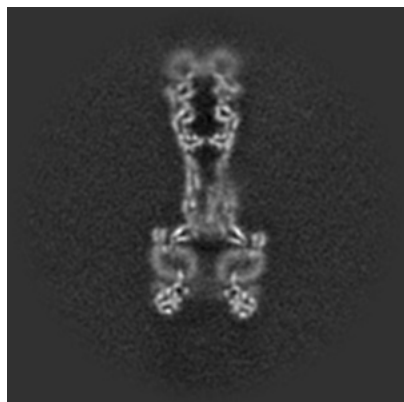


Z

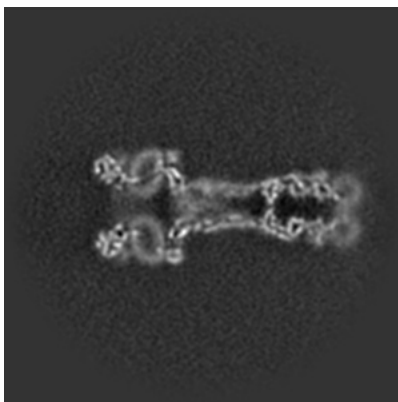
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

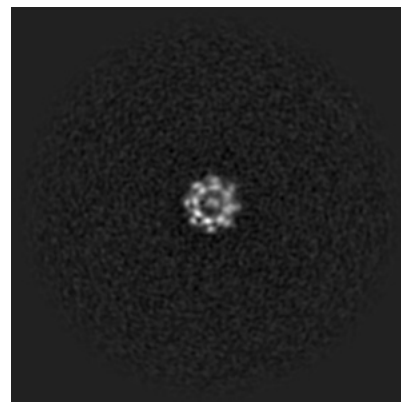
6.2.1 Primary map



X Index: 300

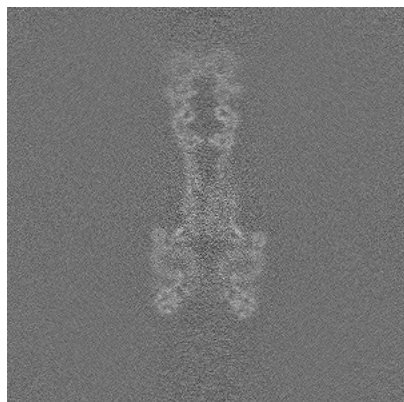


Y Index: 300

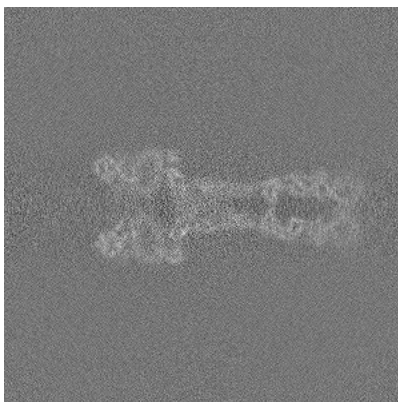


Z Index: 300

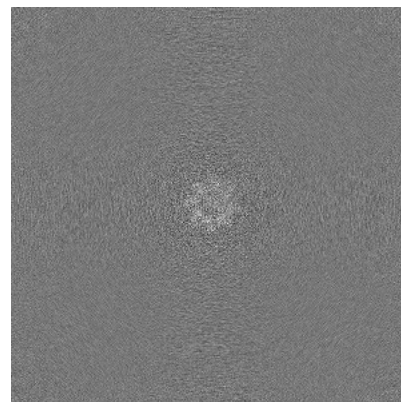
6.2.2 Raw map



X Index: 300



Y Index: 300

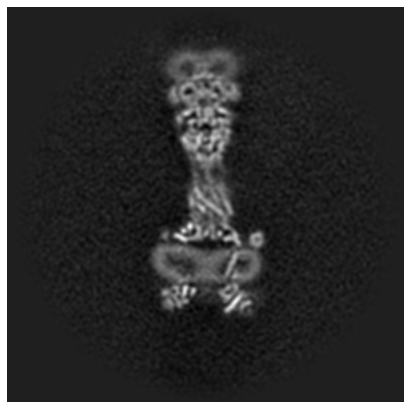


Z Index: 300

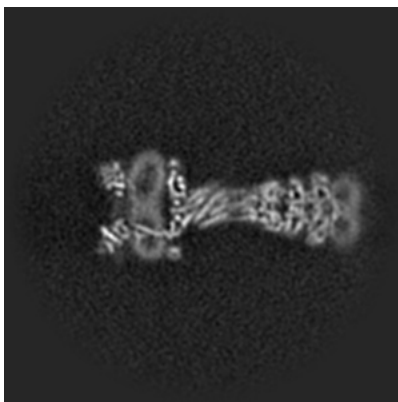
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

