



## Full wwPDB EM Validation Report ⓘ

Nov 21, 2022 – 08:37 PM EST

PDB ID : 7TFC  
EMDB ID : EMD-25869  
Title : B. subtilis GS(14)-Q-GlnR peptide  
Authors : Travis, B.A.; Peck, J.; Schumacher, M.A.  
Deposited on : 2022-01-06  
Resolution : 1.96 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.3

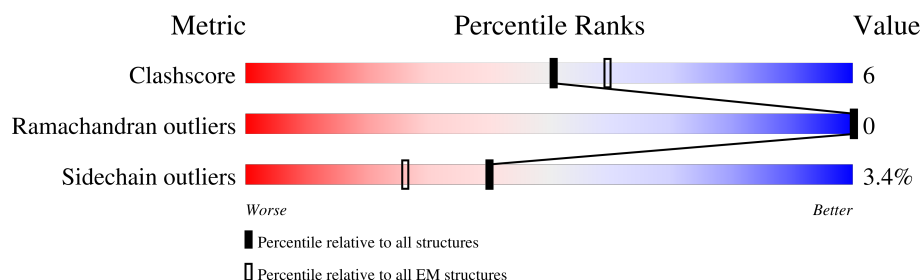
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.96 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	464	<div> <div>12%</div> <div>78%</div> <div>16%</div> <div>• 5%</div> </div>
1	B	464	<div> <div>12%</div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div>
1	C	464	<div> <div>12%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	F	464	<div> <div>12%</div> <div>81%</div> <div>14%</div> <div>• 5%</div> </div>
1	G	464	<div> <div>12%</div> <div>80%</div> <div>15%</div> <div>• 5%</div> </div>
1	H	464	<div> <div>12%</div> <div>79%</div> <div>16%</div> <div>• 5%</div> </div>
1	I	464	<div> <div>12%</div> <div>78%</div> <div>18%</div> <div>5%</div> </div>
1	N	464	<div> <div>12%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	O	464	
1	P	464	
1	Q	464	
1	R	464	
1	S	464	
1	T	464	
2	D	10	
2	E	10	
2	J	10	
2	K	10	
2	L	10	
2	M	10	
2	U	10	
2	V	10	
2	W	10	
2	X	10	
2	Y	10	
2	Z	10	
2	a	10	
2	b	10	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50456 atoms, of which 140 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	B	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	C	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	F	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	G	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	H	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	I	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	N	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	O	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	P	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	Q	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	R	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	S	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		
1	T	443	Total	C	N	O	S	0	0
			3498	2238	587	658	15		

There are 280 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A085CCI2
A	-18	GLY	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	SER	-	expression tag	UNP A0A085CCI2
A	-16	SER	-	expression tag	UNP A0A085CCI2
A	-15	HIS	-	expression tag	UNP A0A085CCI2
A	-14	HIS	-	expression tag	UNP A0A085CCI2
A	-13	HIS	-	expression tag	UNP A0A085CCI2
A	-12	HIS	-	expression tag	UNP A0A085CCI2
A	-11	HIS	-	expression tag	UNP A0A085CCI2
A	-10	HIS	-	expression tag	UNP A0A085CCI2
A	-9	SER	-	expression tag	UNP A0A085CCI2
A	-8	SER	-	expression tag	UNP A0A085CCI2
A	-7	GLY	-	expression tag	UNP A0A085CCI2
A	-6	LEU	-	expression tag	UNP A0A085CCI2
A	-5	VAL	-	expression tag	UNP A0A085CCI2
A	-4	PRO	-	expression tag	UNP A0A085CCI2
A	-3	ARG	-	expression tag	UNP A0A085CCI2
A	-2	GLY	-	expression tag	UNP A0A085CCI2
A	-1	SER	-	expression tag	UNP A0A085CCI2
A	0	HIS	-	expression tag	UNP A0A085CCI2
B	-19	MET	-	initiating methionine	UNP A0A085CCI2
B	-18	GLY	-	expression tag	UNP A0A085CCI2
B	-17	SER	-	expression tag	UNP A0A085CCI2
B	-16	SER	-	expression tag	UNP A0A085CCI2
B	-15	HIS	-	expression tag	UNP A0A085CCI2
B	-14	HIS	-	expression tag	UNP A0A085CCI2
B	-13	HIS	-	expression tag	UNP A0A085CCI2
B	-12	HIS	-	expression tag	UNP A0A085CCI2
B	-11	HIS	-	expression tag	UNP A0A085CCI2
B	-10	HIS	-	expression tag	UNP A0A085CCI2
B	-9	SER	-	expression tag	UNP A0A085CCI2
B	-8	SER	-	expression tag	UNP A0A085CCI2
B	-7	GLY	-	expression tag	UNP A0A085CCI2
B	-6	LEU	-	expression tag	UNP A0A085CCI2
B	-5	VAL	-	expression tag	UNP A0A085CCI2
B	-4	PRO	-	expression tag	UNP A0A085CCI2
B	-3	ARG	-	expression tag	UNP A0A085CCI2
B	-2	GLY	-	expression tag	UNP A0A085CCI2
B	-1	SER	-	expression tag	UNP A0A085CCI2
B	0	HIS	-	expression tag	UNP A0A085CCI2
C	-19	MET	-	initiating methionine	UNP A0A085CCI2
C	-18	GLY	-	expression tag	UNP A0A085CCI2
C	-17	SER	-	expression tag	UNP A0A085CCI2
C	-16	SER	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	HIS	-	expression tag	UNP A0A085CCI2
C	-14	HIS	-	expression tag	UNP A0A085CCI2
C	-13	HIS	-	expression tag	UNP A0A085CCI2
C	-12	HIS	-	expression tag	UNP A0A085CCI2
C	-11	HIS	-	expression tag	UNP A0A085CCI2
C	-10	HIS	-	expression tag	UNP A0A085CCI2
C	-9	SER	-	expression tag	UNP A0A085CCI2
C	-8	SER	-	expression tag	UNP A0A085CCI2
C	-7	GLY	-	expression tag	UNP A0A085CCI2
C	-6	LEU	-	expression tag	UNP A0A085CCI2
C	-5	VAL	-	expression tag	UNP A0A085CCI2
C	-4	PRO	-	expression tag	UNP A0A085CCI2
C	-3	ARG	-	expression tag	UNP A0A085CCI2
C	-2	GLY	-	expression tag	UNP A0A085CCI2
C	-1	SER	-	expression tag	UNP A0A085CCI2
C	0	HIS	-	expression tag	UNP A0A085CCI2
F	-19	MET	-	initiating methionine	UNP A0A085CCI2
F	-18	GLY	-	expression tag	UNP A0A085CCI2
F	-17	SER	-	expression tag	UNP A0A085CCI2
F	-16	SER	-	expression tag	UNP A0A085CCI2
F	-15	HIS	-	expression tag	UNP A0A085CCI2
F	-14	HIS	-	expression tag	UNP A0A085CCI2
F	-13	HIS	-	expression tag	UNP A0A085CCI2
F	-12	HIS	-	expression tag	UNP A0A085CCI2
F	-11	HIS	-	expression tag	UNP A0A085CCI2
F	-10	HIS	-	expression tag	UNP A0A085CCI2
F	-9	SER	-	expression tag	UNP A0A085CCI2
F	-8	SER	-	expression tag	UNP A0A085CCI2
F	-7	GLY	-	expression tag	UNP A0A085CCI2
F	-6	LEU	-	expression tag	UNP A0A085CCI2
F	-5	VAL	-	expression tag	UNP A0A085CCI2
F	-4	PRO	-	expression tag	UNP A0A085CCI2
F	-3	ARG	-	expression tag	UNP A0A085CCI2
F	-2	GLY	-	expression tag	UNP A0A085CCI2
F	-1	SER	-	expression tag	UNP A0A085CCI2
F	0	HIS	-	expression tag	UNP A0A085CCI2
G	-19	MET	-	initiating methionine	UNP A0A085CCI2
G	-18	GLY	-	expression tag	UNP A0A085CCI2
G	-17	SER	-	expression tag	UNP A0A085CCI2
G	-16	SER	-	expression tag	UNP A0A085CCI2
G	-15	HIS	-	expression tag	UNP A0A085CCI2
G	-14	HIS	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A085CCI2
G	-12	HIS	-	expression tag	UNP A0A085CCI2
G	-11	HIS	-	expression tag	UNP A0A085CCI2
G	-10	HIS	-	expression tag	UNP A0A085CCI2
G	-9	SER	-	expression tag	UNP A0A085CCI2
G	-8	SER	-	expression tag	UNP A0A085CCI2
G	-7	GLY	-	expression tag	UNP A0A085CCI2
G	-6	LEU	-	expression tag	UNP A0A085CCI2
G	-5	VAL	-	expression tag	UNP A0A085CCI2
G	-4	PRO	-	expression tag	UNP A0A085CCI2
G	-3	ARG	-	expression tag	UNP A0A085CCI2
G	-2	GLY	-	expression tag	UNP A0A085CCI2
G	-1	SER	-	expression tag	UNP A0A085CCI2
G	0	HIS	-	expression tag	UNP A0A085CCI2
H	-19	MET	-	initiating methionine	UNP A0A085CCI2
H	-18	GLY	-	expression tag	UNP A0A085CCI2
H	-17	SER	-	expression tag	UNP A0A085CCI2
H	-16	SER	-	expression tag	UNP A0A085CCI2
H	-15	HIS	-	expression tag	UNP A0A085CCI2
H	-14	HIS	-	expression tag	UNP A0A085CCI2
H	-13	HIS	-	expression tag	UNP A0A085CCI2
H	-12	HIS	-	expression tag	UNP A0A085CCI2
H	-11	HIS	-	expression tag	UNP A0A085CCI2
H	-10	HIS	-	expression tag	UNP A0A085CCI2
H	-9	SER	-	expression tag	UNP A0A085CCI2
H	-8	SER	-	expression tag	UNP A0A085CCI2
H	-7	GLY	-	expression tag	UNP A0A085CCI2
H	-6	LEU	-	expression tag	UNP A0A085CCI2
H	-5	VAL	-	expression tag	UNP A0A085CCI2
H	-4	PRO	-	expression tag	UNP A0A085CCI2
H	-3	ARG	-	expression tag	UNP A0A085CCI2
H	-2	GLY	-	expression tag	UNP A0A085CCI2
H	-1	SER	-	expression tag	UNP A0A085CCI2
H	0	HIS	-	expression tag	UNP A0A085CCI2
I	-19	MET	-	initiating methionine	UNP A0A085CCI2
I	-18	GLY	-	expression tag	UNP A0A085CCI2
I	-17	SER	-	expression tag	UNP A0A085CCI2
I	-16	SER	-	expression tag	UNP A0A085CCI2
I	-15	HIS	-	expression tag	UNP A0A085CCI2
I	-14	HIS	-	expression tag	UNP A0A085CCI2
I	-13	HIS	-	expression tag	UNP A0A085CCI2
I	-12	HIS	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP A0A085CCI2
I	-10	HIS	-	expression tag	UNP A0A085CCI2
I	-9	SER	-	expression tag	UNP A0A085CCI2
I	-8	SER	-	expression tag	UNP A0A085CCI2
I	-7	GLY	-	expression tag	UNP A0A085CCI2
I	-6	LEU	-	expression tag	UNP A0A085CCI2
I	-5	VAL	-	expression tag	UNP A0A085CCI2
I	-4	PRO	-	expression tag	UNP A0A085CCI2
I	-3	ARG	-	expression tag	UNP A0A085CCI2
I	-2	GLY	-	expression tag	UNP A0A085CCI2
I	-1	SER	-	expression tag	UNP A0A085CCI2
I	0	HIS	-	expression tag	UNP A0A085CCI2
N	-19	MET	-	initiating methionine	UNP A0A085CCI2
N	-18	GLY	-	expression tag	UNP A0A085CCI2
N	-17	SER	-	expression tag	UNP A0A085CCI2
N	-16	SER	-	expression tag	UNP A0A085CCI2
N	-15	HIS	-	expression tag	UNP A0A085CCI2
N	-14	HIS	-	expression tag	UNP A0A085CCI2
N	-13	HIS	-	expression tag	UNP A0A085CCI2
N	-12	HIS	-	expression tag	UNP A0A085CCI2
N	-11	HIS	-	expression tag	UNP A0A085CCI2
N	-10	HIS	-	expression tag	UNP A0A085CCI2
N	-9	SER	-	expression tag	UNP A0A085CCI2
N	-8	SER	-	expression tag	UNP A0A085CCI2
N	-7	GLY	-	expression tag	UNP A0A085CCI2
N	-6	LEU	-	expression tag	UNP A0A085CCI2
N	-5	VAL	-	expression tag	UNP A0A085CCI2
N	-4	PRO	-	expression tag	UNP A0A085CCI2
N	-3	ARG	-	expression tag	UNP A0A085CCI2
N	-2	GLY	-	expression tag	UNP A0A085CCI2
N	-1	SER	-	expression tag	UNP A0A085CCI2
N	0	HIS	-	expression tag	UNP A0A085CCI2
O	-19	MET	-	initiating methionine	UNP A0A085CCI2
O	-18	GLY	-	expression tag	UNP A0A085CCI2
O	-17	SER	-	expression tag	UNP A0A085CCI2
O	-16	SER	-	expression tag	UNP A0A085CCI2
O	-15	HIS	-	expression tag	UNP A0A085CCI2
O	-14	HIS	-	expression tag	UNP A0A085CCI2
O	-13	HIS	-	expression tag	UNP A0A085CCI2
O	-12	HIS	-	expression tag	UNP A0A085CCI2
O	-11	HIS	-	expression tag	UNP A0A085CCI2
O	-10	HIS	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-9	SER	-	expression tag	UNP A0A085CCI2
O	-8	SER	-	expression tag	UNP A0A085CCI2
O	-7	GLY	-	expression tag	UNP A0A085CCI2
O	-6	LEU	-	expression tag	UNP A0A085CCI2
O	-5	VAL	-	expression tag	UNP A0A085CCI2
O	-4	PRO	-	expression tag	UNP A0A085CCI2
O	-3	ARG	-	expression tag	UNP A0A085CCI2
O	-2	GLY	-	expression tag	UNP A0A085CCI2
O	-1	SER	-	expression tag	UNP A0A085CCI2
O	0	HIS	-	expression tag	UNP A0A085CCI2
P	-19	MET	-	initiating methionine	UNP A0A085CCI2
P	-18	GLY	-	expression tag	UNP A0A085CCI2
P	-17	SER	-	expression tag	UNP A0A085CCI2
P	-16	SER	-	expression tag	UNP A0A085CCI2
P	-15	HIS	-	expression tag	UNP A0A085CCI2
P	-14	HIS	-	expression tag	UNP A0A085CCI2
P	-13	HIS	-	expression tag	UNP A0A085CCI2
P	-12	HIS	-	expression tag	UNP A0A085CCI2
P	-11	HIS	-	expression tag	UNP A0A085CCI2
P	-10	HIS	-	expression tag	UNP A0A085CCI2
P	-9	SER	-	expression tag	UNP A0A085CCI2
P	-8	SER	-	expression tag	UNP A0A085CCI2
P	-7	GLY	-	expression tag	UNP A0A085CCI2
P	-6	LEU	-	expression tag	UNP A0A085CCI2
P	-5	VAL	-	expression tag	UNP A0A085CCI2
P	-4	PRO	-	expression tag	UNP A0A085CCI2
P	-3	ARG	-	expression tag	UNP A0A085CCI2
P	-2	GLY	-	expression tag	UNP A0A085CCI2
P	-1	SER	-	expression tag	UNP A0A085CCI2
P	0	HIS	-	expression tag	UNP A0A085CCI2
Q	-19	MET	-	initiating methionine	UNP A0A085CCI2
Q	-18	GLY	-	expression tag	UNP A0A085CCI2
Q	-17	SER	-	expression tag	UNP A0A085CCI2
Q	-16	SER	-	expression tag	UNP A0A085CCI2
Q	-15	HIS	-	expression tag	UNP A0A085CCI2
Q	-14	HIS	-	expression tag	UNP A0A085CCI2
Q	-13	HIS	-	expression tag	UNP A0A085CCI2
Q	-12	HIS	-	expression tag	UNP A0A085CCI2
Q	-11	HIS	-	expression tag	UNP A0A085CCI2
Q	-10	HIS	-	expression tag	UNP A0A085CCI2
Q	-9	SER	-	expression tag	UNP A0A085CCI2
Q	-8	SER	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	-7	GLY	-	expression tag	UNP A0A085CCI2
Q	-6	LEU	-	expression tag	UNP A0A085CCI2
Q	-5	VAL	-	expression tag	UNP A0A085CCI2
Q	-4	PRO	-	expression tag	UNP A0A085CCI2
Q	-3	ARG	-	expression tag	UNP A0A085CCI2
Q	-2	GLY	-	expression tag	UNP A0A085CCI2
Q	-1	SER	-	expression tag	UNP A0A085CCI2
Q	0	HIS	-	expression tag	UNP A0A085CCI2
R	-19	MET	-	initiating methionine	UNP A0A085CCI2
R	-18	GLY	-	expression tag	UNP A0A085CCI2
R	-17	SER	-	expression tag	UNP A0A085CCI2
R	-16	SER	-	expression tag	UNP A0A085CCI2
R	-15	HIS	-	expression tag	UNP A0A085CCI2
R	-14	HIS	-	expression tag	UNP A0A085CCI2
R	-13	HIS	-	expression tag	UNP A0A085CCI2
R	-12	HIS	-	expression tag	UNP A0A085CCI2
R	-11	HIS	-	expression tag	UNP A0A085CCI2
R	-10	HIS	-	expression tag	UNP A0A085CCI2
R	-9	SER	-	expression tag	UNP A0A085CCI2
R	-8	SER	-	expression tag	UNP A0A085CCI2
R	-7	GLY	-	expression tag	UNP A0A085CCI2
R	-6	LEU	-	expression tag	UNP A0A085CCI2
R	-5	VAL	-	expression tag	UNP A0A085CCI2
R	-4	PRO	-	expression tag	UNP A0A085CCI2
R	-3	ARG	-	expression tag	UNP A0A085CCI2
R	-2	GLY	-	expression tag	UNP A0A085CCI2
R	-1	SER	-	expression tag	UNP A0A085CCI2
R	0	HIS	-	expression tag	UNP A0A085CCI2
S	-19	MET	-	initiating methionine	UNP A0A085CCI2
S	-18	GLY	-	expression tag	UNP A0A085CCI2
S	-17	SER	-	expression tag	UNP A0A085CCI2
S	-16	SER	-	expression tag	UNP A0A085CCI2
S	-15	HIS	-	expression tag	UNP A0A085CCI2
S	-14	HIS	-	expression tag	UNP A0A085CCI2
S	-13	HIS	-	expression tag	UNP A0A085CCI2
S	-12	HIS	-	expression tag	UNP A0A085CCI2
S	-11	HIS	-	expression tag	UNP A0A085CCI2
S	-10	HIS	-	expression tag	UNP A0A085CCI2
S	-9	SER	-	expression tag	UNP A0A085CCI2
S	-8	SER	-	expression tag	UNP A0A085CCI2
S	-7	GLY	-	expression tag	UNP A0A085CCI2
S	-6	LEU	-	expression tag	UNP A0A085CCI2

