Full wwPDB EM Validation Report (i)

Nov 12, 2022 – 11:58 AM EST

PDB ID	:	6UIX
EMDB ID	:	EMD-20790
Title	:	Cryo-EM structure of human CALHM2 gap junction
Authors	:	Lu, W.; Du, J.; Choi, W.
Deposited on	:	2019-10-01
Resolution	:	3.50 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 (i) 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 (i)) were used in the production of this report:

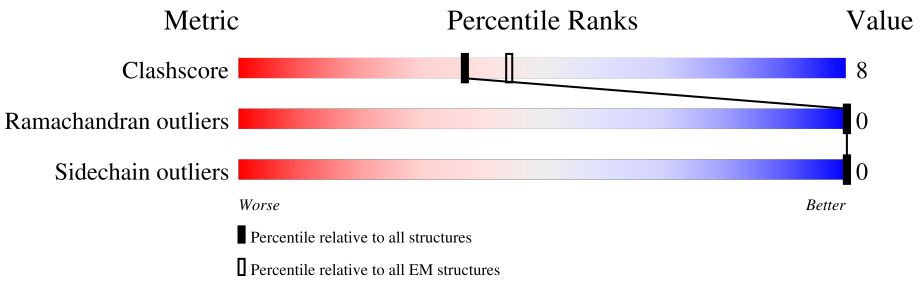
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.50 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 >=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 <=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	331	7% 67% 16% 17%
1	B	331	7% 67% 16% 17%
1	C	331	7% 67% 16% 17%
1	D	331	7% 67% 16% 17%
1	E	331	7% 67% 16% 17%
1	F	331	8% 67% 16% 17%
1	G	331	7% 67% 16% 17%
1	H	331	7% 67% 16% 17%

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Mol	Chain	Length	Quality of chain
1	I	331	8% 66% 17% 17%
1	J	331	8% 66% 17% 17%
1	K	331	8% 67% 16% 17%
1	L	331	9% 67% 16% 17%
1	M	331	10% 66% 17% 17%
1	N	331	9% 67% 16% 17%
1	O	331	9% 66% 17% 17%
1	P	331	10% 67% 16% 17%
1	Q	331	10% 67% 16% 17%
1	R	331	10% 67% 16% 17%
1	S	331	10% 67% 16% 17%
1	T	331	10% 67% 16% 17%
1	U	331	10% 67% 16% 17%
1	V	331	9% 67% 16% 17%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 44198 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 Calcium homeostasis modulator protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	275	2009	1308	365	329	7	0	0
1	B	275	2009	1308	365	329	7	0	0
1	C	275	2009	1308	365	329	7	0	0
1	D	275	2009	1308	365	329	7	0	0
1	E	275	2009	1308	365	329	7	0	0
1	F	275	2009	1308	365	329	7	0	0
1	G	275	2009	1308	365	329	7	0	0
1	H	275	2009	1308	365	329	7	0	0
1	I	275	2009	1308	365	329	7	0	0
1	J	275	2009	1308	365	329	7	0	0
1	K	275	2009	1308	365	329	7	0	0
1	L	275	2009	1308	365	329	7	0	0
1	M	275	2009	1308	365	329	7	0	0
1	N	275	2009	1308	365	329	7	0	0
1	O	275	2009	1308	365	329	7	0	0
1	P	275	2009	1308	365	329	7	0	0
1	Q	275	2009	1308	365	329	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	275	2009	1308	365	329	7	0	0
1	S	275	2009	1308	365	329	7	0	0
1	T	275	2009	1308	365	329	7	0	0
1	U	275	2009	1308	365	329	7	0	0
1	V	275	2009	1308	365	329	7	0	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	PHE	-	expression tag	UNP Q9HA72
A	325	GLU	-	expression tag	UNP Q9HA72
A	326	SER	-	expression tag	UNP Q9HA72
A	327	ARG	-	expression tag	UNP Q9HA72
A	328	LEU	-	expression tag	UNP Q9HA72
A	329	VAL	-	expression tag	UNP Q9HA72
A	330	PRO	-	expression tag	UNP Q9HA72
A	331	ARG	-	expression tag	UNP Q9HA72
B	324	PHE	-	expression tag	UNP Q9HA72
B	325	GLU	-	expression tag	UNP Q9HA72
B	326	SER	-	expression tag	UNP Q9HA72
B	327	ARG	-	expression tag	UNP Q9HA72
B	328	LEU	-	expression tag	UNP Q9HA72
B	329	VAL	-	expression tag	UNP Q9HA72
B	330	PRO	-	expression tag	UNP Q9HA72
B	331	ARG	-	expression tag	UNP Q9HA72
C	324	PHE	-	expression tag	UNP Q9HA72
C	325	GLU	-	expression tag	UNP Q9HA72
C	326	SER	-	expression tag	UNP Q9HA72
C	327	ARG	-	expression tag	UNP Q9HA72
C	328	LEU	-	expression tag	UNP Q9HA72
C	329	VAL	-	expression tag	UNP Q9HA72
C	330	PRO	-	expression tag	UNP Q9HA72
C	331	ARG	-	expression tag	UNP Q9HA72
D	324	PHE	-	expression tag	UNP Q9HA72
D	325	GLU	-	expression tag	UNP Q9HA72
D	326	SER	-	expression tag	UNP Q9HA72
D	327	ARG	-	expression tag	UNP Q9HA72
D	328	LEU	-	expression tag	UNP Q9HA72

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Chain	Residue	Modelled	Actual	Comment	Reference
D	329	VAL	-	expression tag	UNP Q9HA72
D	330	PRO	-	expression tag	UNP Q9HA72
D	331	ARG	-	expression tag	UNP Q9HA72
E	324	PHE	-	expression tag	UNP Q9HA72
E	325	GLU	-	expression tag	UNP Q9HA72
E	326	SER	-	expression tag	UNP Q9HA72
E	327	ARG	-	expression tag	UNP Q9HA72
E	328	LEU	-	expression tag	UNP Q9HA72
E	329	VAL	-	expression tag	UNP Q9HA72
E	330	PRO	-	expression tag	UNP Q9HA72
E	331	ARG	-	expression tag	UNP Q9HA72
F	324	PHE	-	expression tag	UNP Q9HA72
F	325	GLU	-	expression tag	UNP Q9HA72
F	326	SER	-	expression tag	UNP Q9HA72
F	327	ARG	-	expression tag	UNP Q9HA72
F	328	LEU	-	expression tag	UNP Q9HA72
F	329	VAL	-	expression tag	UNP Q9HA72
F	330	PRO	-	expression tag	UNP Q9HA72
F	331	ARG	-	expression tag	UNP Q9HA72
G	324	PHE	-	expression tag	UNP Q9HA72
G	325	GLU	-	expression tag	UNP Q9HA72
G	326	SER	-	expression tag	UNP Q9HA72
G	327	ARG	-	expression tag	UNP Q9HA72
G	328	LEU	-	expression tag	UNP Q9HA72
G	329	VAL	-	expression tag	UNP Q9HA72
G	330	PRO	-	expression tag	UNP Q9HA72
G	331	ARG	-	expression tag	UNP Q9HA72
H	324	PHE	-	expression tag	UNP Q9HA72
H	325	GLU	-	expression tag	UNP Q9HA72
H	326	SER	-	expression tag	UNP Q9HA72
H	327	ARG	-	expression tag	UNP Q9HA72
H	328	LEU	-	expression tag	UNP Q9HA72
H	329	VAL	-	expression tag	UNP Q9HA72
H	330	PRO	-	expression tag	UNP Q9HA72
H	331	ARG	-	expression tag	UNP Q9HA72
I	324	PHE	-	expression tag	UNP Q9HA72
I	325	GLU	-	expression tag	UNP Q9HA72
I	326	SER	-	expression tag	UNP Q9HA72
I	327	ARG	-	expression tag	UNP Q9HA72
I	328	LEU	-	expression tag	UNP Q9HA72
I	329	VAL	-	expression tag	UNP Q9HA72
I	330	PRO	-	expression tag	UNP Q9HA72