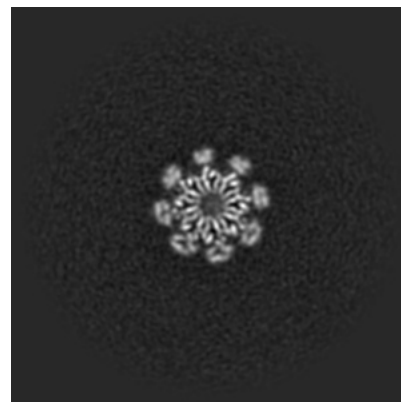
6.3.1 Primary map



X Index: 277

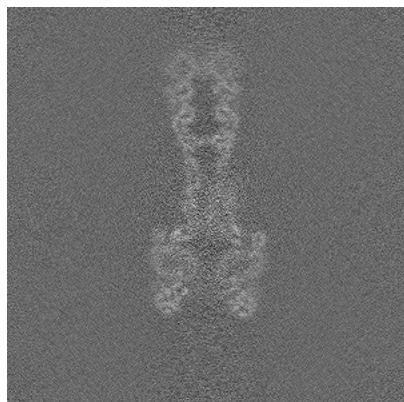


Y Index: 276

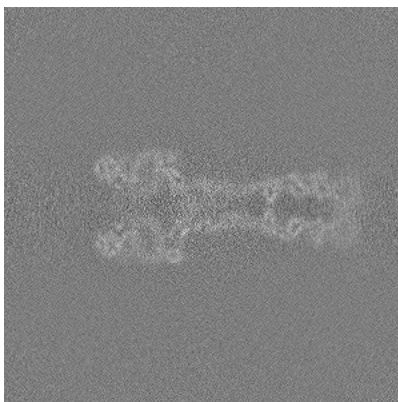


Z Index: 259

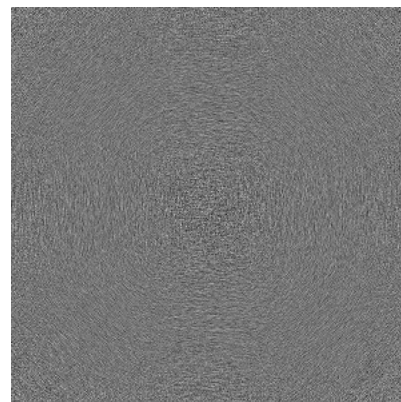
6.3.2 Raw map



X Index: 298



Y Index: 299



Z Index: 0

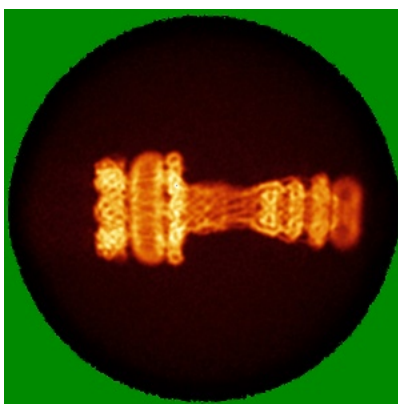
The images above show the largest variance slices of the map in three orthogonal directions.