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-5	VAL	-	expression tag	UNP A0A085CCI2
S	-4	PRO	-	expression tag	UNP A0A085CCI2
S	-3	ARG	-	expression tag	UNP A0A085CCI2
S	-2	GLY	-	expression tag	UNP A0A085CCI2
S	-1	SER	-	expression tag	UNP A0A085CCI2
S	0	HIS	-	expression tag	UNP A0A085CCI2
T	-19	MET	-	initiating methionine	UNP A0A085CCI2
T	-18	GLY	-	expression tag	UNP A0A085CCI2
T	-17	SER	-	expression tag	UNP A0A085CCI2
T	-16	SER	-	expression tag	UNP A0A085CCI2
T	-15	HIS	-	expression tag	UNP A0A085CCI2
T	-14	HIS	-	expression tag	UNP A0A085CCI2
T	-13	HIS	-	expression tag	UNP A0A085CCI2
T	-12	HIS	-	expression tag	UNP A0A085CCI2
T	-11	HIS	-	expression tag	UNP A0A085CCI2
T	-10	HIS	-	expression tag	UNP A0A085CCI2
T	-9	SER	-	expression tag	UNP A0A085CCI2
T	-8	SER	-	expression tag	UNP A0A085CCI2
T	-7	GLY	-	expression tag	UNP A0A085CCI2
T	-6	LEU	-	expression tag	UNP A0A085CCI2
T	-5	VAL	-	expression tag	UNP A0A085CCI2
T	-4	PRO	-	expression tag	UNP A0A085CCI2
T	-3	ARG	-	expression tag	UNP A0A085CCI2
T	-2	GLY	-	expression tag	UNP A0A085CCI2
T	-1	SER	-	expression tag	UNP A0A085CCI2
T	0	HIS	-	expression tag	UNP A0A085CCI2

- Molecule 2 is a protein called GlnR C-tail peptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	E	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	J	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	K	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	L	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	M	10	Total	C	N	O	S	0	0
			84	52	17	14	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	U	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	V	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	W	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	X	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	Y	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	Z	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	a	10	Total	C	N	O	S	0	0
			84	52	17	14	1		
2	b	10	Total	C	N	O	S	0	0
			84	52	17	14	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

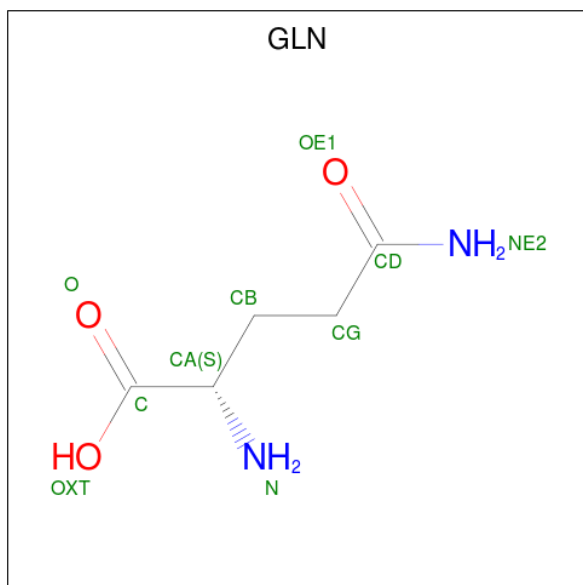
Mol	Chain	Residues	Atoms		AltConf
3	A	2	Total	Mg	0
			2	2	
3	B	2	Total	Mg	0
			2	2	
3	C	2	Total	Mg	0
			2	2	
3	F	2	Total	Mg	0
			2	2	
3	G	2	Total	Mg	0
			2	2	
3	H	2	Total	Mg	0
			2	2	
3	I	2	Total	Mg	0
			2	2	
3	N	2	Total	Mg	0
			2	2	
3	O	2	Total	Mg	0
			2	2	
3	P	2	Total	Mg	0
			2	2	
3	Q	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
3	R	2	Total	Mg	0
			2	2	
3	S	2	Total	Mg	0
			2	2	
3	T	2	Total	Mg	0
			2	2	

- Molecule 4 is GLUTAMINE (three-letter code: GLN) (formula: C<sub>5</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>).




Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	B	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	C	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	F	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	G	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	H	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	I	1	Total	C	H	N	O	0
			20	5	10	2	3	
4	N	1	Total	C	H	N	O	0
			20	5	10	2	3	

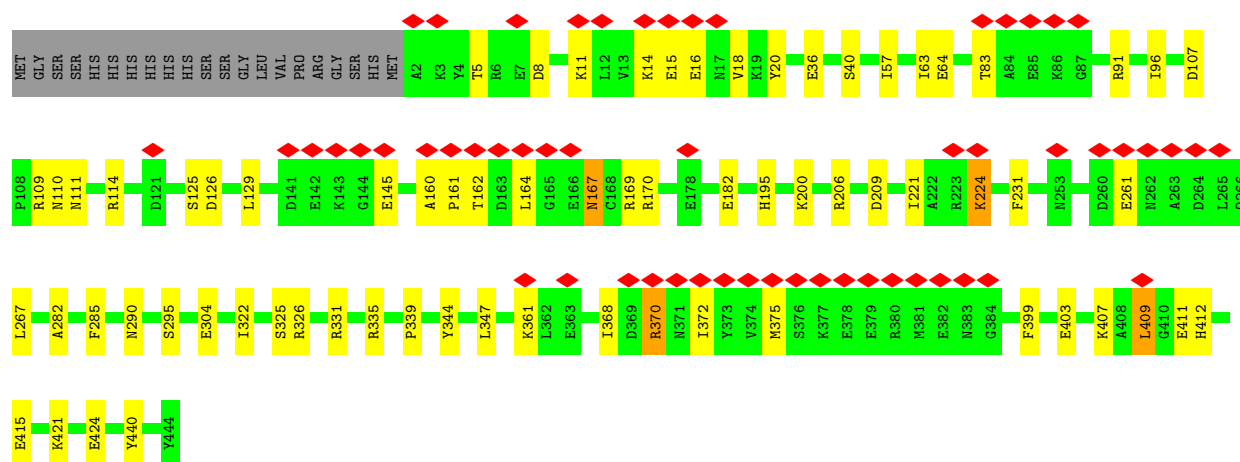
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Mol	Chain	Residues	Atoms					AltConf
4	O	1	Total 20	C 5	H 10	N 2	O 3	0
4	P	1	Total 20	C 5	H 10	N 2	O 3	0
4	Q	1	Total 20	C 5	H 10	N 2	O 3	0
4	R	1	Total 20	C 5	H 10	N 2	O 3	0
4	S	1	Total 20	C 5	H 10	N 2	O 3	0
4	T	1	Total 20	C 5	H 10	N 2	O 3	0

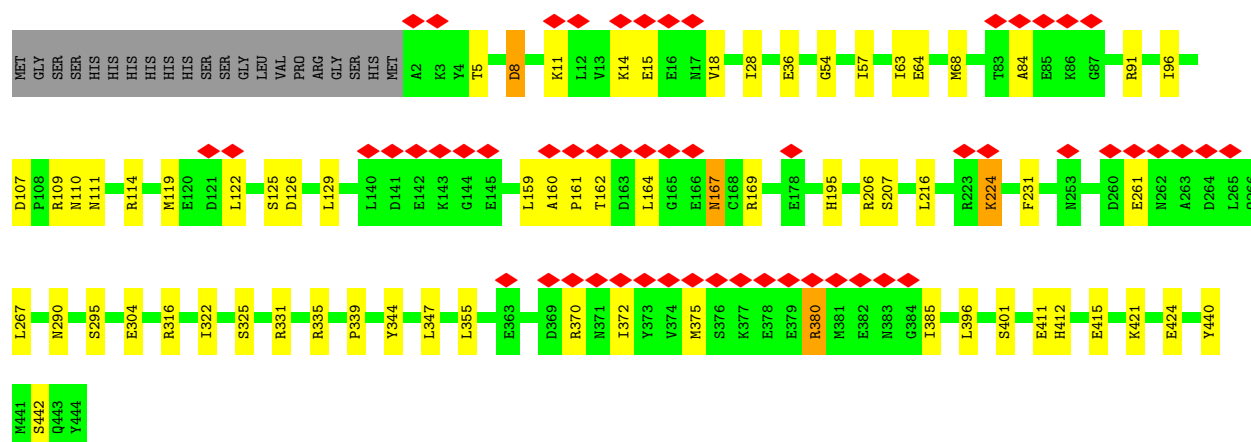


Chain C: 




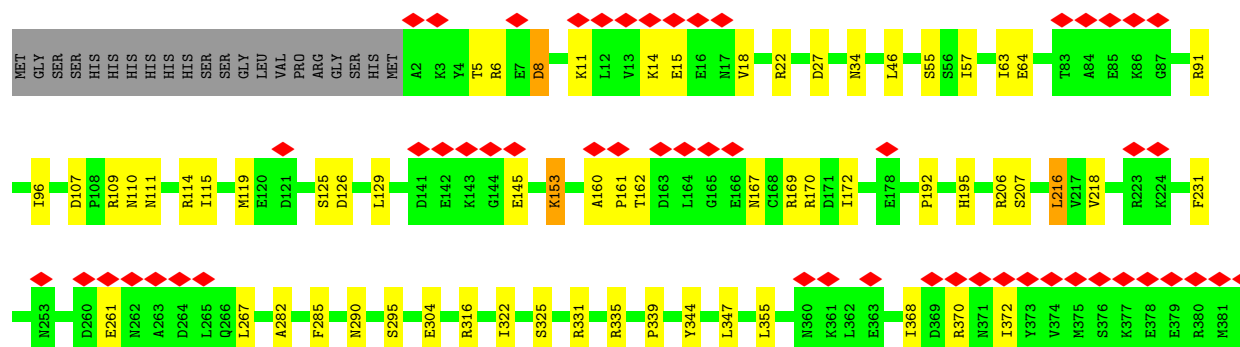
• Molecule 1: Glutamine synthetase

Chain F: 



• Molecule 1: Glutamine synthetase

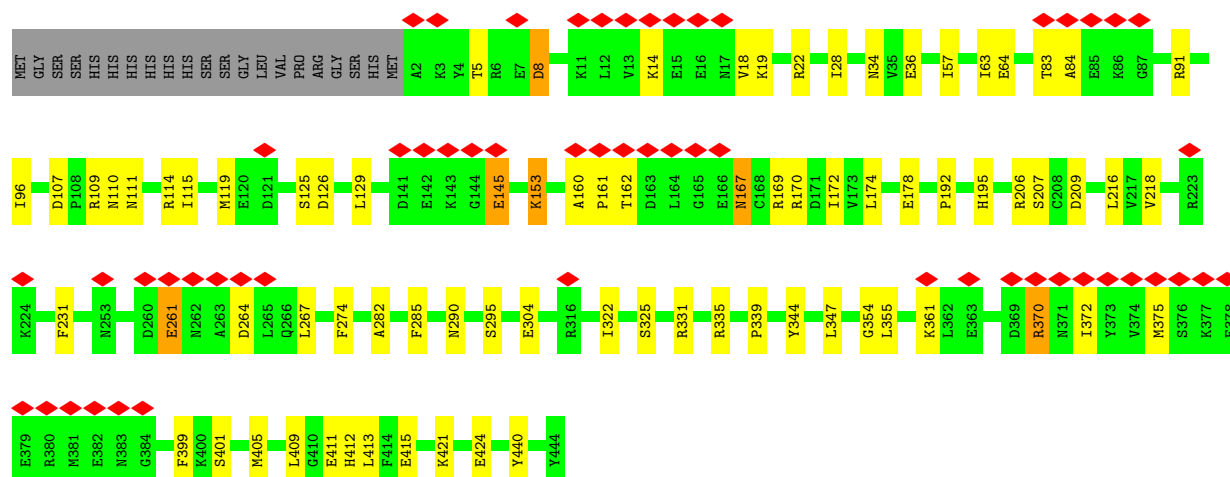
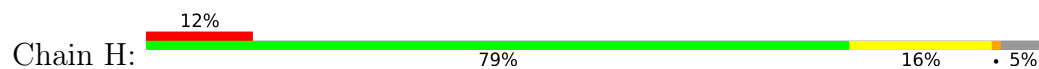
Chain G: 



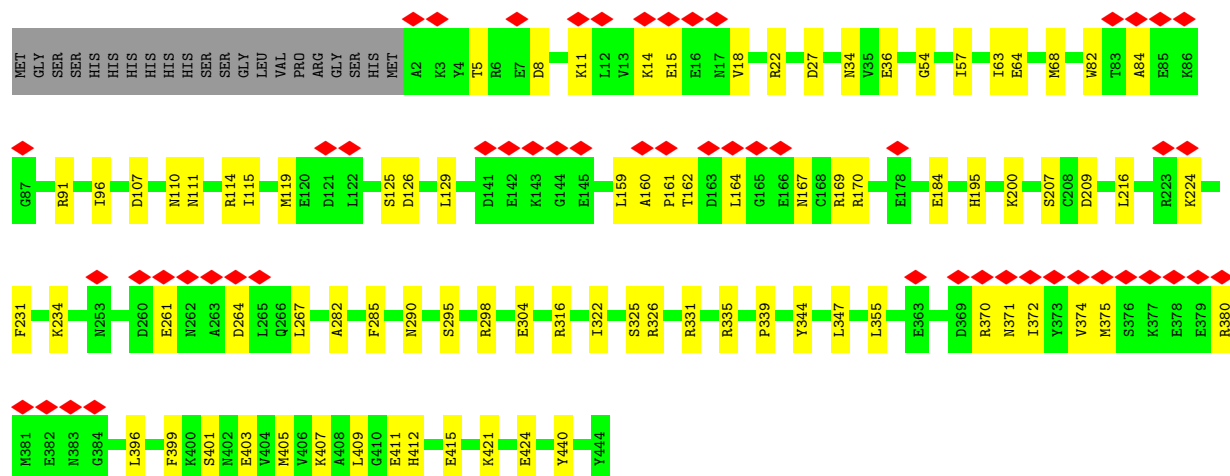
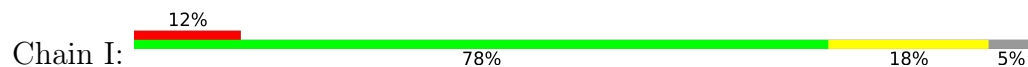