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Chain	Residue	Modelled	Actual	Comment	Reference
I	331	ARG	-	expression tag	UNP Q9HA72
J	324	PHE	-	expression tag	UNP Q9HA72
J	325	GLU	-	expression tag	UNP Q9HA72
J	326	SER	-	expression tag	UNP Q9HA72
J	327	ARG	-	expression tag	UNP Q9HA72
J	328	LEU	-	expression tag	UNP Q9HA72
J	329	VAL	-	expression tag	UNP Q9HA72
J	330	PRO	-	expression tag	UNP Q9HA72
J	331	ARG	-	expression tag	UNP Q9HA72
K	324	PHE	-	expression tag	UNP Q9HA72
K	325	GLU	-	expression tag	UNP Q9HA72
K	326	SER	-	expression tag	UNP Q9HA72
K	327	ARG	-	expression tag	UNP Q9HA72
K	328	LEU	-	expression tag	UNP Q9HA72
K	329	VAL	-	expression tag	UNP Q9HA72
K	330	PRO	-	expression tag	UNP Q9HA72
K	331	ARG	-	expression tag	UNP Q9HA72
L	324	PHE	-	expression tag	UNP Q9HA72
L	325	GLU	-	expression tag	UNP Q9HA72
L	326	SER	-	expression tag	UNP Q9HA72
L	327	ARG	-	expression tag	UNP Q9HA72
L	328	LEU	-	expression tag	UNP Q9HA72
L	329	VAL	-	expression tag	UNP Q9HA72
L	330	PRO	-	expression tag	UNP Q9HA72
L	331	ARG	-	expression tag	UNP Q9HA72
M	324	PHE	-	expression tag	UNP Q9HA72
M	325	GLU	-	expression tag	UNP Q9HA72
M	326	SER	-	expression tag	UNP Q9HA72
M	327	ARG	-	expression tag	UNP Q9HA72
M	328	LEU	-	expression tag	UNP Q9HA72
M	329	VAL	-	expression tag	UNP Q9HA72
M	330	PRO	-	expression tag	UNP Q9HA72
M	331	ARG	-	expression tag	UNP Q9HA72
N	324	PHE	-	expression tag	UNP Q9HA72
N	325	GLU	-	expression tag	UNP Q9HA72
N	326	SER	-	expression tag	UNP Q9HA72
N	327	ARG	-	expression tag	UNP Q9HA72
N	328	LEU	-	expression tag	UNP Q9HA72
N	329	VAL	-	expression tag	UNP Q9HA72
N	330	PRO	-	expression tag	UNP Q9HA72
N	331	ARG	-	expression tag	UNP Q9HA72
O	324	PHE	-	expression tag	UNP Q9HA72

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Chain	Residue	Modelled	Actual	Comment	Reference
O	325	GLU	-	expression tag	UNP Q9HA72
O	326	SER	-	expression tag	UNP Q9HA72
O	327	ARG	-	expression tag	UNP Q9HA72
O	328	LEU	-	expression tag	UNP Q9HA72
O	329	VAL	-	expression tag	UNP Q9HA72
O	330	PRO	-	expression tag	UNP Q9HA72
O	331	ARG	-	expression tag	UNP Q9HA72
P	324	PHE	-	expression tag	UNP Q9HA72
P	325	GLU	-	expression tag	UNP Q9HA72
P	326	SER	-	expression tag	UNP Q9HA72
P	327	ARG	-	expression tag	UNP Q9HA72
P	328	LEU	-	expression tag	UNP Q9HA72
P	329	VAL	-	expression tag	UNP Q9HA72
P	330	PRO	-	expression tag	UNP Q9HA72
P	331	ARG	-	expression tag	UNP Q9HA72
Q	324	PHE	-	expression tag	UNP Q9HA72
Q	325	GLU	-	expression tag	UNP Q9HA72
Q	326	SER	-	expression tag	UNP Q9HA72
Q	327	ARG	-	expression tag	UNP Q9HA72
Q	328	LEU	-	expression tag	UNP Q9HA72
Q	329	VAL	-	expression tag	UNP Q9HA72
Q	330	PRO	-	expression tag	UNP Q9HA72
Q	331	ARG	-	expression tag	UNP Q9HA72
R	324	PHE	-	expression tag	UNP Q9HA72
R	325	GLU	-	expression tag	UNP Q9HA72
R	326	SER	-	expression tag	UNP Q9HA72
R	327	ARG	-	expression tag	UNP Q9HA72
R	328	LEU	-	expression tag	UNP Q9HA72
R	329	VAL	-	expression tag	UNP Q9HA72
R	330	PRO	-	expression tag	UNP Q9HA72
R	331	ARG	-	expression tag	UNP Q9HA72
S	324	PHE	-	expression tag	UNP Q9HA72
S	325	GLU	-	expression tag	UNP Q9HA72
S	326	SER	-	expression tag	UNP Q9HA72
S	327	ARG	-	expression tag	UNP Q9HA72
S	328	LEU	-	expression tag	UNP Q9HA72
S	329	VAL	-	expression tag	UNP Q9HA72
S	330	PRO	-	expression tag	UNP Q9HA72
S	331	ARG	-	expression tag	UNP Q9HA72
T	324	PHE	-	expression tag	UNP Q9HA72
T	325	GLU	-	expression tag	UNP Q9HA72
T	326	SER	-	expression tag	UNP Q9HA72

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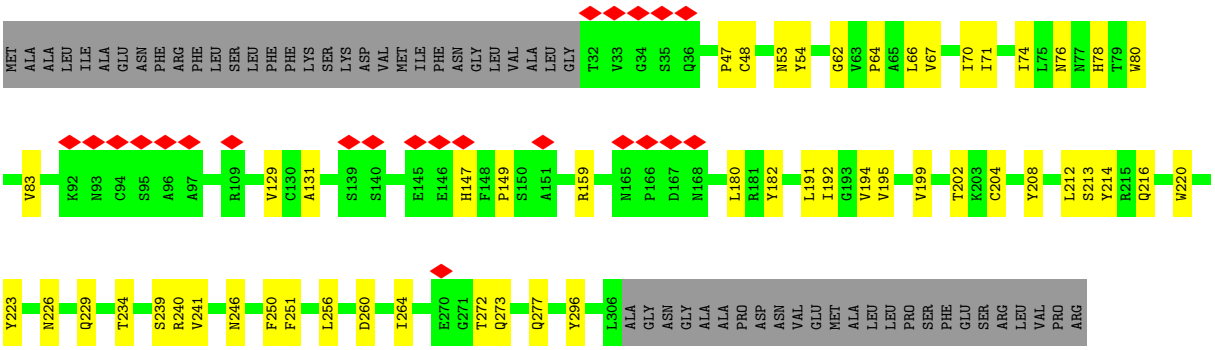
Chain	Residue	Modelled	Actual	Comment	Reference
T	327	ARG	-	expression tag	UNP Q9HA72
T	328	LEU	-	expression tag	UNP Q9HA72
T	329	VAL	-	expression tag	UNP Q9HA72
T	330	PRO	-	expression tag	UNP Q9HA72
T	331	ARG	-	expression tag	UNP Q9HA72
U	324	PHE	-	expression tag	UNP Q9HA72
U	325	GLU	-	expression tag	UNP Q9HA72
U	326	SER	-	expression tag	UNP Q9HA72
U	327	ARG	-	expression tag	UNP Q9HA72
U	328	LEU	-	expression tag	UNP Q9HA72
U	329	VAL	-	expression tag	UNP Q9HA72
U	330	PRO	-	expression tag	UNP Q9HA72
U	331	ARG	-	expression tag	UNP Q9HA72
V	324	PHE	-	expression tag	UNP Q9HA72
V	325	GLU	-	expression tag	UNP Q9HA72
V	326	SER	-	expression tag	UNP Q9HA72
V	327	ARG	-	expression tag	UNP Q9HA72
V	328	LEU	-	expression tag	UNP Q9HA72
V	329	VAL	-	expression tag	UNP Q9HA72
V	330	PRO	-	expression tag	UNP Q9HA72
V	331	ARG	-	expression tag	UNP Q9HA72

