



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 12:41 PM UTC

PDB ID : 8RJL / pdb_00008rjl
EMDB ID : EMD-19251
Title : Structure of a first order Sierpinski triangle formed by the H369R mutant of the citrate synthase from *Synechococcus elongatus*
Authors : Lo, Y.K.; Bohn, S.; Sendker, F.L.; Schuller, J.M.; Hochberg, G.
Deposited on : 2023-12-21
Resolution : 3.34 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:

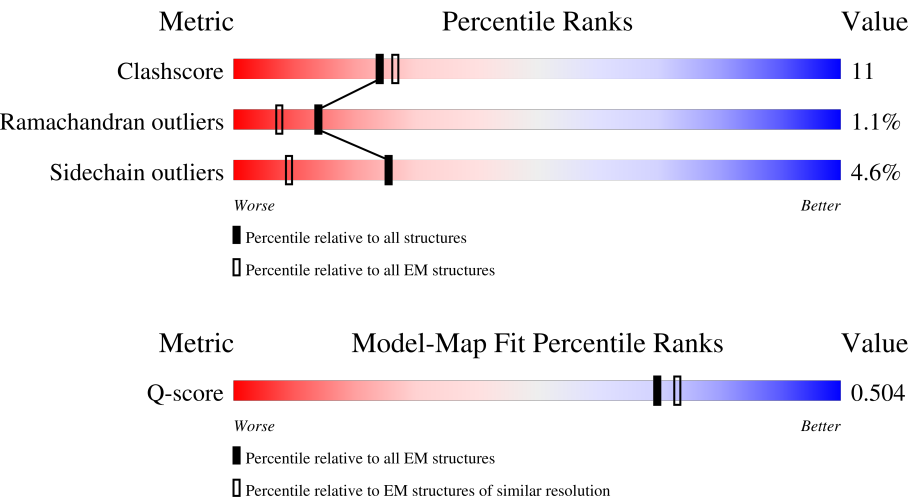
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.34 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	14446 (2.84 - 3.84)

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	13% 42% 11% 45%
1	B	394	11% 43% 12% 44%
1	C	394	58% 9% 31%
1	D	394	52% 15% 31%

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Mol	Chain	Length	Quality of chain
1	E	394	
1	F	394	
1	G	394	
1	H	394	
1	I	394	
1	J	394	
1	K	394	
1	L	394	
1	M	394	
1	N	394	
1	O	394	
1	P	394	
1	Q	394	
1	R	394	

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 36300 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	B	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	C	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	D	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	G	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		
1	H	273	Total	C	N	O	S	0	0
			2162	1389	370	395	8		
1	E	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	I	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	K	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	M	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	O	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		
1	Q	273	Total	C	N	O	S	0	0
			2162	1389	370	395	8		
1	F	218	Total	C	N	O	S	0	0
			1729	1122	291	308	8		
1	J	219	Total	C	N	O	S	0	0
			1740	1126	294	312	8		
1	L	273	Total	C	N	O	S	0	0
			2167	1393	371	395	8		
1	N	272	Total	C	N	O	S	0	0
			2156	1386	373	389	8		
1	P	270	Total	C	N	O	S	0	0
			2146	1380	370	388	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	273	Total	C	N	O	S	0	0
			2162	1389	370	395	8		

There are 162 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	369	ARG	HIS	engineered mutation	UNP Q31QM5
A	387	LEU	-	expression tag	UNP Q31QM5
A	388	GLU	-	expression tag	UNP Q31QM5
A	389	HIS	-	expression tag	UNP Q31QM5
A	390	HIS	-	expression tag	UNP Q31QM5
A	391	HIS	-	expression tag	UNP Q31QM5
A	392	HIS	-	expression tag	UNP Q31QM5
A	393	HIS	-	expression tag	UNP Q31QM5
A	394	HIS	-	expression tag	UNP Q31QM5
B	369	ARG	HIS	engineered mutation	UNP Q31QM5
B	387	LEU	-	expression tag	UNP Q31QM5
B	388	GLU	-	expression tag	UNP Q31QM5
B	389	HIS	-	expression tag	UNP Q31QM5
B	390	HIS	-	expression tag	UNP Q31QM5
B	391	HIS	-	expression tag	UNP Q31QM5
B	392	HIS	-	expression tag	UNP Q31QM5
B	393	HIS	-	expression tag	UNP Q31QM5
B	394	HIS	-	expression tag	UNP Q31QM5
C	369	ARG	HIS	engineered mutation	UNP Q31QM5
C	387	LEU	-	expression tag	UNP Q31QM5
C	388	GLU	-	expression tag	UNP Q31QM5
C	389	HIS	-	expression tag	UNP Q31QM5
C	390	HIS	-	expression tag	UNP Q31QM5
C	391	HIS	-	expression tag	UNP Q31QM5
C	392	HIS	-	expression tag	UNP Q31QM5
C	393	HIS	-	expression tag	UNP Q31QM5
C	394	HIS	-	expression tag	UNP Q31QM5
D	369	ARG	HIS	engineered mutation	UNP Q31QM5
D	387	LEU	-	expression tag	UNP Q31QM5
D	388	GLU	-	expression tag	UNP Q31QM5
D	389	HIS	-	expression tag	UNP Q31QM5
D	390	HIS	-	expression tag	UNP Q31QM5
D	391	HIS	-	expression tag	UNP Q31QM5
D	392	HIS	-	expression tag	UNP Q31QM5
D	393	HIS	-	expression tag	UNP Q31QM5
D	394	HIS	-	expression tag	UNP Q31QM5

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Chain	Residue	Modelled	Actual	Comment	Reference
G	369	ARG	HIS	engineered mutation	UNP Q31QM5
G	387	LEU	-	expression tag	UNP Q31QM5
G	388	GLU	-	expression tag	UNP Q31QM5
G	389	HIS	-	expression tag	UNP Q31QM5
G	390	HIS	-	expression tag	UNP Q31QM5
G	391	HIS	-	expression tag	UNP Q31QM5
G	392	HIS	-	expression tag	UNP Q31QM5
G	393	HIS	-	expression tag	UNP Q31QM5
G	394	HIS	-	expression tag	UNP Q31QM5
H	369	ARG	HIS	engineered mutation	UNP Q31QM5
H	387	LEU	-	expression tag	UNP Q31QM5
H	388	GLU	-	expression tag	UNP Q31QM5
H	389	HIS	-	expression tag	UNP Q31QM5
H	390	HIS	-	expression tag	UNP Q31QM5
H	391	HIS	-	expression tag	UNP Q31QM5
H	392	HIS	-	expression tag	UNP Q31QM5
H	393	HIS	-	expression tag	UNP Q31QM5
H	394	HIS	-	expression tag	UNP Q31QM5
E	369	ARG	HIS	engineered mutation	UNP Q31QM5
E	387	LEU	-	expression tag	UNP Q31QM5
E	388	GLU	-	expression tag	UNP Q31QM5
E	389	HIS	-	expression tag	UNP Q31QM5
E	390	HIS	-	expression tag	UNP Q31QM5
E	391	HIS	-	expression tag	UNP Q31QM5
E	392	HIS	-	expression tag	UNP Q31QM5
E	393	HIS	-	expression tag	UNP Q31QM5
E	394	HIS	-	expression tag	UNP Q31QM5
I	369	ARG	HIS	engineered mutation	UNP Q31QM5
I	387	LEU	-	expression tag	UNP Q31QM5
I	388	GLU	-	expression tag	UNP Q31QM5
I	389	HIS	-	expression tag	UNP Q31QM5
I	390	HIS	-	expression tag	UNP Q31QM5
I	391	HIS	-	expression tag	UNP Q31QM5
I	392	HIS	-	expression tag	UNP Q31QM5
I	393	HIS	-	expression tag	UNP Q31QM5
I	394	HIS	-	expression tag	UNP Q31QM5
K	369	ARG	HIS	engineered mutation	UNP Q31QM5
K	387	LEU	-	expression tag	UNP Q31QM5
K	388	GLU	-	expression tag	UNP Q31QM5
K	389	HIS	-	expression tag	UNP Q31QM5
K	390	HIS	-	expression tag	UNP Q31QM5
K	391	HIS	-	expression tag	UNP Q31QM5

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Chain	Residue	Modelled	Actual	Comment	Reference
K	392	HIS	-	expression tag	UNP Q31QM5
K	393	HIS	-	expression tag	UNP Q31QM5
K	394	HIS	-	expression tag	UNP Q31QM5
M	369	ARG	HIS	engineered mutation	UNP Q31QM5
M	387	LEU	-	expression tag	UNP Q31QM5
M	388	GLU	-	expression tag	UNP Q31QM5
M	389	HIS	-	expression tag	UNP Q31QM5
M	390	HIS	-	expression tag	UNP Q31QM5
M	391	HIS	-	expression tag	UNP Q31QM5
M	392	HIS	-	expression tag	UNP Q31QM5
M	393	HIS	-	expression tag	UNP Q31QM5
M	394	HIS	-	expression tag	UNP Q31QM5
O	369	ARG	HIS	engineered mutation	UNP Q31QM5
O	387	LEU	-	expression tag	UNP Q31QM5
O	388	GLU	-	expression tag	UNP Q31QM5
O	389	HIS	-	expression tag	UNP Q31QM5
O	390	HIS	-	expression tag	UNP Q31QM5
O	391	HIS	-	expression tag	UNP Q31QM5
O	392	HIS	-	expression tag	UNP Q31QM5
O	393	HIS	-	expression tag	UNP Q31QM5
O	394	HIS	-	expression tag	UNP Q31QM5
Q	369	ARG	HIS	engineered mutation	UNP Q31QM5
Q	387	LEU	-	expression tag	UNP Q31QM5
Q	388	GLU	-	expression tag	UNP Q31QM5
Q	389	HIS	-	expression tag	UNP Q31QM5
Q	390	HIS	-	expression tag	UNP Q31QM5
Q	391	HIS	-	expression tag	UNP Q31QM5
Q	392	HIS	-	expression tag	UNP Q31QM5
Q	393	HIS	-	expression tag	UNP Q31QM5
Q	394	HIS	-	expression tag	UNP Q31QM5
F	369	ARG	HIS	engineered mutation	UNP Q31QM5
F	387	LEU	-	expression tag	UNP Q31QM5
F	388	GLU	-	expression tag	UNP Q31QM5
F	389	HIS	-	expression tag	UNP Q31QM5
F	390	HIS	-	expression tag	UNP Q31QM5
F	391	HIS	-	expression tag	UNP Q31QM5
F	392	HIS	-	expression tag	UNP Q31QM5
F	393	HIS	-	expression tag	UNP Q31QM5
F	394	HIS	-	expression tag	UNP Q31QM5
J	369	ARG	HIS	engineered mutation	UNP Q31QM5
J	387	LEU	-	expression tag	UNP Q31QM5
J	388	GLU	-	expression tag	UNP Q31QM5

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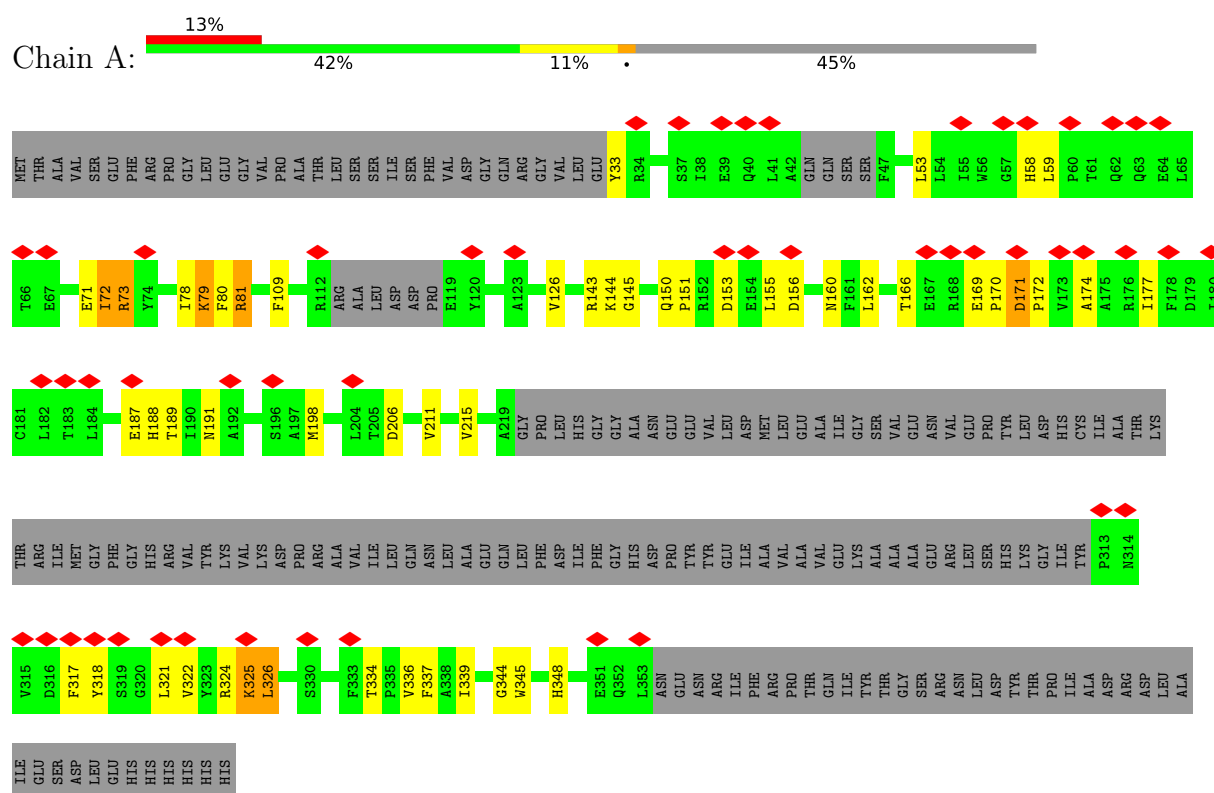
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Chain	Residue	Modelled	Actual	Comment	Reference
J	389	HIS	-	expression tag	UNP Q31QM5
J	390	HIS	-	expression tag	UNP Q31QM5
J	391	HIS	-	expression tag	UNP Q31QM5
J	392	HIS	-	expression tag	UNP Q31QM5
J	393	HIS	-	expression tag	UNP Q31QM5
J	394	HIS	-	expression tag	UNP Q31QM5
L	369	ARG	HIS	engineered mutation	UNP Q31QM5
L	387	LEU	-	expression tag	UNP Q31QM5
L	388	GLU	-	expression tag	UNP Q31QM5
L	389	HIS	-	expression tag	UNP Q31QM5
L	390	HIS	-	expression tag	UNP Q31QM5
L	391	HIS	-	expression tag	UNP Q31QM5
L	392	HIS	-	expression tag	UNP Q31QM5
L	393	HIS	-	expression tag	UNP Q31QM5
L	394	HIS	-	expression tag	UNP Q31QM5
N	369	ARG	HIS	engineered mutation	UNP Q31QM5
N	387	LEU	-	expression tag	UNP Q31QM5
N	388	GLU	-	expression tag	UNP Q31QM5
N	389	HIS	-	expression tag	UNP Q31QM5
N	390	HIS	-	expression tag	UNP Q31QM5
N	391	HIS	-	expression tag	UNP Q31QM5
N	392	HIS	-	expression tag	UNP Q31QM5
N	393	HIS	-	expression tag	UNP Q31QM5
N	394	HIS	-	expression tag	UNP Q31QM5
P	369	ARG	HIS	engineered mutation	UNP Q31QM5
P	387	LEU	-	expression tag	UNP Q31QM5
P	388	GLU	-	expression tag	UNP Q31QM5
P	389	HIS	-	expression tag	UNP Q31QM5
P	390	HIS	-	expression tag	UNP Q31QM5
P	391	HIS	-	expression tag	UNP Q31QM5
P	392	HIS	-	expression tag	UNP Q31QM5
P	393	HIS	-	expression tag	UNP Q31QM5
P	394	HIS	-	expression tag	UNP Q31QM5
R	369	ARG	HIS	engineered mutation	UNP Q31QM5
R	387	LEU	-	expression tag	UNP Q31QM5
R	388	GLU	-	expression tag	UNP Q31QM5
R	389	HIS	-	expression tag	UNP Q31QM5
R	390	HIS	-	expression tag	UNP Q31QM5
R	391	HIS	-	expression tag	UNP Q31QM5
R	392	HIS	-	expression tag	UNP Q31QM5
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R	394	HIS	-	expression tag	UNP Q31QM5

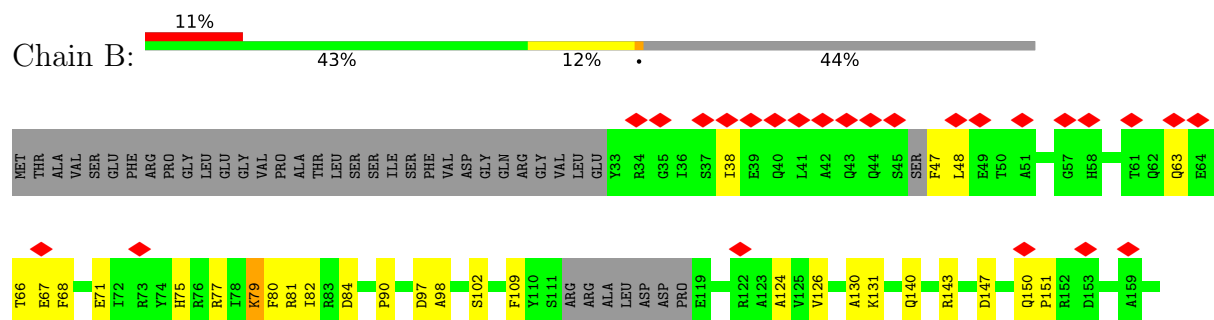
3 Residue-property plots

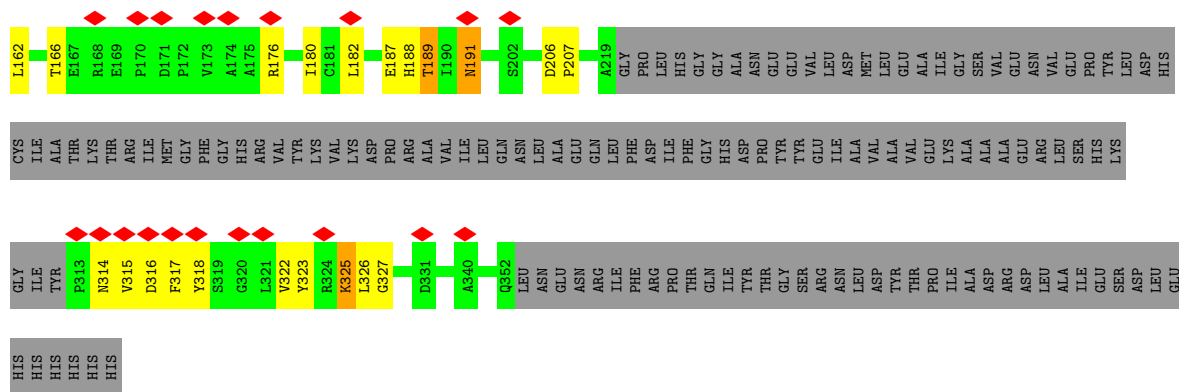
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