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

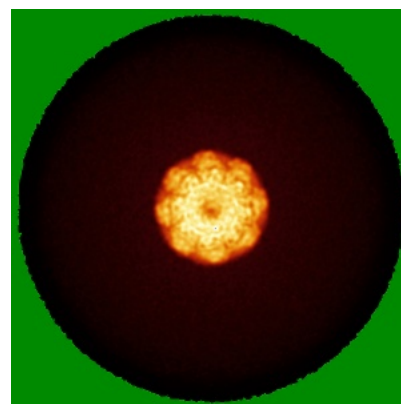
6.4.1 Primary map



X

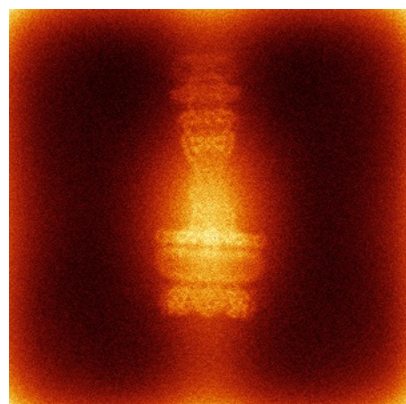


Y

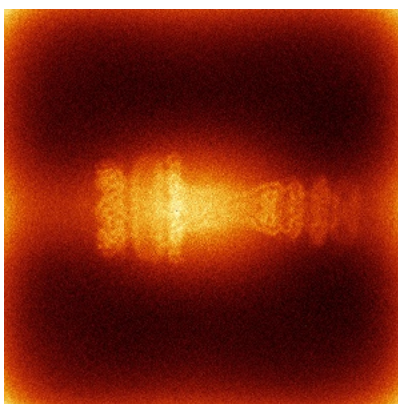


Z

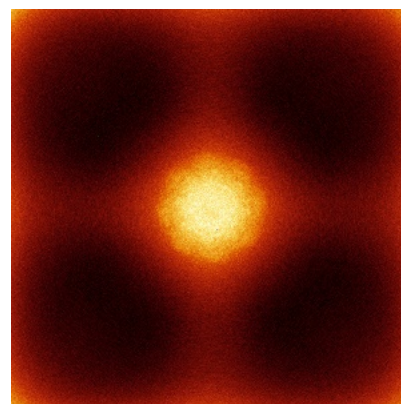
6.4.2 Raw map



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](#)

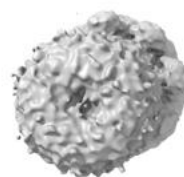
6.5.1 Primary map



X



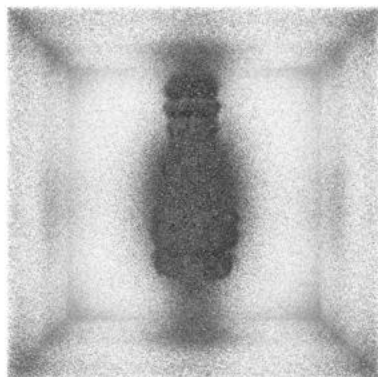
Y



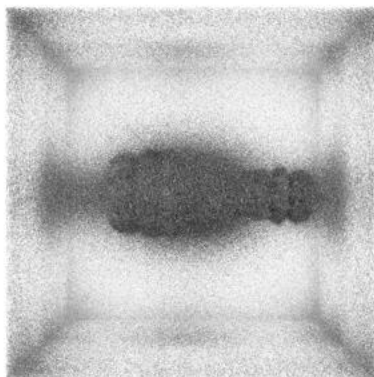
Z

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.

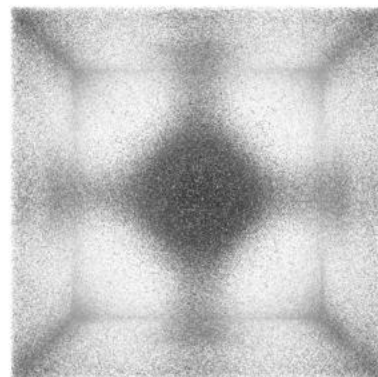
6.5.2 Raw map



X



Y



Z

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.