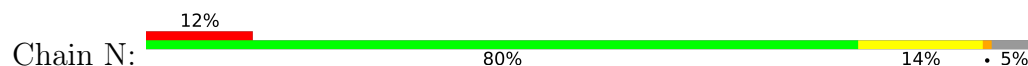
• Molecule 1: Glutamine synthetase

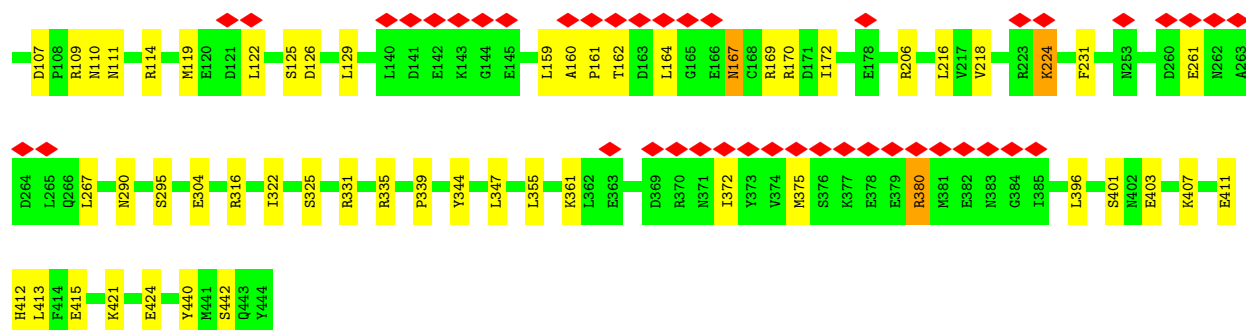


• Molecule 1: Glutamine synthetase

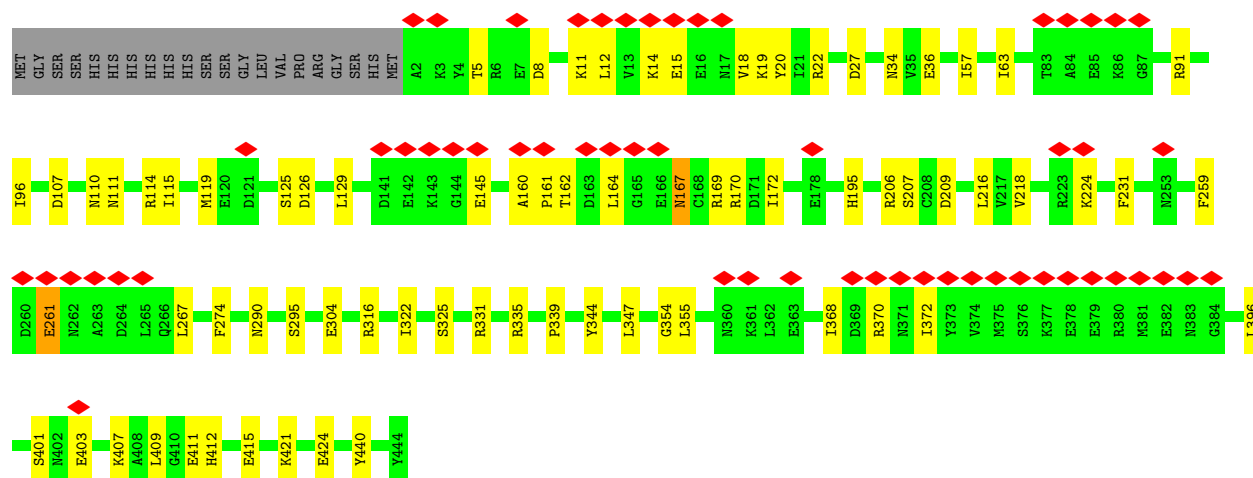
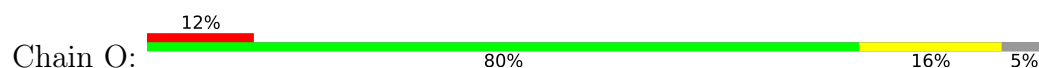


• Molecule 1: Glutamine synthetase

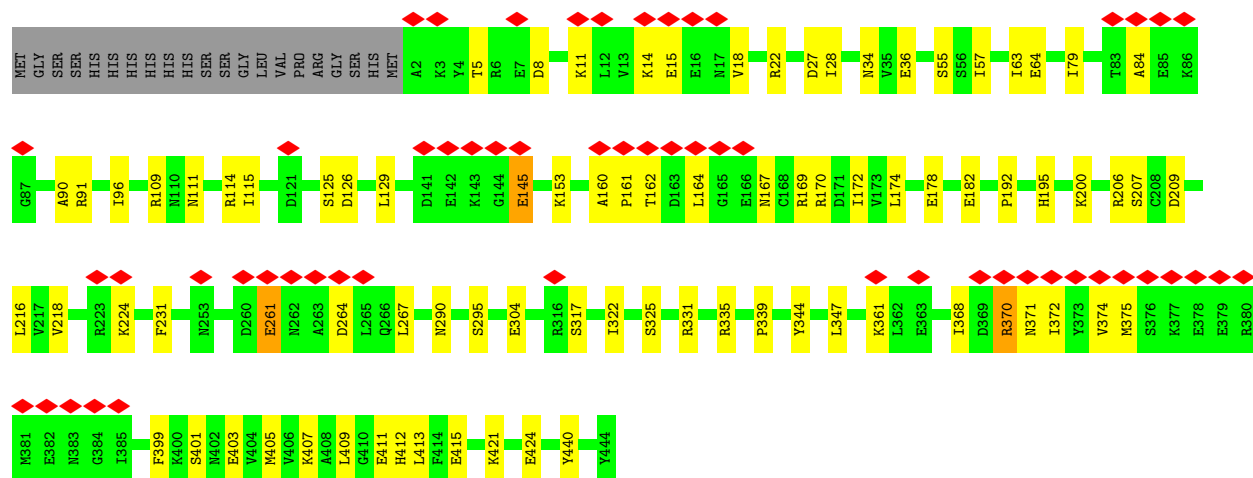
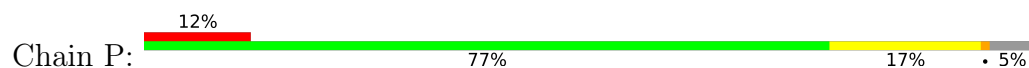




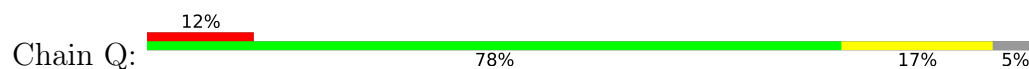
• Molecule 1: Glutamine synthetase



• Molecule 1: Glutamine synthetase

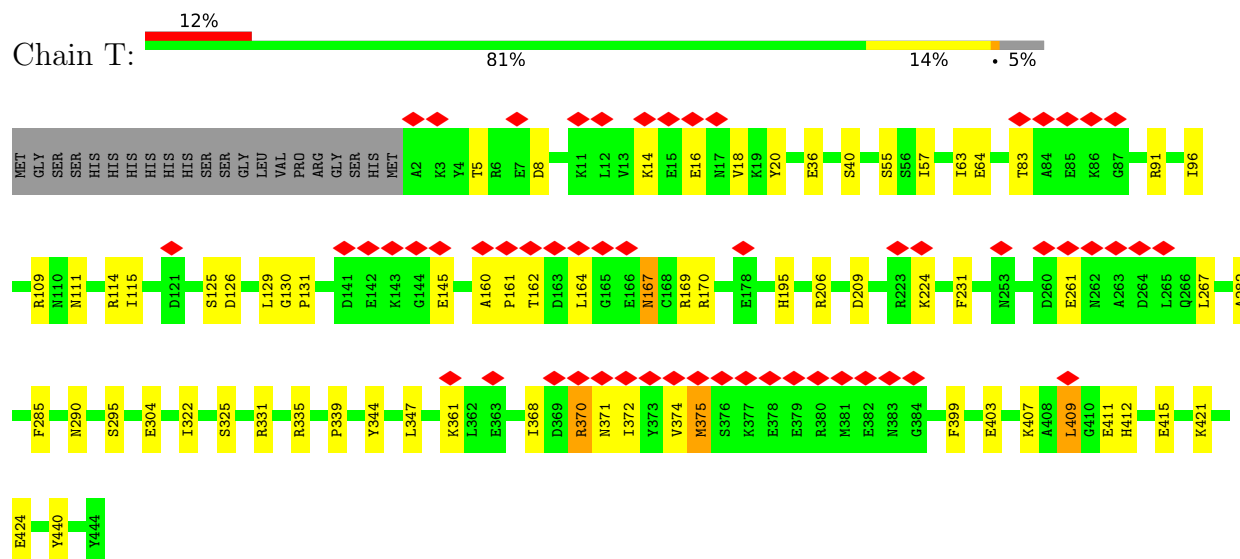


• Molecule 1: Glutamine synthetase

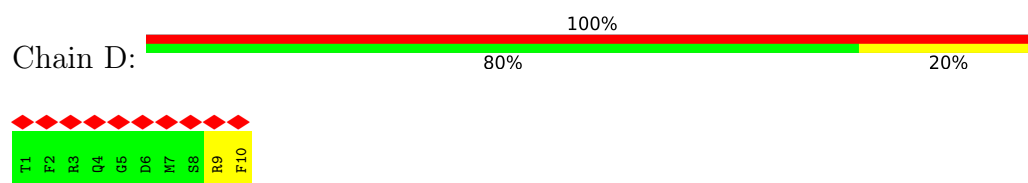




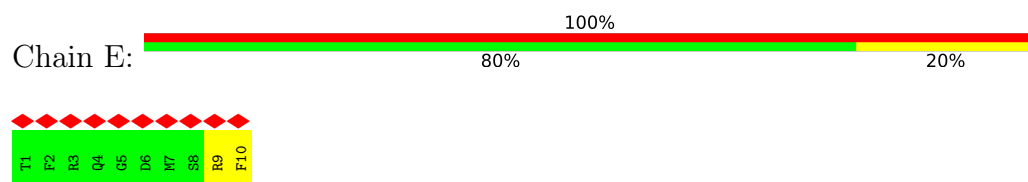
## • Molecule 1: Glutamine synthetase



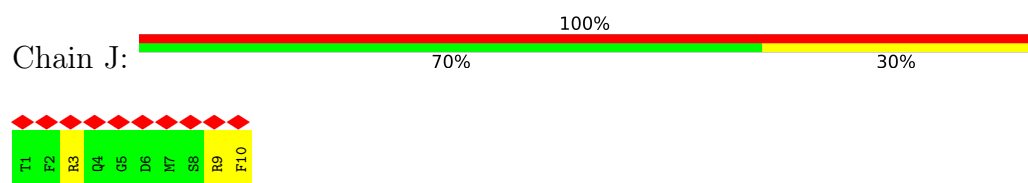
## • Molecule 2: GlnR C-tail peptide



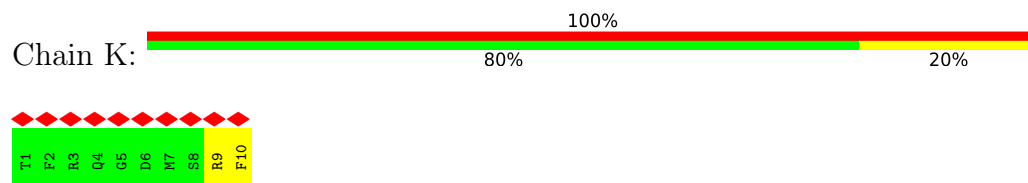
## • Molecule 2: GlnR C-tail peptide



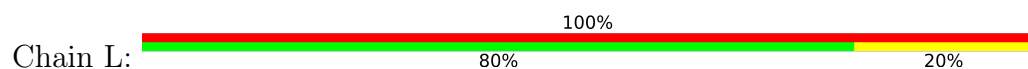
## • Molecule 2: GlnR C-tail peptide



## • Molecule 2: GlnR C-tail peptide

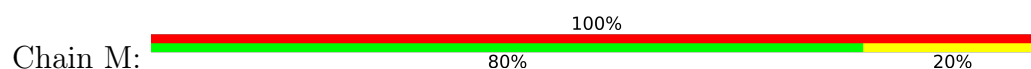


## • Molecule 2: GlnR C-tail peptide





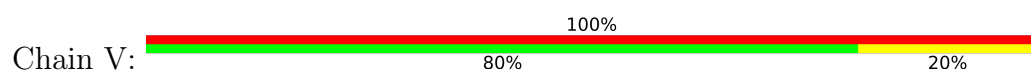
- Molecule 2: GlnR C-tail peptide



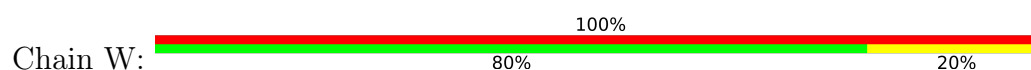
- Molecule 2: GlnR C-tail peptide



- Molecule 2: GlnR C-tail peptide



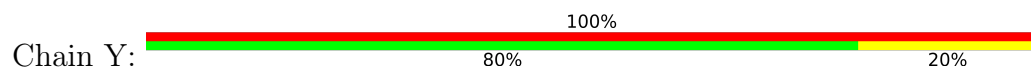
- Molecule 2: GlnR C-tail peptide



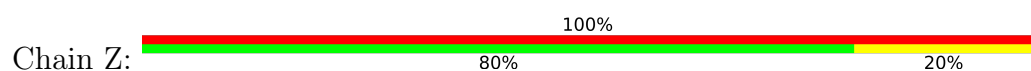
- Molecule 2: GlnR C-tail peptide

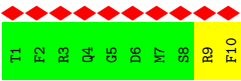


- Molecule 2: GlnR C-tail peptide

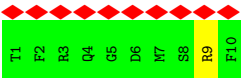
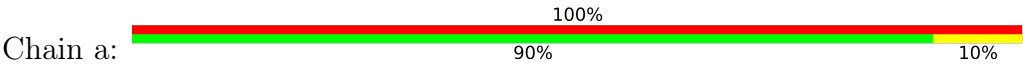


- Molecule 2: GlnR C-tail peptide

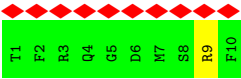
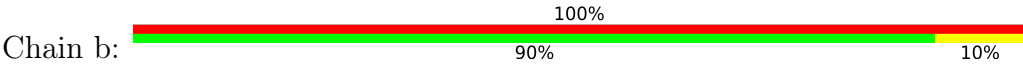




● Molecule 2: GlnR C-tail peptide



● Molecule 2: GlnR C-tail peptide



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D7	Depositor
Number of particles used	1376404	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	43.74	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	5.138	Depositor
Minimum map value	-3.115	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.120	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.26	0/3581	0.48	0/4852
1	B	0.26	0/3581	0.49	0/4852
1	C	0.26	0/3581	0.48	0/4852
1	F	0.26	0/3581	0.48	0/4852
1	G	0.26	0/3581	0.47	0/4852
1	H	0.26	0/3581	0.49	0/4852
1	I	0.26	0/3581	0.48	0/4852
1	N	0.25	0/3581	0.48	0/4852
1	O	0.26	0/3581	0.48	0/4852
1	P	0.26	0/3581	0.48	0/4852
1	Q	0.26	0/3581	0.48	0/4852
1	R	0.26	0/3581	0.49	0/4852
1	S	0.26	0/3581	0.48	0/4852
1	T	0.26	0/3581	0.49	0/4852
2	D	0.33	0/85	0.56	0/110
2	E	0.26	0/85	0.60	0/110
2	J	0.25	0/85	0.60	0/110
2	K	0.25	0/85	0.60	0/110
2	L	0.26	0/85	0.59	0/110
2	M	0.26	0/85	0.60	0/110
2	U	0.25	0/85	0.59	0/110
2	V	0.26	0/85	0.59	0/110
2	W	0.25	0/85	0.60	0/110
2	X	0.33	0/85	0.53	0/110
2	Y	0.25	0/85	0.60	0/110
2	Z	0.26	0/85	0.60	0/110
2	a	0.26	0/85	0.60	0/110
2	b	0.26	0/85	0.58	0/110
All	All	0.26	0/51324	0.48	0/69468

There are no bond length outliers.



There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3498	0	3406	50	0
1	B	3498	0	3406	45	0
1	C	3498	0	3406	42	0
1	F	3498	0	3406	38	0
1	G	3498	0	3406	45	0
1	H	3498	0	3406	47	0
1	I	3498	0	3406	49	0
1	N	3498	0	3406	42	0
1	O	3498	0	3406	47	0
1	P	3498	0	3406	52	0
1	Q	3498	0	3406	50	0
1	R	3498	0	3406	49	0
1	S	3498	0	3406	43	0
1	T	3498	0	3406	44	0
2	D	84	0	77	1	0
2	E	84	0	77	1	0
2	J	84	0	77	2	0
2	K	84	0	77	1	0
2	L	84	0	77	1	0
2	M	84	0	77	1	0
2	U	84	0	77	2	0
2	V	84	0	77	1	0
2	W	84	0	77	1	0
2	X	84	0	77	2	0
2	Y	84	0	77	1	0
2	Z	84	0	77	1	0
2	a	84	0	77	0	0
2	b	84	0	77	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	2	0	0	0	0
3	S	2	0	0	0	0
3	T	2	0	0	0	0
4	A	10	10	7	0	0
4	B	10	10	7	0	0
4	C	10	10	7	0	0
4	F	10	10	7	0	0
4	G	10	10	7	0	0
4	H	10	10	7	0	0
4	I	10	10	7	0	0
4	N	10	10	7	0	0
4	O	10	10	7	0	0
4	P	10	10	7	0	0
4	Q	10	10	7	0	0
4	R	10	10	7	0	0
4	S	10	10	7	0	0
4	T	10	10	7	0	0
All	All	50316	140	48860	584	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 6.