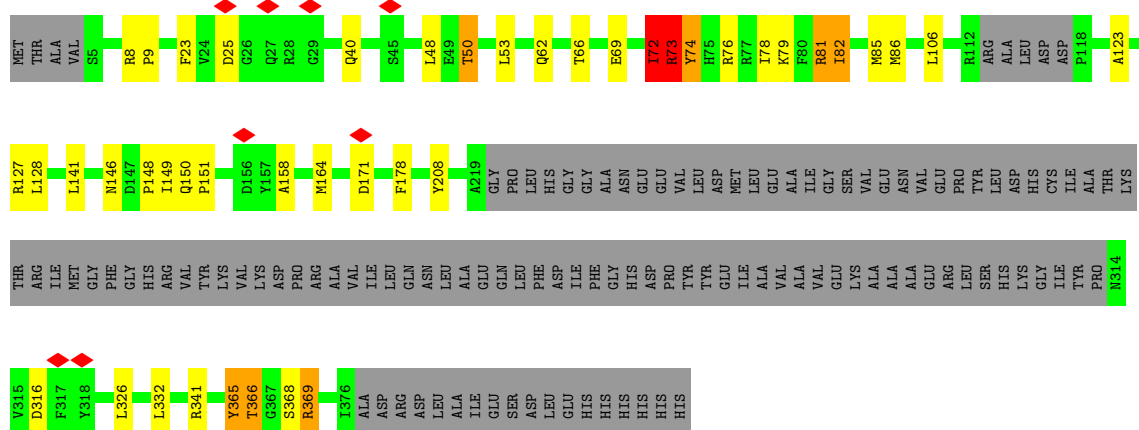


• Molecule 1: Citrate synthase

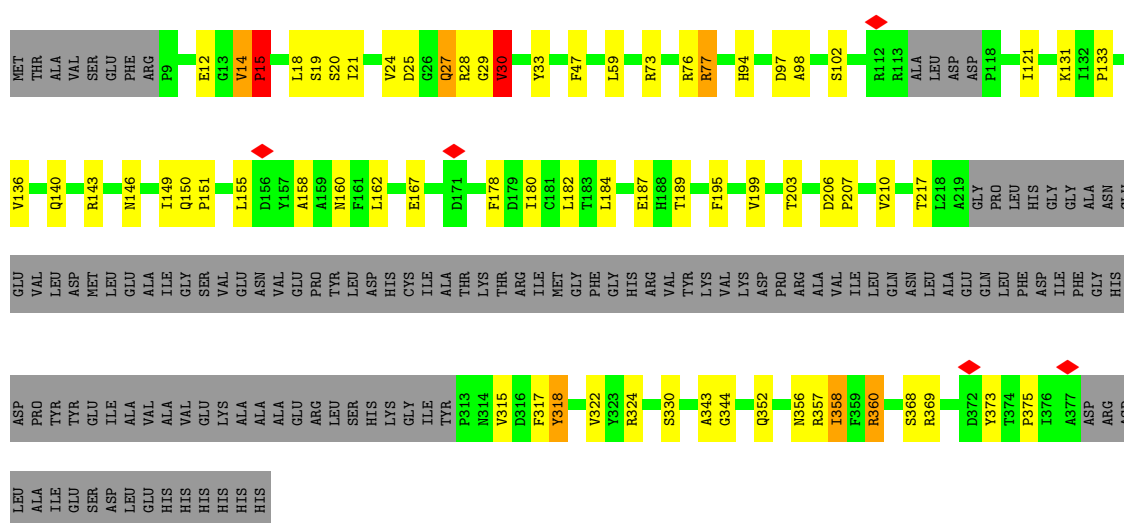




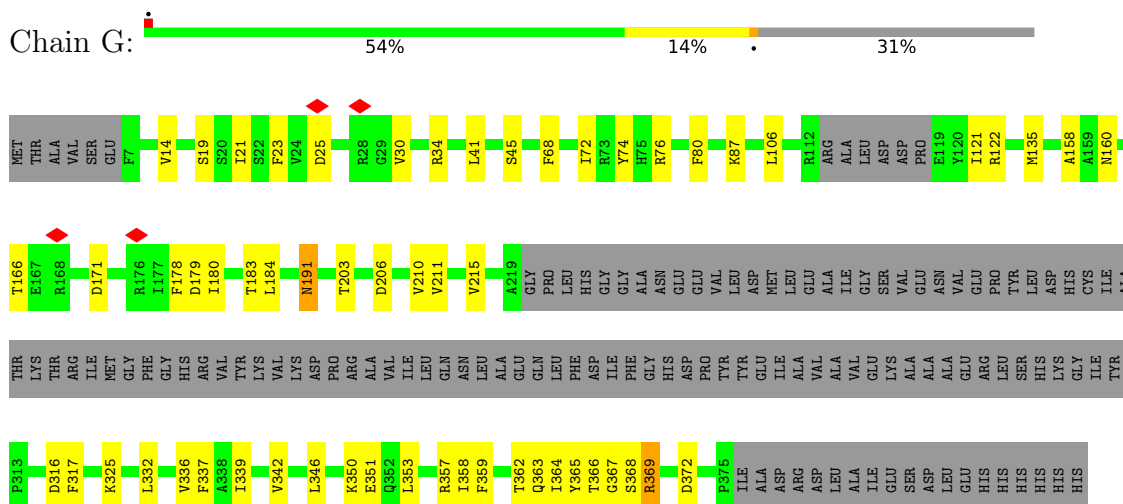
• Molecule 1: Citrate synthase



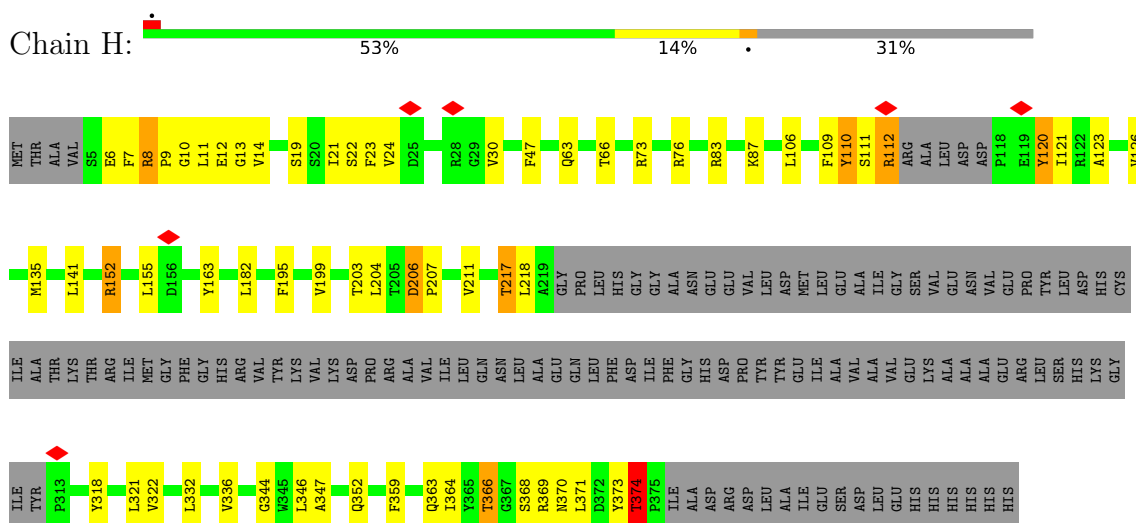
• Molecule 1: Citrate synthase



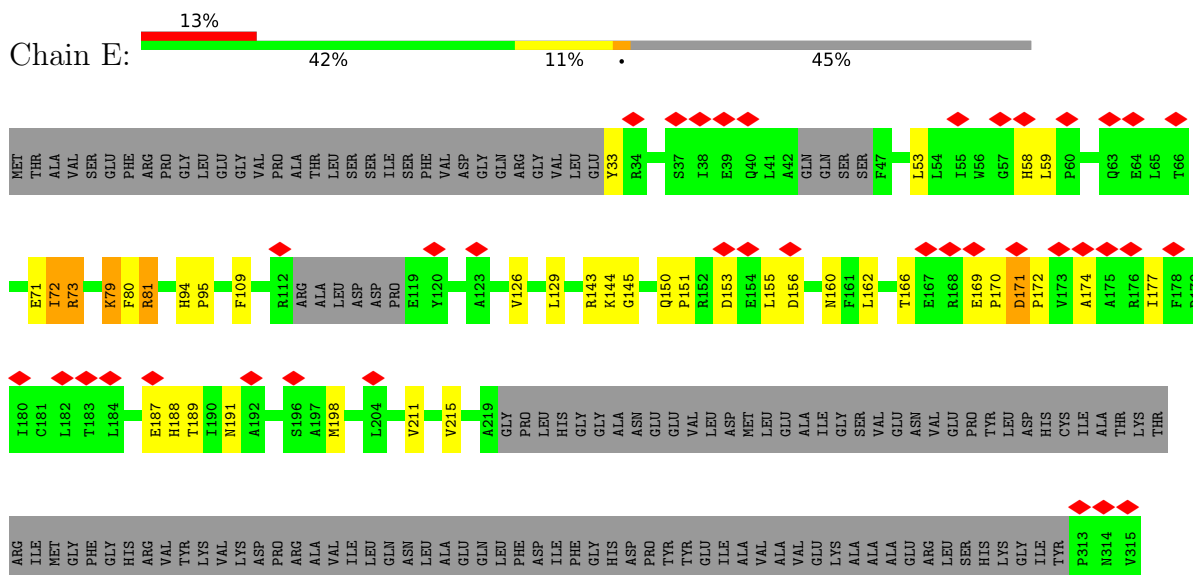
• Molecule 1: Citrate synthase

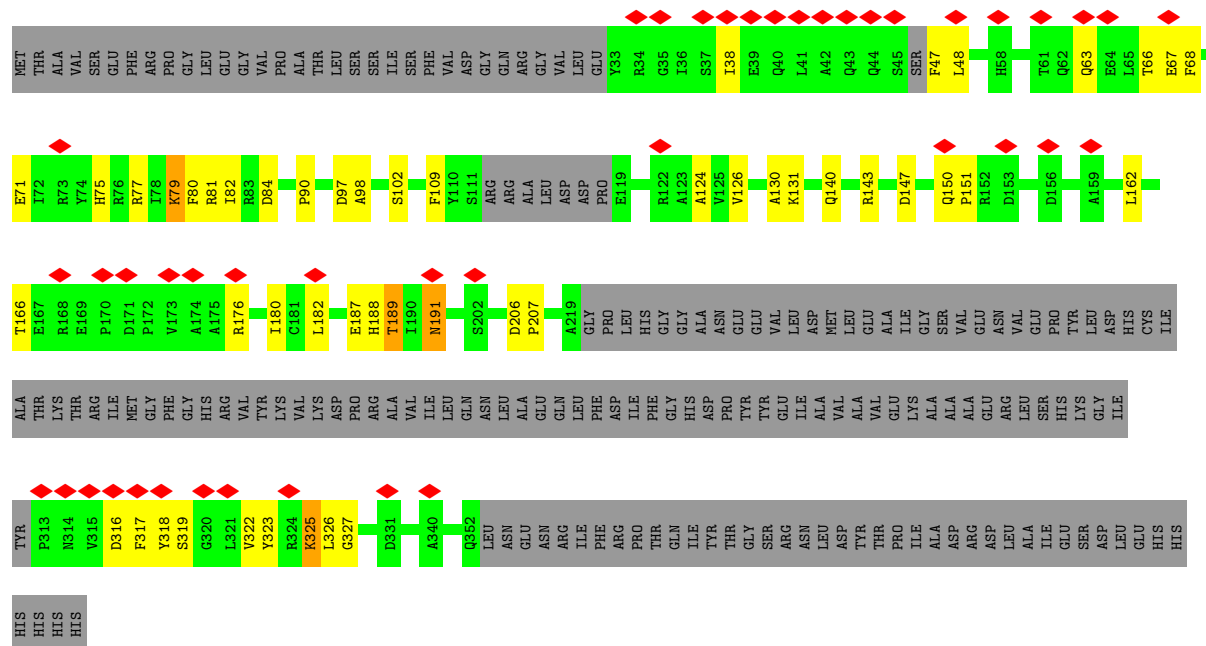


- Molecule 1: Citrate synthase

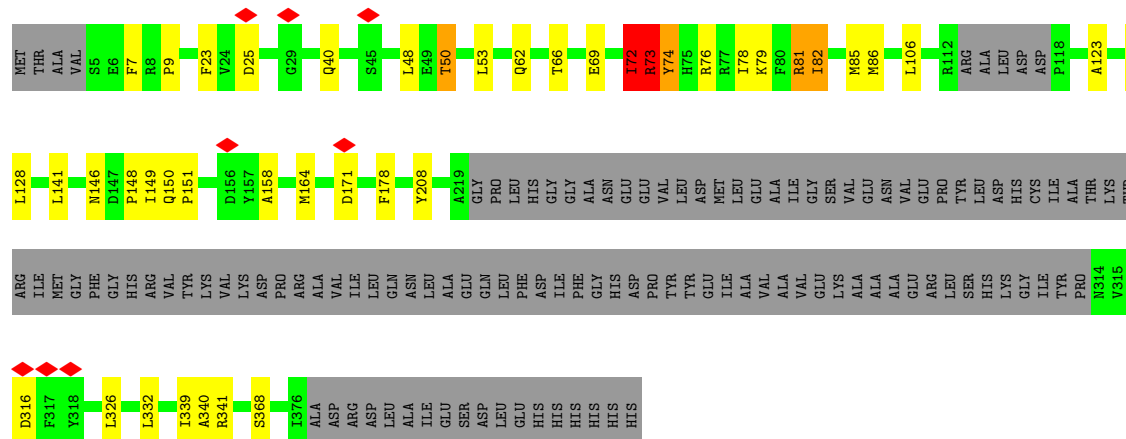


- Molecule 1: Citrate synthase



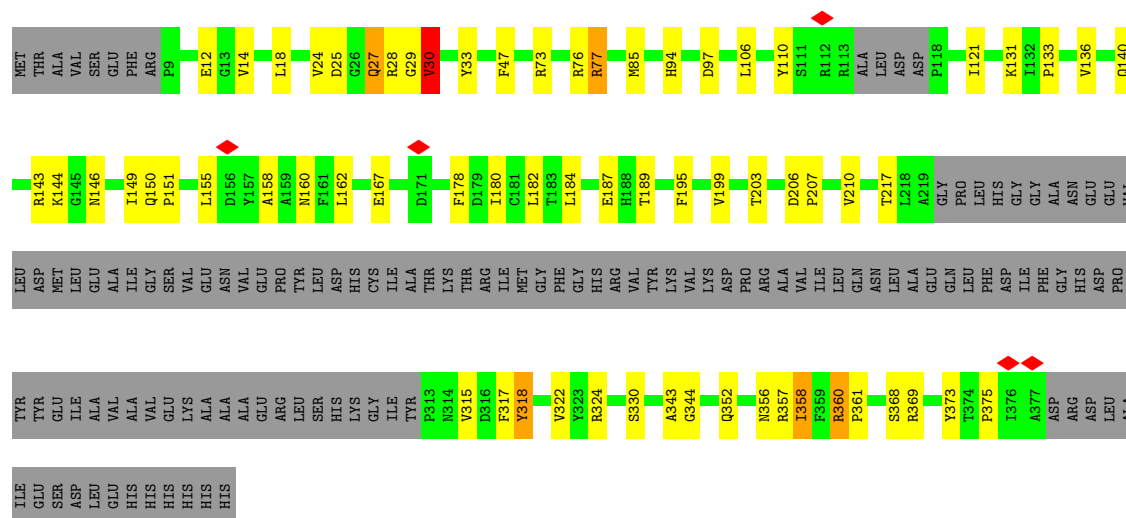


- Molecule 1: Citrate synthase

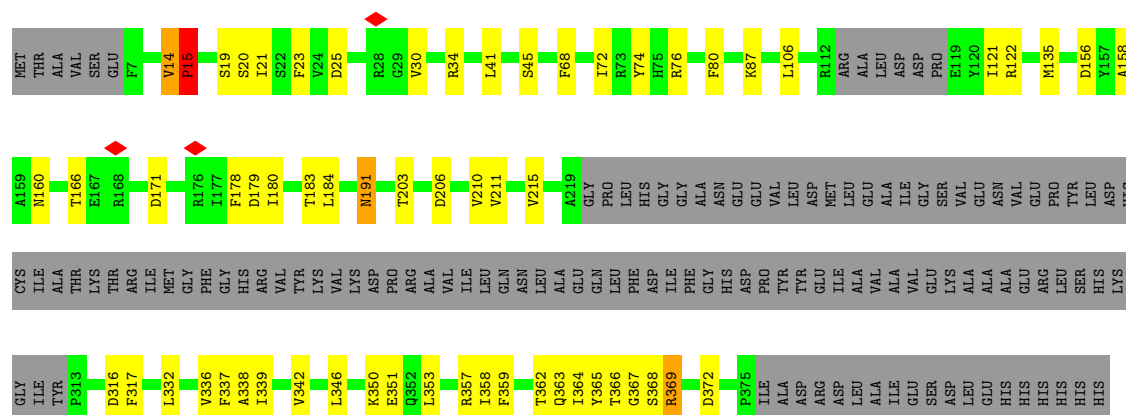


- Molecule 1: Citrate synthase

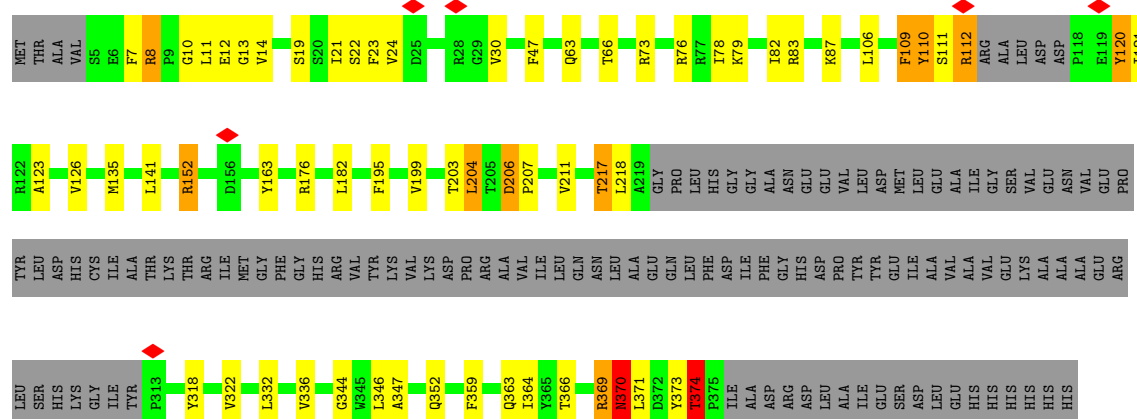




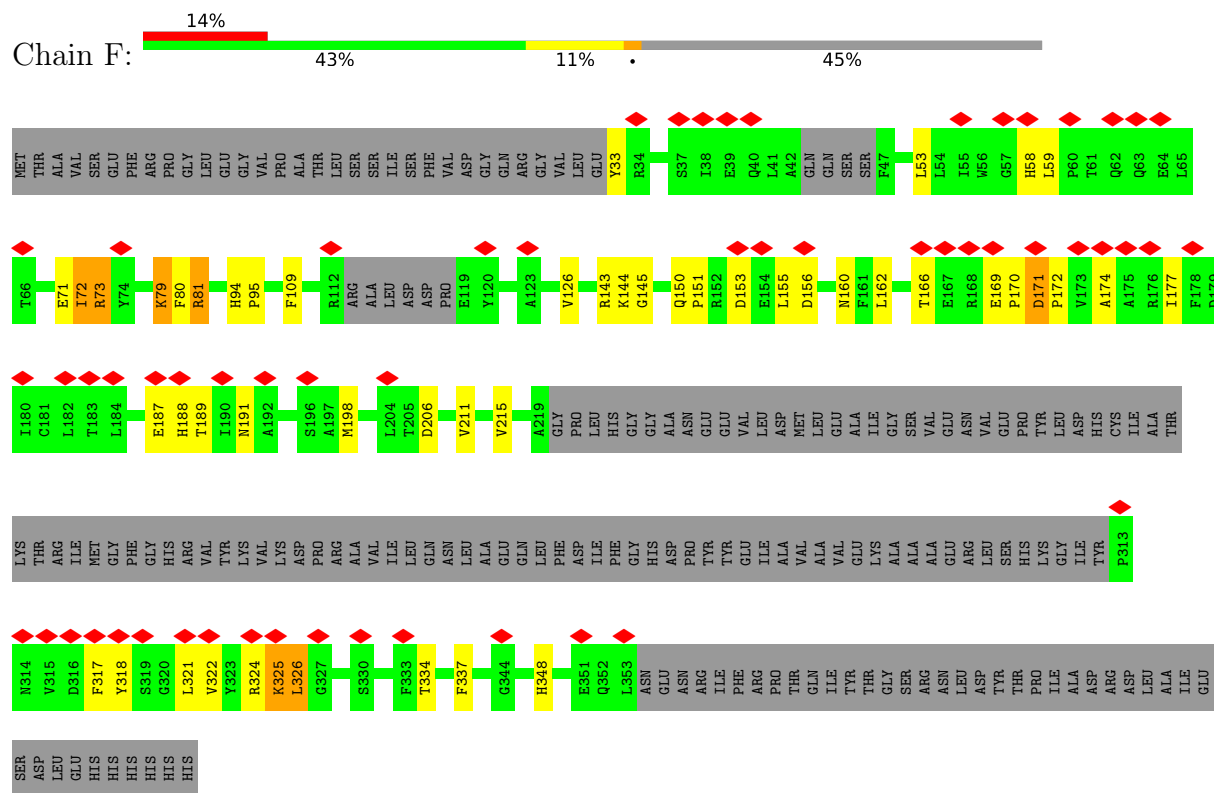
• Molecule 1: Citrate synthase



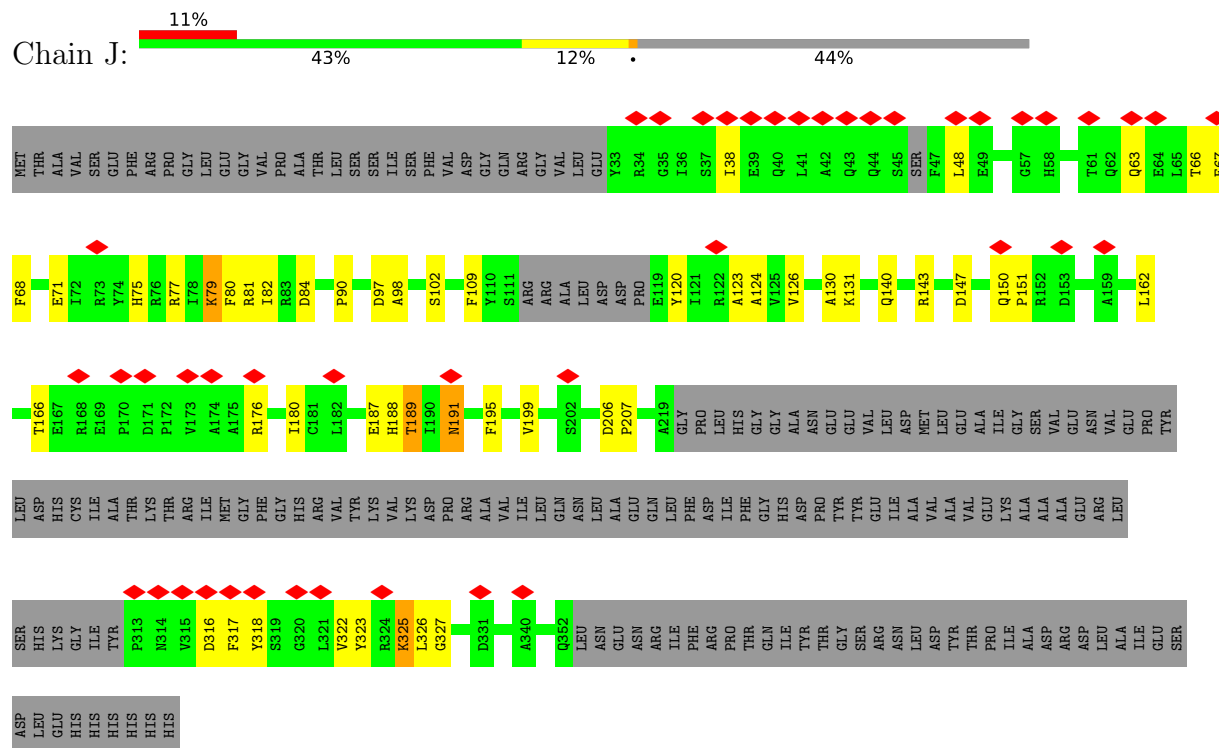
• Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