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

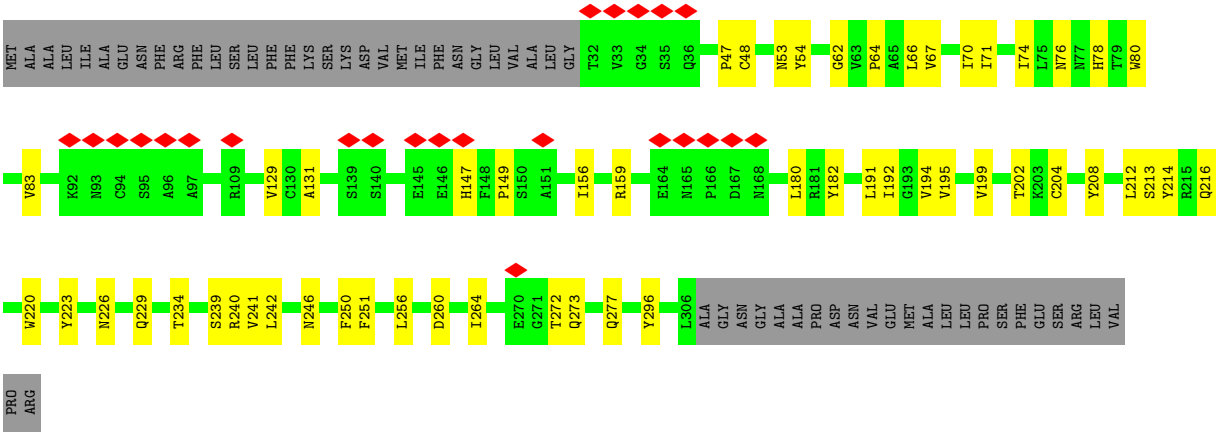
• Molecule 1: Calcium homeostasis modulator protein 2

Chain A:



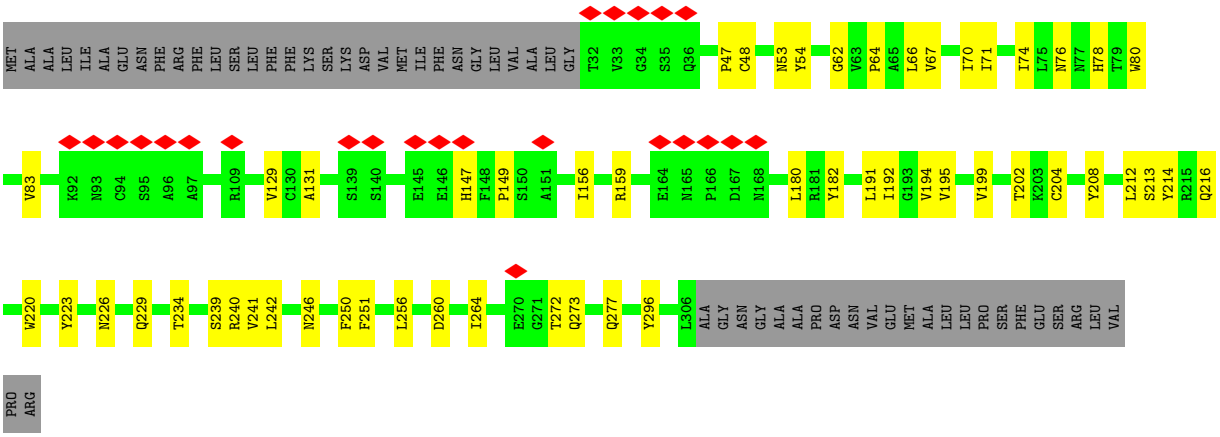
• Molecule 1: Calcium homeostasis modulator protein 2

Chain B:



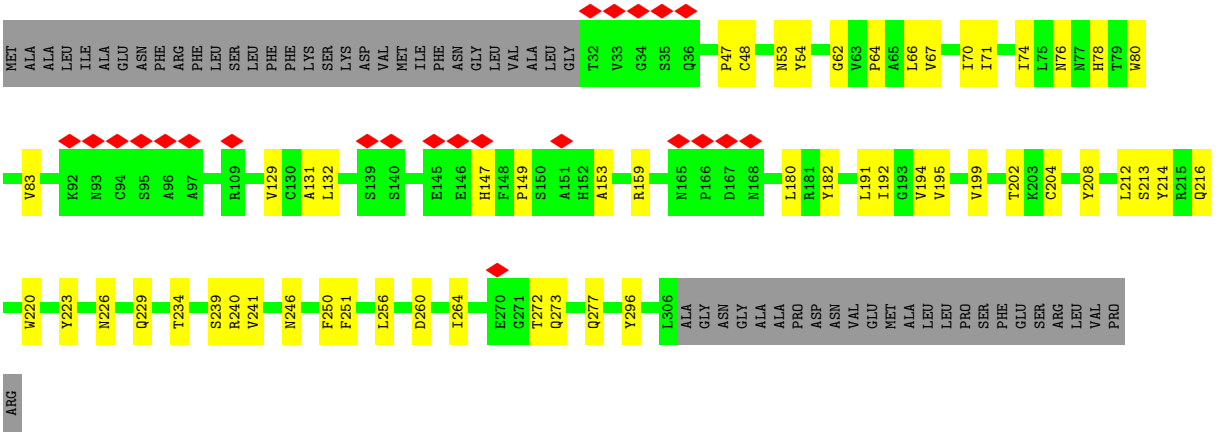
• Molecule 1: Calcium homeostasis modulator protein 2

Chain C:



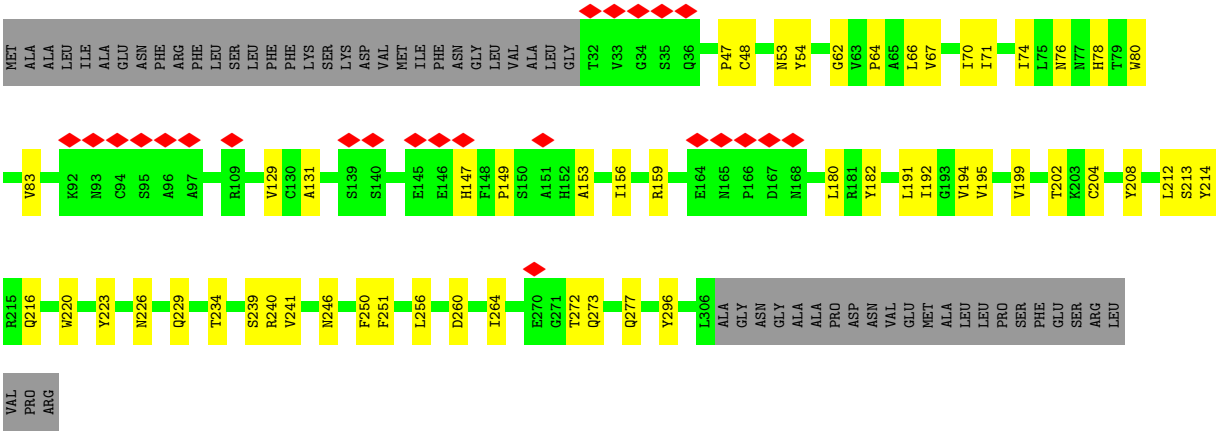
• Molecule 1: Calcium homeostasis modulator protein 2