All (584) 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:R:11:LYS:NZ	1:R:15:GLU:OE2	2.20	0.75
1:R:403:GLU:OE2	1:R:407:LYS:NZ	2.20	0.75
1:I:11:LYS:NZ	1:I:15:GLU:OE2	2.22	0.73
1:A:370:ARG:HH22	1:A:372:ILE:HA	1.54	0.72
1:P:403:GLU:OE2	1:P:407:LYS:NZ	2.20	0.72
1:T:370:ARG:NH2	1:T:375:MET:SD	2.63	0.71
1:Q:22:ARG:HH11	1:Q:34:ASN:HD21	1.39	0.71
1:B:403:GLU:OE2	1:B:407:LYS:NZ	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:ILE:HD11	1:N:413:LEU:HD22	1.75	0.69
1:G:11:LYS:NZ	1:G:15:GLU:OE2	2.25	0.68
1:H:22:ARG:HH11	1:H:34:ASN:HD21	1.42	0.68
1:P:5:THR:OG1	1:P:8:ASP:OD1	2.13	0.67
1:B:11:LYS:NZ	1:B:15:GLU:OE2	2.27	0.66
1:I:5:THR:OG1	1:I:8:ASP:OD1	2.14	0.66
1:H:5:THR:OG1	1:H:8:ASP:OD1	2.14	0.66
1:R:191:ALA:HB2	1:R:240:ASN:HB2	1.77	0.65
1:G:5:THR:OG1	1:G:8:ASP:OD1	2.14	0.65
1:C:5:THR:OG1	1:C:8:ASP:OD1	2.13	0.65
1:P:22:ARG:HH11	1:P:34:ASN:HD21	1.42	0.65
1:O:5:THR:OG1	1:O:8:ASP:OD1	2.14	0.64
1:S:5:THR:OG1	1:S:8:ASP:OD1	2.13	0.64
1:R:5:THR:OG1	1:R:8:ASP:OD1	2.15	0.64
1:S:169:ARG:NH1	1:T:36:GLU:OE1	2.31	0.64
1:R:304:GLU:O	1:R:335:ARG:NH2	2.31	0.64
1:Q:5:THR:OG1	1:Q:8:ASP:OD1	2.15	0.64
1:C:11:LYS:NZ	1:C:15:GLU:OE2	2.26	0.63
1:A:63:ILE:HG22	1:A:64:GLU:HG3	1.81	0.63
1:B:169:ARG:NH1	1:C:36:GLU:OE1	2.31	0.63
1:I:224:LYS:HZ1	1:T:164:LEU:HD21	1.63	0.63
1:T:162:THR:O	1:T:167:ASN:ND2	2.31	0.63
1:H:304:GLU:O	1:H:335:ARG:NH2	2.32	0.63
1:P:304:GLU:O	1:P:335:ARG:NH2	2.32	0.62
1:A:231:PHE:HB3	1:A:339:PRO:HB2	1.80	0.62
1:C:162:THR:O	1:C:167:ASN:ND2	2.31	0.62
1:I:304:GLU:O	1:I:335:ARG:NH2	2.33	0.62
1:S:231:PHE:HB3	1:S:339:PRO:HB2	1.80	0.62
1:Q:304:GLU:O	1:Q:335:ARG:NH2	2.32	0.62
1:T:5:THR:OG1	1:T:8:ASP:OD1	2.14	0.62
1:B:231:PHE:HB3	1:B:339:PRO:HB2	1.80	0.62
1:C:164:LEU:HD21	1:Q:224:LYS:HZ1	1.62	0.62
1:F:5:THR:OG1	1:F:8:ASP:OD1	2.18	0.62
1:H:231:PHE:HB3	1:H:339:PRO:HB2	1.81	0.62
1:R:267:LEU:HD11	1:R:322:ILE:HD13	1.82	0.62
1:B:5:THR:OG1	1:B:8:ASP:OD1	2.15	0.61
1:S:267:LEU:HD11	1:S:322:ILE:HD13	1.82	0.61
1:G:368:ILE:HG21	1:G:372:ILE:HG23	1.81	0.61
1:G:304:GLU:O	1:G:335:ARG:NH2	2.33	0.61
1:T:63:ILE:HG22	1:T:64:GLU:HG3	1.82	0.61
1:T:399:PHE:HZ	1:T:409:LEU:HD21	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:GLU:O	1:C:335:ARG:NH2	2.34	0.61
1:O:304:GLU:O	1:O:335:ARG:NH2	2.33	0.61
1:Q:231:PHE:HB3	1:Q:339:PRO:HB2	1.81	0.61
1:C:63:ILE:HG22	1:C:64:GLU:HG3	1.82	0.61
1:A:267:LEU:HD11	1:A:322:ILE:HD13	1.83	0.61
1:O:231:PHE:HB3	1:O:339:PRO:HB2	1.83	0.61
1:P:11:LYS:NZ	1:P:15:GLU:OE2	2.33	0.61
1:P:162:THR:O	1:P:167:ASN:ND2	2.33	0.61
1:P:231:PHE:HB3	1:P:339:PRO:HB2	1.81	0.61
1:T:304:GLU:O	1:T:335:ARG:NH2	2.34	0.61
1:I:231:PHE:HB3	1:I:339:PRO:HB2	1.82	0.60
1:B:304:GLU:O	1:B:335:ARG:NH2	2.34	0.60
1:S:304:GLU:O	1:S:335:ARG:NH2	2.34	0.60
1:B:267:LEU:HD11	1:B:322:ILE:HD13	1.82	0.60
1:O:267:LEU:HD11	1:O:322:ILE:HD13	1.83	0.60
1:A:5:THR:OG1	1:A:8:ASP:OD1	2.18	0.60
1:A:304:GLU:O	1:A:335:ARG:NH2	2.35	0.60
1:F:122:LEU:HD12	1:F:355:LEU:HD22	1.84	0.60
1:B:63:ILE:HG22	1:B:64:GLU:HG3	1.84	0.60
1:G:231:PHE:HB3	1:G:339:PRO:HB2	1.83	0.60
1:T:267:LEU:HD11	1:T:322:ILE:HD13	1.83	0.60
1:R:231:PHE:HB3	1:R:339:PRO:HB2	1.83	0.60
1:C:231:PHE:HB3	1:C:339:PRO:HB2	1.83	0.60
1:S:403:GLU:OE2	1:S:407:LYS:NZ	2.32	0.59
1:N:122:LEU:HD12	1:N:355:LEU:HD22	1.84	0.59
1:N:5:THR:OG1	1:N:8:ASP:OD1	2.19	0.59
1:S:63:ILE:HG22	1:S:64:GLU:HG3	1.84	0.59
1:N:304:GLU:O	1:N:335:ARG:NH2	2.36	0.59
1:Q:63:ILE:HG22	1:Q:64:GLU:HG3	1.84	0.59
1:G:267:LEU:HD11	1:G:322:ILE:HD13	1.84	0.58
1:G:411:GLU:O	1:G:415:GLU:HG3	2.03	0.58
1:I:63:ILE:HG22	1:I:64:GLU:HG3	1.84	0.58
1:I:403:GLU:OE2	1:I:407:LYS:NZ	2.31	0.58
1:O:169:ARG:NH1	1:P:36:GLU:OE1	2.37	0.58
1:H:267:LEU:HD11	1:H:322:ILE:HD13	1.86	0.58
1:Q:267:LEU:HD11	1:Q:322:ILE:HD13	1.84	0.58
1:Q:411:GLU:O	1:Q:415:GLU:HG3	2.04	0.58
1:A:403:GLU:OE2	1:A:407:LYS:NZ	2.33	0.58
1:B:370:ARG:HH21	1:B:372:ILE:HA	1.68	0.58
1:F:304:GLU:O	1:F:335:ARG:NH2	2.36	0.58
1:F:411:GLU:O	1:F:415:GLU:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:411:GLU:O	1:T:415:GLU:HG3	2.04	0.58
1:T:231:PHE:HB3	1:T:339:PRO:HB2	1.84	0.58
1:A:28:ILE:HD11	1:A:413:LEU:HD22	1.86	0.57
1:Q:54:GLY:HA3	1:Q:68:MET:HG3	1.86	0.57
1:S:325:SER:OG	1:S:331:ARG:NH1	2.37	0.57
1:S:411:GLU:O	1:S:415:GLU:HG3	2.04	0.57
1:N:411:GLU:O	1:N:415:GLU:HG3	2.05	0.57
1:B:411:GLU:O	1:B:415:GLU:HG3	2.04	0.57
1:P:267:LEU:HD11	1:P:322:ILE:HD13	1.86	0.57
1:I:267:LEU:HD11	1:I:322:ILE:HD13	1.85	0.57
1:C:399:PHE:HZ	1:C:409:LEU:HD21	1.69	0.57
1:A:325:SER:OG	1:A:331:ARG:NH1	2.38	0.57
1:I:169:ARG:NH1	1:R:36:GLU:OE1	2.38	0.57
1:C:411:GLU:O	1:C:415:GLU:HG3	2.04	0.56
1:P:411:GLU:O	1:P:415:GLU:HG3	2.05	0.56
1:G:169:ARG:NH1	1:H:36:GLU:OE1	2.37	0.56
1:I:36:GLU:OE1	1:T:169:ARG:NH1	2.38	0.56
1:B:325:SER:OG	1:B:331:ARG:NH1	2.37	0.56
1:H:411:GLU:O	1:H:415:GLU:HG3	2.05	0.56
1:H:162:THR:O	1:H:167:ASN:ND2	2.38	0.56
1:I:370:ARG:HH12	1:I:372:ILE:HA	1.70	0.56
1:I:411:GLU:O	1:I:415:GLU:HG3	2.04	0.56
1:O:411:GLU:O	1:O:415:GLU:HG3	2.05	0.56
1:Q:370:ARG:HH12	1:Q:372:ILE:HA	1.70	0.56
1:I:325:SER:OG	1:I:331:ARG:NH1	2.38	0.56
1:I:54:GLY:HA3	1:I:68:MET:HG3	1.87	0.56
1:R:325:SER:OG	1:R:331:ARG:NH1	2.38	0.56
1:N:169:ARG:NH1	1:O:36:GLU:OE1	2.39	0.56
1:A:169:ARG:NH1	1:N:36:GLU:OE1	2.38	0.55
1:A:36:GLU:OE1	1:Q:169:ARG:NH1	2.38	0.55
1:H:169:ARG:NH1	1:S:36:GLU:OE1	2.39	0.55
1:C:169:ARG:NH1	1:Q:36:GLU:OE1	2.38	0.55
1:F:231:PHE:HB3	1:F:339:PRO:HB2	1.87	0.55
1:N:231:PHE:HB3	1:N:339:PRO:HB2	1.87	0.55
1:F:36:GLU:OE1	1:R:169:ARG:NH1	2.39	0.55
1:O:325:SER:OG	1:O:331:ARG:NH1	2.39	0.55
1:S:54:GLY:HA3	1:S:68:MET:HG3	1.88	0.55
1:B:54:GLY:HA3	1:B:68:MET:HG3	1.88	0.55
1:C:368:ILE:HG21	1:C:372:ILE:HG23	1.88	0.55
1:B:224:LYS:HZ3	1:P:164:LEU:HD11	1.72	0.55
1:Q:370:ARG:NH1	1:Q:375:MET:SD	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:HD11	1:C:322:ILE:HD13	1.87	0.55
1:H:63:ILE:HG22	1:H:64:GLU:HG3	1.89	0.55
1:S:368:ILE:HG21	1:S:372:ILE:HG23	1.88	0.55
1:O:403:GLU:OE2	1:O:407:LYS:HE2	2.07	0.54
1:Q:325:SER:OG	1:Q:331:ARG:NH1	2.38	0.54
1:Q:424:GLU:OE2	1:R:440:TYR:OH	2.18	0.54
1:S:264:ASP:OD1	1:S:264:ASP:N	2.37	0.54
1:A:411:GLU:O	1:A:415:GLU:HG3	2.06	0.54
1:R:22:ARG:HH11	1:R:34:ASN:HD21	1.55	0.54
1:A:440:TYR:OH	1:I:424:GLU:OE2	2.18	0.54
1:A:55:SER:OG	1:A:64:GLU:O	2.21	0.54
1:I:22:ARG:HH11	1:I:34:ASN:HD21	1.56	0.54
1:O:22:ARG:HH11	1:O:34:ASN:HD21	1.56	0.54
1:R:370:ARG:O	1:R:370:ARG:HG2	2.08	0.54
1:C:325:SER:OG	1:C:331:ARG:NH1	2.40	0.54
1:G:325:SER:OG	1:G:331:ARG:NH1	2.40	0.54
1:B:440:TYR:OH	1:G:424:GLU:OE2	2.18	0.53
1:I:370:ARG:NH1	1:I:375:MET:SD	2.81	0.53
1:S:22:ARG:HH11	1:S:34:ASN:HD21	1.55	0.53
1:C:261:GLU:OE1	1:C:261:GLU:N	2.29	0.53
1:B:36:GLU:OE1	1:P:169:ARG:NH1	2.41	0.53
1:H:111:ASN:OD1	1:H:114:ARG:NH2	2.42	0.53
1:I:200:LYS:NZ	1:I:200:LYS:HB3	2.24	0.53
1:A:22:ARG:HH11	1:A:34:ASN:HD21	1.56	0.53
1:C:403:GLU:OE2	1:C:407:LYS:HE2	2.09	0.53
1:G:22:ARG:HH11	1:G:34:ASN:HD21	1.56	0.53
1:Q:200:LYS:NZ	1:Q:200:LYS:HB3	2.24	0.53
1:R:209:ASP:OD1	1:R:344:TYR:OH	2.25	0.53
1:P:368:ILE:HG21	1:P:372:ILE:HG23	1.91	0.53
1:H:325:SER:OG	1:H:331:ARG:NH1	2.41	0.53
1:I:209:ASP:OD1	1:I:344:TYR:OH	2.26	0.53
1:B:162:THR:O	1:B:167:ASN:ND2	2.41	0.52
1:N:162:THR:O	1:N:167:ASN:ND2	2.43	0.52
1:F:325:SER:OG	1:F:331:ARG:NH1	2.41	0.52
1:H:28:ILE:HD11	1:H:413:LEU:HD22	1.91	0.52
1:S:162:THR:O	1:S:167:ASN:ND2	2.41	0.52
1:P:129:LEU:HD22	1:P:347:LEU:HD21	1.91	0.52
1:G:111:ASN:OD1	1:G:114:ARG:NH2	2.42	0.52
1:P:209:ASP:OD1	1:P:344:TYR:OH	2.27	0.52
1:C:440:TYR:OH	1:F:424:GLU:OE2	2.18	0.52
1:R:411:GLU:O	1:R:415:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:325:SER:OG	1:T:331:ARG:NH1	2.40	0.52
1:N:325:SER:OG	1:N:331:ARG:NH1	2.40	0.52
1:P:182:GLU:HB3	1:P:200:LYS:HD3	1.92	0.52
1:P:325:SER:OG	1:P:331:ARG:NH1	2.42	0.52
1:R:162:THR:O	1:R:167:ASN:ND2	2.40	0.52
1:A:162:THR:O	1:A:167:ASN:ND2	2.41	0.52
1:B:169:ARG:HD3	1:B:195:HIS:HB3	1.92	0.52
1:N:424:GLU:HG3	2:U:10:PHE:HZ	1.75	0.51
1:T:368:ILE:HG21	1:T:372:ILE:HG23	1.92	0.51
1:H:424:GLU:OE2	1:P:440:TYR:OH	2.18	0.51
1:P:111:ASN:OD1	1:P:114:ARG:NH2	2.42	0.51
1:S:22:ARG:HB3	1:S:34:ASN:HD22	1.74	0.51
1:H:129:LEU:HD22	1:H:347:LEU:HD21	1.91	0.51
1:F:224:LYS:HG3	1:R:164:LEU:HD11	1.93	0.51
1:O:111:ASN:OD1	1:O:114:ARG:NH2	2.43	0.51
1:Q:403:GLU:OE2	1:Q:407:LYS:NZ	2.35	0.51
1:P:63:ILE:HG22	1:P:64:GLU:HG3	1.91	0.51
1:H:290:ASN:HB3	1:H:295:SER:HB3	1.92	0.51
1:Q:111:ASN:OD1	1:Q:114:ARG:NH2	2.44	0.51
1:Q:440:TYR:OH	1:R:424:GLU:OE2	2.19	0.51
1:R:28:ILE:HD11	1:R:413:LEU:HD22	1.91	0.51
1:C:125:SER:OG	1:C:126:ASP:OD1	2.25	0.51
1:C:129:LEU:HD22	1:C:347:LEU:HD21	1.93	0.51
1:F:129:LEU:HD22	1:F:347:LEU:HD21	1.93	0.51
1:S:169:ARG:HD3	1:S:195:HIS:HB3	1.92	0.51
1:N:63:ILE:HG22	1:N:64:GLU:HG3	1.93	0.50
1:N:375:MET:HG3	1:N:380:ARG:HB3	1.92	0.50
1:A:164:LEU:HD11	1:N:224:LYS:HG3	1.93	0.50
1:B:28:ILE:HG22	1:B:29:LEU:HD23	1.94	0.50
1:I:162:THR:O	1:I:167:ASN:ND2	2.42	0.50
1:A:111:ASN:OD1	1:A:114:ARG:NH2	2.45	0.50
1:F:372:ILE:HG21	1:F:385:ILE:HD13	1.94	0.50
1:Q:162:THR:O	1:Q:167:ASN:ND2	2.42	0.50
1:R:370:ARG:NH2	1:R:372:ILE:HA	2.26	0.50
1:A:170:ARG:NH1	1:N:84:ALA:HB1	2.27	0.50
1:I:129:LEU:HD22	1:I:347:LEU:HD21	1.93	0.50
1:R:129:LEU:HD22	1:R:347:LEU:HD21	1.93	0.50
1:P:290:ASN:HB3	1:P:295:SER:HB3	1.93	0.50
1:A:290:ASN:HB3	1:A:295:SER:HB3	1.93	0.50
1:B:209:ASP:OD1	1:B:344:TYR:OH	2.28	0.50
1:B:424:GLU:OE2	1:G:440:TYR:OH	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:169:ARG:HD3	1:P:195:HIS:HB3	1.94	0.50
1:T:129:LEU:HD22	1:T:347:LEU:HD21	1.93	0.50
1:N:11:LYS:NZ	1:N:15:GLU:OE2	2.45	0.49
1:B:129:LEU:HD22	1:B:347:LEU:HD21	1.95	0.49
1:C:290:ASN:HB3	1:C:295:SER:HB3	1.93	0.49
1:F:63:ILE:HG22	1:F:64:GLU:HG3	1.94	0.49
1:N:119:MET:HB2	1:N:355:LEU:HD11	1.94	0.49
1:N:129:LEU:HD22	1:N:347:LEU:HD21	1.94	0.49
1:N:164:LEU:HD11	1:O:224:LYS:HG3	1.93	0.49
1:O:209:ASP:OD1	1:O:344:TYR:OH	2.27	0.49
1:H:370:ARG:HH21	1:H:372:ILE:HA	1.76	0.49
1:S:290:ASN:HB3	1:S:295:SER:HB3	1.93	0.49
1:A:189:GLU:HB3	1:A:194:GLN:HB3	1.94	0.49
1:B:22:ARG:HH11	1:B:34:ASN:HD21	1.60	0.49
1:P:370:ARG:NH2	1:P:371:ASN:O	2.46	0.49
1:R:290:ASN:HB3	1:R:295:SER:HB3	1.92	0.49
1:T:290:ASN:HB3	1:T:295:SER:HB3	1.93	0.49
1:F:267:LEU:HD11	1:F:322:ILE:HD13	1.93	0.49
1:I:111:ASN:OD1	1:I:114:ARG:NH2	2.45	0.49
1:A:370:ARG:O	1:A:370:ARG:HG2	2.11	0.49
1:F:119:MET:HB2	1:F:355:LEU:HD11	1.94	0.49
1:H:174:LEU:O	1:H:178:GLU:HG3	2.12	0.49
1:B:290:ASN:HB3	1:B:295:SER:HB3	1.93	0.49
1:H:261:GLU:CD	1:H:261:GLU:H	2.16	0.49
1:I:22:ARG:HB3	1:I:34:ASN:HD22	1.76	0.49
1:N:267:LEU:HD11	1:N:322:ILE:HD13	1.93	0.49
1:Q:129:LEU:HD22	1:Q:347:LEU:HD21	1.93	0.49
1:I:84:ALA:HB1	1:T:170:ARG:NH1	2.28	0.49
1:G:22:ARG:HB3	1:G:34:ASN:HD22	1.78	0.49
1:G:129:LEU:HD22	1:G:347:LEU:HD21	1.95	0.49
1:H:440:TYR:OH	1:P:424:GLU:OE2	2.19	0.49
1:S:129:LEU:HD22	1:S:347:LEU:HD21	1.94	0.49
1:T:424:GLU:HG3	2:V:10:PHE:HZ	1.77	0.49
1:T:403:GLU:OE2	1:T:407:LYS:HE2	2.13	0.48
1:Q:22:ARG:HB3	1:Q:34:ASN:HD22	1.79	0.48
1:C:170:ARG:NH1	1:Q:84:ALA:HB1	2.28	0.48
1:F:54:GLY:HA3	1:F:68:MET:HG3	1.94	0.48
1:O:22:ARG:HB3	1:O:34:ASN:HD22	1.77	0.48
1:O:125:SER:OG	1:O:126:ASP:OD1	2.24	0.48
1:R:189:GLU:HB3	1:R:194:GLN:HB3	1.95	0.48
1:P:28:ILE:HD11	1:P:413:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:370:ARG:HH22	1:C:372:ILE:HA	1.78	0.48
1:N:125:SER:OG	1:N:126:ASP:OD1	2.25	0.48
1:Q:125:SER:OG	1:Q:126:ASP:OD1	2.25	0.48
1:C:411:GLU:HG3	1:C:412:HIS:N	2.29	0.48
1:G:55:SER:OG	1:G:64:GLU:O	2.22	0.48
1:C:209:ASP:OD1	1:C:344:TYR:OH	2.26	0.48
1:G:162:THR:O	1:G:167:ASN:ND2	2.46	0.48
1:I:411:GLU:HG3	1:I:412:HIS:N	2.29	0.48
1:R:111:ASN:OD1	1:R:114:ARG:NH2	2.46	0.48
1:C:261:GLU:H	1:C:261:GLU:CD	2.14	0.48
1:F:169:ARG:HD3	1:F:195:HIS:HB3	1.96	0.48
1:G:63:ILE:HG12	2:J:3:ARG:HD3	1.96	0.48
1:T:411:GLU:HG3	1:T:412:HIS:N	2.29	0.48
1:G:290:ASN:HB3	1:G:295:SER:HB3	1.95	0.48
1:N:403:GLU:OE2	1:N:407:LYS:HE2	2.13	0.48
1:O:170:ARG:NH1	1:P:84:ALA:HB1	2.29	0.48
1:F:84:ALA:HB1	1:R:170:ARG:NH1	2.28	0.47
1:O:119:MET:HB2	1:O:355:LEU:HD11	1.96	0.47
1:O:290:ASN:HB3	1:O:295:SER:HB3	1.95	0.47
1:P:261:GLU:CD	1:P:261:GLU:H	2.17	0.47
1:P:370:ARG:HH22	1:P:374:VAL:HB	1.79	0.47
1:R:22:ARG:HB3	1:R:34:ASN:HD22	1.78	0.47
1:A:129:LEU:HD22	1:A:347:LEU:HD21	1.94	0.47
1:A:370:ARG:O	1:A:370:ARG:NH1	2.48	0.47
1:B:411:GLU:HG3	1:B:412:HIS:N	2.30	0.47
1:F:162:THR:O	1:F:167:ASN:ND2	2.44	0.47
1:G:170:ARG:NH1	1:H:84:ALA:HB1	2.28	0.47
1:Q:411:GLU:HG3	1:Q:412:HIS:N	2.29	0.47
1:R:174:LEU:O	1:R:178:GLU:HG3	2.14	0.47
1:T:370:ARG:NH2	1:T:371:ASN:O	2.46	0.47
1:A:169:ARG:HD3	1:A:195:HIS:HB3	1.97	0.47
1:F:125:SER:OG	1:F:126:ASP:OD1	2.25	0.47
1:O:129:LEU:HD22	1:O:347:LEU:HD21	1.95	0.47
1:P:174:LEU:O	1:P:178:GLU:HG3	2.14	0.47
1:A:22:ARG:HB3	1:A:34:ASN:HD22	1.79	0.47
1:P:125:SER:OG	1:P:126:ASP:OD1	2.26	0.47
1:N:63:ILE:HD13	2:U:3:ARG:HD3	1.97	0.47
1:A:145:GLU:N	1:A:145:GLU:OE1	2.47	0.47
1:Q:11:LYS:NZ	1:Q:15:GLU:OE2	2.47	0.47
1:F:224:LYS:HE2	1:F:224:LYS:HB3	1.75	0.47
1:O:411:GLU:HG3	1:O:412:HIS:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:370:ARG:HH22	1:T:374:VAL:HB	1.79	0.47
1:B:368:ILE:HG21	1:B:372:ILE:HG23	1.95	0.47
1:F:411:GLU:HG3	1:F:412:HIS:N	2.30	0.47
1:H:264:ASP:OD1	1:H:264:ASP:N	2.42	0.47
1:P:411:GLU:HG3	1:P:412:HIS:N	2.30	0.47
1:T:261:GLU:OE1	1:T:261:GLU:N	2.31	0.47
1:C:57:ILE:HD11	1:C:96:ILE:HG13	1.97	0.47
1:C:424:GLU:HG3	2:D:10:PHE:HZ	1.79	0.47
1:T:55:SER:OG	1:T:64:GLU:O	2.24	0.47
1:A:174:LEU:O	1:A:178:GLU:HG3	2.15	0.46
1:G:411:GLU:HG3	1:G:412:HIS:N	2.30	0.46
1:P:424:GLU:HG3	2:Y:10:PHE:HZ	1.80	0.46
1:S:111:ASN:OD1	1:S:114:ARG:NH2	2.48	0.46
1:G:125:SER:OG	1:G:126:ASP:OD1	2.24	0.46
1:F:375:MET:HG3	1:F:380:ARG:HB3	1.96	0.46
1:H:153:LYS:HA	1:H:192:PRO:HB3	1.96	0.46
1:N:411:GLU:HG3	1:N:412:HIS:N	2.30	0.46
1:O:368:ILE:HG21	1:O:372:ILE:HG23	1.96	0.46
1:R:153:LYS:HA	1:R:192:PRO:HB3	1.97	0.46
1:B:125:SER:OG	1:B:126:ASP:OD1	2.25	0.46
1:C:424:GLU:OE2	1:F:440:TYR:OH	2.22	0.46
1:N:54:GLY:HA3	1:N:68:MET:HG3	1.97	0.46
1:H:370:ARG:O	1:H:370:ARG:NH1	2.49	0.46
1:A:234:LYS:HD3	1:A:298:ARG:HA	1.97	0.46
1:P:370:ARG:O	1:P:370:ARG:NH1	2.48	0.46
1:S:411:GLU:HG3	1:S:412:HIS:N	2.29	0.46
1:T:57:ILE:HD11	1:T:96:ILE:HG13	1.98	0.46
1:A:421:LYS:HA	1:A:421:LYS:HD3	1.78	0.46
2:E:10:PHE:HZ	1:Q:424:GLU:HG3	1.80	0.46
1:O:162:THR:O	1:O:167:ASN:ND2	2.45	0.46
1:A:411:GLU:HG3	1:A:412:HIS:N	2.30	0.46
1:N:440:TYR:OH	1:T:424:GLU:OE2	2.19	0.46