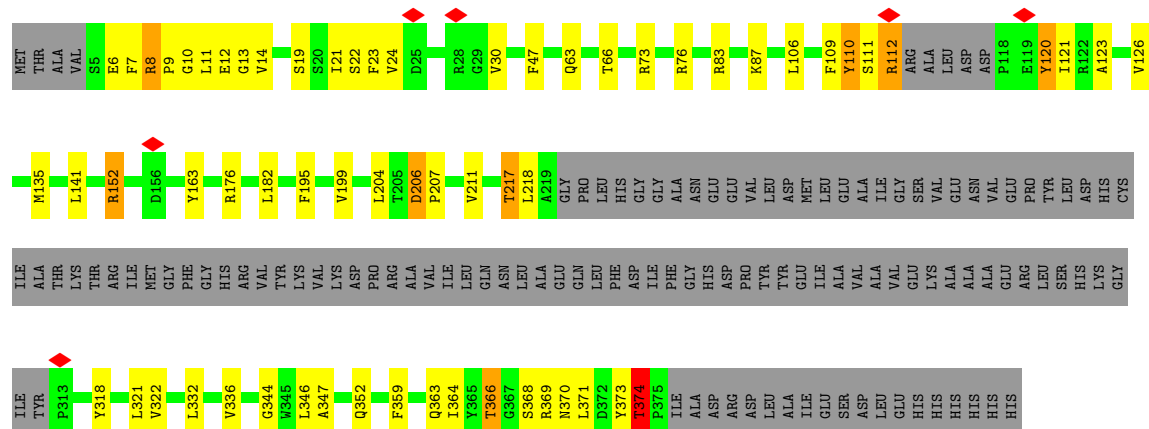
- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	178751	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.855	Depositor
Minimum map value	-0.625	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.1	Depositor
Map size ($\text{\AA}$)	395.0, 395.0, 395.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.79, 0.79, 0.79	Depositor

5 Model quality

5.1 Standard geometry

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	0.42	0/1772	0.69	0/2408
1	B	0.41	0/1783	0.73	1/2422 (0.0%)
1	C	0.59	2/2220 (0.1%)	0.81	2/3017 (0.1%)
1	D	0.74	2/2209 (0.1%)	0.97	8/3001 (0.3%)
1	E	0.42	0/1772	0.69	0/2408
1	F	0.42	0/1772	0.69	0/2408
1	G	0.57	0/2199	0.87	4/2988 (0.1%)
1	H	0.58	0/2216	0.87	7/3013 (0.2%)
1	I	0.41	0/1783	0.74	1/2422 (0.0%)
1	J	0.41	0/1783	0.74	1/2422 (0.0%)
1	K	0.58	2/2220 (0.1%)	0.82	2/3017 (0.1%)
1	L	0.58	2/2220 (0.1%)	0.83	2/3017 (0.1%)
1	M	0.61	1/2209 (0.0%)	0.88	5/3001 (0.2%)
1	N	0.61	0/2209	0.88	5/3001 (0.2%)
1	O	0.70	2/2199 (0.1%)	0.96	7/2988 (0.2%)
1	P	0.57	0/2199	0.87	4/2988 (0.1%)
1	Q	0.58	0/2216	0.85	3/3013 (0.1%)
1	R	0.59	0/2216	0.87	7/3013 (0.2%)
All	All	0.56	11/37197 (0.0%)	0.83	59/50547 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
1	G	0	1
1	I	0	1
1	J	0	1
1	M	0	1
1	N	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	1
1	P	0	1
All	All	0	9

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	15	PRO	N-CA	18.67	1.71	1.47
1	O	15	PRO	N-CA	18.43	1.71	1.47
1	L	146	ASN	C-N	-5.62	1.24	1.33
1	C	146	ASN	C-N	-5.57	1.24	1.33
1	K	146	ASN	C-N	-5.54	1.24	1.33
1	K	72	ILE	N-CA	5.36	1.53	1.46
1	L	72	ILE	N-CA	5.35	1.53	1.46
1	C	72	ILE	N-CA	5.33	1.53	1.46
1	O	14	VAL	C-N	5.11	1.45	1.33
1	D	14	VAL	C-N	5.11	1.45	1.33
1	M	361	PRO	N-CD	-5.02	1.40	1.47

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	14	VAL	CA-C-N	14.69	138.21	119.84
1	O	14	VAL	C-N-CA	14.69	138.21	119.84
1	D	14	VAL	CA-C-N	14.61	138.10	119.84
1	D	14	VAL	C-N-CA	14.61	138.10	119.84
1	O	15	PRO	CA-N-CD	-8.92	99.52	112.00
1	D	15	PRO	CA-N-CD	-8.57	100.00	112.00
1	K	74	TYR	N-CA-C	-8.13	103.08	113.16
1	C	74	TYR	N-CA-C	-8.12	103.10	113.16
1	L	74	TYR	N-CA-C	-8.09	103.12	113.16
1	I	67	GLU	N-CA-C	-7.27	104.94	113.88
1	B	67	GLU	N-CA-C	-7.24	104.97	113.88
1	N	121	ILE	N-CA-C	-7.24	106.84	113.71
1	M	121	ILE	N-CA-C	-7.22	106.85	113.71
1	D	121	ILE	N-CA-C	-7.21	106.86	113.71
1	J	67	GLU	N-CA-C	-7.21	105.01	113.88
1	Q	109	PHE	CA-C-O	-6.50	111.21	120.51
1	R	109	PHE	CA-C-O	-6.48	111.25	120.51
1	H	109	PHE	CA-C-O	-6.47	111.26	120.51
1	R	366	THR	CA-C-N	-6.15	116.99	122.47
1	R	366	THR	C-N-CA	-6.15	116.99	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	120	TYR	CB-CA-C	-6.06	100.38	110.68
1	H	120	TYR	CB-CA-C	-6.05	100.39	110.68
1	Q	120	TYR	CB-CA-C	-6.04	100.41	110.68
1	L	50	THR	CA-C-O	-5.96	114.74	121.00
1	C	50	THR	CA-C-O	-5.94	114.76	121.00
1	K	50	THR	CA-C-O	-5.91	114.80	121.00
1	N	356	ASN	CA-C-N	-5.89	110.29	121.54
1	N	356	ASN	C-N-CA	-5.89	110.29	121.54
1	M	356	ASN	CA-C-N	-5.88	110.32	121.54
1	M	356	ASN	C-N-CA	-5.88	110.32	121.54
1	D	356	ASN	CA-C-N	-5.87	110.32	121.54
1	D	356	ASN	C-N-CA	-5.87	110.32	121.54
1	Q	374	THR	CB-CA-C	-5.39	103.71	109.85
1	R	374	THR	CB-CA-C	-5.38	103.72	109.85
1	H	374	THR	CB-CA-C	-5.37	103.72	109.85
1	G	179	ASP	CA-C-N	-5.37	112.80	120.42
1	G	179	ASP	C-N-CA	-5.37	112.80	120.42
1	P	179	ASP	CA-C-N	-5.35	112.82	120.42
1	P	179	ASP	C-N-CA	-5.35	112.82	120.42
1	R	364	ILE	CA-C-N	5.35	128.30	120.71
1	R	364	ILE	C-N-CA	5.35	128.30	120.71
1	O	179	ASP	CA-C-N	-5.34	112.83	120.42
1	O	179	ASP	C-N-CA	-5.34	112.83	120.42
1	H	364	ILE	CA-C-N	5.33	128.28	120.71
1	H	364	ILE	C-N-CA	5.33	128.28	120.71
1	D	30	VAL	CA-C-O	-5.20	116.83	121.09
1	G	80	PHE	CA-C-O	-5.18	113.22	119.59
1	O	80	PHE	CA-C-O	-5.18	113.22	119.59
1	N	30	VAL	CA-C-O	-5.18	116.84	121.09
1	P	80	PHE	CA-C-O	-5.15	113.25	119.59
1	M	30	VAL	CA-C-O	-5.12	116.89	121.09
1	G	80	PHE	N-CA-C	-5.10	107.22	112.93
1	O	80	PHE	N-CA-C	-5.09	107.23	112.93
1	P	80	PHE	N-CA-C	-5.08	107.24	112.93
1	H	366	THR	CA-C-N	-5.05	117.24	122.69
1	H	366	THR	C-N-CA	-5.05	117.24	122.69
1	D	318	TYR	N-CA-C	-5.05	107.25	113.41
1	M	318	TYR	N-CA-C	-5.04	107.26	113.41
1	N	318	TYR	N-CA-C	-5.03	107.27	113.41

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	79	LYS	Peptide
1	D	189	THR	Peptide
1	G	367	GLY	Mainchain
1	I	79	LYS	Peptide
1	J	79	LYS	Peptide
1	M	189	THR	Peptide
1	N	189	THR	Peptide
1	O	367	GLY	Mainchain
1	P	367	GLY	Mainchain

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	1729	0	1714	41	0
1	B	1740	0	1722	30	0
1	C	2167	0	2144	56	0
1	D	2156	0	2147	58	0
1	E	1729	0	1714	41	0
1	F	1729	0	1714	38	0
1	G	2146	0	2127	45	0
1	H	2162	0	2130	56	0
1	I	1740	0	1722	30	0
1	J	1740	0	1722	31	0
1	K	2167	0	2144	41	0
1	L	2167	0	2144	47	0
1	M	2156	0	2147	42	0
1	N	2156	0	2147	51	0
1	O	2146	0	2127	49	0
1	P	2146	0	2127	43	0
1	Q	2162	0	2130	61	0
1	R	2162	0	2130	57	0
All	All	36300	0	35952	760	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 11.