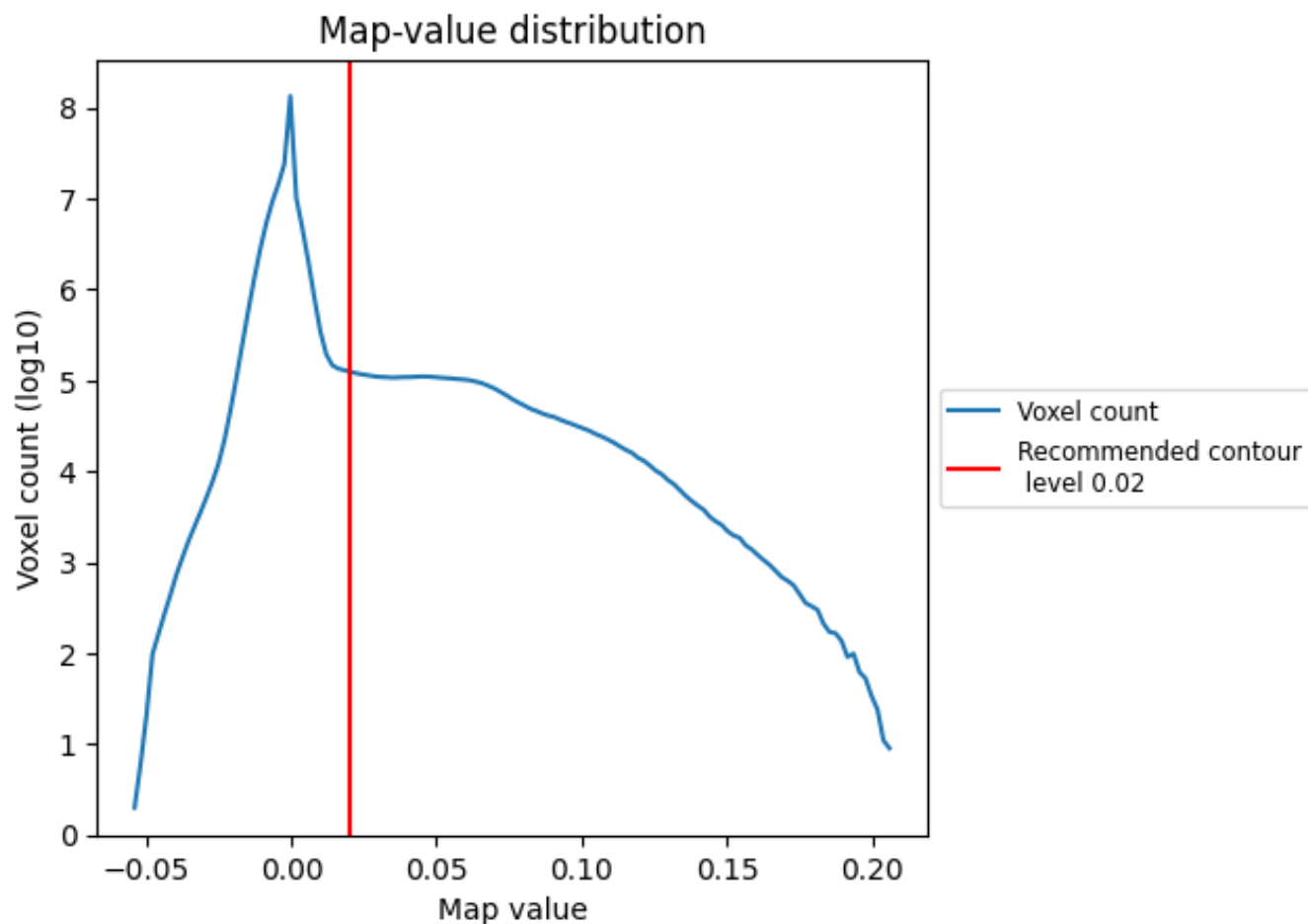
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

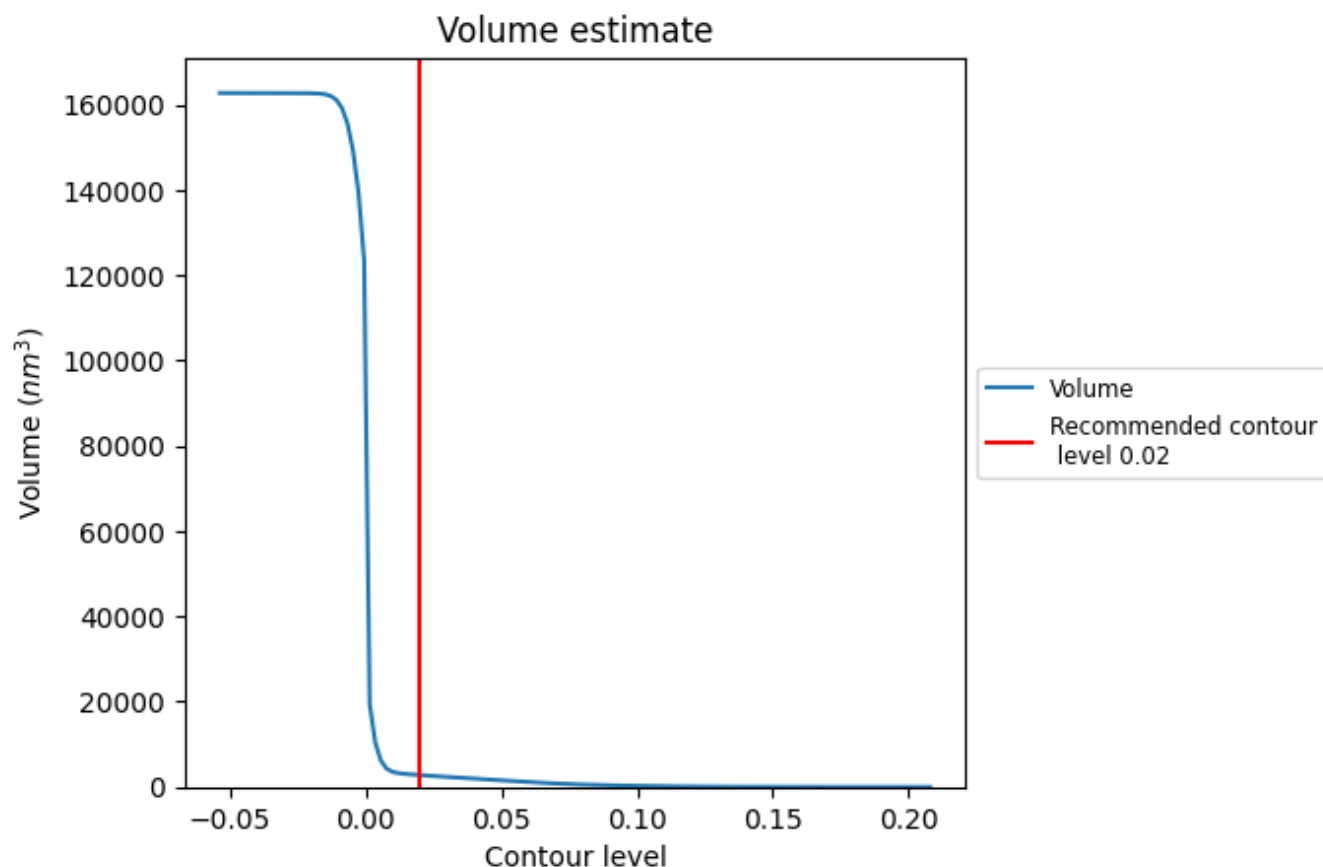
This section contains the results of statistical analysis of the map.