1:Q:290:ASN:HB3	1:Q:295:SER:HB3	1.98	0.46
1:B:111:ASN:OD1	1:B:114:ARG:NH2	2.48	0.46
1:H:424:GLU:HG3	2:K:10:PHE:HZ	1.81	0.46
1:T:261:GLU:H	1:T:261:GLU:CD	2.17	0.46
1:N:424:GLU:OE2	1:T:440:TYR:OH	2.19	0.45
1:O:259:PHE:CZ	1:O:261:GLU:HG2	2.51	0.45
1:G:424:GLU:HG3	2:J:10:PHE:HZ	1.80	0.45
1:R:145:GLU:N	1:R:145:GLU:OE1	2.47	0.45
1:R:368:ILE:HG21	1:R:372:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:424:GLU:HG3	2:W:10:PHE:HZ	1.82	0.45
2:M:10:PHE:HZ	1:R:424:GLU:HG3	1.81	0.45
1:B:424:GLU:HG3	2:Z:10:PHE:HZ	1.81	0.45
1:O:424:GLU:HG3	2:X:10:PHE:HZ	1.80	0.45
1:P:55:SER:OG	1:P:64:GLU:O	2.22	0.45
1:H:411:GLU:HG3	1:H:412:HIS:N	2.30	0.45
1:N:111:ASN:OD1	1:N:114:ARG:NH2	2.50	0.45
1:N:421:LYS:HA	1:N:421:LYS:HD3	1.79	0.45
1:S:107:ASP:HB3	1:S:110:ASN:HB2	1.99	0.45
1:G:57:ILE:HD11	1:G:96:ILE:HG13	1.97	0.45
1:P:317:SER:O	1:P:317:SER:OG	2.33	0.45
1:Q:399:PHE:HE1	1:Q:405:MET:HB3	1.81	0.45
1:R:326:ARG:HG2	1:R:326:ARG:HH11	1.81	0.45
1:B:107:ASP:HB3	1:B:110:ASN:HB2	1.99	0.45
1:C:169:ARG:HD3	1:C:195:HIS:HB3	1.99	0.45
1:I:234:LYS:HG3	1:I:298:ARG:HA	1.99	0.45
1:Q:234:LYS:HG3	1:Q:298:ARG:HA	1.99	0.45
1:A:129:LEU:HD23	1:A:207:SER:HB3	1.99	0.45
1:P:57:ILE:HD11	1:P:96:ILE:HG13	1.99	0.45
1:P:399:PHE:HE1	1:P:405:MET:HB3	1.81	0.45
1:R:160:ALA:HB3	1:R:161:PRO:HD3	1.99	0.45
1:S:125:SER:OG	1:S:126:ASP:OD1	2.25	0.45
1:O:11:LYS:NZ	1:O:15:GLU:OE2	2.50	0.44
1:P:264:ASP:OD1	1:P:264:ASP:N	2.42	0.44
1:F:370:ARG:HH21	1:F:372:ILE:HA	1.82	0.44
2:L:10:PHE:HZ	1:S:424:GLU:HG3	1.82	0.44
1:N:224:LYS:HE2	1:N:224:LYS:HB3	1.75	0.44
1:P:370:ARG:HH21	1:P:372:ILE:HA	1.82	0.44
1:T:370:ARG:O	1:T:370:ARG:NH1	2.50	0.44
1:H:399:PHE:HE1	1:H:405:MET:HB3	1.81	0.44
1:I:290:ASN:HB3	1:I:295:SER:HB3	1.98	0.44
1:I:316:ARG:HD3	1:R:63:ILE:O	2.18	0.44
1:T:111:ASN:OD1	1:T:114:ARG:NH2	2.50	0.44
1:B:160:ALA:HB3	1:B:161:PRO:HD3	1.99	0.44
1:H:170:ARG:HG3	1:S:20:TYR:CD2	2.53	0.44
1:N:107:ASP:HB3	1:N:110:ASN:HB2	2.00	0.44
1:R:169:ARG:HD3	1:R:195:HIS:HB3	1.98	0.44
1:T:169:ARG:HD3	1:T:195:HIS:HB3	1.99	0.44
1:A:209:ASP:OD1	1:A:344:TYR:OH	2.25	0.44
1:A:261:GLU:CD	1:A:261:GLU:H	2.21	0.44
1:G:119:MET:HB2	1:G:355:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:261:GLU:CD	1:R:261:GLU:H	2.21	0.44
1:C:111:ASN:OD1	1:C:114:ARG:NH2	2.50	0.44
1:I:371:ASN:O	1:I:374:VAL:HG12	2.18	0.44
1:P:160:ALA:HB3	1:P:161:PRO:HD3	1.99	0.44
1:Q:371:ASN:O	1:Q:374:VAL:HG12	2.18	0.44
1:A:160:ALA:HB3	1:A:161:PRO:HD3	1.99	0.44
1:I:184:GLU:HG3	1:I:200:LYS:HG2	1.99	0.44
1:Q:119:MET:HB2	1:Q:355:LEU:HD11	2.00	0.44
1:Q:184:GLU:HG3	1:Q:200:LYS:HG2	1.99	0.44
1:B:421:LYS:HA	1:B:421:LYS:HD3	1.78	0.43
1:G:153:LYS:H	1:G:153:LYS:HG2	1.68	0.43
1:G:169:ARG:HD3	1:G:195:HIS:HB3	1.99	0.43
1:H:421:LYS:HD3	1:H:421:LYS:HA	1.81	0.43
1:N:57:ILE:HD11	1:N:96:ILE:HG13	2.00	0.43
1:O:63:ILE:HG12	2:X:3:ARG:HD3	2.00	0.43
1:F:107:ASP:HB3	1:F:110:ASN:HB2	2.00	0.43
1:R:129:LEU:HD23	1:R:207:SER:HB3	2.00	0.43
1:S:145:GLU:OE1	1:S:145:GLU:N	2.51	0.43
1:B:326:ARG:HG2	1:B:326:ARG:HH11	1.82	0.43
1:C:221:ILE:HA	1:C:224:LYS:HD3	2.00	0.43
1:F:316:ARG:HD3	1:G:63:ILE:O	2.18	0.43
1:O:57:ILE:HD11	1:O:96:ILE:HG13	1.99	0.43
1:P:421:LYS:HA	1:P:421:LYS:HD3	1.80	0.43
1:T:16:GLU:HA	1:T:16:GLU:OE1	2.19	0.43
1:C:16:GLU:HA	1:C:16:GLU:OE1	2.18	0.43
1:C:145:GLU:N	1:C:145:GLU:OE1	2.51	0.43
1:C:160:ALA:HB3	1:C:161:PRO:HD3	2.00	0.43
1:F:111:ASN:OD1	1:F:114:ARG:NH2	2.51	0.43
1:G:421:LYS:HA	1:G:421:LYS:HD3	1.79	0.43
1:N:396:LEU:HD11	1:N:421:LYS:HB3	2.00	0.43
1:O:169:ARG:HD3	1:O:195:HIS:HB3	2.00	0.43
1:Q:421:LYS:HA	1:Q:421:LYS:HD3	1.80	0.43
1:T:370:ARG:HH21	1:T:372:ILE:HA	1.83	0.43
1:G:316:ARG:HD3	1:H:63:ILE:O	2.19	0.43
1:I:107:ASP:HB3	1:I:110:ASN:HB2	2.01	0.43
1:I:399:PHE:HE1	1:I:405:MET:HB3	1.83	0.43
1:S:160:ALA:HB3	1:S:161:PRO:HD3	1.99	0.43
1:A:224:LYS:HG3	1:Q:164:LEU:HD11	2.01	0.43
1:C:326:ARG:HH11	1:C:326:ARG:HG2	1.83	0.43
1:I:125:SER:OG	1:I:126:ASP:OD1	2.25	0.43
1:H:125:SER:OG	1:H:126:ASP:OD1	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:MET:HB2	1:I:355:LEU:HD11	2.00	0.43
1:N:316:ARG:HD3	1:O:63:ILE:O	2.19	0.43
1:O:316:ARG:HD3	1:P:63:ILE:O	2.19	0.43
1:R:107:ASP:HB3	1:R:110:ASN:HB2	2.01	0.43
1:S:326:ARG:HG2	1:S:326:ARG:HH11	1.83	0.43
1:H:22:ARG:HB3	1:H:34:ASN:HD22	1.84	0.43
1:A:11:LYS:NZ	1:A:15:GLU:OE2	2.38	0.43
1:H:145:GLU:N	1:H:145:GLU:OE1	2.52	0.43
1:I:159:LEU:HG	1:R:34:ASN:ND2	2.34	0.43
1:O:27:ASP:HA	1:O:57:ILE:HG23	2.01	0.43
1:S:396:LEU:HD11	1:S:421:LYS:HB3	2.01	0.43
1:A:153:LYS:HA	1:A:192:PRO:HB3	2.01	0.43
1:B:109:ARG:NH2	1:B:209:ASP:OD2	2.43	0.43
1:F:57:ILE:HD11	1:F:96:ILE:HG13	2.00	0.43
1:F:396:LEU:HD11	1:F:421:LYS:HB3	2.00	0.43
1:N:109:ARG:HG3	1:N:344:TYR:CE1	2.54	0.43
1:A:107:ASP:HB3	1:A:110:ASN:HB2	2.01	0.42
1:F:372:ILE:O	1:F:375:MET:HG2	2.19	0.42
1:F:421:LYS:HA	1:F:421:LYS:HD3	1.79	0.42
1:P:145:GLU:N	1:P:145:GLU:OE1	2.51	0.42
1:B:145:GLU:OE1	1:B:145:GLU:N	2.51	0.42
1:G:172:ILE:HD13	1:G:218:VAL:HG22	2.01	0.42
1:S:109:ARG:NH2	1:S:209:ASP:OD2	2.44	0.42
1:B:396:LEU:HD11	1:B:421:LYS:HB3	2.01	0.42
1:F:109:ARG:HG3	1:F:344:TYR:CE1	2.54	0.42
1:Q:200:LYS:HB3	1:Q:200:LYS:HZ2	1.84	0.42
1:R:396:LEU:HD11	1:R:421:LYS:HB3	2.01	0.42
1:H:160:ALA:HB3	1:H:161:PRO:HD3	2.01	0.42
1:I:160:ALA:HB3	1:I:161:PRO:HD3	2.01	0.42
1:O:129:LEU:HD23	1:O:207:SER:HB3	2.01	0.42
1:T:111:ASN:ND2	1:T:409:LEU:HA	2.34	0.42
1:A:34:ASN:ND2	1:Q:159:LEU:HG	2.35	0.42
1:C:182:GLU:HB3	1:C:200:LYS:HD3	2.02	0.42
1:G:27:ASP:HA	1:G:57:ILE:HG23	2.01	0.42
1:P:153:LYS:HA	1:P:192:PRO:HB3	2.02	0.42
1:T:209:ASP:OD1	1:T:344:TYR:OH	2.26	0.42
1:C:109:ARG:HG3	1:C:344:TYR:CE1	2.55	0.42
1:G:129:LEU:HD23	1:G:207:SER:HB3	2.02	0.42
1:G:160:ALA:HB3	1:G:161:PRO:HD3	2.01	0.42
1:N:290:ASN:HB3	1:N:295:SER:HB3	2.00	0.42
1:T:160:ALA:HB3	1:T:161:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:ASN:HB3	1:F:295:SER:HB3	2.00	0.42
1:H:19:LYS:HA	1:H:19:LYS:HD3	1.89	0.42
1:H:57:ILE:HD11	1:H:96:ILE:HG13	2.01	0.42
1:I:129:LEU:HD23	1:I:207:SER:HB3	2.02	0.42
1:O:160:ALA:HB3	1:O:161:PRO:HD3	2.01	0.42
1:Q:107:ASP:HB3	1:Q:110:ASN:HB2	2.01	0.42
1:G:403:GLU:OE2	1:G:407:LYS:NZ	2.45	0.42
1:H:172:ILE:HD13	1:H:218:VAL:HG22	2.02	0.42
1:N:159:LEU:HG	1:O:34:ASN:ND2	2.35	0.42
1:N:372:ILE:O	1:N:375:MET:HG2	2.20	0.42
1:P:172:ILE:HD13	1:P:218:VAL:HG22	2.01	0.42
1:Q:160:ALA:HB3	1:Q:161:PRO:HD3	2.01	0.42
1:Q:282:ALA:HA	1:Q:285:PHE:CZ	2.55	0.42
1:S:11:LYS:HG2	1:S:15:GLU:OE2	2.19	0.42
1:A:150:LEU:HD13	1:A:192:PRO:HB2	2.01	0.42
1:O:107:ASP:HB3	1:O:110:ASN:HB2	2.02	0.42
1:F:160:ALA:HB3	1:F:161:PRO:HD3	2.01	0.42
1:I:164:LEU:HD11	1:R:224:LYS:HG3	2.02	0.42
1:N:19:LYS:HA	1:N:19:LYS:HD3	1.91	0.42
1:R:111:ASN:O	1:R:115:ILE:HG12	2.20	0.42
1:H:169:ARG:HD3	1:H:195:HIS:HB3	2.01	0.41
1:P:79:ILE:HD13	1:P:90:ALA:HB2	2.02	0.41
1:Q:28:ILE:HG22	1:Q:29:LEU:HD23	2.02	0.41
1:Q:111:ASN:O	1:Q:115:ILE:HG12	2.20	0.41
1:S:170:ARG:HG3	1:T:20:TYR:CD2	2.55	0.41
1:S:370:ARG:HH22	1:S:372:ILE:HA	1.85	0.41
1:H:153:LYS:H	1:H:153:LYS:HG2	1.64	0.41
1:H:209:ASP:OD1	1:H:344:TYR:OH	2.27	0.41
1:I:111:ASN:O	1:I:115:ILE:HG12	2.20	0.41
1:O:424:GLU:OE2	1:S:440:TYR:OH	2.18	0.41
1:R:63:ILE:HG22	1:R:64:GLU:HG3	2.02	0.41
1:T:109:ARG:HG3	1:T:344:TYR:CE1	2.55	0.41
1:B:170:ARG:HG3	1:C:20:TYR:CD2	2.55	0.41
1:G:109:ARG:HG3	1:G:344:TYR:CE1	2.56	0.41
1:I:27:ASP:HA	1:I:57:ILE:HG23	2.03	0.41
1:Q:169:ARG:HD3	1:Q:195:HIS:HB3	2.03	0.41
1:G:11:LYS:O	1:G:15:GLU:OE1	2.38	0.41
1:O:164:LEU:HD11	1:P:224:LYS:HG3	2.03	0.41
1:P:109:ARG:HG3	1:P:344:TYR:CE1	2.55	0.41
1:R:27:ASP:HA	1:R:57:ILE:HG23	2.03	0.41
1:T:130:GLY:HA2	1:T:131:PRO:HD3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ASN:O	1:A:115:ILE:HG12	2.20	0.41
1:C:282:ALA:HA	1:C:285:PHE:CZ	2.55	0.41
1:G:153:LYS:HA	1:G:192:PRO:HB3	2.03	0.41
1:N:160:ALA:HB3	1:N:161:PRO:HD3	2.01	0.41
1:O:19:LYS:HD3	1:O:19:LYS:HA	1.89	0.41
1:B:111:ASN:O	1:B:115:ILE:HG12	2.21	0.41
1:H:119:MET:HB2	1:H:355:LEU:HD11	2.02	0.41
1:S:109:ARG:HG3	1:S:344:TYR:CE1	2.55	0.41
1:T:125:SER:OG	1:T:126:ASP:OD1	2.25	0.41
1:A:282:ALA:HA	1:A:285:PHE:CZ	2.56	0.41
1:B:109:ARG:HG3	1:B:344:TYR:CE1	2.55	0.41
1:B:264:ASP:OD1	1:B:265:LEU:N	2.53	0.41
1:F:159:LEU:HG	1:G:34:ASN:ND2	2.36	0.41
1:H:111:ASN:O	1:H:115:ILE:HG12	2.21	0.41
1:I:326:ARG:HG2	1:I:326:ARG:HH11	1.85	0.41
1:P:111:ASN:O	1:P:115:ILE:HG12	2.21	0.41
1:R:212:GLN:HA	1:R:212:GLN:HE21	1.86	0.41
1:A:181:PHE:HZ	1:A:213:THR:HB	1.86	0.41
1:B:20:TYR:CD2	1:P:170:ARG:HG3	2.56	0.41
1:G:399:PHE:HE1	1:G:405:MET:HB3	1.86	0.41
1:I:169:ARG:HD3	1:I:195:HIS:HB3	2.03	0.41
1:I:282:ALA:HA	1:I:285:PHE:CZ	2.55	0.41
1:S:206:ARG:HG3	1:S:206:ARG:HH11	1.86	0.41
1:F:11:LYS:NZ	1:F:15:GLU:OE2	2.53	0.41
1:G:282:ALA:HA	1:G:285:PHE:CZ	2.56	0.41
1:H:274:PHE:CE1	1:H:354:GLY:HA3	2.56	0.41
1:H:282:ALA:HA	1:H:285:PHE:CZ	2.56	0.41
1:I:261:GLU:OE1	1:I:261:GLU:N	2.35	0.41
1:O:12:LEU:HA	1:O:15:GLU:OE1	2.21	0.41
1:O:172:ILE:HD13	1:O:218:VAL:HG22	2.03	0.41
1:O:396:LEU:HD11	1:O:421:LYS:HB3	2.03	0.41
1:Q:55:SER:OG	1:Q:64:GLU:O	2.22	0.41
1:Q:129:LEU:HD23	1:Q:207:SER:HB3	2.02	0.41
1:R:109:ARG:HG3	1:R:344:TYR:CE1	2.56	0.41
1:T:421:LYS:HA	1:T:421:LYS:HD3	1.79	0.41
1:A:396:LEU:HD11	1:A:421:LYS:HB3	2.02	0.41
1:C:107:ASP:HB3	1:C:110:ASN:HB2	2.03	0.41
1:F:164:LEU:HD23	1:F:164:LEU:HA	1.91	0.41
1:H:129:LEU:HD23	1:H:207:SER:HB3	2.03	0.41
1:P:27:ASP:HA	1:P:57:ILE:HG23	2.03	0.41
1:P:129:LEU:HD23	1:P:207:SER:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:209:ASP:OD1	1:Q:344:TYR:OH	2.26	0.41
1:R:14:LYS:NZ	1:R:14:LYS:HB2	2.36	0.41
1:S:55:SER:OG	1:S:64:GLU:O	2.21	0.41
1:T:111:ASN:O	1:T:115:ILE:HG12	2.21	0.41
1:T:282:ALA:HA	1:T:285:PHE:CZ	2.56	0.41
1:A:27:ASP:HA	1:A:57:ILE:HG23	2.02	0.40
1:B:282:ALA:HA	1:B:285:PHE:CZ	2.56	0.40
1:C:421:LYS:HD3	1:C:421:LYS:HA	1.78	0.40
1:F:129:LEU:HD23	1:F:207:SER:HB3	2.03	0.40
1:G:107:ASP:HB3	1:G:110:ASN:HB2	2.02	0.40
1:N:170:ARG:HG3	1:O:20:TYR:CD2	2.56	0.40
1:O:421:LYS:HD3	1:O:421:LYS:HA	1.79	0.40
1:S:19:LYS:HA	1:S:19:LYS:HD3	1.91	0.40
1:S:111:ASN:O	1:S:115:ILE:HG12	2.21	0.40
1:S:170:ARG:HG3	1:T:20:TYR:CE2	2.56	0.40
1:B:57:ILE:HD11	1:B:96:ILE:HG13	2.03	0.40
1:B:206:ARG:HH11	1:B:206:ARG:HG3	1.86	0.40
1:I:170:ARG:HG3	1:R:20:TYR:CD2	2.57	0.40
1:Q:216:LEU:HD23	1:Q:216:LEU:HA	1.94	0.40
1:S:282:ALA:HA	1:S:285:PHE:CZ	2.56	0.40
1:G:216:LEU:HD23	1:G:216:LEU:HA	1.93	0.40
1:H:107:ASP:HB3	1:H:110:ASN:HB2	2.03	0.40
1:I:57:ILE:HD11	1:I:96:ILE:HG13	2.02	0.40
1:O:111:ASN:O	1:O:115:ILE:HG12	2.21	0.40
1:O:111:ASN:HD21	1:O:409:LEU:HA	1.87	0.40
1:Q:12:LEU:HA	1:Q:15:GLU:OE1	2.21	0.40
1:Q:326:ARG:HG2	1:Q:326:ARG:HH11	1.85	0.40
1:A:212:GLN:HA	1:A:212:GLN:HE21	1.86	0.40
1:A:368:ILE:HG21	1:A:372:ILE:CG2	2.51	0.40
1:B:170:ARG:HG3	1:C:20:TYR:CE2	2.57	0.40
1:B:274:PHE:CE1	1:B:354:GLY:HA3	2.56	0.40
1:G:6:ARG:HG3	1:G:46:LEU:HD13	2.04	0.40
1:G:111:ASN:O	1:G:115:ILE:HG12	2.21	0.40
1:H:109:ARG:HG3	1:H:344:TYR:CE1	2.56	0.40
1:I:396:LEU:HD11	1:I:421:LYS:HB3	2.03	0.40
1:N:172:ILE:HD13	1:N:218:VAL:HG22	2.04	0.40
1:O:274:PHE:CE1	1:O:354:GLY:HA3	2.57	0.40
1:O:440:TYR:OH	1:S:424:GLU:OE2	2.18	0.40
1:A:130:GLY:HA2	1:A:131:PRO:HD3	1.93	0.40
1:A:424:GLU:OE2	1:I:440:TYR:OH	2.19	0.40
1:Q:57:ILE:HD11	1:Q:96:ILE:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:55:SER:OG	1:R:64:GLU:O	2.19	0.40
1:S:172:ILE:HD13	1:S:218:VAL:HG22	2.03	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	441/464 (95%)	422 (96%)	19 (4%)	0	100	100
1	B	441/464 (95%)	424 (96%)	17 (4%)	0	100	100
1	C	441/464 (95%)	424 (96%)	17 (4%)	0	100	100
1	F	441/464 (95%)	426 (97%)	15 (3%)	0	100	100
1	G	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	H	441/464 (95%)	424 (96%)	17 (4%)	0	100	100
1	I	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	N	441/464 (95%)	425 (96%)	16 (4%)	0	100	100
1	O	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	P	441/464 (95%)	424 (96%)	17 (4%)	0	100	100
1	Q	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	R	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	S	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
1	T	441/464 (95%)	423 (96%)	18 (4%)	0	100	100
2	D	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	E	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	J	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	K	8/10 (80%)	7 (88%)	1 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	M	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	U	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
2	V	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	W	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	X	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	Y	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	Z	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	a	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
2	b	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	6286/6636 (95%)	6027 (96%)	259 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/400 (93%)	356 (96%)	16 (4%)	29	16
1	B	372/400 (93%)	362 (97%)	10 (3%)	44	34
1	C	372/400 (93%)	360 (97%)	12 (3%)	39	27
1	F	372/400 (93%)	359 (96%)	13 (4%)	36	24
1	G	372/400 (93%)	361 (97%)	11 (3%)	41	30
1	H	372/400 (93%)	356 (96%)	16 (4%)	29	16
1	I	372/400 (93%)	363 (98%)	9 (2%)	49	40
1	N	372/400 (93%)	359 (96%)	13 (4%)	36	24
1	O	372/400 (93%)	362 (97%)	10 (3%)	44	34
1	P	372/400 (93%)	360 (97%)	12 (3%)	39	27
1	Q	372/400 (93%)	364 (98%)	8 (2%)	52	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	372/400 (93%)	356 (96%)	16 (4%)	29	16
1	S	372/400 (93%)	361 (97%)	11 (3%)	41	30
1	T	372/400 (93%)	359 (96%)	13 (4%)	36	24
2	D	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	E	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	J	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	K	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	L	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	M	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	U	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	V	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	W	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	X	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	Y	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	Z	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	a	8/9 (89%)	7 (88%)	1 (12%)	4	0
2	b	8/9 (89%)	7 (88%)	1 (12%)	4	0
All	All	5320/5726 (93%)	5136 (96%)	184 (4%)	40	24