All (760) 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:D:15:PRO:N	1:D:15:PRO:CA	1.71	1.34
1:O:15:PRO:N	1:O:15:PRO:CA	1.70	1.33
1:C:365:TYR:CE1	1:D:20:SER:HA	1.80	1.17
1:C:365:TYR:OH	1:D:20:SER:O	1.63	1.13
1:P:369:ARG:HH21	1:P:369:ARG:HG3	1.13	1.13
1:G:369:ARG:HG3	1:G:369:ARG:HH21	1.13	1.11
1:E:72:ILE:HD11	1:E:126:VAL:HG12	1.33	1.11
1:O:369:ARG:HH21	1:O:369:ARG:HG3	1.13	1.08
1:F:72:ILE:HD11	1:F:126:VAL:HG12	1.33	1.06
1:A:72:ILE:HD11	1:A:126:VAL:HG12	1.33	1.04
1:C:365:TYR:CE1	1:D:20:SER:CA	2.41	1.03
1:L:369:ARG:HG3	1:L:369:ARG:HH11	1.24	1.00
1:C:365:TYR:CE1	1:D:20:SER:C	2.41	0.98
1:A:72:ILE:HD11	1:A:126:VAL:CG1	1.95	0.97
1:E:72:ILE:HD11	1:E:126:VAL:CG1	1.95	0.96
1:F:72:ILE:HD11	1:F:126:VAL:CG1	1.95	0.96
1:C:365:TYR:HH	1:D:20:SER:C	1.74	0.94
1:C:365:TYR:OH	1:D:20:SER:C	2.11	0.94
1:R:152:ARG:CD	1:R:163:TYR:CE2	2.53	0.92
1:H:152:ARG:CD	1:H:163:TYR:CE2	2.53	0.92
1:H:369:ARG:HG2	1:H:369:ARG:HH11	1.34	0.91
1:H:8:ARG:HG3	1:H:9:PRO:HD2	1.50	0.91
1:Q:152:ARG:CD	1:Q:163:TYR:CE2	2.53	0.91
1:R:8:ARG:HG3	1:R:9:PRO:HD2	1.51	0.91
1:L:73:ARG:HG3	1:L:76:ARG:HH21	1.36	0.90
1:K:73:ARG:HG3	1:K:76:ARG:HH21	1.36	0.89
1:C:365:TYR:HE1	1:D:20:SER:CA	1.85	0.89
1:E:325:LYS:O	1:E:325:LYS:HD2	1.73	0.88
1:F:325:LYS:HD2	1:F:325:LYS:O	1.73	0.88
1:C:73:ARG:HG3	1:C:76:ARG:HH21	1.36	0.88
1:R:369:ARG:HG2	1:R:369:ARG:HH11	1.37	0.88
1:A:325:LYS:HD2	1:A:325:LYS:O	1.73	0.88
1:Q:369:ARG:HH21	1:Q:369:ARG:HG3	1.41	0.85
1:C:365:TYR:CZ	1:D:20:SER:C	2.55	0.83
1:H:152:ARG:CG	1:H:163:TYR:CE2	2.62	0.82
1:Q:152:ARG:CG	1:Q:163:TYR:CE2	2.62	0.82
1:R:152:ARG:CG	1:R:163:TYR:CE2	2.62	0.82
1:B:322:VAL:HG22	1:B:326:LEU:HD11	1.63	0.81
1:G:369:ARG:HG3	1:G:369:ARG:NH2	1.93	0.81
1:C:73:ARG:CG	1:C:76:ARG:HH21	1.94	0.81
1:I:322:VAL:HG22	1:I:326:LEU:HD11	1.63	0.80
1:J:322:VAL:HG22	1:J:326:LEU:HD11	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:ARG:CG	1:K:76:ARG:HH21	1.94	0.80
1:L:73:ARG:CG	1:L:76:ARG:HH21	1.94	0.80
1:K:9:PRO:HB2	1:M:357:ARG:HH12	1.47	0.79
1:R:152:ARG:HD3	1:R:163:TYR:CE2	2.18	0.78
1:C:369:ARG:HG3	1:C:369:ARG:HH11	1.47	0.78
1:H:152:ARG:HD3	1:H:163:TYR:CE2	2.18	0.77
1:Q:152:ARG:HD3	1:Q:163:TYR:CE2	2.18	0.77
1:O:369:ARG:HG3	1:O:369:ARG:NH2	1.93	0.77
1:L:369:ARG:HG3	1:L:369:ARG:NH1	1.96	0.77
1:C:365:TYR:HE1	1:D:20:SER:C	1.87	0.76
1:J:326:LEU:H	1:J:326:LEU:HD12	1.51	0.75
1:H:152:ARG:HG2	1:H:163:TYR:HE2	1.51	0.75
1:Q:152:ARG:HG2	1:Q:163:TYR:HE2	1.51	0.75
1:B:326:LEU:HD12	1:B:326:LEU:H	1.51	0.74
1:R:152:ARG:CD	1:R:163:TYR:CZ	2.71	0.74
1:A:72:ILE:HD11	1:A:126:VAL:CB	2.18	0.74
1:I:326:LEU:HD12	1:I:326:LEU:H	1.51	0.74
1:A:72:ILE:CD1	1:A:126:VAL:HB	2.18	0.74
1:F:80:PHE:CE2	1:P:87:LYS:NZ	2.56	0.74
1:A:80:PHE:CE2	1:G:87:LYS:NZ	2.56	0.74
1:E:72:ILE:HD11	1:E:126:VAL:CB	2.18	0.74
1:R:152:ARG:HG2	1:R:163:TYR:HE2	1.51	0.73
1:E:80:PHE:CE2	1:O:87:LYS:NZ	2.56	0.73
1:E:72:ILE:CD1	1:E:126:VAL:HB	2.18	0.73
1:Q:152:ARG:CD	1:Q:163:TYR:CZ	2.71	0.73
1:F:72:ILE:CD1	1:F:126:VAL:HB	2.18	0.73
1:H:152:ARG:CD	1:H:163:TYR:CZ	2.71	0.73
1:K:40:GLN:HE21	1:M:373:TYR:HB3	1.54	0.73
1:F:72:ILE:HD11	1:F:126:VAL:CB	2.18	0.73
1:D:360:ARG:HH11	1:D:360:ARG:HG2	1.54	0.73
1:N:360:ARG:HH11	1:N:360:ARG:HG2	1.54	0.72
1:L:40:GLN:HE21	1:N:373:TYR:HB3	1.54	0.72
1:Q:369:ARG:HG3	1:Q:369:ARG:NH2	2.00	0.72
1:M:360:ARG:HG2	1:M:360:ARG:HH11	1.54	0.72
1:M:25:ASP:HB3	1:M:30:VAL:CG2	2.20	0.72
1:D:25:ASP:HB3	1:D:30:VAL:CG2	2.20	0.71
1:N:25:ASP:HB3	1:N:30:VAL:CG2	2.20	0.71
1:C:40:GLN:HE21	1:D:373:TYR:HB3	1.54	0.71
1:B:63:GLN:HA	1:B:66:THR:HG22	1.73	0.71
1:L:7:PHE:CE1	1:N:18:LEU:CD1	2.73	0.71
1:D:140:GLN:HE22	1:D:143:ARG:HH21	1.37	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ILE:O	1:G:183:THR:N	2.24	0.71
1:L:151:PRO:HB3	1:L:164:MET:HE2	1.73	0.71
1:I:63:GLN:HA	1:I:66:THR:HG22	1.73	0.71
1:C:151:PRO:HB3	1:C:164:MET:HE2	1.73	0.70
1:C:369:ARG:HG3	1:C:369:ARG:NH1	2.04	0.70
1:K:81:ARG:HB3	1:K:81:ARG:HH11	1.56	0.70
1:C:81:ARG:HH11	1:C:81:ARG:HB3	1.56	0.70
1:E:73:ARG:NH2	1:E:155:LEU:O	2.25	0.70
1:F:73:ARG:NH2	1:F:155:LEU:O	2.25	0.70
1:P:180:ILE:O	1:P:183:THR:N	2.24	0.70
1:A:325:LYS:HD2	1:A:325:LYS:C	2.14	0.70
1:O:180:ILE:O	1:O:183:THR:N	2.24	0.70
1:M:140:GLN:HE22	1:M:143:ARG:HH21	1.37	0.70
1:Q:152:ARG:CG	1:Q:163:TYR:HE2	2.04	0.70
1:K:151:PRO:HB3	1:K:164:MET:HE2	1.73	0.69
1:R:369:ARG:HG2	1:R:369:ARG:NH1	2.03	0.69
1:F:325:LYS:HD2	1:F:325:LYS:C	2.14	0.69
1:N:140:GLN:HE22	1:N:143:ARG:HH21	1.37	0.69
1:A:73:ARG:NH2	1:A:155:LEU:O	2.25	0.69
1:J:63:GLN:HA	1:J:66:THR:HG22	1.73	0.69
1:H:152:ARG:HD3	1:H:163:TYR:CZ	2.28	0.69
1:E:326:LEU:O	1:E:326:LEU:HD12	1.93	0.69
1:L:81:ARG:HH11	1:L:81:ARG:HB3	1.56	0.69
1:R:106:LEU:CD1	1:R:110:TYR:HE1	2.06	0.69
1:F:326:LEU:HD12	1:F:326:LEU:O	1.93	0.68
1:R:152:ARG:HD3	1:R:163:TYR:CZ	2.28	0.68
1:A:326:LEU:HD12	1:A:326:LEU:O	1.93	0.68
1:C:78:ILE:HD11	1:C:82:ILE:HD12	1.76	0.68
1:Q:112:ARG:HB2	1:Q:112:ARG:CZ	2.24	0.68
1:Q:152:ARG:HD2	1:Q:163:TYR:OH	1.94	0.68
1:K:78:ILE:HD11	1:K:82:ILE:HD12	1.76	0.68
1:Q:106:LEU:CD1	1:Q:110:TYR:HE1	2.06	0.68
1:H:152:ARG:HD2	1:H:163:TYR:OH	1.94	0.68
1:C:72:ILE:HG22	1:C:72:ILE:O	1.94	0.68
1:C:365:TYR:CZ	1:D:20:SER:O	2.46	0.68
1:G:369:ARG:HH21	1:G:369:ARG:CG	2.01	0.67
1:K:50:THR:O	1:K:53:LEU:N	2.27	0.67
1:H:152:ARG:CG	1:H:163:TYR:HE2	2.04	0.67
1:Q:152:ARG:HD3	1:Q:163:TYR:CZ	2.28	0.67
1:P:76:ARG:NH1	1:P:160:ASN:HD22	1.92	0.67
1:G:76:ARG:NH1	1:G:160:ASN:HD22	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:152:ARG:HD2	1:R:163:TYR:OH	1.94	0.67
1:R:112:ARG:HB2	1:R:112:ARG:CZ	2.24	0.67
1:H:106:LEU:CD1	1:H:110:TYR:HE1	2.06	0.67
1:K:72:ILE:HG22	1:K:72:ILE:O	1.94	0.67
1:O:76:ARG:NH1	1:O:160:ASN:HD22	1.92	0.67
1:L:50:THR:O	1:L:53:LEU:N	2.27	0.67
1:C:50:THR:O	1:C:53:LEU:N	2.27	0.67
1:C:9:PRO:HB2	1:D:357:ARG:HH12	1.59	0.66
1:H:112:ARG:CZ	1:H:112:ARG:HB2	2.24	0.66
1:O:369:ARG:HH21	1:O:369:ARG:CG	2.01	0.66
1:L:78:ILE:HD11	1:L:82:ILE:HD12	1.76	0.66
1:L:369:ARG:HH11	1:L:369:ARG:CG	2.05	0.66
1:L:72:ILE:O	1:L:72:ILE:HG22	1.94	0.66
1:H:369:ARG:HG2	1:H:369:ARG:NH1	2.02	0.65
1:D:25:ASP:HB3	1:D:30:VAL:HG23	1.78	0.65
1:Q:369:ARG:HH21	1:Q:369:ARG:CG	2.09	0.65
1:C:366:THR:HG23	1:Q:7:PHE:HB3	1.78	0.65
1:D:73:ARG:NH2	1:D:155:LEU:O	2.30	0.65
1:M:25:ASP:HB3	1:M:30:VAL:HG23	1.78	0.65
1:N:73:ARG:NH2	1:N:155:LEU:O	2.30	0.65
1:P:21:ILE:HD13	1:P:34:ARG:HH21	1.63	0.64
1:G:21:ILE:HD13	1:G:34:ARG:HH21	1.63	0.64
1:E:325:LYS:HD2	1:E:325:LYS:C	2.14	0.64
1:M:73:ARG:NH2	1:M:155:LEU:O	2.30	0.64
1:O:21:ILE:HD13	1:O:34:ARG:HH21	1.63	0.64
1:K:73:ARG:HG3	1:K:76:ARG:NH2	2.12	0.64
1:N:25:ASP:HB3	1:N:30:VAL:HG23	1.78	0.64
1:J:322:VAL:CG2	1:J:326:LEU:HD11	2.29	0.63
1:P:369:ARG:HG3	1:P:369:ARG:NH2	1.93	0.63
1:Q:106:LEU:HD12	1:Q:110:TYR:HE1	1.64	0.63
1:E:72:ILE:CD1	1:E:126:VAL:CB	2.77	0.62
1:R:152:ARG:HD2	1:R:163:TYR:CZ	2.34	0.62
1:B:322:VAL:CG2	1:B:326:LEU:HD11	2.28	0.62
1:D:150:GLN:HG2	1:D:151:PRO:HD2	1.82	0.62
1:N:150:GLN:HG2	1:N:151:PRO:HD2	1.82	0.62
1:M:150:GLN:HG2	1:M:151:PRO:HD2	1.82	0.62
1:R:106:LEU:HD12	1:R:110:TYR:HE1	1.64	0.62
1:A:72:ILE:CD1	1:A:126:VAL:CB	2.77	0.62
1:L:73:ARG:HG3	1:L:76:ARG:NH2	2.12	0.62
1:D:158:ALA:HB1	1:D:178:PHE:HD2	1.65	0.61
1:H:106:LEU:HD12	1:H:110:TYR:HE1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ARG:HD2	1:H:163:TYR:CZ	2.34	0.61
1:F:72:ILE:HG22	1:F:72:ILE:O	2.00	0.61
1:M:158:ALA:HB1	1:M:178:PHE:HD2	1.65	0.61
1:N:158:ALA:HB1	1:N:178:PHE:HD2	1.65	0.61
1:A:72:ILE:HG22	1:A:72:ILE:O	2.00	0.61
1:C:48:LEU:HD22	1:C:69:GLU:HG2	1.82	0.61
1:I:322:VAL:CG2	1:I:326:LEU:HD11	2.28	0.61
1:R:366:THR:O	1:R:366:THR:HG22	2.01	0.61
1:Q:152:ARG:HD2	1:Q:163:TYR:CZ	2.34	0.60
1:L:48:LEU:HD22	1:L:69:GLU:HG2	1.82	0.60
1:F:33:TYR:HE1	1:F:187:GLU:HB3	1.67	0.60
1:E:72:ILE:HG22	1:E:72:ILE:O	2.00	0.60
1:K:48:LEU:HD22	1:K:69:GLU:HG2	1.82	0.60
1:B:38:ILE:H	1:B:38:ILE:HD12	1.67	0.60
1:J:38:ILE:HD12	1:J:38:ILE:H	1.67	0.60
1:I:38:ILE:HD12	1:I:38:ILE:H	1.67	0.60
1:L:73:ARG:O	1:L:73:ARG:HG2	2.02	0.60
1:C:73:ARG:HG2	1:C:73:ARG:O	2.02	0.59
1:C:369:ARG:HH11	1:C:369:ARG:CG	2.10	0.59
1:M:76:ARG:NH1	1:M:160:ASN:HD22	2.01	0.59
1:E:33:TYR:HE1	1:E:187:GLU:HB3	1.67	0.59
1:K:73:ARG:O	1:K:73:ARG:HG2	2.02	0.59
1:A:326:LEU:HD12	1:A:326:LEU:C	2.28	0.59
1:C:73:ARG:HG3	1:C:76:ARG:NH2	2.12	0.59
1:F:72:ILE:CD1	1:F:126:VAL:CB	2.77	0.59
1:P:211:VAL:O	1:P:215:VAL:HG12	2.03	0.59
1:D:76:ARG:NH1	1:D:160:ASN:HD22	2.01	0.59
1:Q:366:THR:HG22	1:Q:366:THR:O	2.02	0.59
1:A:33:TYR:HE1	1:A:187:GLU:HB3	1.67	0.58
1:G:211:VAL:O	1:G:215:VAL:HG12	2.03	0.58
1:H:47:PHE:CE2	1:H:182:LEU:HB3	2.39	0.58
1:F:326:LEU:HD12	1:F:326:LEU:C	2.28	0.58
1:A:188:HIS:CD2	1:A:189:THR:HG22	2.39	0.58
1:N:76:ARG:NH1	1:N:160:ASN:HD22	2.00	0.58
1:O:211:VAL:O	1:O:215:VAL:HG12	2.03	0.58
1:R:47:PHE:CE2	1:R:182:LEU:HB3	2.39	0.58
1:F:188:HIS:CD2	1:F:189:THR:HG22	2.39	0.58
1:E:188:HIS:CD2	1:E:189:THR:HG22	2.39	0.57
1:Q:47:PHE:CE2	1:Q:182:LEU:HB3	2.39	0.57
1:E:326:LEU:HD12	1:E:326:LEU:C	2.28	0.57
1:M:360:ARG:HG2	1:M:360:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:217:THR:O	1:M:217:THR:OG1	2.21	0.57
1:N:315:VAL:O	1:N:315:VAL:HG22	2.05	0.57
1:H:369:ARG:HD2	1:H:369:ARG:O	2.05	0.56
1:D:315:VAL:O	1:D:315:VAL:HG22	2.05	0.56
1:M:315:VAL:HG22	1:M:315:VAL:O	2.05	0.56
1:N:360:ARG:HG2	1:N:360:ARG:NH1	2.19	0.56
1:P:342:VAL:O	1:P:346:LEU:HD13	2.05	0.56
1:O:342:VAL:O	1:O:346:LEU:HD13	2.05	0.56
1:F:318:TYR:O	1:F:322:VAL:HG23	2.06	0.56
1:R:206:ASP:OD1	1:R:206:ASP:N	2.38	0.56
1:H:195:PHE:O	1:H:199:VAL:HG23	2.06	0.56
1:O:365:TYR:CD2	1:Q:23:PHE:HD2	2.24	0.56
1:Q:195:PHE:O	1:Q:199:VAL:HG23	2.06	0.55
1:R:110:TYR:CD1	1:R:110:TYR:N	2.74	0.55
1:E:318:TYR:O	1:E:322:VAL:HG23	2.06	0.55
1:A:318:TYR:O	1:A:322:VAL:HG23	2.06	0.55
1:G:363:GLN:NE2	1:H:19:SER:OG	2.37	0.55
1:N:217:THR:O	1:N:217:THR:OG1	2.21	0.55
1:R:195:PHE:O	1:R:199:VAL:HG23	2.06	0.55
1:H:206:ASP:OD1	1:H:206:ASP:N	2.39	0.55
1:G:342:VAL:O	1:G:346:LEU:HD13	2.05	0.55
1:K:158:ALA:HB1	1:K:178:PHE:HD2	1.71	0.55
1:O:191:ASN:N	1:O:191:ASN:OD1	2.39	0.55
1:J:80:PHE:O	1:J:84:ASP:HB2	2.07	0.55
1:P:365:TYR:CD2	1:R:23:PHE:HD2	2.24	0.55
1:R:369:ARG:HD2	1:R:369:ARG:O	2.06	0.55
1:H:110:TYR:N	1:H:110:TYR:CD1	2.74	0.55
1:P:363:GLN:NE2	1:R:19:SER:OG	2.36	0.55
1:G:365:TYR:CD2	1:H:23:PHE:HD2	2.24	0.55
1:H:106:LEU:HD22	1:H:135:MET:HE1	1.89	0.55
1:H:12:GLU:O	1:H:14:VAL:HG23	2.07	0.55
1:R:21:ILE:HG13	1:R:22:SER:N	2.22	0.55
1:R:106:LEU:HD22	1:R:135:MET:HE1	1.89	0.55
1:Q:12:GLU:O	1:Q:14:VAL:HG23	2.07	0.55
1:H:8:ARG:HG3	1:H:9:PRO:CD	2.30	0.54
1:E:156:ASP:O	1:E:160:ASN:HB2	2.07	0.54
1:B:66:THR:O	1:B:66:THR:OG1	2.21	0.54
1:H:112:ARG:CZ	1:H:112:ARG:CB	2.86	0.54
1:D:217:THR:O	1:D:217:THR:OG1	2.21	0.54
1:Q:73:ARG:HG2	1:Q:76:ARG:HH21	1.72	0.54
1:F:156:ASP:O	1:F:160:ASN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:158:ALA:HB1	1:L:178:PHE:HD2	1.71	0.54
1:C:158:ALA:HB1	1:C:178:PHE:HD2	1.71	0.54
1:R:12:GLU:O	1:R:14:VAL:HG23	2.07	0.54
1:G:191:ASN:N	1:G:191:ASN:OD1	2.39	0.54
1:E:58:HIS:ND1	1:E:59:LEU:O	2.39	0.54
1:O:15:PRO:N	1:O:15:PRO:C	2.62	0.54
1:H:73:ARG:HG2	1:H:76:ARG:HH21	1.73	0.54
1:D:360:ARG:HG2	1:D:360:ARG:NH1	2.19	0.54
1:Q:206:ASP:N	1:Q:206:ASP:OD1	2.40	0.54
1:P:121:ILE:HG21	1:P:350:LYS:HE2	1.90	0.54
1:R:73:ARG:HG2	1:R:76:ARG:HH21	1.72	0.54
1:K:7:PHE:CD1	1:K:7:PHE:C	2.85	0.54
1:O:121:ILE:HG21	1:O:350:LYS:HE2	1.90	0.54
1:Q:112:ARG:CZ	1:Q:112:ARG:CB	2.85	0.54
1:R:112:ARG:CZ	1:R:112:ARG:CB	2.86	0.54
1:H:21:ILE:HG13	1:H:22:SER:N	2.22	0.53
1:H:217:THR:O	1:H:217:THR:OG1	2.27	0.53
1:L:149:ILE:HG22	1:L:150:GLN:H	1.73	0.53
1:P:191:ASN:OD1	1:P:191:ASN:N	2.39	0.53
1:A:156:ASP:O	1:A:160:ASN:HB2	2.07	0.53
1:Q:106:LEU:HD22	1:Q:135:MET:HE1	1.89	0.53
1:A:153:ASP:OD1	1:A:153:ASP:N	2.41	0.53
1:A:317:PHE:O	1:A:321:LEU:HG	2.09	0.53
1:I:80:PHE:O	1:I:84:ASP:HB2	2.07	0.53
1:G:121:ILE:HG21	1:G:350:LYS:HE2	1.90	0.53
1:N:360:ARG:HD2	1:N:360:ARG:O	2.09	0.53
1:F:53:LEU:HD13	1:F:59:LEU:HD12	1.91	0.53
1:Q:110:TYR:CD1	1:Q:110:TYR:N	2.74	0.53
1:F:153:ASP:OD1	1:F:153:ASP:N	2.41	0.53
1:F:317:PHE:O	1:F:321:LEU:HG	2.09	0.53
1:H:366:THR:O	1:H:366:THR:HG22	2.09	0.53
1:E:53:LEU:HD13	1:E:59:LEU:HD12	1.91	0.53
1:Q:21:ILE:HG13	1:Q:22:SER:N	2.22	0.53
1:B:80:PHE:O	1:B:84:ASP:HB2	2.07	0.53
1:D:330:SER:O	1:D:330:SER:OG	2.25	0.52
1:D:360:ARG:HD2	1:D:360:ARG:O	2.09	0.52
1:E:317:PHE:O	1:E:321:LEU:HG	2.09	0.52
1:M:360:ARG:HD2	1:M:360:ARG:O	2.09	0.52
1:M:373:TYR:CZ	1:M:375:PRO:HD3	2.45	0.52
1:J:140:GLN:NE2	1:J:143:ARG:HH12	2.07	0.52
1:D:373:TYR:CZ	1:D:375:PRO:HD3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:373:TYR:CZ	1:N:375:PRO:HD3	2.45	0.52
1:D:195:PHE:O	1:D:199:VAL:HG23	2.10	0.52
1:H:332:LEU:O	1:H:336:VAL:HG23	2.10	0.52
1:Q:217:THR:O	1:Q:217:THR:OG1	2.27	0.52
1:R:217:THR:O	1:R:217:THR:OG1	2.26	0.52
1:C:149:ILE:HG22	1:C:150:GLN:H	1.73	0.52
1:G:203:THR:O	1:G:203:THR:OG1	2.28	0.52
1:I:140:GLN:NE2	1:I:143:ARG:HH12	2.07	0.52
1:K:149:ILE:HG22	1:K:150:GLN:H	1.73	0.52
1:P:19:SER:OG	1:R:363:GLN:HG3	2.10	0.52
1:L:7:PHE:CE1	1:N:18:LEU:HD11	2.45	0.52
1:R:8:ARG:HG3	1:R:9:PRO:CD	2.32	0.52
1:Q:374:THR:HG23	1:Q:374:THR:O	2.10	0.52
1:D:357:ARG:O	1:D:358:ILE:HB	2.10	0.52
1:A:53:LEU:HD13	1:A:59:LEU:HD12	1.91	0.51
1:H:369:ARG:NH1	1:H:369:ARG:CG	2.72	0.51
1:O:19:SER:OG	1:Q:363:GLN:HG3	2.10	0.51
1:Q:332:LEU:O	1:Q:336:VAL:HG23	2.10	0.51
1:Q:369:ARG:HD2	1:Q:370:ASN:H	1.74	0.51
1:H:63:GLN:O	1:H:66:THR:HG22	2.10	0.51
1:O:363:GLN:NE2	1:Q:19:SER:OG	2.37	0.51
1:R:63:GLN:O	1:R:66:THR:HG22	2.10	0.51
1:G:362:THR:HG22	1:G:363:GLN:H	1.75	0.51
1:H:374:THR:HG23	1:H:374:THR:O	2.10	0.51
1:N:195:PHE:O	1:N:199:VAL:HG23	2.10	0.51
1:M:195:PHE:O	1:M:199:VAL:HG23	2.10	0.51
1:R:332:LEU:O	1:R:336:VAL:HG23	2.10	0.51
1:R:374:THR:HG23	1:R:374:THR:O	2.10	0.51
1:B:140:GLN:NE2	1:B:143:ARG:HH12	2.07	0.51
1:C:85:MET:O	1:C:85:MET:HG2	2.11	0.51
1:N:357:ARG:O	1:N:358:ILE:HB	2.10	0.51
1:G:316:ASP:OD1	1:G:317:PHE:N	2.44	0.51
1:E:153:ASP:OD1	1:E:153:ASP:N	2.41	0.51
1:K:141:LEU:HD13	1:K:148:PRO:HA	1.93	0.51
1:Q:352:GLN:O	1:Q:352:GLN:HG3	2.10	0.51
1:Q:373:TYR:CD1	1:Q:373:TYR:C	2.89	0.51
1:C:9:PRO:HB2	1:D:357:ARG:NH1	2.25	0.51
1:M:33:TYR:CZ	1:M:187:GLU:HB3	2.46	0.51
1:D:149:ILE:HD13	1:D:167:GLU:OE2	2.11	0.50
1:G:106:LEU:HD21	1:G:135:MET:HE1	1.94	0.50
1:O:203:THR:O	1:O:203:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:63:GLN:O	1:Q:66:THR:HG22	2.10	0.50
1:P:362:THR:HG22	1:P:363:GLN:H	1.75	0.50
1:D:206:ASP:OD1	1:D:206:ASP:N	2.40	0.50
1:O:106:LEU:HD21	1:O:135:MET:HE1	1.94	0.50
1:R:352:GLN:O	1:R:352:GLN:HG3	2.11	0.50
1:K:85:MET:O	1:K:85:MET:HG2	2.11	0.50
1:N:33:TYR:CZ	1:N:187:GLU:HB3	2.46	0.50
1:G:19:SER:OG	1:H:363:GLN:HG3	2.10	0.50
1:O:316:ASP:OD1	1:O:317:PHE:N	2.44	0.50
1:R:373:TYR:CD1	1:R:373:TYR:C	2.89	0.50
1:H:352:GLN:O	1:H:352:GLN:HG3	2.11	0.50
1:C:141:LEU:HD13	1:C:148:PRO:HA	1.93	0.50
1:P:106:LEU:HD21	1:P:135:MET:HE1	1.94	0.50
1:L:128:LEU:HD21	1:L:208:TYR:CE1	2.47	0.50
1:D:33:TYR:CZ	1:D:187:GLU:HB3	2.46	0.50
1:Q:106:LEU:HD11	1:Q:110:TYR:HE1	1.77	0.50
1:L:141:LEU:HD13	1:L:148:PRO:HA	1.93	0.50
1:P:316:ASP:OD1	1:P:317:PHE:N	2.44	0.50
1:H:373:TYR:C	1:H:373:TYR:CD1	2.89	0.50
1:E:198:MET:HE2	1:E:348:HIS:HB3	1.94	0.50
1:O:41:LEU:O	1:O:45:SER:HB2	2.12	0.50
1:P:41:LEU:O	1:P:45:SER:HB2	2.12	0.50
1:A:58:HIS:ND1	1:A:59:LEU:O	2.39	0.49
1:M:149:ILE:HD13	1:M:167:GLU:OE2	2.12	0.49
1:L:85:MET:O	1:L:85:MET:HG2	2.11	0.49
1:C:128:LEU:HD21	1:C:208:TYR:CE1	2.47	0.49
1:M:357:ARG:O	1:M:358:ILE:HB	2.10	0.49
1:O:362:THR:HG22	1:O:363:GLN:H	1.75	0.49
1:A:198:MET:HE2	1:A:348:HIS:HB3	1.94	0.49
1:K:128:LEU:HD21	1:K:208:TYR:CE1	2.47	0.49
1:J:79:LYS:O	1:J:81:ARG:N	2.45	0.49
1:P:23:PHE:CD1	1:P:23:PHE:C	2.91	0.49
1:F:191:ASN:OD1	1:F:191:ASN:N	2.46	0.49
1:M:12:GLU:O	1:M:14:VAL:HG23	2.13	0.49
1:P:369:ARG:HH21	1:P:369:ARG:CG	2.01	0.49
1:B:79:LYS:O	1:B:81:ARG:N	2.45	0.49
1:L:7:PHE:CD2	1:L:7:PHE:C	2.90	0.49
1:L:79:LYS:HB3	1:L:81:ARG:HD3	1.95	0.49
1:N:149:ILE:HD13	1:N:167:GLU:OE2	2.12	0.49
1:R:106:LEU:HD11	1:R:110:TYR:HE1	1.77	0.49
1:B:176:ARG:O	1:B:180:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:GLU:O	1:D:14:VAL:HG23	2.13	0.49
1:I:79:LYS:O	1:I:81:ARG:N	2.45	0.49
1:J:176:ARG:O	1:J:180:ILE:HG13	2.13	0.49
1:P:25:ASP:HB3	1:P:30:VAL:CG1	2.43	0.49
1:D:98:ALA:O	1:D:102:SER:OG	2.25	0.48
1:N:94:HIS:HB2	1:N:97:ASP:OD2	2.13	0.48
1:G:41:LEU:O	1:G:45:SER:HB2	2.12	0.48
1:Q:152:ARG:HG2	1:Q:163:TYR:CE2	2.34	0.48
1:F:58:HIS:ND1	1:F:59:LEU:O	2.40	0.48
1:F:198:MET:HE2	1:F:348:HIS:HB3	1.94	0.48
1:G:23:PHE:CD1	1:G:23:PHE:C	2.91	0.48
1:G:25:ASP:HB3	1:G:30:VAL:CG1	2.43	0.48
1:N:12:GLU:O	1:N:14:VAL:HG23	2.13	0.48
1:B:98:ALA:O	1:B:102:SER:OG	2.24	0.48
1:H:106:LEU:HD11	1:H:110:TYR:HE1	1.77	0.48
1:I:176:ARG:O	1:I:180:ILE:HG13	2.13	0.48
1:C:79:LYS:HB3	1:C:81:ARG:HD3	1.95	0.48
1:D:94:HIS:HB2	1:D:97:ASP:OD2	2.13	0.48
1:D:352:GLN:HG3	1:D:352:GLN:O	2.14	0.48