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.

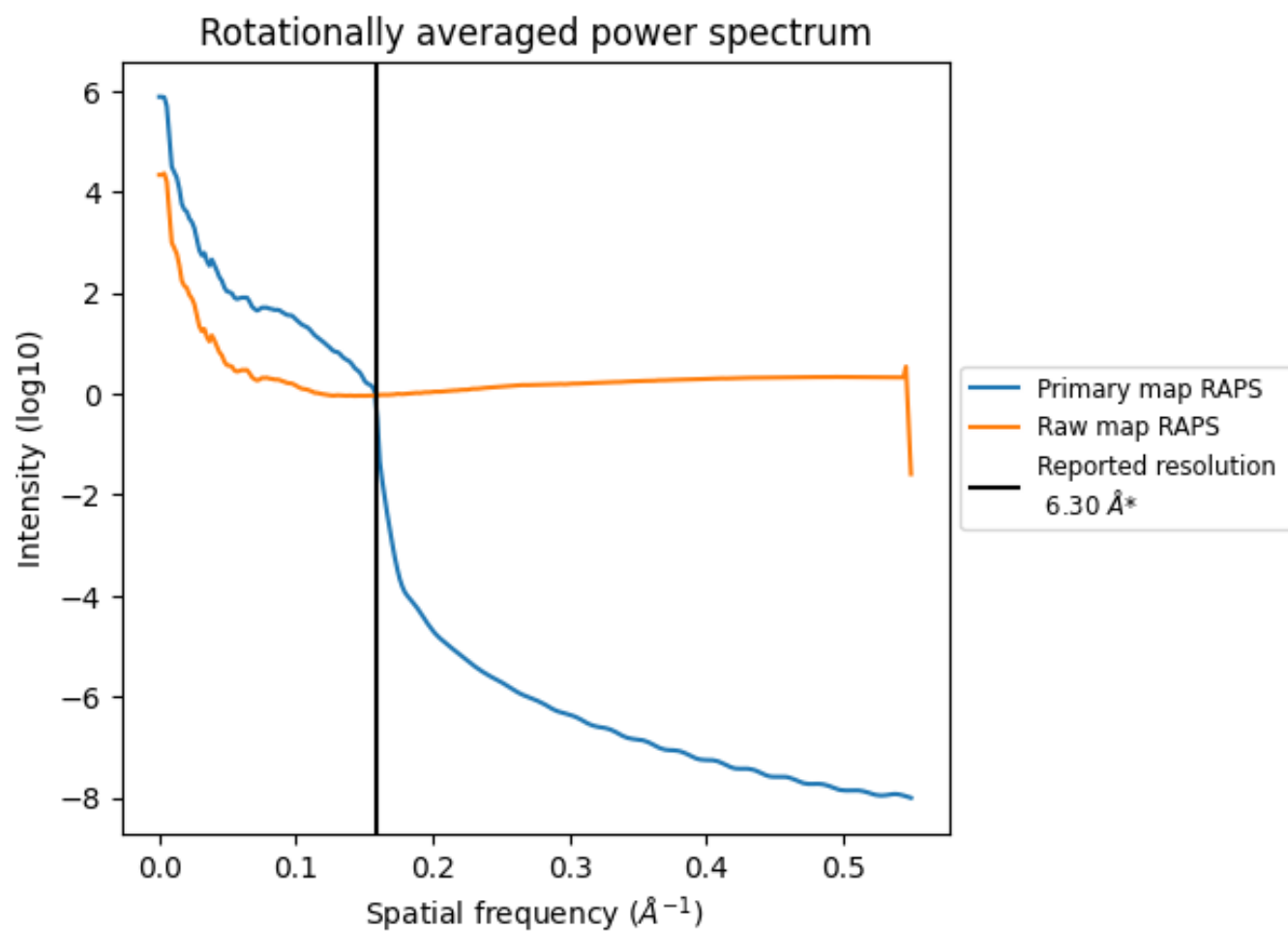
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2782 nm^3 ; this corresponds to an approximate mass of 2513 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 ⓘ