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	14	LYS
1	A	18	VAL
1	A	20	TYR
1	A	36	GLU
1	A	91	ARG
1	A	145	GLU
1	A	167	ASN
1	A	206	ARG
1	A	212	GLN
1	A	216	LEU
1	A	224	LYS
1	A	361	LYS
1	A	370	ARG

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Mol	Chain	Res	Type
1	A	375	MET
1	A	409	LEU
1	B	14	LYS
1	B	18	VAL
1	B	20	TYR
1	B	40	SER
1	B	91	ARG
1	B	145	GLU
1	B	206	ARG
1	B	361	LYS
1	B	370	ARG
1	B	409	LEU
1	C	14	LYS
1	C	18	VAL
1	C	40	SER
1	C	83	THR
1	C	91	ARG
1	C	167	ASN
1	C	206	ARG
1	C	224	LYS
1	C	361	LYS
1	C	370	ARG
1	C	375	MET
1	C	409	LEU
2	D	9	ARG
2	E	9	ARG
1	F	8	ASP
1	F	14	LYS
1	F	18	VAL
1	F	28	ILE
1	F	91	ARG
1	F	167	ASN
1	F	206	ARG
1	F	216	LEU
1	F	224	LYS
1	F	261	GLU
1	F	380	ARG
1	F	401	SER
1	F	442	SER
1	G	8	ASP
1	G	14	LYS
1	G	18	VAL

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Mol	Chain	Res	Type
1	G	91	ARG
1	G	145	GLU
1	G	153	LYS
1	G	206	ARG
1	G	216	LEU
1	G	261	GLU
1	G	370	ARG
1	G	401	SER
1	H	8	ASP
1	H	14	LYS
1	H	18	VAL
1	H	83	THR
1	H	91	ARG
1	H	145	GLU
1	H	153	LYS
1	H	167	ASN
1	H	206	ARG
1	H	216	LEU
1	H	261	GLU
1	H	361	LYS
1	H	370	ARG
1	H	375	MET
1	H	401	SER
1	H	409	LEU
1	I	14	LYS
1	I	18	VAL
1	I	82	TRP
1	I	91	ARG
1	I	216	LEU
1	I	264	ASP
1	I	380	ARG
1	I	401	SER
1	I	409	LEU
2	J	9	ARG
2	K	9	ARG
2	L	9	ARG
2	M	9	ARG
1	N	8	ASP
1	N	14	LYS
1	N	18	VAL
1	N	91	ARG
1	N	167	ASN

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Mol	Chain	Res	Type
1	N	206	ARG
1	N	216	LEU
1	N	224	LYS
1	N	261	GLU
1	N	361	LYS
1	N	380	ARG
1	N	401	SER
1	N	442	SER
1	O	14	LYS
1	O	18	VAL
1	O	91	ARG
1	O	145	GLU
1	O	167	ASN
1	O	206	ARG
1	O	216	LEU
1	O	261	GLU
1	O	370	ARG
1	O	401	SER
1	P	14	LYS
1	P	18	VAL
1	P	91	ARG
1	P	145	GLU
1	P	206	ARG
1	P	216	LEU
1	P	261	GLU
1	P	361	LYS
1	P	370	ARG
1	P	375	MET
1	P	401	SER
1	P	409	LEU
1	Q	14	LYS
1	Q	18	VAL
1	Q	91	ARG
1	Q	216	LEU
1	Q	264	ASP
1	Q	380	ARG
1	Q	401	SER
1	Q	409	LEU
1	R	8	ASP
1	R	14	LYS
1	R	18	VAL
1	R	20	TYR

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Mol	Chain	Res	Type
1	R	36	GLU
1	R	91	ARG
1	R	145	GLU
1	R	153	LYS
1	R	167	ASN
1	R	206	ARG
1	R	212	GLN
1	R	216	LEU
1	R	224	LYS
1	R	261	GLU
1	R	361	LYS
1	R	409	LEU
1	S	14	LYS
1	S	18	VAL
1	S	40	SER
1	S	91	ARG
1	S	145	GLU
1	S	206	ARG
1	S	361	LYS
1	S	370	ARG
1	S	375	MET
1	S	401	SER
1	S	409	LEU
1	T	14	LYS
1	T	18	VAL
1	T	40	SER
1	T	83	THR
1	T	91	ARG
1	T	145	GLU
1	T	167	ASN
1	T	206	ARG
1	T	224	LYS
1	T	361	LYS
1	T	370	ARG
1	T	375	MET
1	T	409	LEU
2	U	9	ARG
2	V	9	ARG
2	W	9	ARG
2	X	9	ARG
2	Y	9	ARG
2	Z	9	ARG

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Mol	Chain	Res	Type
2	a	9	ARG
2	b	9	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	B	34	ASN
1	G	34	ASN
1	H	34	ASN
1	I	34	ASN
1	N	34	ASN
1	O	34	ASN
1	P	34	ASN
1	Q	34	ASN
1	R	34	ASN
1	S	34	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 28 are monoatomic - leaving 14 for Mogul analysis.