1:O:23:PHE:CD1	1:O:23:PHE:C	2.91	0.48
1:J:98:ALA:O	1:J:102:SER:OG	2.24	0.48
1:J:63:GLN:HA	1:J:66:THR:CG2	2.43	0.48
1:M:352:GLN:O	1:M:352:GLN:HG3	2.14	0.48
1:J:66:THR:O	1:J:66:THR:OG1	2.21	0.48
1:L:7:PHE:CE1	1:N:18:LEU:HD13	2.47	0.48
1:K:79:LYS:HB3	1:K:81:ARG:HD3	1.95	0.48
1:O:76:ARG:NH1	1:O:160:ASN:ND2	2.62	0.48
1:L:7:PHE:HE1	1:N:18:LEU:CD1	2.26	0.48
1:L:7:PHE:O	1:L:7:PHE:CG	2.67	0.48
1:H:344:GLY:O	1:H:347:ALA:HB3	2.14	0.47
1:Q:344:GLY:O	1:Q:347:ALA:HB3	2.14	0.47
1:R:344:GLY:O	1:R:347:ALA:HB3	2.14	0.47
1:C:171:ASP:OD1	1:C:171:ASP:N	2.40	0.47
1:M:94:HIS:HB2	1:M:97:ASP:OD2	2.13	0.47
1:O:25:ASP:HB3	1:O:30:VAL:CG1	2.43	0.47
1:O:357:ARG:C	1:O:358:ILE:HG13	2.39	0.47
1:M:360:ARG:NH1	1:M:360:ARG:CG	2.78	0.47
1:O:351:GLU:C	1:O:353:LEU:H	2.22	0.47
1:P:357:ARG:C	1:P:358:ILE:HG13	2.40	0.47
1:A:211:VAL:O	1:A:215:VAL:HG12	2.15	0.47
1:B:206:ASP:HB3	1:B:207:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:203:THR:HG22	1:D:203:THR:O	2.15	0.47
1:L:171:ASP:OD1	1:L:171:ASP:N	2.40	0.47
1:C:365:TYR:CD1	1:D:20:SER:HA	2.43	0.47
1:G:351:GLU:C	1:G:353:LEU:H	2.22	0.47
1:G:357:ARG:C	1:G:358:ILE:HG13	2.40	0.47
1:J:206:ASP:HB3	1:J:207:PRO:HD2	1.97	0.47
1:N:352:GLN:O	1:N:352:GLN:HG3	2.14	0.47
1:C:365:TYR:CD1	1:D:19:SER:O	2.68	0.47
1:Q:47:PHE:HE2	1:Q:182:LEU:HB3	1.79	0.47
1:F:162:LEU:O	1:F:166:THR:HG22	2.15	0.47
1:D:206:ASP:HB2	1:D:207:PRO:HD2	1.97	0.47
1:A:191:ASN:OD1	1:A:191:ASN:N	2.45	0.46
1:E:162:LEU:O	1:E:166:THR:HG22	2.15	0.46
1:E:191:ASN:N	1:E:191:ASN:OD1	2.45	0.46
1:I:206:ASP:HB3	1:I:207:PRO:HD2	1.97	0.46
1:N:206:ASP:OD1	1:N:206:ASP:N	2.40	0.46
1:P:76:ARG:NH1	1:P:160:ASN:ND2	2.62	0.46
1:B:162:LEU:O	1:B:166:THR:HG22	2.15	0.46
1:I:63:GLN:HA	1:I:66:THR:CG2	2.44	0.46
1:I:162:LEU:O	1:I:166:THR:HG22	2.15	0.46
1:O:15:PRO:HB2	1:Q:7:PHE:CE1	2.50	0.46
1:N:360:ARG:NH1	1:N:360:ARG:CG	2.77	0.46
1:H:47:PHE:HE2	1:H:182:LEU:HB3	1.79	0.46
1:E:33:TYR:CE1	1:E:187:GLU:HB3	2.50	0.46
1:M:206:ASP:HB2	1:M:207:PRO:HD2	1.97	0.46
1:P:351:GLU:C	1:P:353:LEU:H	2.22	0.46
1:A:150:GLN:HG3	1:A:151:PRO:HD2	1.98	0.46
1:A:162:LEU:O	1:A:166:THR:HG22	2.15	0.46
1:C:123:ALA:O	1:C:127:ARG:HG3	2.16	0.46
1:R:8:ARG:HE	1:R:8:ARG:HB2	1.55	0.46
1:Q:8:ARG:HA	1:Q:8:ARG:HD3	1.61	0.46
1:M:203:THR:HG22	1:M:203:THR:O	2.15	0.46
1:E:211:VAL:O	1:E:215:VAL:HG12	2.15	0.46
1:L:123:ALA:O	1:L:127:ARG:HG3	2.16	0.46
1:N:203:THR:HG22	1:N:203:THR:O	2.15	0.46
1:R:47:PHE:HE2	1:R:182:LEU:HB3	1.79	0.46
1:G:76:ARG:NH1	1:G:160:ASN:ND2	2.62	0.46
1:O:171:ASP:OD1	1:O:171:ASP:N	2.49	0.46
1:N:206:ASP:HB2	1:N:207:PRO:HD2	1.97	0.46
1:B:316:ASP:OD1	1:B:317:PHE:N	2.49	0.46
1:C:74:TYR:CD1	1:C:74:TYR:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:74:TYR:O	1:K:74:TYR:CG	2.69	0.46
1:J:162:LEU:O	1:J:166:THR:HG22	2.15	0.46
1:Q:11:LEU:HD12	1:Q:11:LEU:HA	1.71	0.46
1:F:109:PHE:CE1	1:J:90:PRO:HG3	2.51	0.46
1:L:10:GLY:C	1:L:12:GLU:N	2.72	0.46
1:L:74:TYR:O	1:L:74:TYR:CD1	2.69	0.46
1:C:74:TYR:O	1:C:74:TYR:CG	2.69	0.45
1:M:180:ILE:O	1:M:184:LEU:HD23	2.16	0.45
1:Q:364:ILE:HG22	1:Q:364:ILE:O	2.15	0.45
1:E:109:PHE:CE1	1:I:90:PRO:HG3	2.51	0.45
1:E:150:GLN:HG3	1:E:151:PRO:HD2	1.98	0.45
1:O:372:ASP:OD1	1:O:372:ASP:N	2.50	0.45
1:N:180:ILE:O	1:N:184:LEU:HD23	2.16	0.45
1:I:98:ALA:O	1:I:102:SER:OG	2.24	0.45
1:M:315:VAL:O	1:M:315:VAL:HG13	2.17	0.45
1:F:211:VAL:O	1:F:215:VAL:HG12	2.15	0.45
1:F:150:GLN:HG3	1:F:151:PRO:HD2	1.98	0.45
1:D:315:VAL:O	1:D:315:VAL:HG13	2.17	0.45
1:I:323:TYR:HA	1:I:326:LEU:HD13	1.98	0.45
1:K:123:ALA:O	1:K:127:ARG:HG3	2.16	0.45
1:Q:318:TYR:O	1:Q:322:VAL:HG12	2.16	0.45
1:C:62:GLN:O	1:C:66:THR:HG23	2.17	0.45
1:C:365:TYR:HE1	1:D:21:ILE:N	2.15	0.45
1:I:66:THR:O	1:I:66:THR:OG1	2.21	0.45
1:K:74:TYR:O	1:K:74:TYR:CD1	2.69	0.45
1:C:50:THR:O	1:C:53:LEU:HB3	2.16	0.45
1:Q:24:VAL:HA	1:Q:30:VAL:O	2.17	0.45
1:Q:370:ASN:C	1:Q:370:ASN:HD22	2.25	0.45
1:J:316:ASP:OD1	1:J:317:PHE:N	2.49	0.45
1:G:171:ASP:OD1	1:G:171:ASP:N	2.49	0.45
1:E:326:LEU:C	1:E:326:LEU:CD1	2.90	0.45
1:I:316:ASP:OD1	1:I:317:PHE:N	2.49	0.45
1:P:171:ASP:N	1:P:171:ASP:OD1	2.49	0.45
1:K:171:ASP:OD1	1:K:171:ASP:N	2.40	0.45
1:J:323:TYR:HA	1:J:326:LEU:HD13	1.98	0.45
1:R:7:PHE:O	1:R:7:PHE:CD2	2.70	0.45
1:B:48:LEU:HD12	1:B:48:LEU:H	1.82	0.45
1:D:180:ILE:O	1:D:184:LEU:HD23	2.16	0.45
1:H:24:VAL:HA	1:H:30:VAL:O	2.17	0.45
1:L:50:THR:O	1:L:53:LEU:HB3	2.17	0.45
1:R:318:TYR:O	1:R:322:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PHE:CE1	1:B:90:PRO:HG3	2.51	0.44
1:C:365:TYR:CE1	1:D:21:ILE:N	2.85	0.44
1:L:62:GLN:O	1:L:66:THR:HG23	2.17	0.44
1:R:141:LEU:HA	1:R:141:LEU:HD23	1.81	0.44
1:D:25:ASP:HB3	1:D:30:VAL:HG21	1.99	0.44
1:K:50:THR:O	1:K:53:LEU:HB3	2.16	0.44
1:R:152:ARG:CG	1:R:163:TYR:HE2	2.04	0.44
1:C:341:ARG:HA	1:C:341:ARG:HD3	1.79	0.44
1:H:11:LEU:HA	1:H:11:LEU:HD12	1.71	0.44
1:I:48:LEU:HD12	1:I:48:LEU:H	1.82	0.44
1:N:162:LEU:HD23	1:N:162:LEU:HA	1.59	0.44
1:P:74:TYR:O	1:P:74:TYR:CG	2.71	0.44
1:H:7:PHE:O	1:H:7:PHE:CD2	2.70	0.44
1:H:141:LEU:HD23	1:H:141:LEU:HA	1.81	0.44
1:Q:204:LEU:HD12	1:Q:204:LEU:HA	1.82	0.44
1:J:82:ILE:HG13	1:J:109:PHE:HE2	1.83	0.44
1:R:24:VAL:HA	1:R:30:VAL:O	2.17	0.44
1:A:80:PHE:O	1:A:80:PHE:CD1	2.70	0.44
1:H:318:TYR:O	1:H:322:VAL:HG12	2.17	0.44
1:E:80:PHE:O	1:E:80:PHE:CD1	2.70	0.44
1:K:341:ARG:HA	1:K:341:ARG:HD3	1.79	0.44
1:M:133:PRO:HA	1:M:136:VAL:HG12	2.00	0.44
1:O:332:LEU:HD12	1:O:332:LEU:HA	1.83	0.44
1:C:316:ASP:OD1	1:C:316:ASP:N	2.50	0.44
1:F:33:TYR:CE1	1:F:187:GLU:HB3	2.50	0.44
1:F:79:LYS:HG3	1:F:81:ARG:H	1.83	0.44
1:L:316:ASP:OD1	1:L:316:ASP:N	2.50	0.44
1:P:366:THR:HG22	1:P:366:THR:O	2.18	0.44
1:B:75:HIS:O	1:B:130:ALA:HB1	2.18	0.44
1:B:325:LYS:C	1:B:327:GLY:N	2.75	0.44
1:G:166:THR:O	1:G:166:THR:HG22	2.17	0.44
1:K:62:GLN:O	1:K:66:THR:HG23	2.17	0.44
1:O:337:PHE:CD1	1:O:337:PHE:C	2.96	0.44
1:J:325:LYS:C	1:J:327:GLY:N	2.75	0.44
1:N:315:VAL:O	1:N:315:VAL:HG13	2.17	0.44
1:P:372:ASP:N	1:P:372:ASP:OD1	2.50	0.44
1:C:78:ILE:HD11	1:C:82:ILE:HG21	1.99	0.44
1:G:372:ASP:OD1	1:G:372:ASP:N	2.50	0.44
1:B:323:TYR:HA	1:B:326:LEU:HD13	1.98	0.44
1:Q:141:LEU:HD23	1:Q:141:LEU:HA	1.81	0.44
1:J:48:LEU:H	1:J:48:LEU:HD12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:74:TYR:O	1:L:74:TYR:CG	2.69	0.44
1:P:166:THR:HG22	1:P:166:THR:O	2.18	0.44
1:I:77:ARG:O	1:I:131:LYS:HE2	2.18	0.43
1:F:80:PHE:O	1:F:80:PHE:CD1	2.70	0.43
1:L:78:ILE:HD11	1:L:82:ILE:HG21	1.99	0.43
1:L:341:ARG:HA	1:L:341:ARG:HD3	1.79	0.43
1:P:337:PHE:CD1	1:P:337:PHE:C	2.96	0.43
1:B:63:GLN:HA	1:B:66:THR:CG2	2.44	0.43
1:B:77:ARG:O	1:B:131:LYS:HE2	2.18	0.43
1:C:73:ARG:HG3	1:C:73:ARG:HH11	1.83	0.43
1:G:74:TYR:O	1:G:74:TYR:CG	2.71	0.43
1:E:79:LYS:HG3	1:E:81:ARG:H	1.83	0.43
1:O:366:THR:HG22	1:O:366:THR:O	2.18	0.43
1:L:7:PHE:CD2	1:L:7:PHE:O	2.70	0.43
1:C:366:THR:CG2	1:Q:7:PHE:HB3	2.47	0.43
1:D:15:PRO:N	1:D:15:PRO:C	2.66	0.43
1:D:133:PRO:HA	1:D:136:VAL:HG12	2.00	0.43
1:H:346:LEU:O	1:H:347:ALA:C	2.62	0.43
1:K:149:ILE:HG22	1:K:150:GLN:N	2.33	0.43
1:M:85:MET:O	1:M:85:MET:HG2	2.19	0.43
1:J:75:HIS:O	1:J:130:ALA:HB1	2.18	0.43
1:J:77:ARG:O	1:J:131:LYS:HE2	2.18	0.43
1:A:33:TYR:CE1	1:A:187:GLU:HB3	2.50	0.43
1:A:326:LEU:C	1:A:326:LEU:CD1	2.90	0.43
1:B:318:TYR:O	1:B:322:VAL:HG12	2.18	0.43
1:C:149:ILE:HG22	1:C:150:GLN:N	2.33	0.43
1:E:174:ALA:HA	1:E:177:ILE:HD12	2.00	0.43
1:K:73:ARG:HG3	1:K:73:ARG:HH11	1.83	0.43
1:O:158:ALA:HB1	1:O:178:PHE:HD2	1.84	0.43
1:O:166:THR:HG22	1:O:166:THR:O	2.18	0.43
1:Q:207:PRO:O	1:Q:211:VAL:HG23	2.19	0.43
1:A:188:HIS:CG	1:A:189:THR:H	2.37	0.43
1:G:337:PHE:CD1	1:G:337:PHE:C	2.96	0.43
1:G:366:THR:HG22	1:G:366:THR:O	2.18	0.43
1:K:72:ILE:HD13	1:K:72:ILE:HG21	1.70	0.43
1:K:316:ASP:N	1:K:316:ASP:OD1	2.50	0.43
1:F:188:HIS:CG	1:F:189:THR:H	2.37	0.43
1:L:73:ARG:HG3	1:L:73:ARG:HH11	1.83	0.43
1:N:38:ILE:HD12	1:N:38:ILE:HA	1.88	0.43
1:A:79:LYS:HG3	1:A:81:ARG:H	1.83	0.43
1:G:357:ARG:O	1:G:358:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:HIS:HA	1:E:95:PRO:HD3	1.85	0.43
1:K:78:ILE:HD11	1:K:82:ILE:HG21	1.99	0.43
1:O:74:TYR:O	1:O:74:TYR:CG	2.71	0.43
1:Q:176:ARG:HA	1:Q:176:ARG:HD2	1.77	0.43
1:R:83:ARG:O	1:R:87:LYS:HG3	2.19	0.43
1:A:334:THR:O	1:A:337:PHE:HB3	2.19	0.43
1:G:365:TYR:CE2	1:H:23:PHE:HB2	2.54	0.43
1:L:149:ILE:HG22	1:L:150:GLN:N	2.33	0.43
1:C:332:LEU:HD23	1:C:332:LEU:HA	1.81	0.43
1:H:83:ARG:O	1:H:87:LYS:HG3	2.19	0.43
1:E:79:LYS:HE2	1:E:79:LYS:HB3	1.78	0.43
1:I:82:ILE:HG13	1:I:109:PHE:HE2	1.82	0.43
1:A:79:LYS:HE2	1:A:79:LYS:HB3	1.77	0.43
1:A:174:ALA:HA	1:A:177:ILE:HD12	2.00	0.43
1:M:25:ASP:HB3	1:M:30:VAL:HG21	1.99	0.43
1:Q:83:ARG:O	1:Q:87:LYS:HG3	2.19	0.43
1:L:73:ARG:HG2	1:L:76:ARG:HH21	1.81	0.43
1:N:133:PRO:HA	1:N:136:VAL:HG12	2.00	0.43
1:R:207:PRO:O	1:R:211:VAL:HG23	2.18	0.43
1:G:158:ALA:HB1	1:G:178:PHE:HD2	1.83	0.43
1:H:123:ALA:O	1:H:126:VAL:N	2.52	0.43
1:O:206:ASP:OD1	1:O:206:ASP:N	2.52	0.43
1:F:334:THR:O	1:F:337:PHE:HB3	2.19	0.43
1:B:82:ILE:HG13	1:B:109:PHE:HE2	1.83	0.42
1:Q:123:ALA:O	1:Q:126:VAL:N	2.52	0.42
1:F:174:ALA:HA	1:F:177:ILE:HD12	2.00	0.42
1:R:366:THR:O	1:R:366:THR:CG2	2.67	0.42
1:O:336:VAL:O	1:O:339:ILE:HB	2.19	0.42
1:O:365:TYR:CE2	1:Q:23:PHE:HB2	2.54	0.42
1:D:77:ARG:O	1:D:131:LYS:HE2	2.19	0.42
1:M:77:ARG:O	1:M:131:LYS:HE2	2.19	0.42
1:O:357:ARG:O	1:O:358:ILE:HG13	2.19	0.42
1:N:25:ASP:HB3	1:N:30:VAL:HG21	1.99	0.42
1:C:128:LEU:HD21	1:C:208:TYR:CD1	2.55	0.42
1:C:326:LEU:HA	1:C:326:LEU:HD23	1.79	0.42
1:D:360:ARG:NH1	1:D:360:ARG:CG	2.77	0.42
1:E:188:HIS:CG	1:E:189:THR:H	2.37	0.42
1:E:334:THR:O	1:E:337:PHE:HB3	2.19	0.42
1:Q:152:ARG:HE	1:Q:152:ARG:HB3	1.51	0.42
1:J:318:TYR:O	1:J:322:VAL:HG12	2.18	0.42
1:N:77:ARG:O	1:N:131:LYS:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:330:SER:O	1:N:330:SER:OG	2.25	0.42
1:R:123:ALA:O	1:R:126:VAL:N	2.52	0.42
1:R:346:LEU:O	1:R:347:ALA:C	2.62	0.42
1:J:68:PHE:O	1:J:71:GLU:N	2.53	0.42
1:L:128:LEU:HD21	1:L:208:TYR:CD1	2.55	0.42
1:P:158:ALA:HB1	1:P:178:PHE:HD2	1.84	0.42
1:P:336:VAL:O	1:P:339:ILE:HB	2.19	0.42
1:D:47:PHE:HE1	1:D:182:LEU:O	2.02	0.42
1:G:363:GLN:HG2	1:G:364:ILE:N	2.34	0.42
1:I:75:HIS:O	1:I:130:ALA:HB1	2.18	0.42
1:I:318:TYR:O	1:I:322:VAL:HG12	2.18	0.42
1:K:9:PRO:HB2	1:M:357:ARG:NH1	2.23	0.42
1:L:23:PHE:HE1	1:L:25:ASP:HB2	1.84	0.42
1:P:365:TYR:CE2	1:R:23:PHE:HB2	2.54	0.42
1:B:68:PHE:O	1:B:71:GLU:N	2.53	0.42
1:B:188:HIS:ND1	1:B:189:THR:HG23	2.35	0.42
1:I:325:LYS:C	1:I:327:GLY:N	2.75	0.42
1:M:167:GLU:O	1:M:167:GLU:HG3	2.19	0.42
1:F:94:HIS:HA	1:F:95:PRO:HD3	1.85	0.42
1:N:59:LEU:HA	1:N:59:LEU:HD23	1.76	0.42
1:M:330:SER:O	1:M:330:SER:OG	2.25	0.42
1:J:188:HIS:ND1	1:J:189:THR:HG23	2.35	0.42
1:N:318:TYR:O	1:N:322:VAL:HG23	2.20	0.42
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.76	0.42
1:D:167:GLU:O	1:D:167:GLU:HG3	2.19	0.42
1:H:155:LEU:HD23	1:H:155:LEU:HA	1.86	0.42
1:L:326:LEU:HD23	1:L:326:LEU:HA	1.79	0.42
1:R:176:ARG:HD2	1:R:176:ARG:HA	1.77	0.42
1:A:318:TYR:HA	1:A:321:LEU:HD12	2.02	0.42
1:D:318:TYR:O	1:D:322:VAL:HG23	2.20	0.42
1:I:150:GLN:HG3	1:I:151:PRO:HD2	2.02	0.42
1:I:188:HIS:ND1	1:I:189:THR:HG23	2.35	0.42
1:K:128:LEU:HD21	1:K:208:TYR:CD1	2.55	0.42
1:K:332:LEU:HD23	1:K:332:LEU:HA	1.81	0.42
1:M:343:ALA:O	1:M:344:GLY:C	2.63	0.42
1:N:85:MET:O	1:N:85:MET:HG2	2.18	0.42
1:P:357:ARG:O	1:P:358:ILE:HG13	2.19	0.42
1:B:124:ALA:C	1:B:126:VAL:N	2.78	0.41
1:C:73:ARG:CG	1:C:73:ARG:O	2.68	0.41
1:D:343:ALA:O	1:D:344:GLY:C	2.63	0.41
1:G:206:ASP:OD1	1:G:206:ASP:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:LEU:HD12	1:G:332:LEU:HA	1.83	0.41
1:K:23:PHE:HE1	1:K:25:ASP:HB2	1.84	0.41
1:M:162:LEU:HA	1:M:162:LEU:HD23	1.58	0.41
1:Q:346:LEU:O	1:Q:347:ALA:C	2.62	0.41
1:C:23:PHE:HE1	1:C:25:ASP:HB2	1.84	0.41
1:H:206:ASP:HB3	1:H:207:PRO:HD2	2.02	0.41
1:K:7:PHE:CE2	1:M:18:LEU:CD1	3.03	0.41
1:J:120:TYR:O	1:J:123:ALA:N	2.50	0.41
1:N:141:LEU:HD23	1:N:141:LEU:HA	1.73	0.41
1:A:78:ILE:HD12	1:A:78:ILE:HA	1.93	0.41
1:N:47:PHE:HE1	1:N:182:LEU:O	2.02	0.41
1:G:206:ASP:O	1:G:210:VAL:HG23	2.20	0.41
1:G:351:GLU:C	1:G:353:LEU:N	2.78	0.41
1:M:47:PHE:HE1	1:M:182:LEU:O	2.03	0.41
1:M:318:TYR:O	1:M:322:VAL:HG23	2.20	0.41
1:O:68:PHE:HD1	1:O:122:ARG:HH21	1.68	0.41
1:F:72:ILE:O	1:F:72:ILE:CG2	2.69	0.41
1:L:10:GLY:O	1:L:12:GLU:N	2.53	0.41
1:R:359:PHE:N	1:R:359:PHE:CD1	2.88	0.41
1:A:71:GLU:C	1:A:73:ARG:H	2.28	0.41
1:H:359:PHE:N	1:H:359:PHE:CD1	2.88	0.41
1:O:363:GLN:HG2	1:O:364:ILE:N	2.34	0.41
1:P:206:ASP:O	1:P:210:VAL:HG23	2.20	0.41
1:P:206:ASP:OD1	1:P:206:ASP:N	2.52	0.41
1:C:40:GLN:HE21	1:D:373:TYR:CB	2.29	0.41
1:G:357:ARG:HH21	1:H:10:GLY:HA3	1.85	0.41
1:K:326:LEU:HD23	1:K:326:LEU:HA	1.79	0.41
1:O:351:GLU:C	1:O:353:LEU:N	2.78	0.41
1:N:144:LYS:HA	1:N:144:LYS:HD3	1.77	0.41
1:N:167:GLU:O	1:N:167:GLU:HG3	2.19	0.41
1:N:343:ALA:O	1:N:344:GLY:C	2.63	0.41
1:H:207:PRO:O	1:H:211:VAL:HG23	2.20	0.41
1:E:129:LEU:HD23	1:E:129:LEU:HA	1.96	0.41
1:I:68:PHE:O	1:I:71:GLU:N	2.53	0.41
1:K:73:ARG:CG	1:K:73:ARG:O	2.68	0.41
1:M:144:LYS:HA	1:M:144:LYS:HD3	1.77	0.41
1:O:363:GLN:HG3	1:Q:19:SER:OG	2.21	0.41
1:F:71:GLU:C	1:F:73:ARG:H	2.28	0.41
1:L:50:THR:O	1:L:53:LEU:CB	2.69	0.41
1:P:40:GLN:O	1:R:373:TYR:CD2	2.74	0.41
1:P:203:THR:O	1:P:203:THR:OG1	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:PHE:CE1	1:A:321:LEU:HD21	2.56	0.41
1:E:71:GLU:C	1:E:73:ARG:H	2.28	0.41
1:J:162:LEU:HD23	1:J:162:LEU:HA	1.91	0.41
1:N:180:ILE:HD13	1:N:180:ILE:HG21	1.87	0.41
1:B:150:GLN:HG3	1:B:151:PRO:HD2	2.02	0.41
1:G:68:PHE:HD1	1:G:122:ARG:HH21	1.68	0.41
1:G:336:VAL:O	1:G:339:ILE:HB	2.19	0.41
1:G:363:GLN:HG3	1:H:19:SER:OG	2.21	0.41
1:E:317:PHE:CE1	1:E:321:LEU:HD21	2.56	0.41
1:E:318:TYR:HA	1:E:321:LEU:HD12	2.02	0.41
1:E:336:VAL:O	1:E:339:ILE:HG22	2.21	0.41
1:I:47:PHE:CE1	1:I:182:LEU:HB3	2.56	0.41
1:I:124:ALA:C	1:I:126:VAL:H	2.29	0.41
1:K:50:THR:O	1:K:53:LEU:CB	2.69	0.41
1:O:156:ASP:O	1:O:160:ASN:HB2	2.21	0.41
1:O:206:ASP:O	1:O:210:VAL:HG23	2.20	0.41
1:O:338:ALA:O	1:O:342:VAL:HG23	2.21	0.41
1:L:40:GLN:HE21	1:N:373:TYR:CB	2.29	0.41
1:N:98:ALA:O	1:N:102:SER:OG	2.25	0.41
1:H:321:LEU:HD13	1:H:321:LEU:HA	1.74	0.41
1:P:357:ARG:HH21	1:R:10:GLY:HA3	1.85	0.41
1:P:363:GLN:HG2	1:P:364:ILE:N	2.34	0.41
1:R:321:LEU:HD13	1:R:321:LEU:HA	1.74	0.41
1:A:336:VAL:O	1:A:339:ILE:HG22	2.21	0.40
1:D:162:LEU:HA	1:D:162:LEU:HD23	1.59	0.40
1:I:124:ALA:C	1:I:126:VAL:N	2.78	0.40
1:O:357:ARG:HH21	1:Q:10:GLY:HA3	1.85	0.40
1:F:317:PHE:CE1	1:F:321:LEU:HD21	2.56	0.40
1:F:318:TYR:HA	1:F:321:LEU:HD12	2.02	0.40
1:P:23:PHE:CZ	1:P:25:ASP:HB2	2.56	0.40
1:P:121:ILE:HG22	1:P:121:ILE:O	2.21	0.40
1:B:47:PHE:CE1	1:B:182:LEU:HB3	2.56	0.40
1:O:20:SER:O	1:O:20:SER:OG	2.29	0.40
1:J:124:ALA:C	1:J:126:VAL:H	2.29	0.40
1:C:73:ARG:HG2	1:C:76:ARG:HH21	1.81	0.40
1:D:357:ARG:HB3	1:D:358:ILE:H	1.67	0.40
1:G:135:MET:HE3	1:G:135:MET:HB2	1.95	0.40
1:I:316:ASP:HA	1:I:319:SER:OG	2.22	0.40
1:Q:359:PHE:N	1:Q:359:PHE:CD1	2.88	0.40
1:J:124:ALA:C	1:J:126:VAL:N	2.78	0.40
1:J:195:PHE:O	1:J:199:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:LEU:HD11	1:N:110:TYR:HE2	1.87	0.40
1:P:363:GLN:HG3	1:R:19:SER:OG	2.21	0.40
1:A:344:GLY:O	1:A:345:TRP:C	2.64	0.40
1:B:326:LEU:H	1:B:326:LEU:CD1	2.29	0.40
1:K:339:ILE:O	1:K:340:ALA:C	2.64	0.40
1:M:206:ASP:OD1	1:M:206:ASP:N	2.40	0.40
1:O:121:ILE:HG22	1:O:121:ILE:O	2.21	0.40
1:J:150:GLN:HG3	1:J:151:PRO:HD2	2.02	0.40
1:L:7:PHE:HE1	1:N:18:LEU:HD13	1.87	0.40
1:P:351:GLU:C	1:P:353:LEU:N	2.78	0.40
1:R:11:LEU:HD12	1:R:11:LEU:HA	1.71	0.40
1:A:206:ASP:OD1	1:A:206:ASP:N	2.53	0.40
1:B:314:ASN:OD1	1:B:315:VAL:N	2.55	0.40
1:G:23:PHE:CZ	1:G:25:ASP:HB2	2.56	0.40
1:G:325:LYS:HA	1:G:325:LYS:HD3	1.88	0.40
1:E:72:ILE:O	1:E:72:ILE:CG2	2.69	0.40
1:K:81:ARG:HB3	1:K:81:ARG:NH1	2.32	0.40
1:M:106:LEU:HD11	1:M:110:TYR:HE2	1.87	0.40
1:Q:82:ILE:HD11	1:Q:109:PHE:CE2	2.57	0.40
1:F:206:ASP:OD1	1:F:206:ASP:N	2.53	0.40
1:N:106:LEU:HD22	1:N:135:MET:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	4	24
1	B	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	14	43
1	C	267/394 (68%)	228 (85%)	37 (14%)	2 (1%)	18	49
1	D	266/394 (68%)	222 (84%)	39 (15%)	5 (2%)	6	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	4	24
1	F	210/394 (53%)	190 (90%)	15 (7%)	5 (2%)	4	24
1	G	264/394 (67%)	225 (85%)	39 (15%)	0	100	100
1	H	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	18	49
1	I	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	14	43
1	J	211/394 (54%)	184 (87%)	25 (12%)	2 (1%)	14	43
1	K	267/394 (68%)	228 (85%)	37 (14%)	2 (1%)	18	49
1	L	267/394 (68%)	227 (85%)	37 (14%)	3 (1%)	11	40
1	M	266/394 (68%)	223 (84%)	39 (15%)	4 (2%)	8	33
1	N	266/394 (68%)	222 (84%)	40 (15%)	4 (2%)	8	33
1	O	264/394 (67%)	224 (85%)	39 (15%)	1 (0%)	30	59
1	P	264/394 (67%)	225 (85%)	39 (15%)	0	100	100
1	Q	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	18	49
1	R	267/394 (68%)	234 (88%)	31 (12%)	2 (1%)	18	49
All	All	4455/7092 (63%)	3848 (86%)	559 (12%)	48 (1%)	14	40