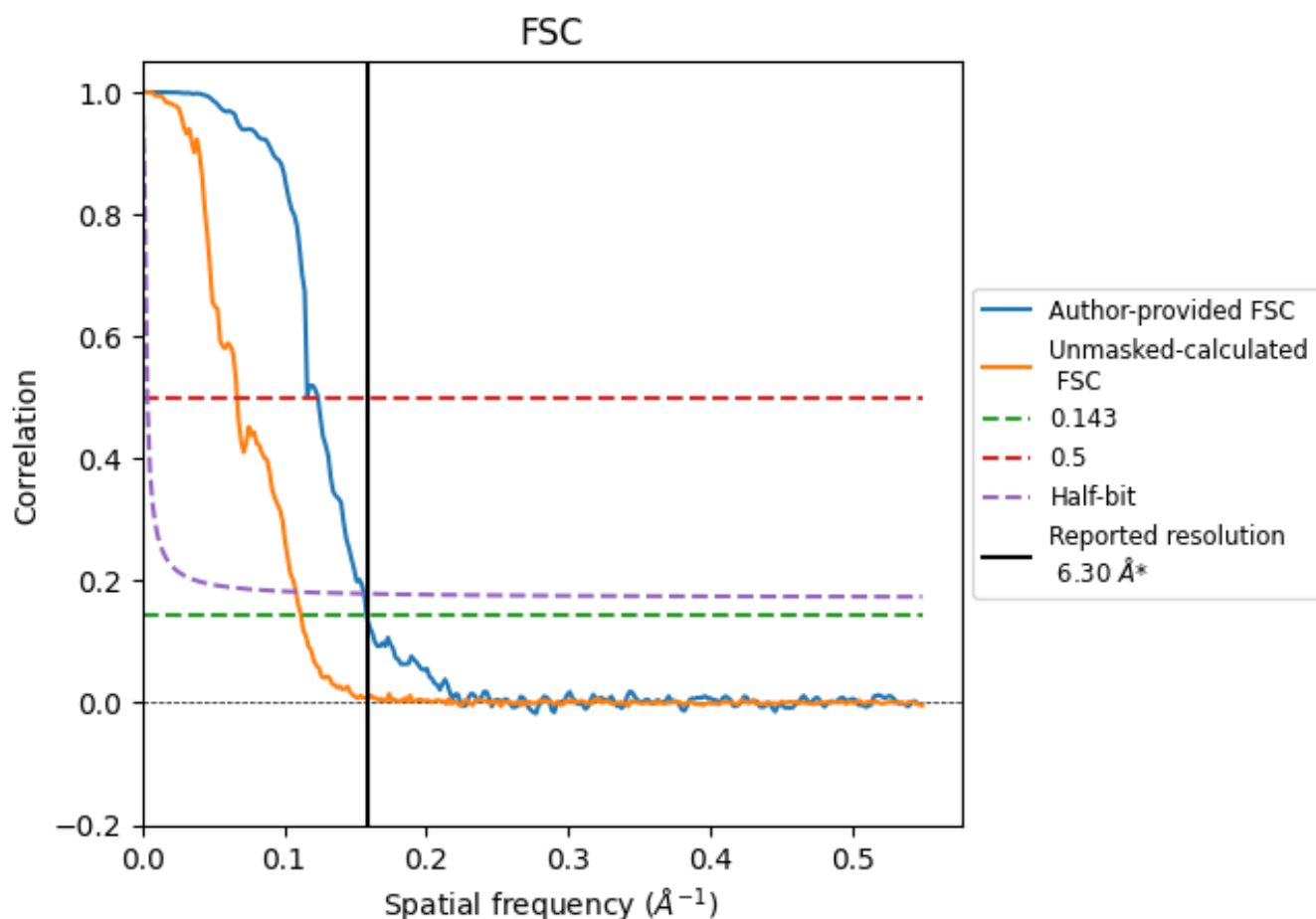


*Reported resolution corresponds to spatial frequency of 0.159 $\text{\AA}^{-1}$

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 $0.159 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.30	-	-
Author-provided FSC curve	6.32	8.08	6.40
Unmasked-calculated*	8.94	14.97	9.24