Chain D:



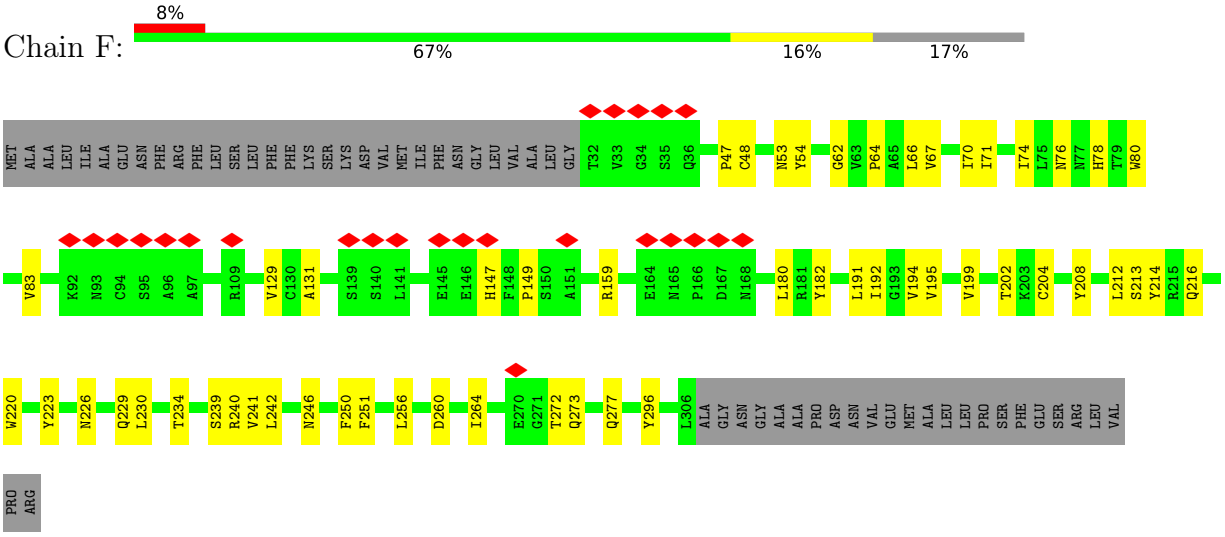
• Molecule 1: Calcium homeostasis modulator protein 2

Chain E:



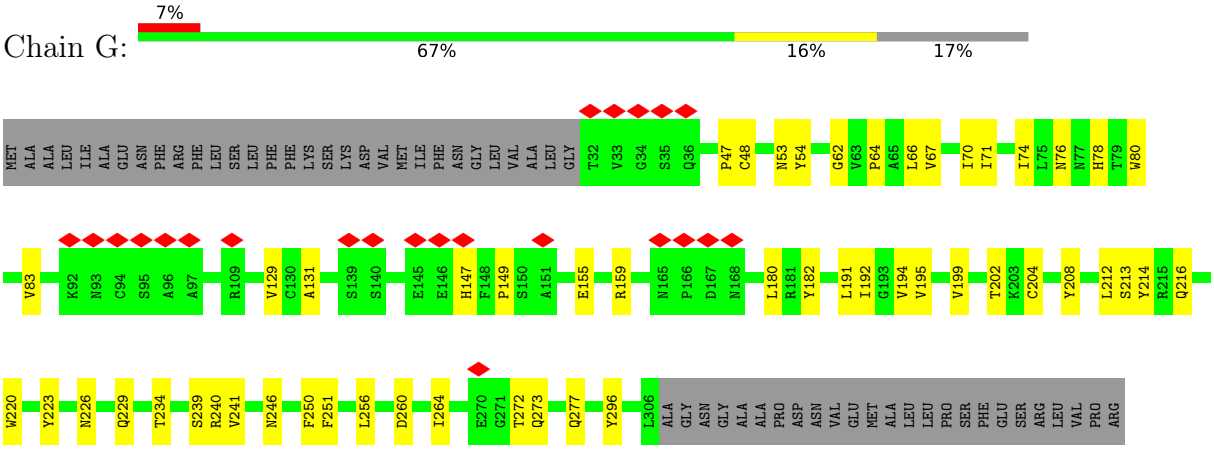
• Molecule 1: Calcium homeostasis modulator protein 2

Chain F:



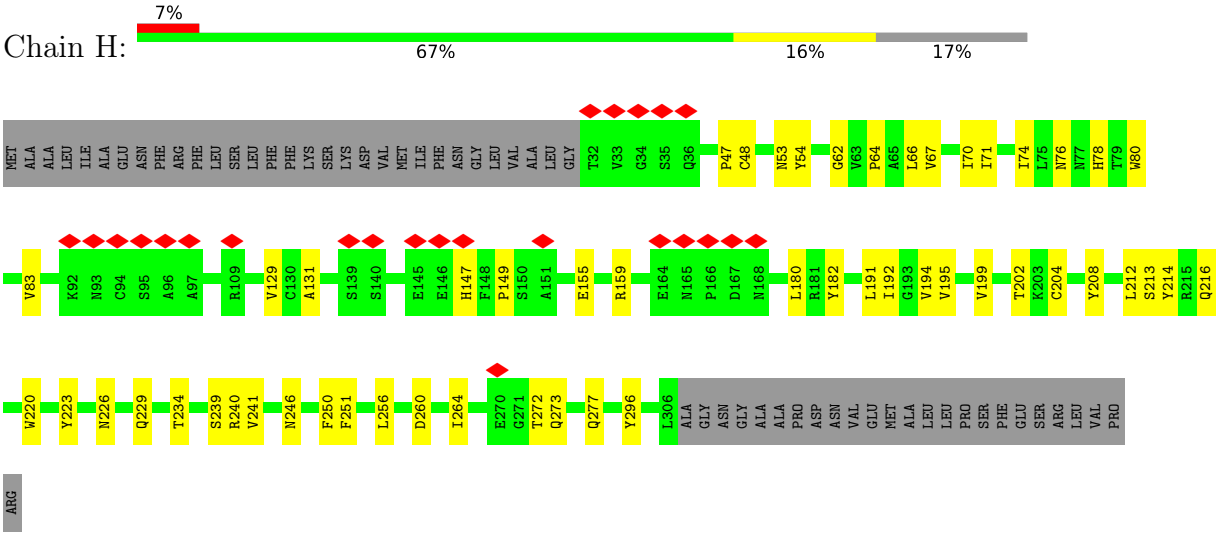
• Molecule 1: Calcium homeostasis modulator protein 2

Chain G:



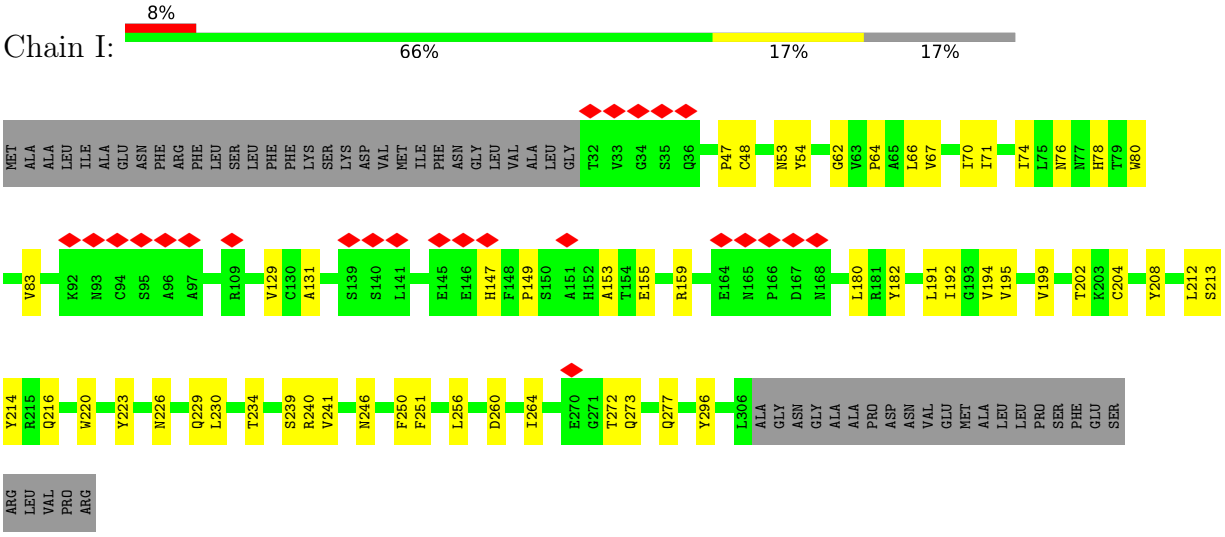
• Molecule 1: Calcium homeostasis modulator protein 2

Chain H:



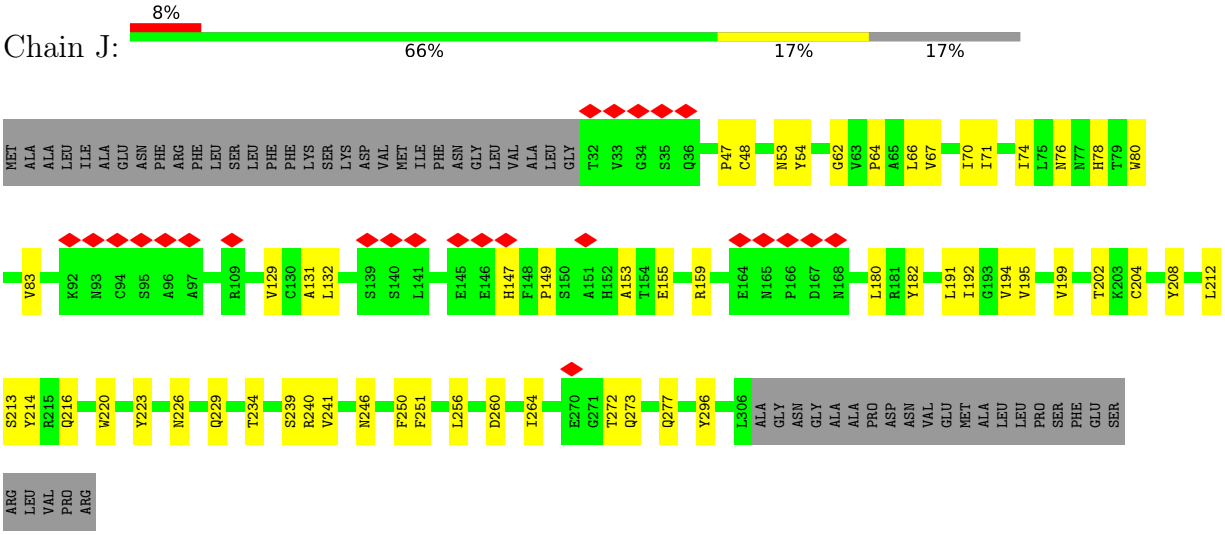
• Molecule 1: Calcium homeostasis modulator protein 2

Chain I:



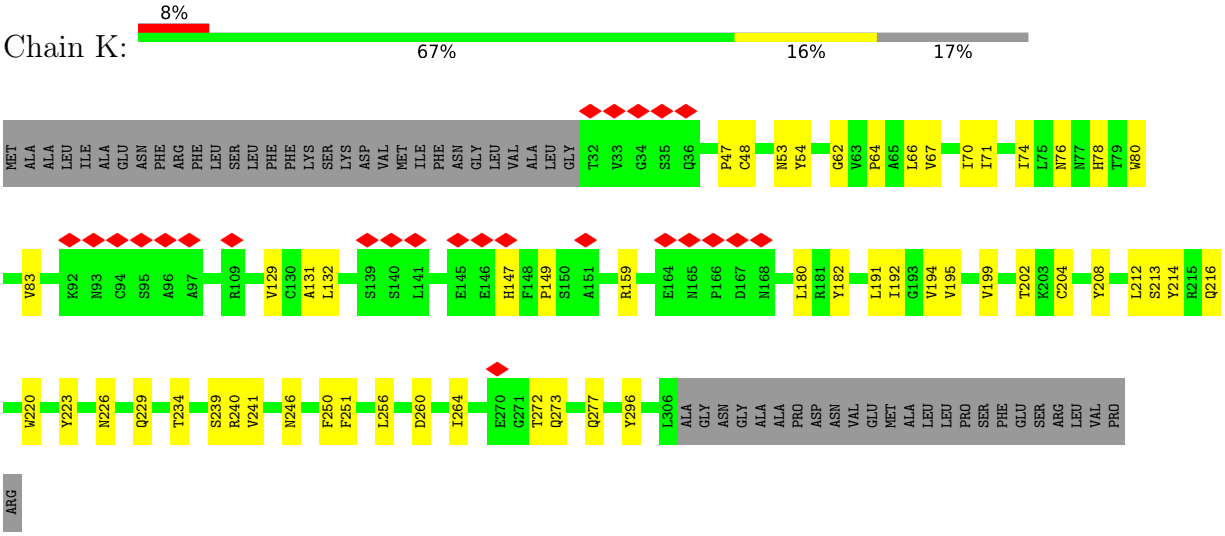
• Molecule 1: Calcium homeostasis modulator protein 2

Chain J:



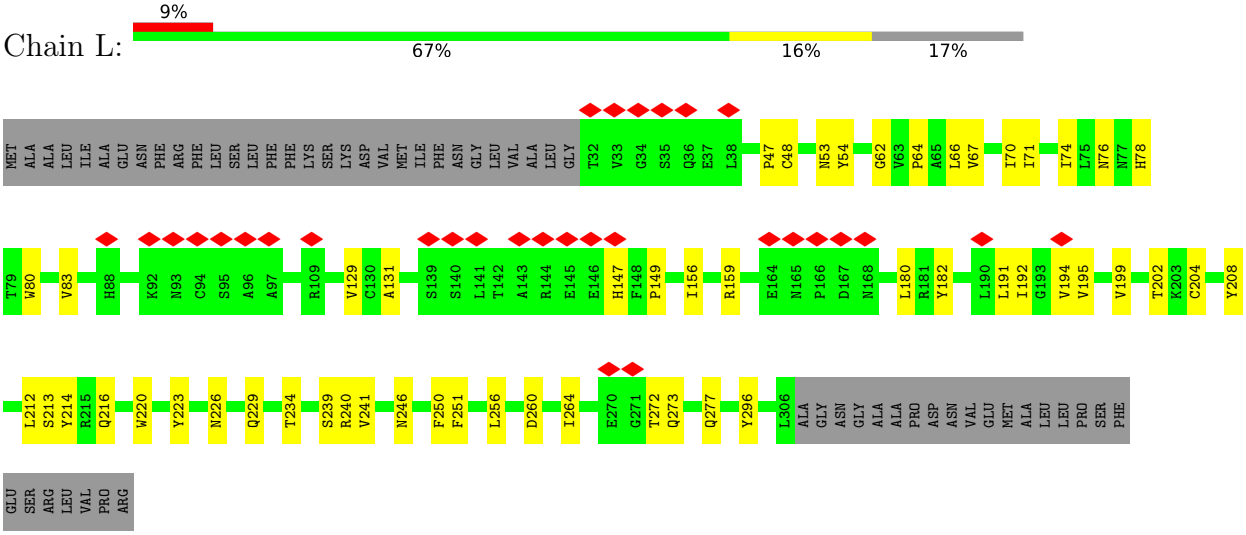
• Molecule 1: Calcium homeostasis modulator protein 2