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	11	LEU
1	B	191	ASN
1	C	72	ILE
1	D	27	GLN
1	D	317	PHE
1	D	358	ILE
1	I	191	ASN
1	K	72	ILE
1	M	27	GLN
1	M	317	PHE
1	M	358	ILE
1	Q	370	ASN
1	J	191	ASN
1	L	72	ILE
1	N	27	GLN
1	N	317	PHE
1	N	358	ILE
1	B	189	THR

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Mol	Chain	Res	Type
1	H	368	SER
1	I	189	THR
1	J	189	THR
1	R	368	SER
1	A	145	GLY
1	E	145	GLY
1	O	15	PRO
1	F	145	GLY
1	D	15	PRO
1	A	170	PRO
1	C	73	ARG
1	E	170	PRO
1	K	73	ARG
1	F	170	PRO
1	L	73	ARG
1	A	172	PRO
1	E	172	PRO
1	F	172	PRO
1	R	13	GLY
1	A	171	ASP
1	H	13	GLY
1	E	171	ASP
1	Q	13	GLY
1	F	171	ASP
1	A	72	ILE
1	D	29	GLY
1	E	72	ILE
1	M	29	GLY
1	F	72	ILE
1	N	29	GLY

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	179/329 (54%)	169 (94%)	10 (6%)	19 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	181/329 (55%)	176 (97%)	5 (3%)	38	62
1	C	229/329 (70%)	219 (96%)	10 (4%)	25	53
1	D	227/329 (69%)	215 (95%)	12 (5%)	20	49
1	E	179/329 (54%)	169 (94%)	10 (6%)	19	47
1	F	179/329 (54%)	169 (94%)	10 (6%)	19	47
1	G	226/329 (69%)	219 (97%)	7 (3%)	35	61
1	H	228/329 (69%)	212 (93%)	16 (7%)	14	41
1	I	181/329 (55%)	176 (97%)	5 (3%)	38	62
1	J	181/329 (55%)	176 (97%)	5 (3%)	38	62
1	K	229/329 (70%)	223 (97%)	6 (3%)	40	63
1	L	229/329 (70%)	219 (96%)	10 (4%)	25	53
1	M	227/329 (69%)	216 (95%)	11 (5%)	23	52
1	N	227/329 (69%)	216 (95%)	11 (5%)	23	52
1	O	226/329 (69%)	219 (97%)	7 (3%)	35	61
1	P	226/329 (69%)	219 (97%)	7 (3%)	35	61
1	Q	228/329 (69%)	210 (92%)	18 (8%)	11	37
1	R	228/329 (69%)	213 (93%)	15 (7%)	15	44
All	All	3810/5922 (64%)	3635 (95%)	175 (5%)	25	53

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	A	79	LYS
1	A	81	ARG
1	A	143	ARG
1	A	144	LYS
1	A	169	GLU
1	A	171	ASP
1	A	324	ARG
1	A	325	LYS
1	A	326	LEU
1	B	97	ASP
1	B	147	ASP
1	B	187	GLU
1	B	191	ASN

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Mol	Chain	Res	Type
1	B	325	LYS
1	C	8	ARG
1	C	73	ARG
1	C	81	ARG
1	C	82	ILE
1	C	86	MET
1	C	106	LEU
1	C	365	TYR
1	C	366	THR
1	C	368	SER
1	C	369	ARG
1	D	18	LEU
1	D	24	VAL
1	D	27	GLN
1	D	28	ARG
1	D	30	VAL
1	D	77	ARG
1	D	146	ASN
1	D	210	VAL
1	D	324	ARG
1	D	360	ARG
1	D	368	SER
1	D	369	ARG
1	G	14	VAL
1	G	72	ILE
1	G	184	LEU
1	G	191	ASN
1	G	359	PHE
1	G	368	SER
1	G	369	ARG
1	H	6	GLU
1	H	8	ARG
1	H	110	TYR
1	H	111	SER
1	H	112	ARG
1	H	120	TYR
1	H	121	ILE
1	H	152	ARG
1	H	203	THR
1	H	204	LEU
1	H	206	ASP
1	H	217	THR

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Mol	Chain	Res	Type
1	H	218	LEU
1	H	370	ASN
1	H	371	LEU
1	H	374	THR
1	E	73	ARG
1	E	79	LYS
1	E	81	ARG
1	E	143	ARG
1	E	144	LYS
1	E	169	GLU
1	E	171	ASP
1	E	324	ARG
1	E	325	LYS
1	E	326	LEU
1	I	97	ASP
1	I	147	ASP
1	I	187	GLU
1	I	191	ASN
1	I	325	LYS
1	K	73	ARG
1	K	81	ARG
1	K	82	ILE
1	K	86	MET
1	K	106	LEU
1	K	368	SER
1	M	24	VAL
1	M	27	GLN
1	M	28	ARG
1	M	30	VAL
1	M	77	ARG
1	M	146	ASN
1	M	210	VAL
1	M	324	ARG
1	M	360	ARG
1	M	368	SER
1	M	369	ARG
1	O	14	VAL
1	O	72	ILE
1	O	184	LEU
1	O	191	ASN
1	O	359	PHE
1	O	368	SER

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Mol	Chain	Res	Type
1	O	369	ARG
1	Q	8	ARG
1	Q	78	ILE
1	Q	79	LYS
1	Q	110	TYR
1	Q	111	SER
1	Q	112	ARG
1	Q	120	TYR
1	Q	121	ILE
1	Q	152	ARG
1	Q	203	THR
1	Q	204	LEU
1	Q	206	ASP
1	Q	217	THR
1	Q	218	LEU
1	Q	369	ARG
1	Q	370	ASN
1	Q	371	LEU
1	Q	374	THR
1	F	73	ARG
1	F	79	LYS
1	F	81	ARG
1	F	143	ARG
1	F	144	LYS
1	F	169	GLU
1	F	171	ASP
1	F	324	ARG
1	F	325	LYS
1	F	326	LEU
1	J	97	ASP
1	J	147	ASP
1	J	187	GLU
1	J	191	ASN
1	J	325	LYS
1	L	5	SER
1	L	6	GLU
1	L	8	ARG
1	L	73	ARG
1	L	81	ARG
1	L	82	ILE
1	L	86	MET
1	L	106	LEU

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Mol	Chain	Res	Type
1	L	368	SER
1	L	369	ARG
1	N	24	VAL
1	N	27	GLN
1	N	28	ARG
1	N	30	VAL
1	N	77	ARG
1	N	146	ASN
1	N	210	VAL
1	N	324	ARG
1	N	360	ARG
1	N	368	SER
1	N	369	ARG
1	P	14	VAL
1	P	72	ILE
1	P	184	LEU
1	P	191	ASN
1	P	359	PHE
1	P	368	SER
1	P	369	ARG
1	R	6	GLU
1	R	8	ARG
1	R	110	TYR
1	R	111	SER
1	R	112	ARG
1	R	120	TYR
1	R	121	ILE
1	R	152	ARG
1	R	204	LEU
1	R	206	ASP
1	R	217	THR
1	R	218	LEU
1	R	370	ASN
1	R	371	LEU
1	R	374	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	188	HIS
1	B	140	GLN

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Mol	Chain	Res	Type
1	B	150	GLN
1	C	40	GLN
1	C	58	HIS
1	C	94	HIS
1	C	354	ASN
1	D	40	GLN
1	D	58	HIS
1	D	75	HIS
1	D	94	HIS
1	D	140	GLN
1	D	160	ASN
1	D	188	HIS
1	D	354	ASN
1	D	356	ASN
1	G	58	HIS
1	G	100	GLN
1	G	160	ASN
1	G	188	HIS
1	G	363	GLN
1	H	58	HIS
1	E	94	HIS
1	E	188	HIS
1	I	140	GLN
1	I	146	ASN
1	K	40	GLN
1	K	58	HIS
1	K	94	HIS
1	K	191	ASN
1	K	354	ASN
1	M	58	HIS
1	M	75	HIS
1	M	140	GLN
1	M	160	ASN
1	M	188	HIS
1	M	354	ASN
1	M	356	ASN
1	O	58	HIS
1	O	100	GLN
1	O	160	ASN
1	O	188	HIS
1	O	363	GLN
1	Q	58	HIS

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Mol	Chain	Res	Type
1	Q	370	ASN
1	F	94	HIS
1	F	188	HIS
1	J	140	GLN
1	J	150	GLN
1	L	40	GLN
1	L	58	HIS
1	L	94	HIS
1	L	354	ASN
1	N	40	GLN
1	N	58	HIS
1	N	75	HIS
1	N	94	HIS
1	N	140	GLN
1	N	160	ASN
1	N	188	HIS
1	N	354	ASN
1	P	58	HIS
1	P	100	GLN
1	P	160	ASN
1	P	188	HIS
1	P	363	GLN
1	R	58	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

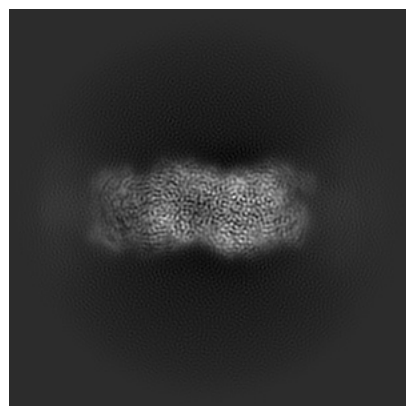
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19251. These allow visual inspection of the internal detail of the map and identification of artifacts.