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	$\# Z  > 2$
4	GLN	O	503	-	8,9,9	0.82	1 (12%)	10,11,11	0.67	0
4	GLN	B	503	-	8,9,9	0.82	1 (12%)	10,11,11	0.67	0
4	GLN	Q	503	-	8,9,9	0.82	1 (12%)	10,11,11	0.66	0
4	GLN	R	503	-	8,9,9	0.72	0	10,11,11	0.56	0
4	GLN	P	503	-	8,9,9	0.81	1 (12%)	10,11,11	0.66	0
4	GLN	T	503	-	8,9,9	0.71	0	10,11,11	0.56	0
4	GLN	H	503	-	8,9,9	0.71	0	10,11,11	0.55	0
4	GLN	I	503	-	8,9,9	0.71	0	10,11,11	0.56	0
4	GLN	N	503	-	8,9,9	0.81	1 (12%)	10,11,11	0.67	0
4	GLN	S	503	-	8,9,9	0.70	0	10,11,11	0.53	0
4	GLN	A	503	-	8,9,9	0.82	1 (12%)	10,11,11	0.67	0
4	GLN	G	503	-	8,9,9	0.70	0	10,11,11	0.54	0
4	GLN	C	503	-	8,9,9	0.81	1 (12%)	10,11,11	0.67	0
4	GLN	F	503	-	8,9,9	0.71	0	10,11,11	0.54	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GLN	O	503	-	-	5/9/9/9	-
4	GLN	B	503	-	-	4/9/9/9	-
4	GLN	Q	503	-	-	5/9/9/9	-
4	GLN	R	503	-	-	4/9/9/9	-
4	GLN	P	503	-	-	5/9/9/9	-
4	GLN	T	503	-	-	4/9/9/9	-
4	GLN	H	503	-	-	4/9/9/9	-
4	GLN	I	503	-	-	4/9/9/9	-
4	GLN	N	503	-	-	5/9/9/9	-
4	GLN	S	503	-	-	2/9/9/9	-
4	GLN	A	503	-	-	5/9/9/9	-
4	GLN	G	503	-	-	4/9/9/9	-
4	GLN	C	503	-	-	4/9/9/9	-
4	GLN	F	503	-	-	3/9/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	Q	503	GLN	OXT-C	-2.21	1.23	1.30
4	A	503	GLN	OXT-C	-2.20	1.23	1.30
4	O	503	GLN	OXT-C	-2.19	1.23	1.30
4	B	503	GLN	OXT-C	-2.19	1.23	1.30
4	C	503	GLN	OXT-C	-2.19	1.23	1.30
4	P	503	GLN	OXT-C	-2.18	1.23	1.30
4	N	503	GLN	OXT-C	-2.18	1.23	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	503	GLN	CA-CB-CG-CD
4	S	503	GLN	CA-CB-CG-CD
4	A	503	GLN	CA-CB-CG-CD
4	B	503	GLN	CA-CB-CG-CD
4	H	503	GLN	CA-CB-CG-CD
4	Q	503	GLN	CA-CB-CG-CD
4	A	503	GLN	OXT-C-CA-CB
4	O	503	GLN	OXT-C-CA-CB
4	C	503	GLN	CA-CB-CG-CD
4	P	503	GLN	OXT-C-CA-CB
4	Q	503	GLN	OXT-C-CA-CB
4	C	503	GLN	OXT-C-CA-CB
4	N	503	GLN	OXT-C-CA-CB
4	N	503	GLN	CA-CB-CG-CD
4	O	503	GLN	CA-CB-CG-CD
4	P	503	GLN	CA-CB-CG-CD
4	T	503	GLN	CA-CB-CG-CD
4	A	503	GLN	O-C-CA-CB
4	B	503	GLN	OXT-C-CA-CB
4	C	503	GLN	O-C-CA-CB
4	N	503	GLN	O-C-CA-CB
4	O	503	GLN	O-C-CA-CB
4	P	503	GLN	O-C-CA-CB
4	Q	503	GLN	O-C-CA-CB
4	B	503	GLN	O-C-CA-CB
4	R	503	GLN	OXT-C-CA-CB
4	G	503	GLN	CA-CB-CG-CD
4	R	503	GLN	O-C-CA-CB

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	T	503	GLN	OXT-C-CA-CB
4	F	503	GLN	CA-CB-CG-CD
4	I	503	GLN	CA-CB-CG-CD
4	G	503	GLN	OXT-C-CA-CB
4	I	503	GLN	OXT-C-CA-CB
4	T	503	GLN	O-C-CA-CB
4	H	503	GLN	OXT-C-CA-CB
4	Q	503	GLN	OXT-C-CA-N
4	I	503	GLN	O-C-CA-CB
4	F	503	GLN	OXT-C-CA-CB
4	G	503	GLN	O-C-CA-CB
4	H	503	GLN	O-C-CA-CB
4	A	503	GLN	OXT-C-CA-N
4	O	503	GLN	OXT-C-CA-N
4	P	503	GLN	OXT-C-CA-N
4	N	503	GLN	OXT-C-CA-N
4	A	503	GLN	N-CA-CB-CG
4	B	503	GLN	N-CA-CB-CG
4	C	503	GLN	N-CA-CB-CG
4	F	503	GLN	N-CA-CB-CG
4	G	503	GLN	N-CA-CB-CG
4	H	503	GLN	N-CA-CB-CG
4	I	503	GLN	N-CA-CB-CG
4	N	503	GLN	N-CA-CB-CG
4	O	503	GLN	N-CA-CB-CG
4	P	503	GLN	N-CA-CB-CG
4	Q	503	GLN	N-CA-CB-CG
4	R	503	GLN	N-CA-CB-CG
4	S	503	GLN	N-CA-CB-CG
4	T	503	GLN	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

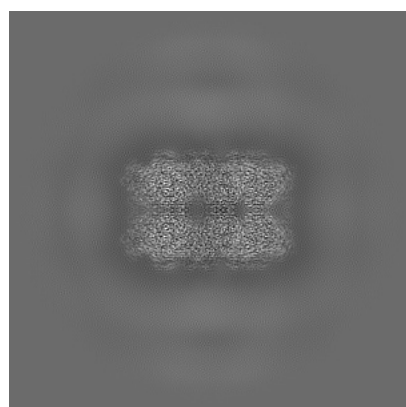
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25869. These allow visual inspection of the internal detail of the map and identification of artifacts.

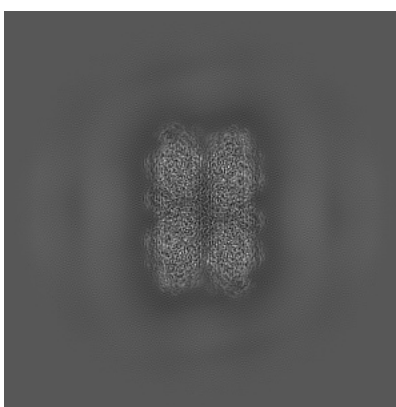
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

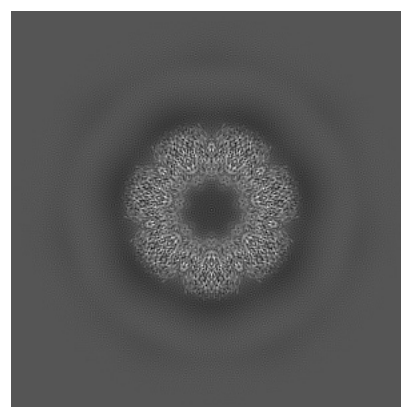
#### 6.1.1 Primary map



X



Y

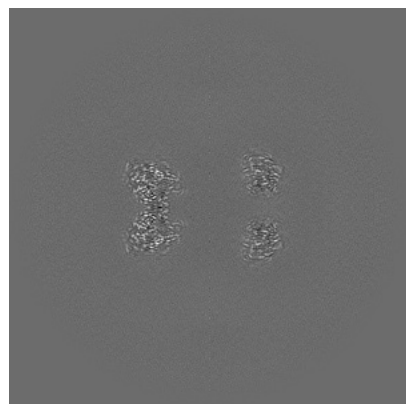


Z

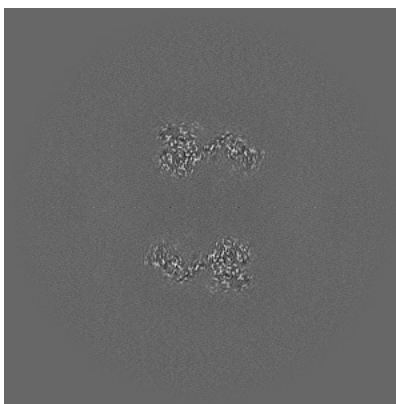
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

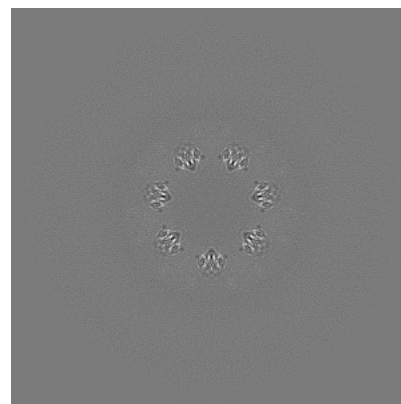
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

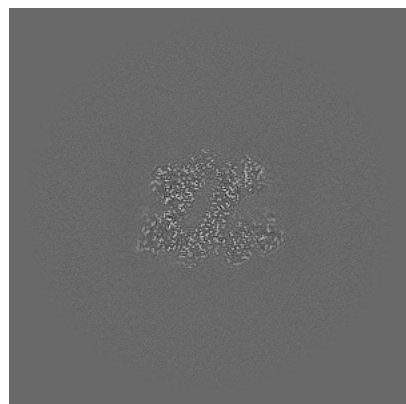


Z Index: 200

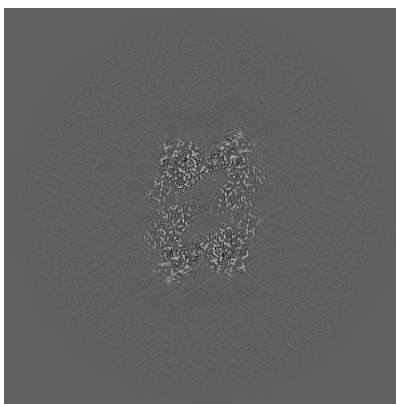
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

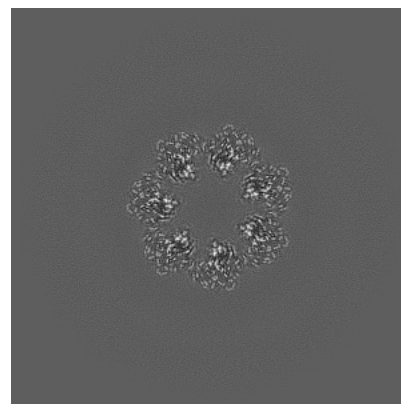
### 6.3.1 Primary map



X Index: 248



Y Index: 159

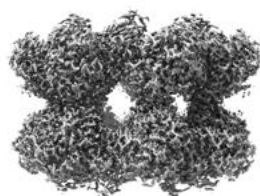


Z Index: 222

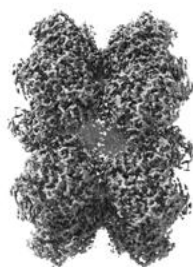
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

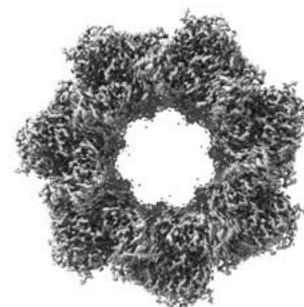
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

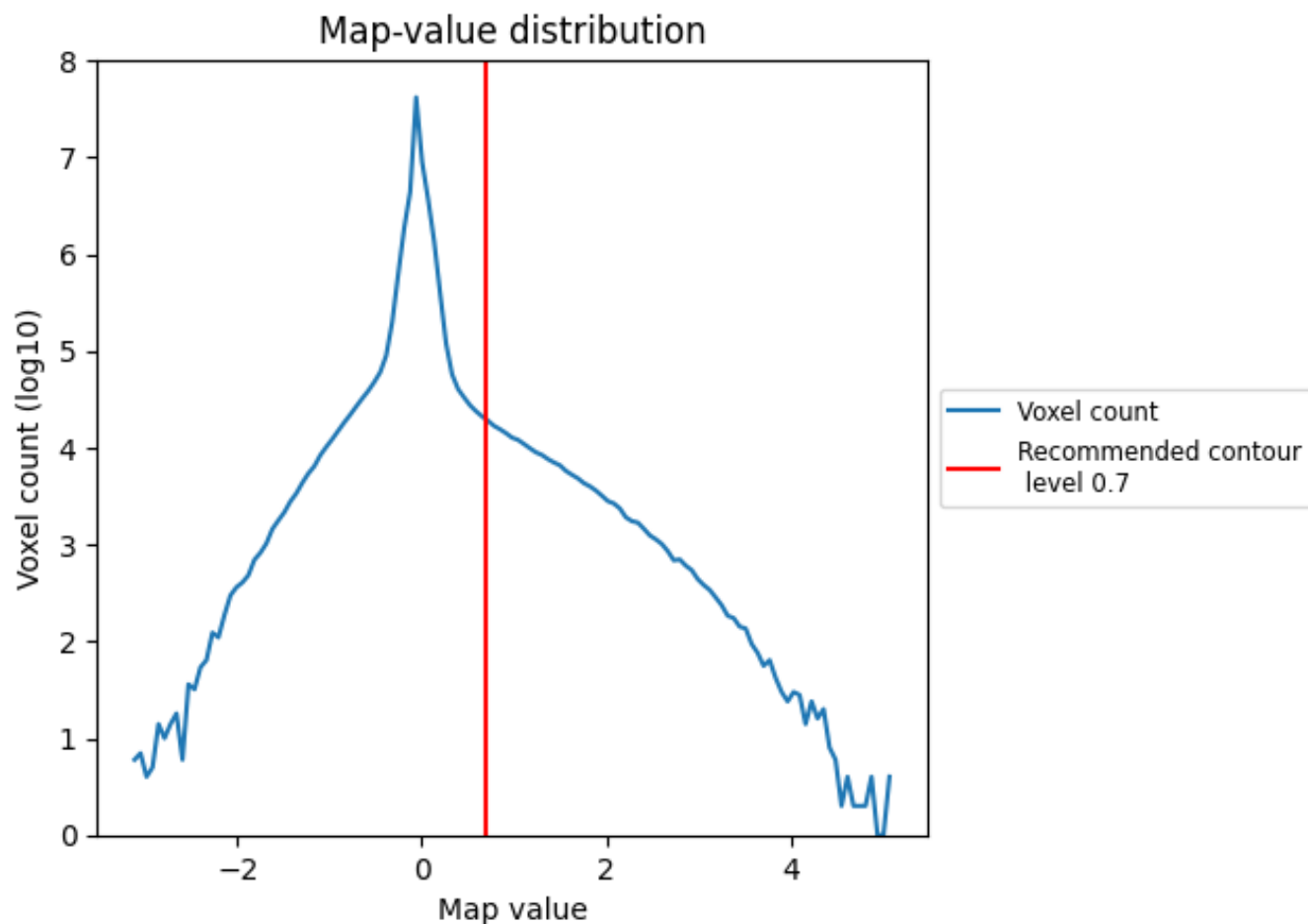
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