Chain K:



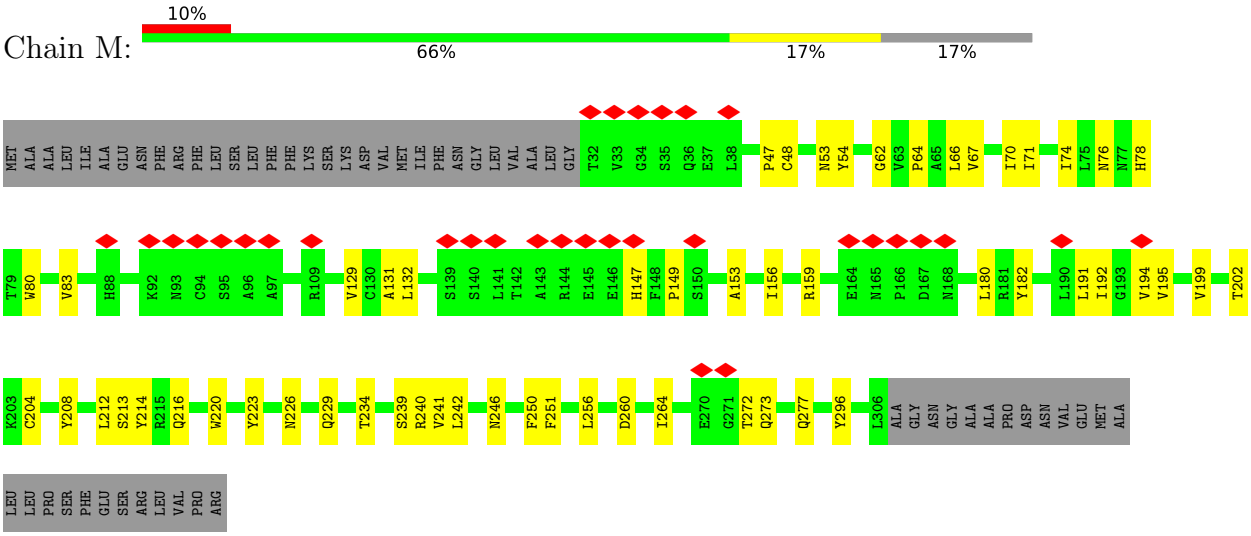
• Molecule 1: Calcium homeostasis modulator protein 2

Chain L:



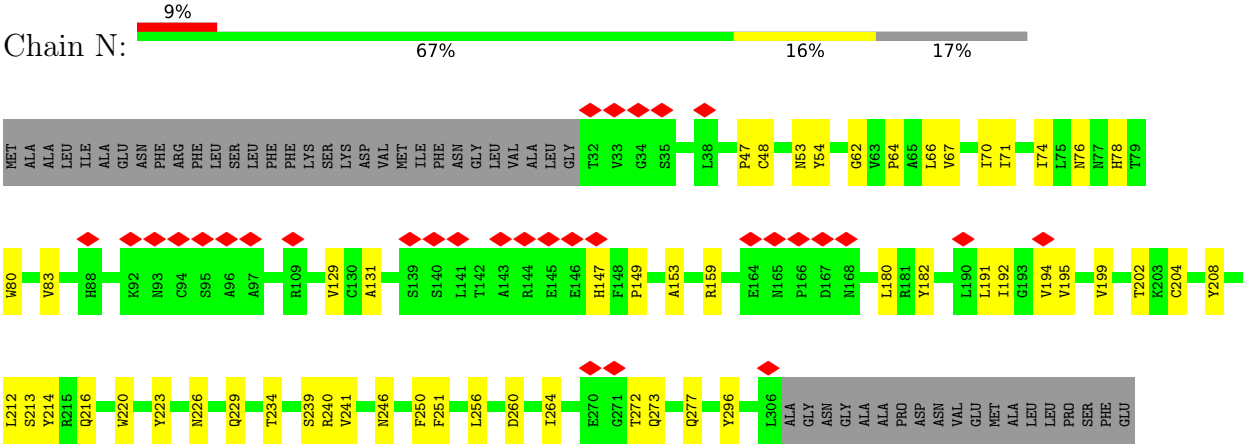
• Molecule 1: Calcium homeostasis modulator protein 2

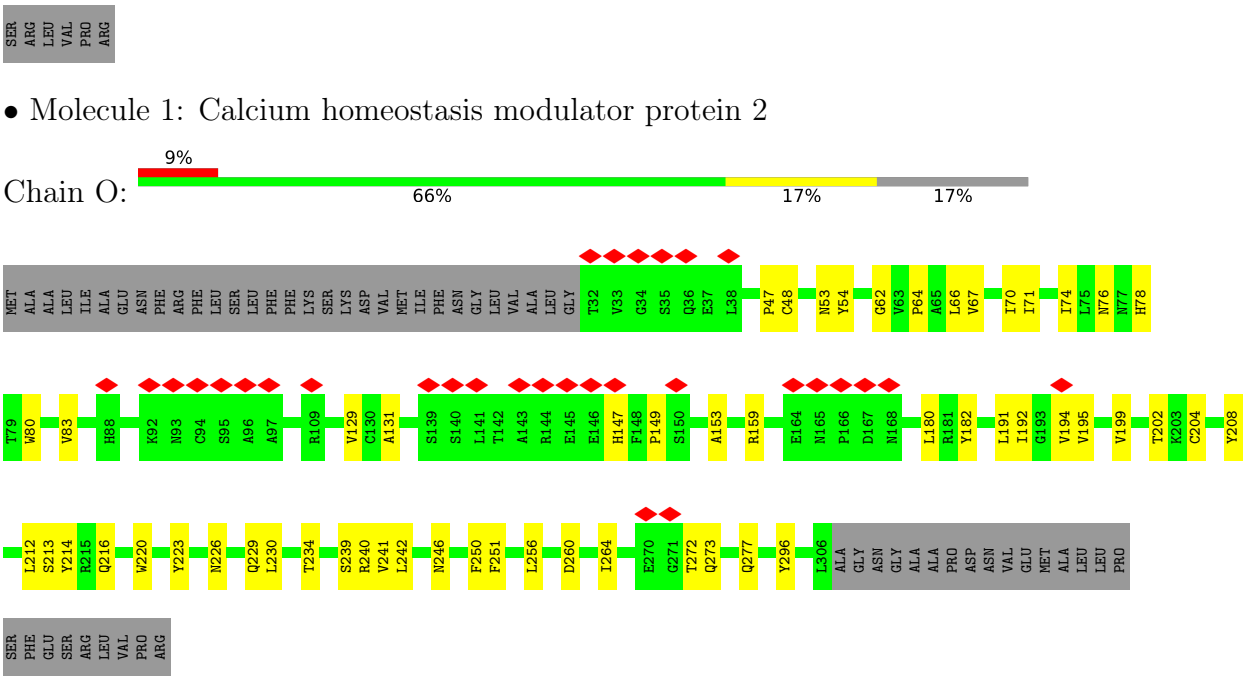
Chain M:

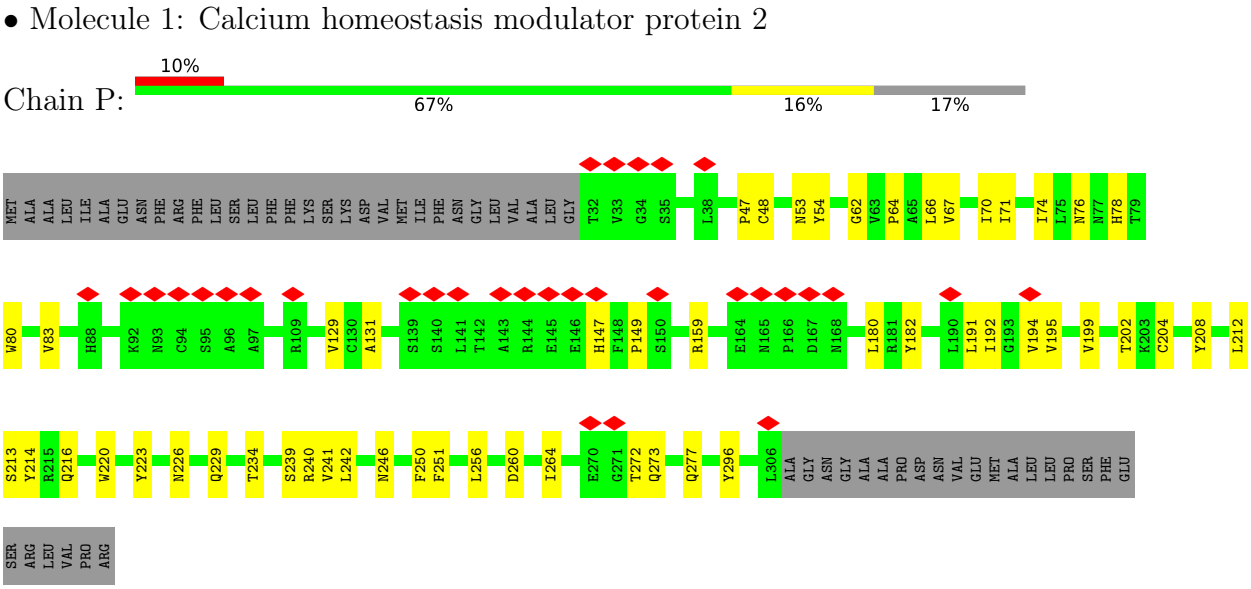


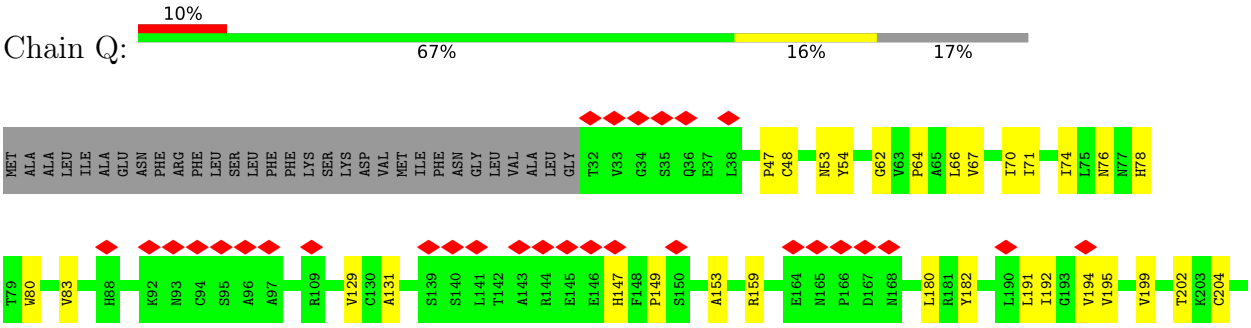
• Molecule 1: Calcium homeostasis modulator protein 2

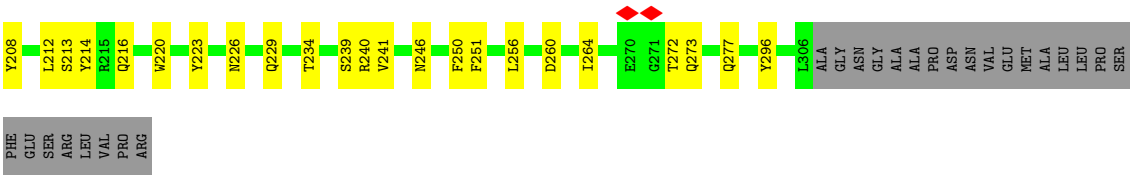
Chain N:




SER ARG LEU VAL PRO ARG
• Molecule 1: Calcium homeostasis modulator protein 2
Chain O:
9%
66%
17%
17%
MET ALA ALA LEU ILE ALA GLU ASN PHE ARG PHE LEU SER LEU PHE PHE LYS SER LYS ASP VAL MET ILE PHE ASN GLY LEU VAL ALA LEU GLY T32 V33 G34 S35 Q36 E37 L38 P47 C48 N53 Y54 G62 V63 P64 A65 L66 V67 I70 I71 I74 L75 N76 N77 H78
T79 W80 V83 H88 K92 N93 C94 S95 A96 A97 R109 V129 C130 A131 S139 S140 L141 T142 A143 R144 E145 E146 H147 F148 P149 S150 A153 R159 E164 N165 P166 D167 N168 L180 R181 Y182 L191 I192 G193 V194 V195 V199 T202 K203 C204 Y208
L212 S213 Y214 R215 Q216 W220 Y223 N226 Q229 L230 T234 S239 R240 V241 L242 N246 F250 F251 L256 D260 I264 E270 G271 T272 Q273 Q277 Y296 L306 ALA GLY ASN GLY ALA ALA PRO ASP ASN VAL GLU MET ALA LEU LEU PRO
SER PHE GLU SER ARG LEU VAL PRO ARG