*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 8.94 differs from the reported value 6.3 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53608 and PDB model 9R6A. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

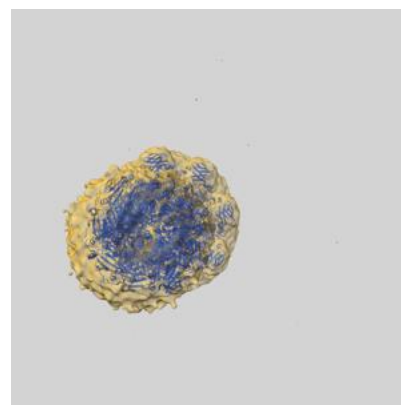
9.1 Map-model overlay [i](#)



X



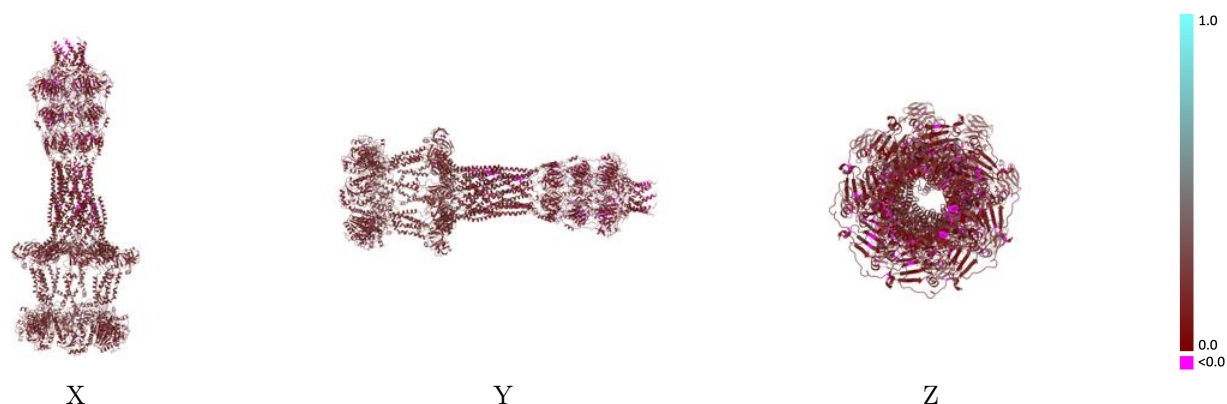
Y



Z

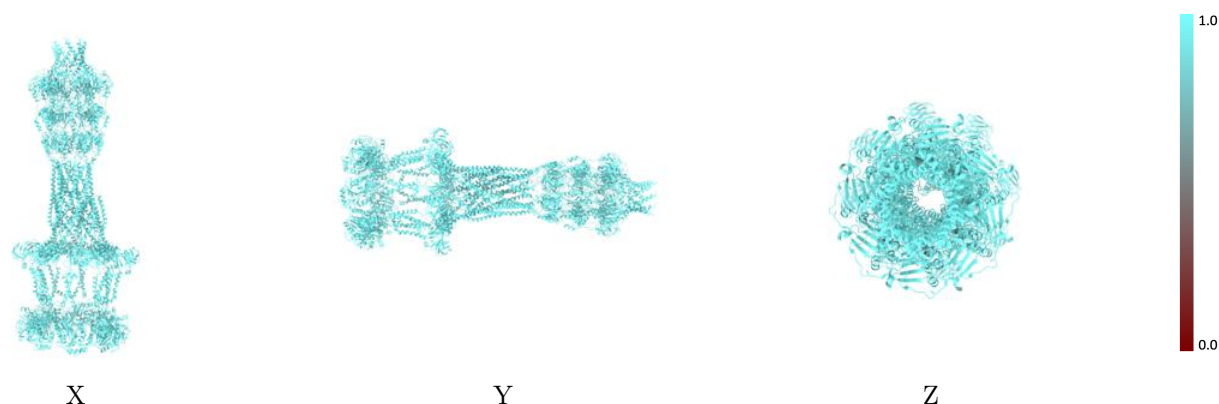
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