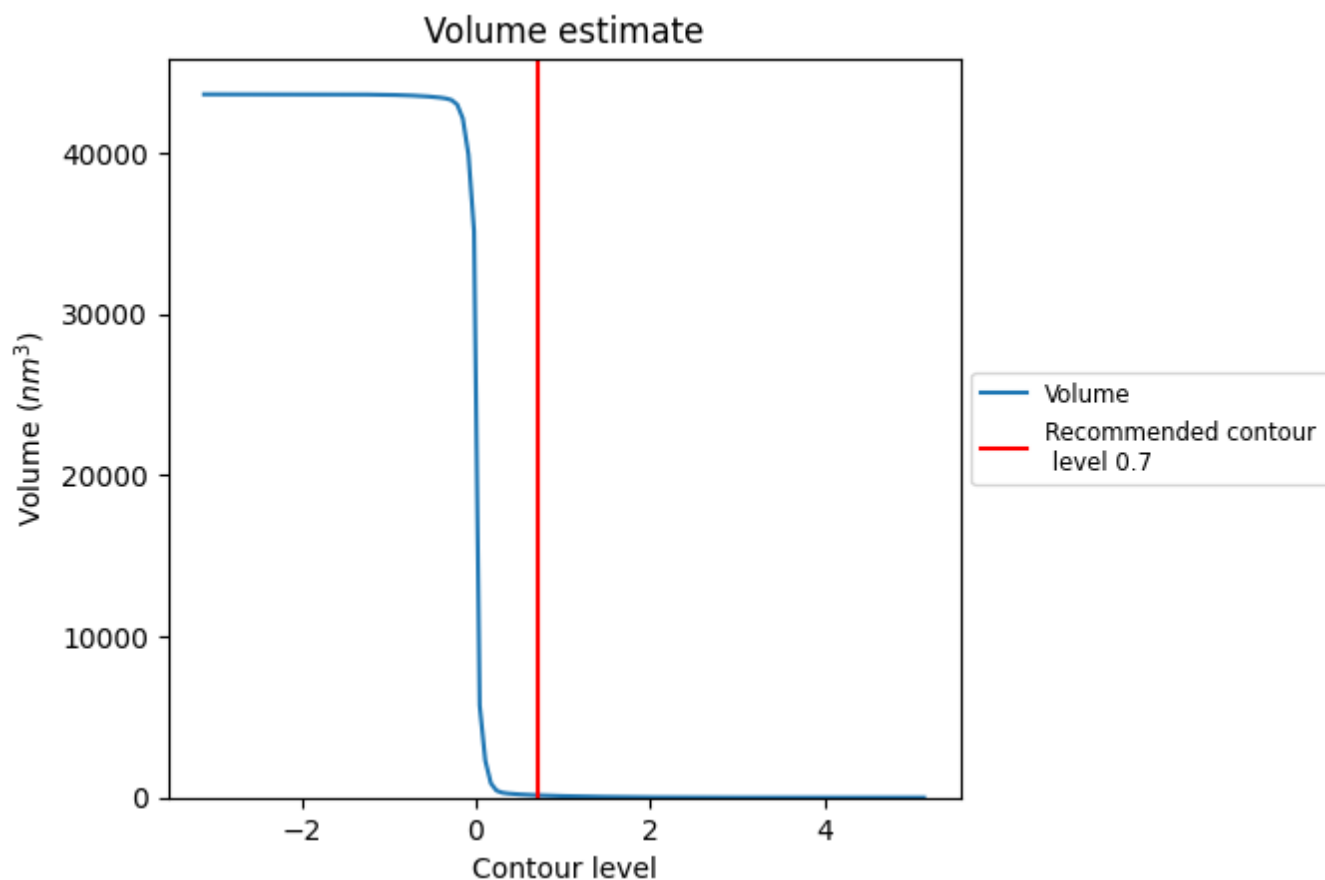
This section contains the results of statistical analysis of the map.

### 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](#)

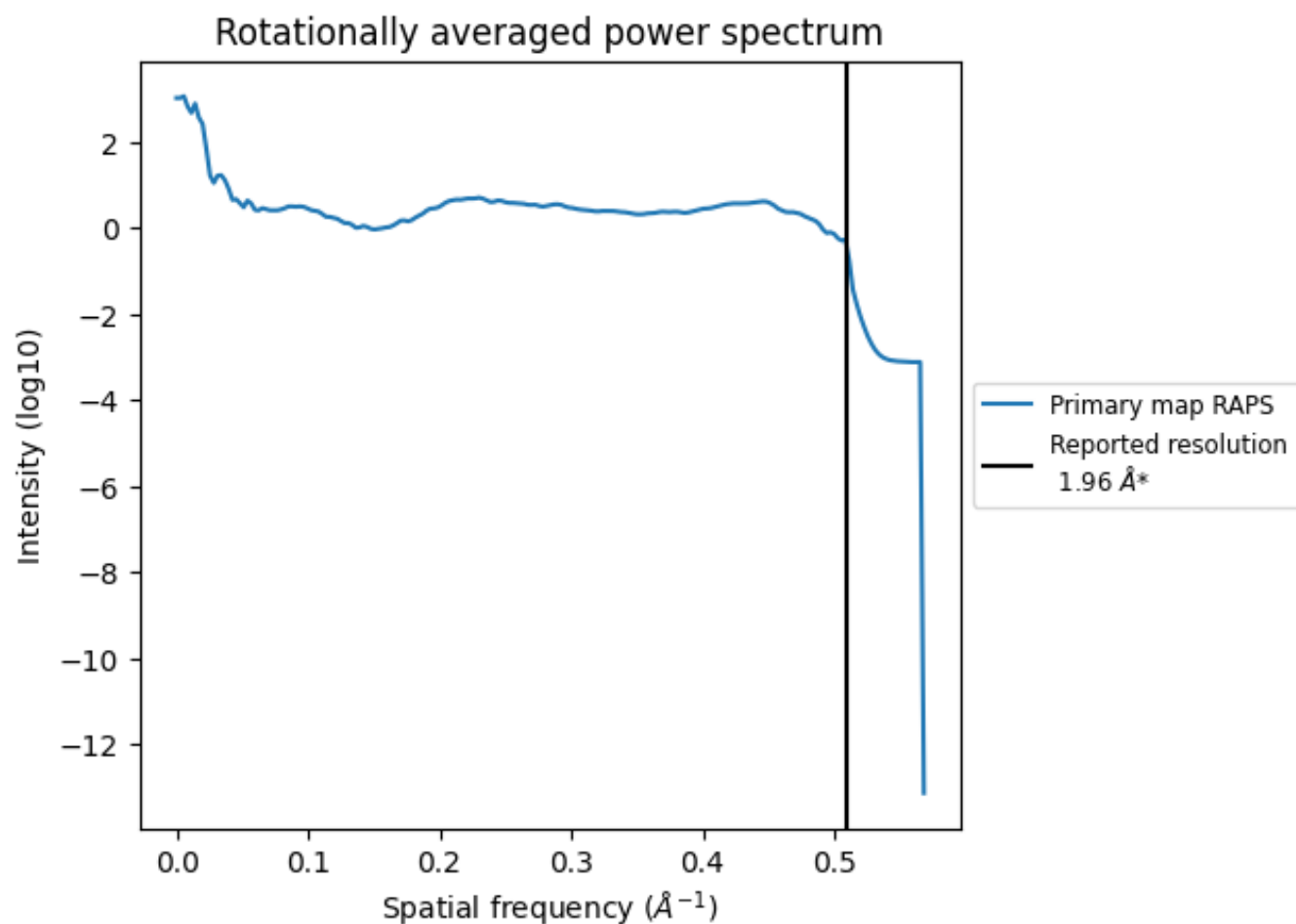


The volume at the recommended contour level is 144 nm<sup>3</sup>; this corresponds to an approximate mass of 130 kDa.

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

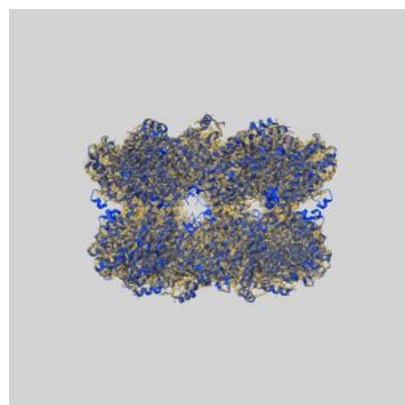
## 8 Fourier-Shell correlation ⓘ

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

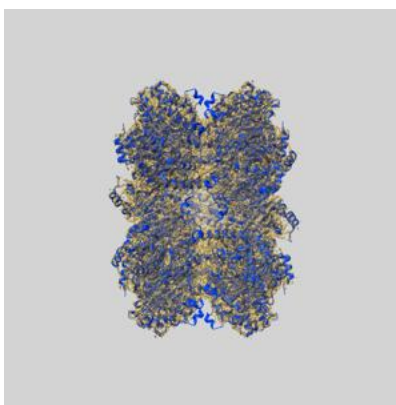
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25869 and PDB model 7TFC. Per-residue inclusion information can be found in section 3 on page 15.

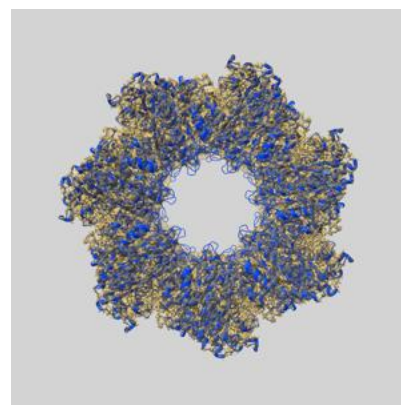
### 9.1 Map-model overlay [i](#)



X



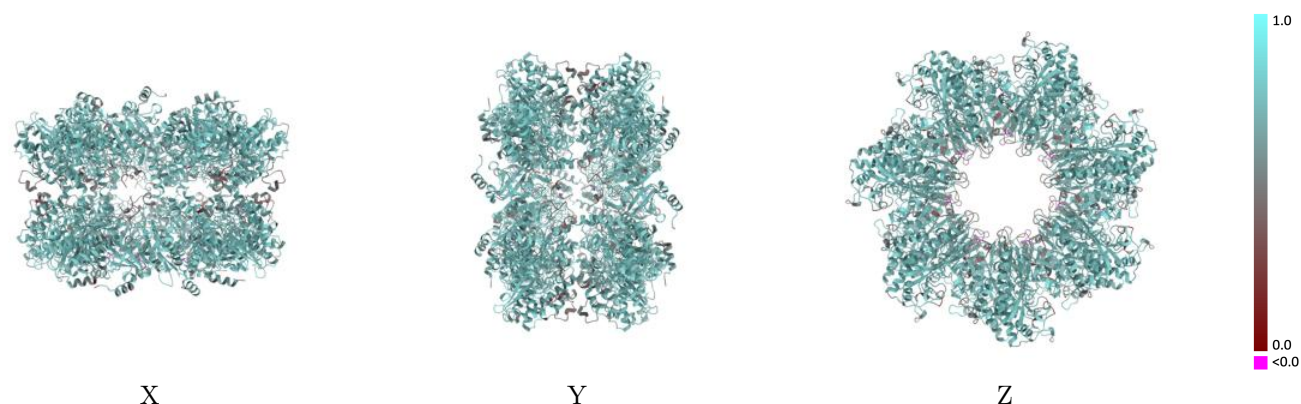
Y



Z

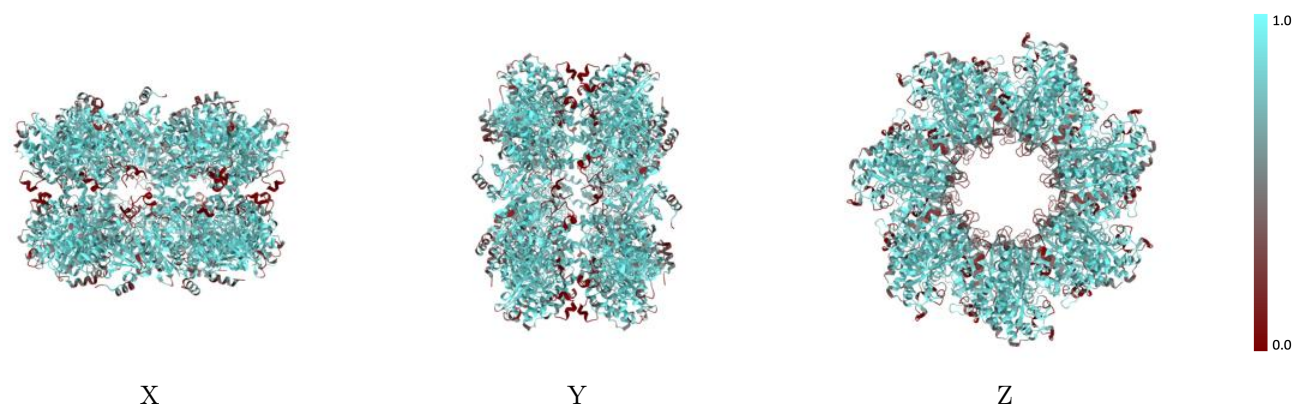
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



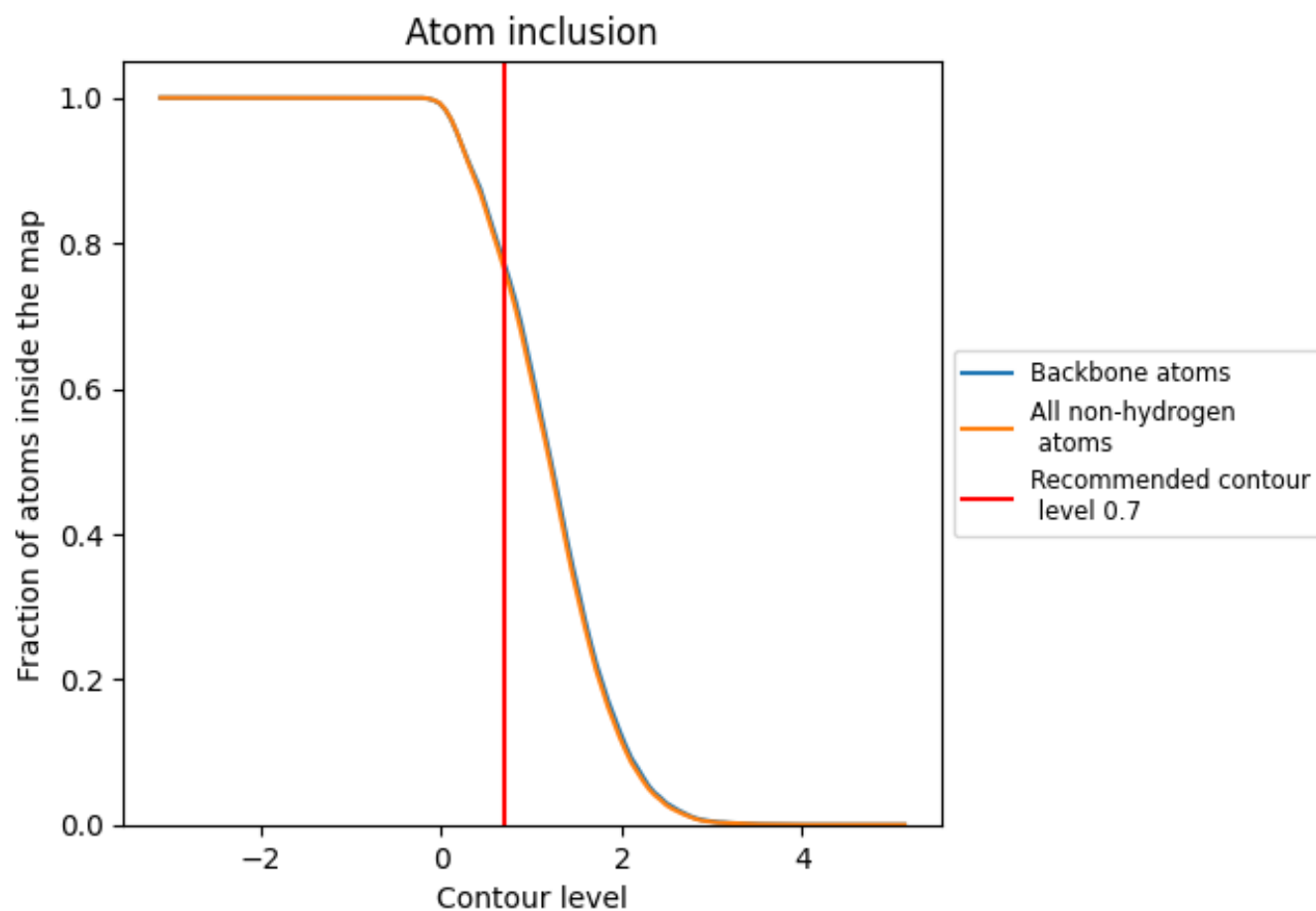
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).



























































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7633	 0.7010
A	 0.7813	 0.7080
B	 0.7816	 0.7110
C	 0.7853	 0.7090
D	 0.0375	 0.4080
E	 0.0250	 0.4150
F	 0.7848	 0.7090
G	 0.7845	 0.7080
H	 0.7830	 0.7080
I	 0.7842	 0.7090
J	 0.0250	 0.4200
K	 0.0500	 0.4070
L	 0.0125	 0.3880
M	 0.0125	 0.4020
N	 0.7827	 0.7080
O	 0.7833	 0.7080
P	 0.7836	 0.7090
Q	 0.7833	 0.7070
R	 0.7810	 0.7080
S	 0.7798	 0.7090
T	 0.7848	 0.7090
U	 0.0000	 0.3710
V	 0.0375	 0.4200
W	 0.0250	 0.3950
X	 0.0250	 0.4230
Y	 0.0125	 0.4000
Z	 0.0375	 0.4220
a	 0.0125	 0.3860
b	 0.0375	 0.3860