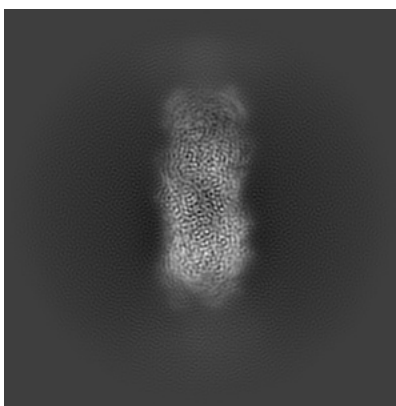
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

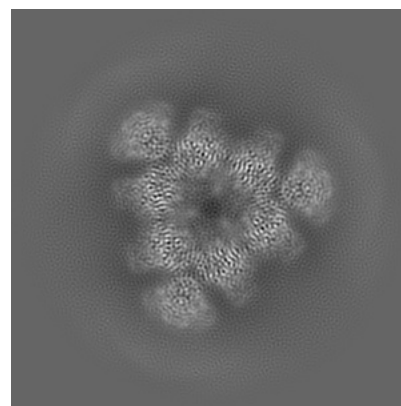
6.1.1 Primary map



X

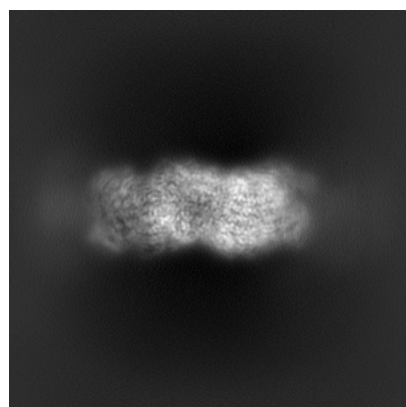


Y

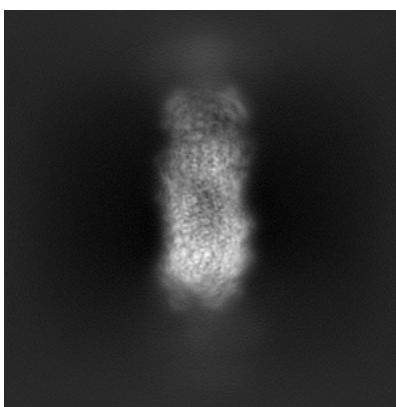


Z

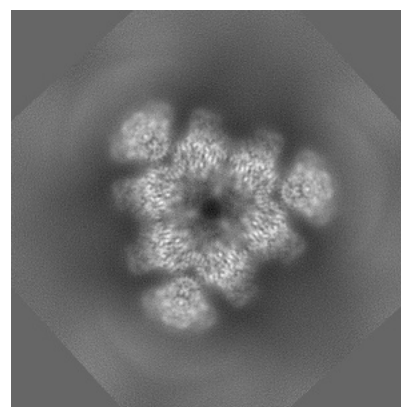
6.1.2 Raw map



X



Y

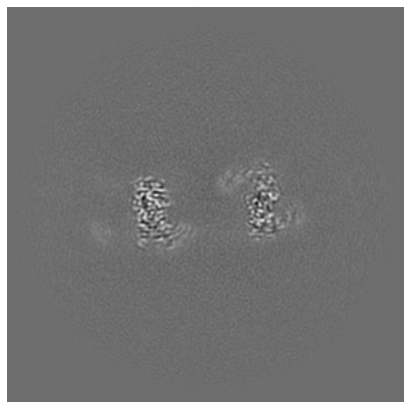


Z

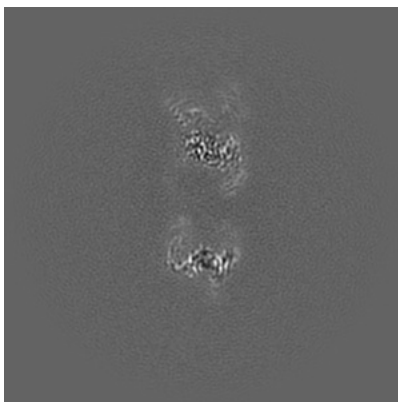
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

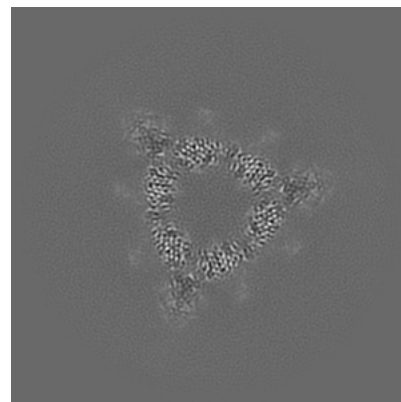
6.2.1 Primary map



X Index: 250

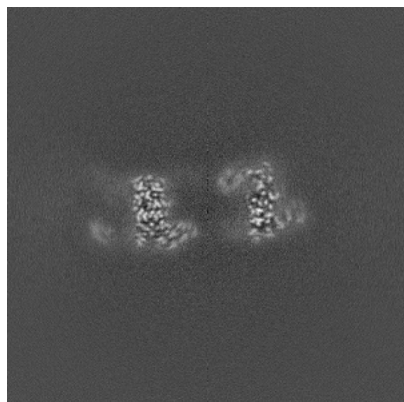


Y Index: 250

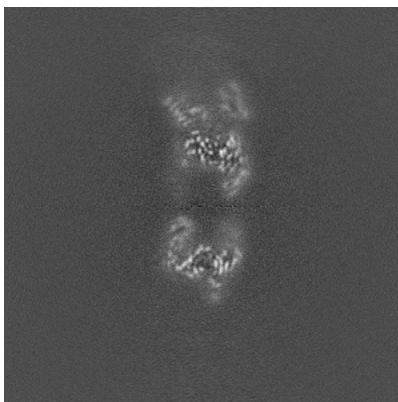


Z Index: 250

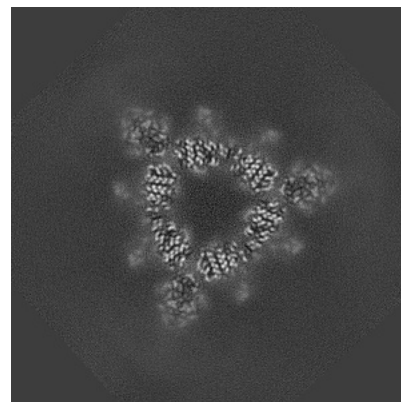
6.2.2 Raw map



X Index: 250



Y Index: 250

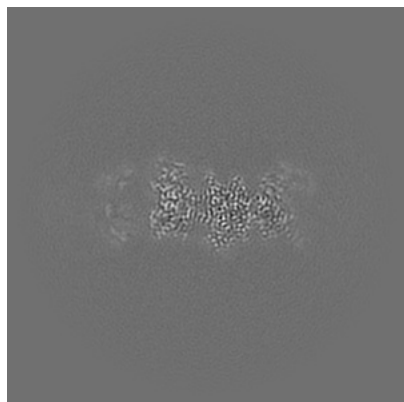


Z Index: 250

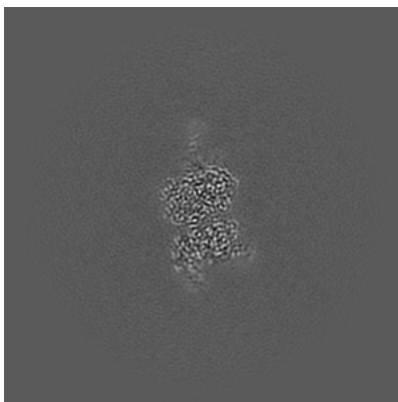
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

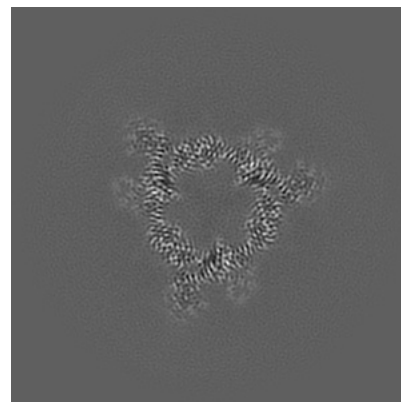
6.3.1 Primary map



X Index: 187

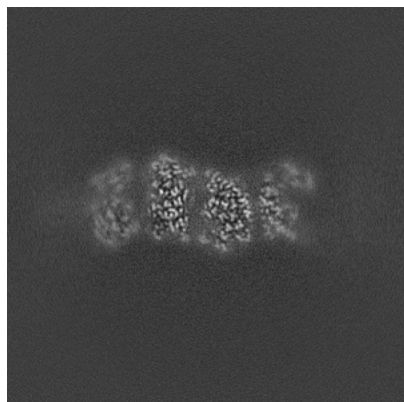


Y Index: 191

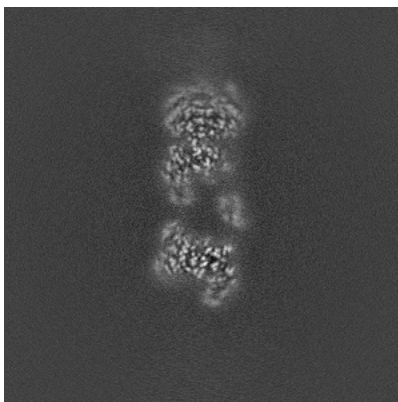


Z Index: 261

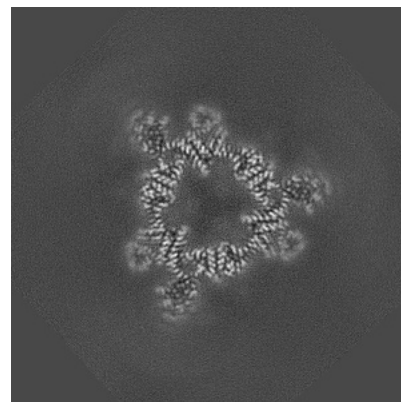
6.3.2 Raw map



X Index: 193



Y Index: 275

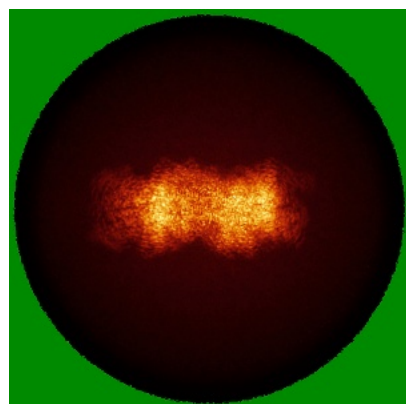


Z Index: 239

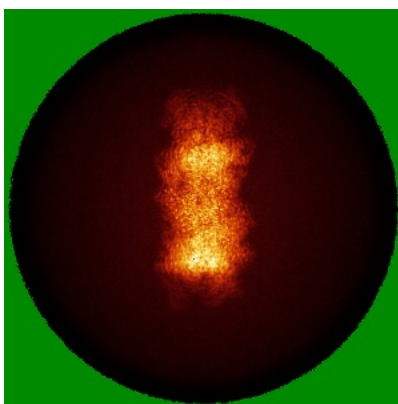
The images above show the largest variance slices of the map in three orthogonal directions.

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

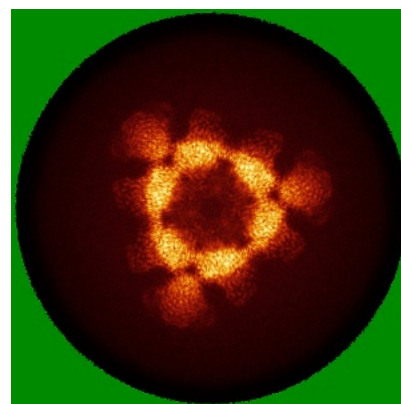
6.4.1 Primary map



X

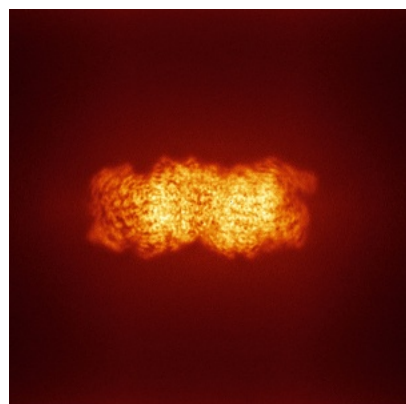


Y

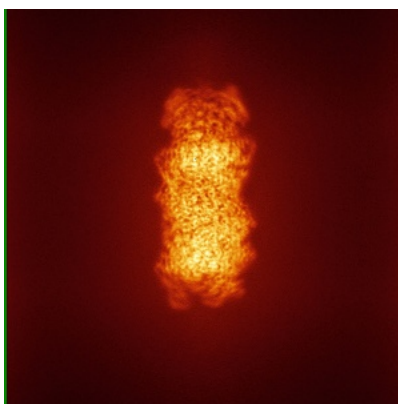


Z

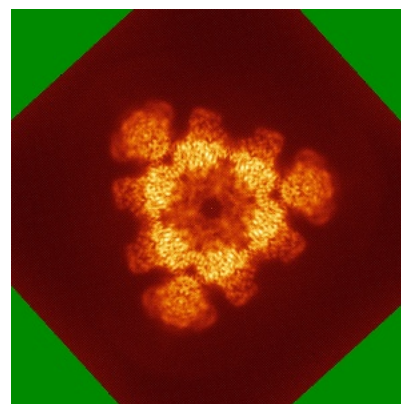
6.4.2 Raw map



X



Y

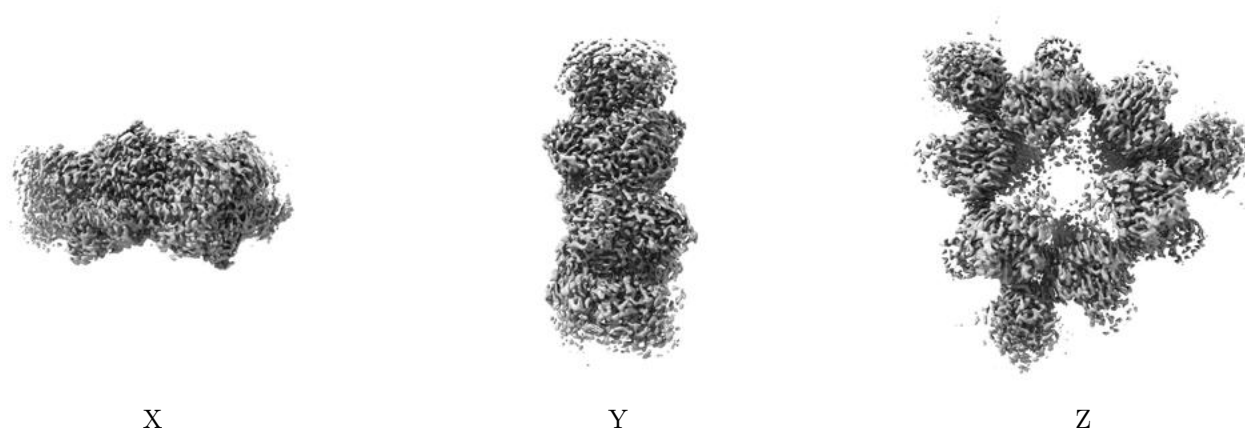


Z

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

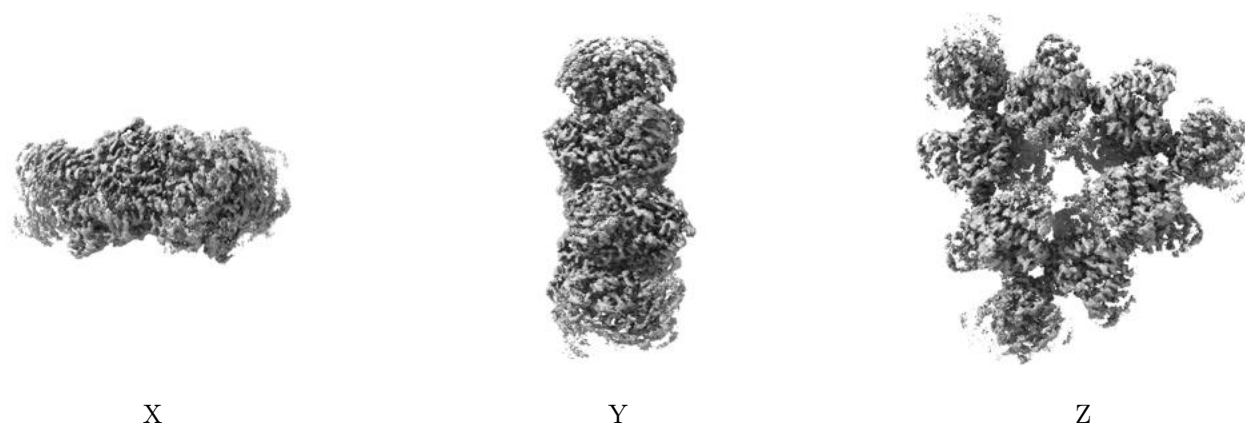
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

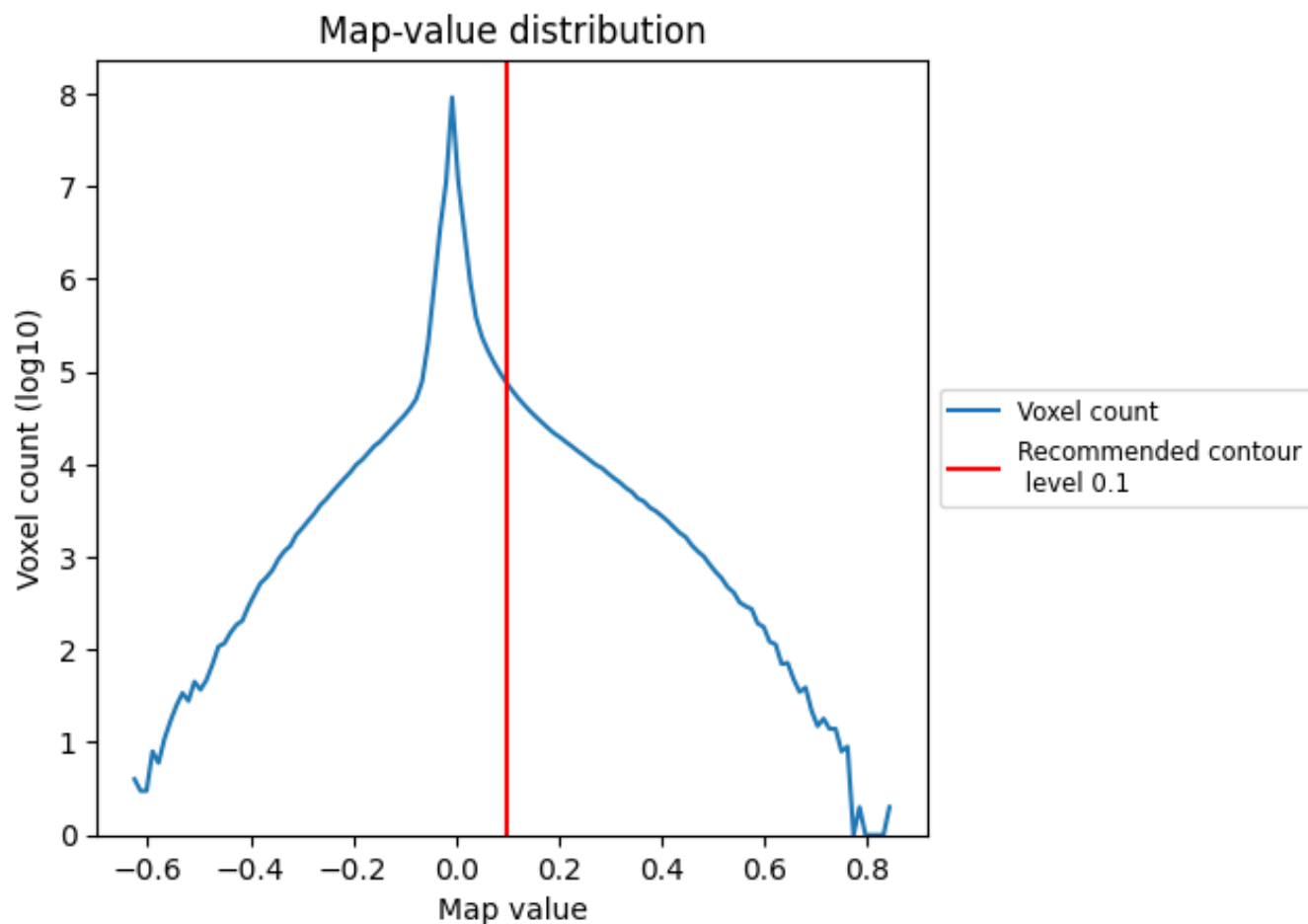
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