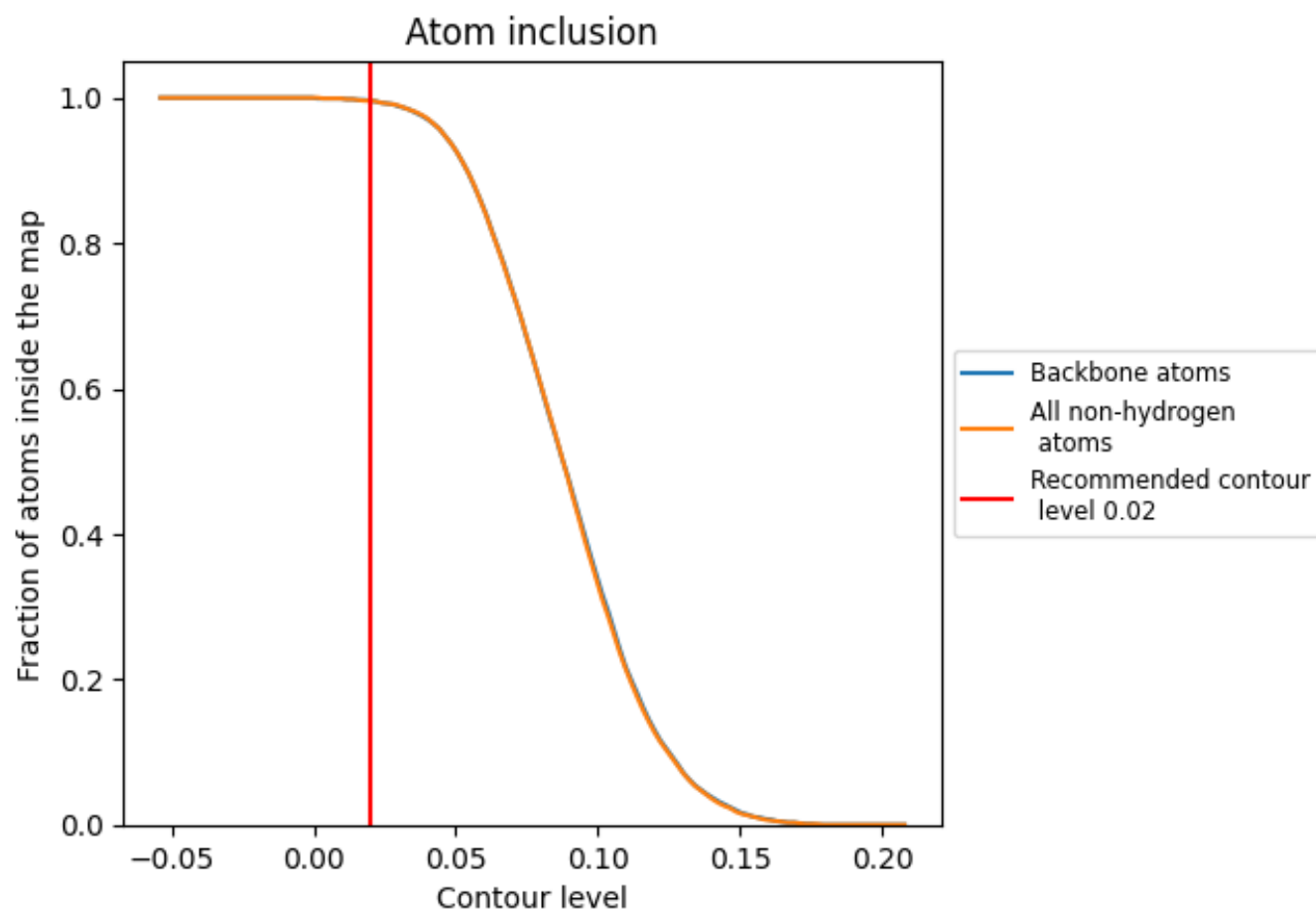
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 100% of all backbone atoms, 100% 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	 0.9960	 0.1870
A	 0.9890	 0.1570
B	 0.9880	 0.1590
C	 0.9880	 0.1640
D	 0.9880	 0.1650
E	 0.9890	 0.1590
F	 0.9890	 0.1630
G	 0.9890	 0.1670
H	 0.9890	 0.1570
I	 0.9980	 0.2050
J	 0.9990	 0.2050
K	 0.9980	 0.2050
L	 0.9990	 0.1990
M	 0.9990	 0.1950
N	 0.9990	 0.1910
O	 0.9990	 0.1990
P	 0.9980	 0.2060