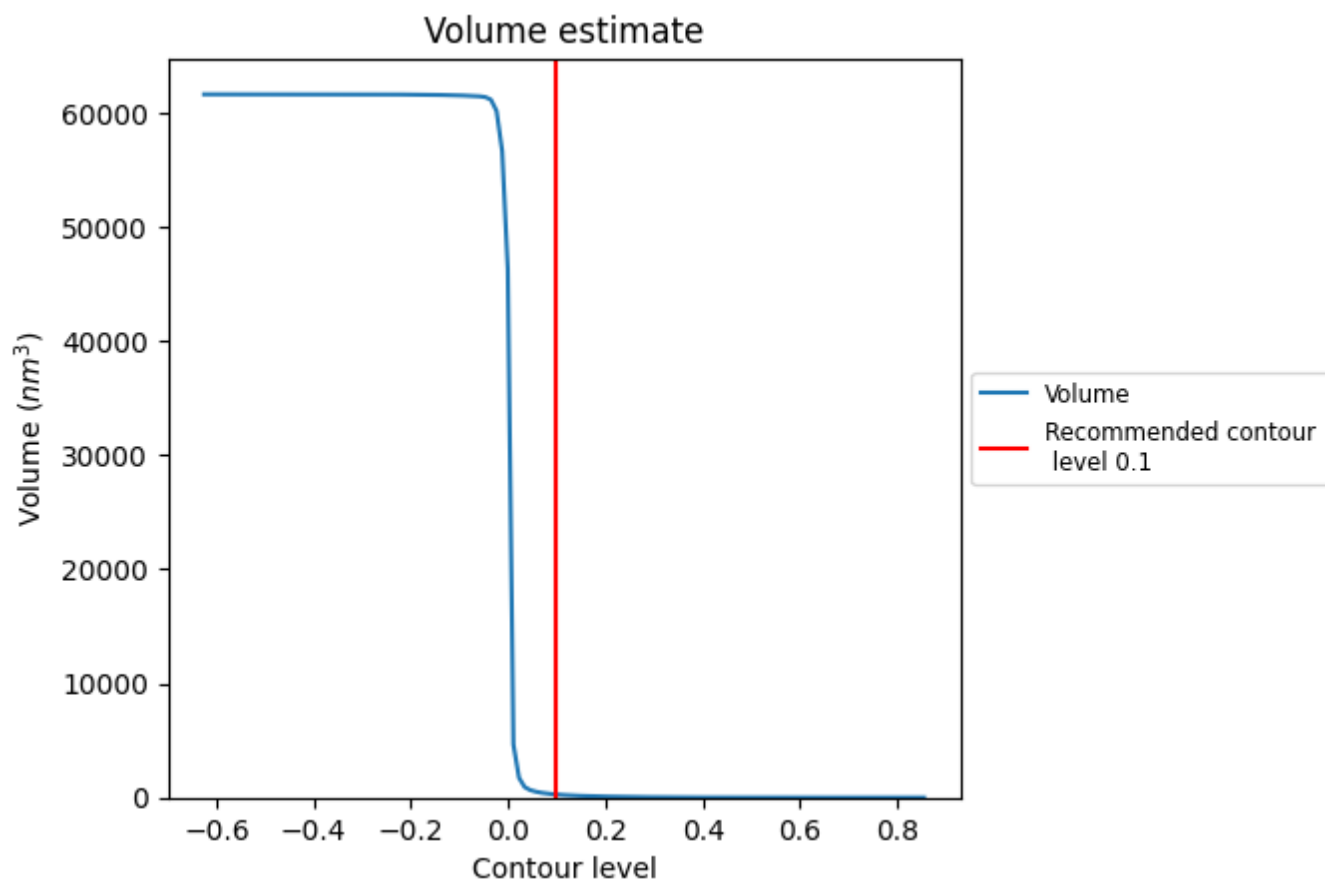
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

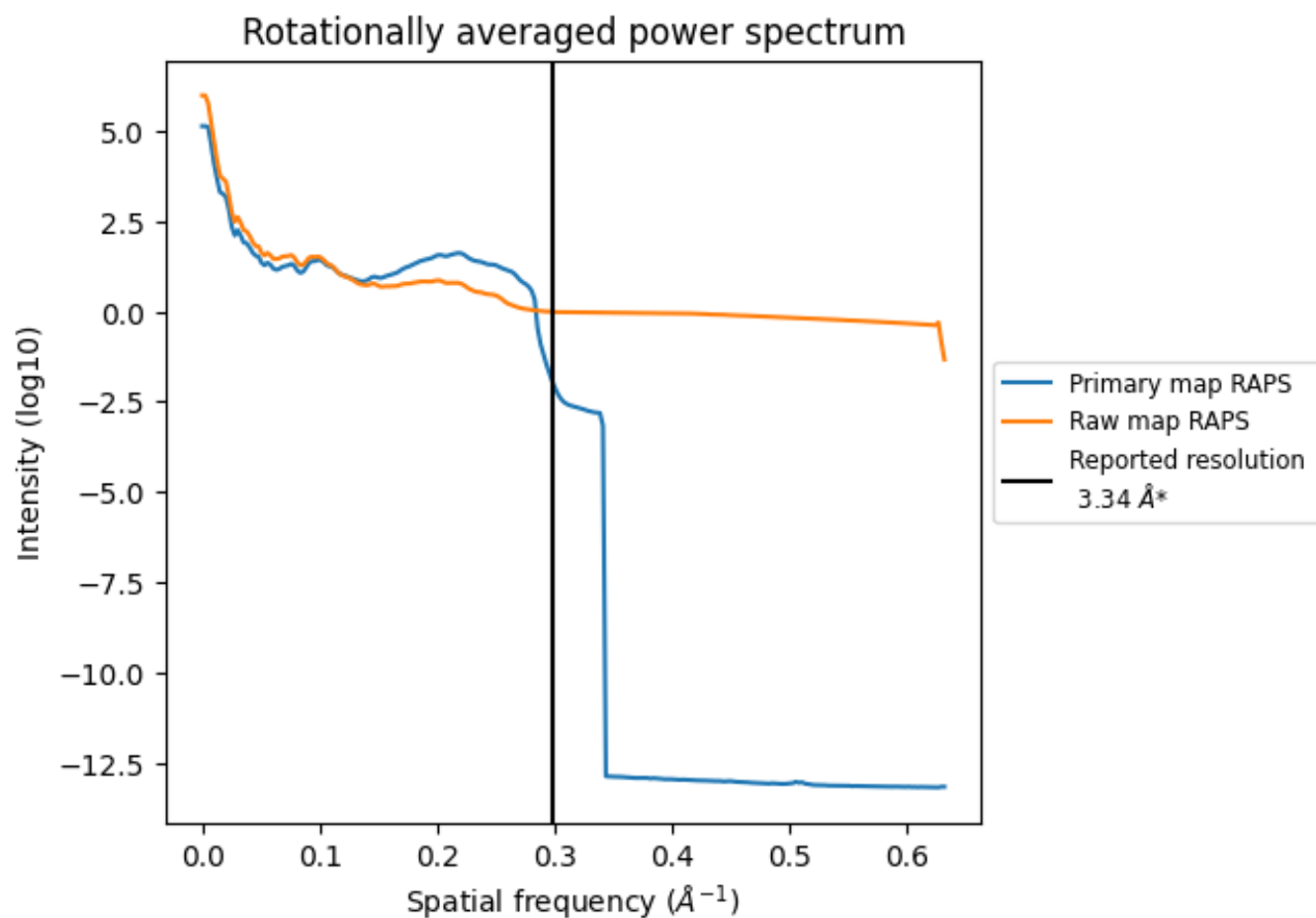
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 266 nm³; this corresponds to an approximate mass of 241 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 ⓘ

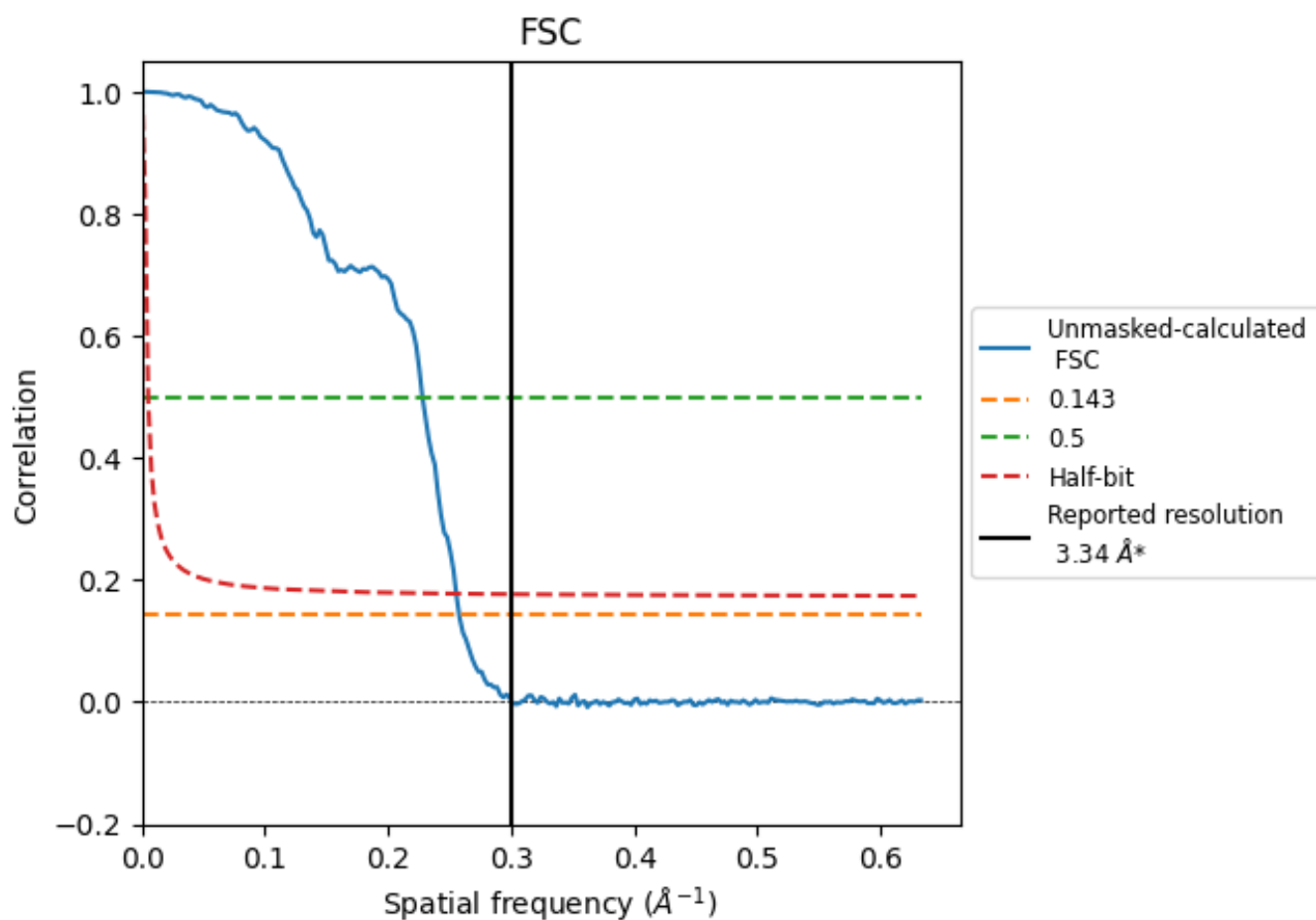


*Reported resolution corresponds to spatial frequency of 0.299 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.299 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

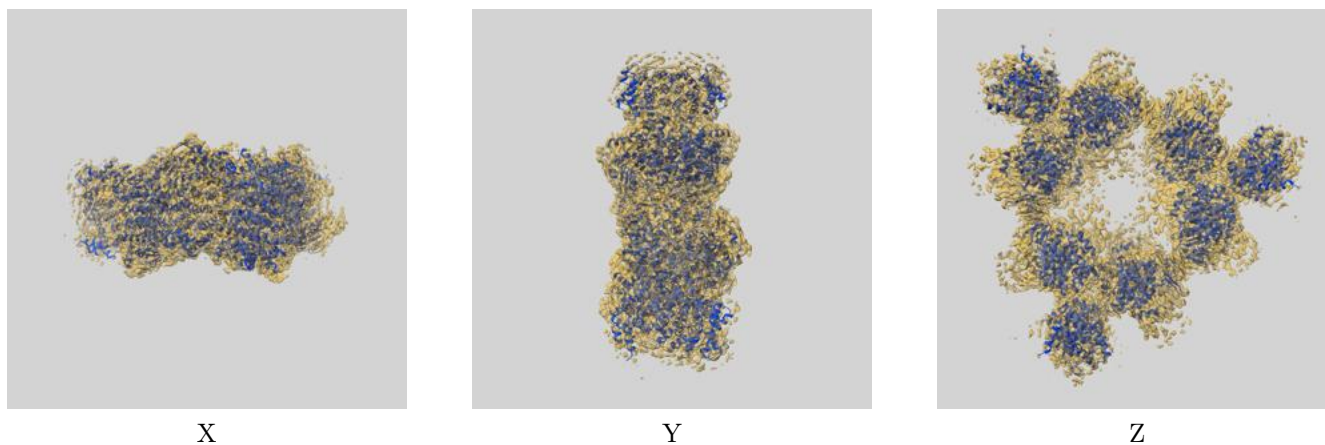
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.34	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.88	4.39	3.92

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.34 by more than 10 %

9 Map-model fit [i](#)

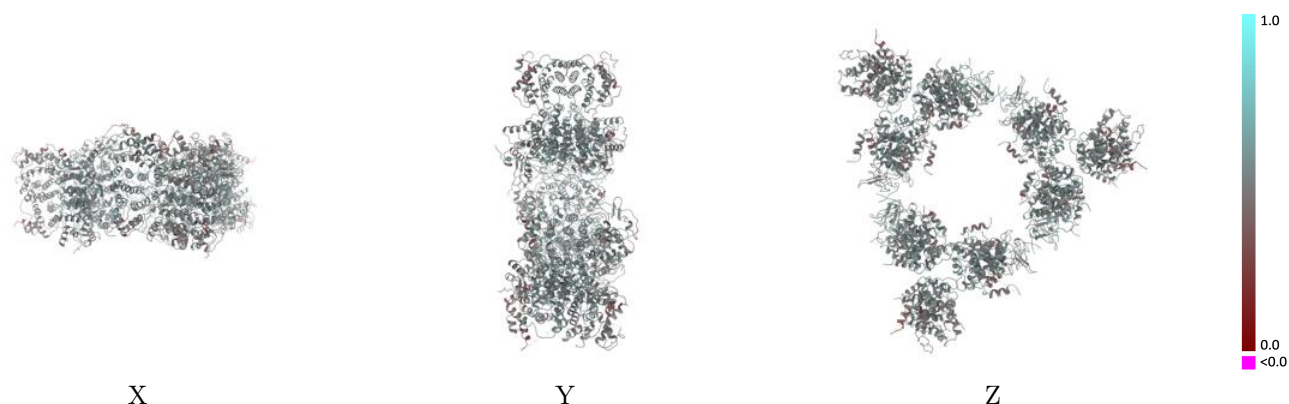
This section contains information regarding the fit between EMDB map EMD-19251 and PDB model 8RJL. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.1 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](#)

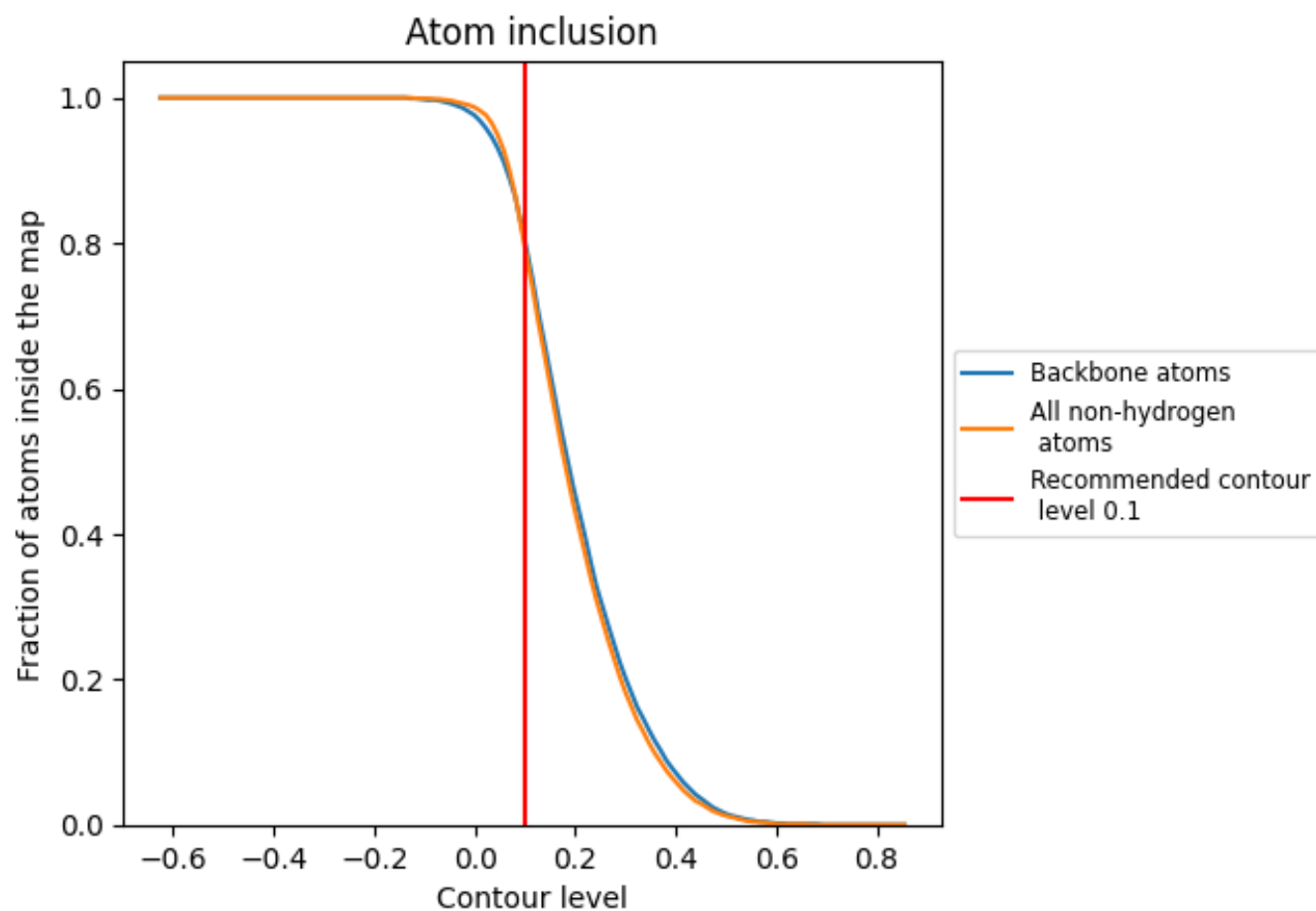


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 80% of all backbone atoms, 79% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7940	 0.5040
A	 0.6240	 0.4820
B	 0.6560	 0.4850
C	 0.8430	 0.5100
D	 0.8660	 0.5220
E	 0.6210	 0.4780
F	 0.6170	 0.4780
G	 0.8650	 0.5150
H	 0.8570	 0.5070
I	 0.6570	 0.4840
J	 0.6530	 0.4840
K	 0.8450	 0.5130
L	 0.8460	 0.5110
M	 0.8640	 0.5220
N	 0.8640	 0.5210
O	 0.8630	 0.5120
P	 0.8670	 0.5120
Q	 0.8530	 0.5030
R	 0.8530	 0.5060