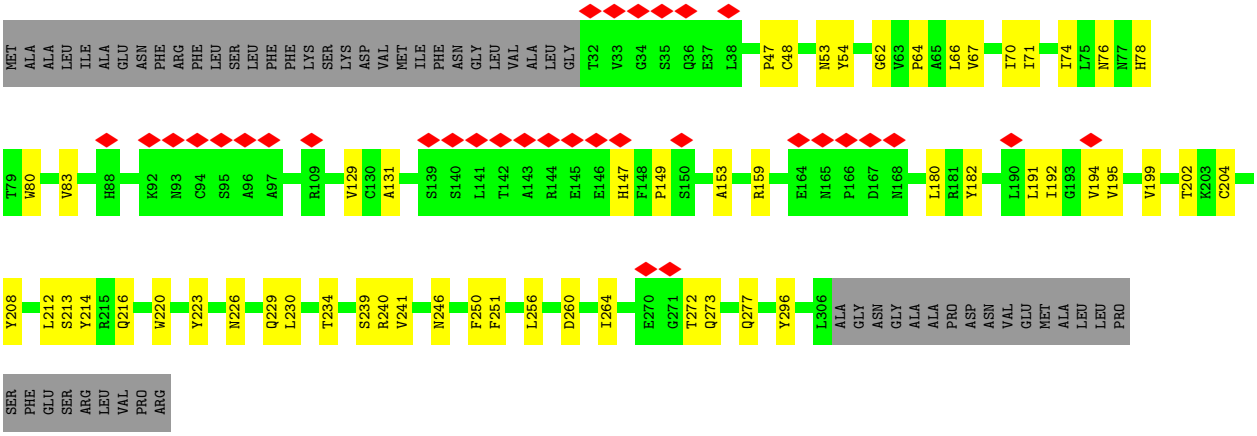

• Molecule 1: Calcium homeostasis modulator protein 2
Chain P:
10%
67%
16%
17%
MET ALA ALA LEU ILE ALA GLU ASN PHE ARG PHE LEU SER LEU PHE PHE LYS SER LYS ASP VAL MET ILE PHE ASN GLY LEU VAL ALA LEU GLY T32 V33 G34 S35 L38 P47 C48 N53 Y54 G62 V63 P64 A65 L66 V67 I70 I71 I74 L75 N76 N77 H78 T79
W80 V83 H88 K92 N93 C94 S95 A96 A97 R109 V129 C130 A131 S139 S140 L141 T142 A143 R144 E145 E146 H147 F148 P149 S150 R159 E164 N165 P166 D167 N168 L180 R181 Y182 L190 L191 I192 G193 V194 V195 V199 T202 K203 C204 Y208 L212
S213 Y214 R215 Q216 W220 Y223 N226 Q229 T234 S239 R240 V241 L242 N246 F250 F251 L256 D260 I264 E270 G271 T272 Q273 Q277 Y296 L306 ALA GLY ASN GLY ALA ALA PRO ASP ASN VAL GLU MET ALA LEU LEU PRO SER PHE GLU
SER ARG LEU VAL PRO ARG


• Molecule 1: Calcium homeostasis modulator protein 2
Chain Q:
10%
67%
16%
17%
MET ALA ALA LEU ILE ALA GLU ASN PHE ARG PHE LEU SER LEU PHE PHE LYS SER LYS ASP VAL MET ILE PHE ASN GLY LEU VAL ALA LEU GLY T32 V33 G34 S35 Q36 E37 L38 P47 C48 N53 Y54 G62 V63 P64 A65 L66 V67 I70 I71 I74 L75 N76 N77 H78
T79 W80 V83 H88 K92 N93 C94 S95 A96 A97 R109 V129 C130 A131 S139 S140 L141 T142 A143 R144 E145 E146 H147 F148 P149 S150 A153 R159 E164 N165 P166 D167 N168 L180 R181 Y182 L190 L191 I192 G193 V194 V195 V199 T202 K203 C204



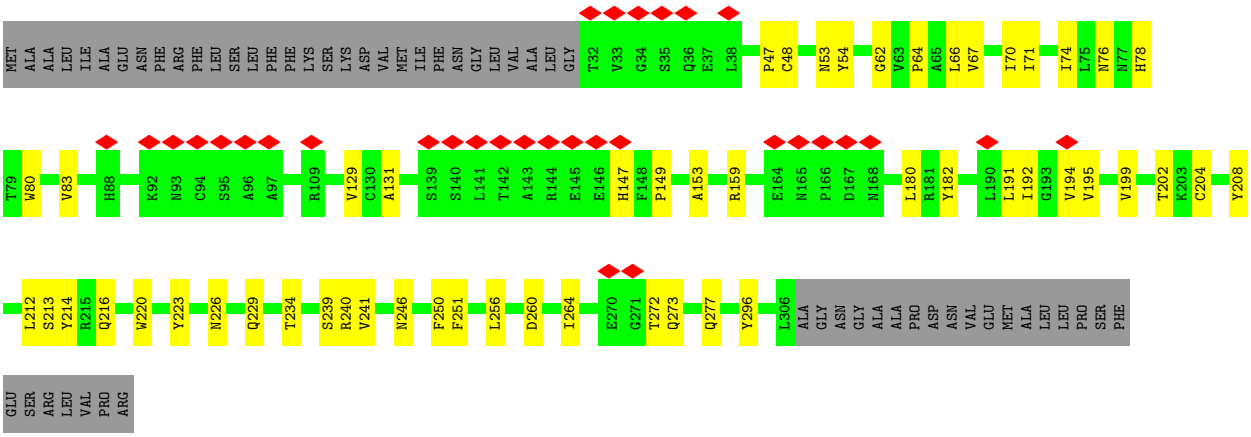
• Molecule 1: Calcium homeostasis modulator protein 2

Chain R:



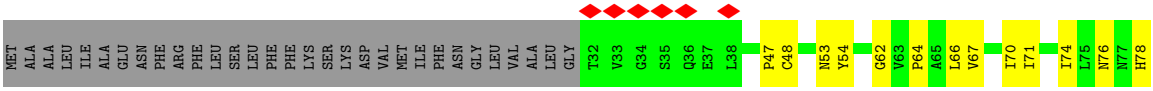
• Molecule 1: Calcium homeostasis modulator protein 2

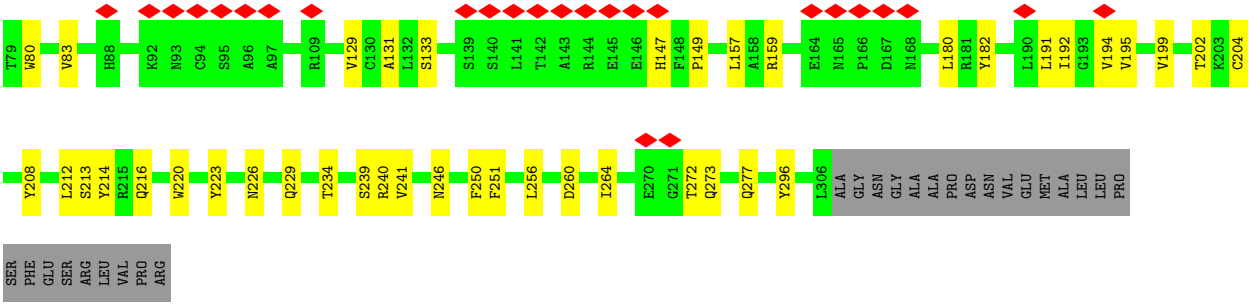
Chain S:



• Molecule 1: Calcium homeostasis modulator protein 2

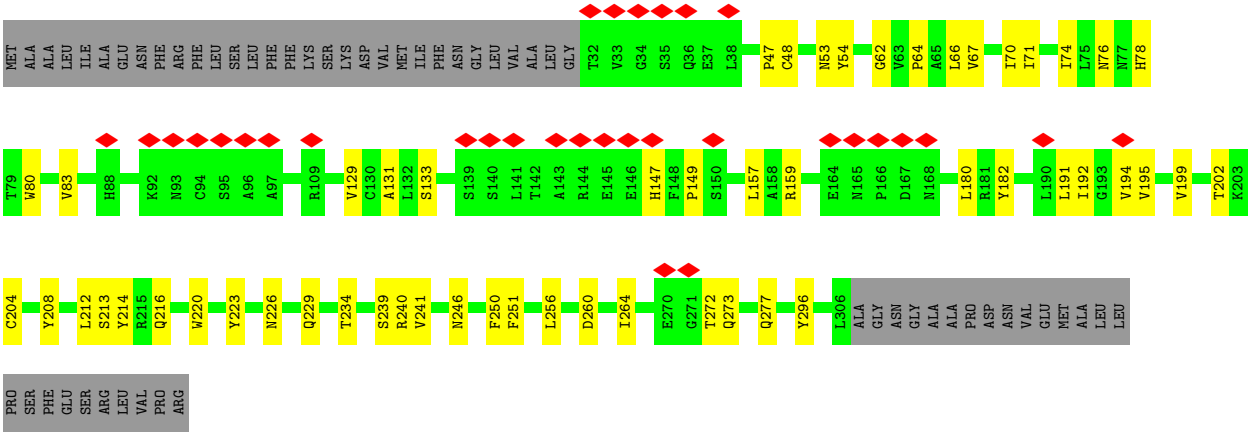
Chain T:





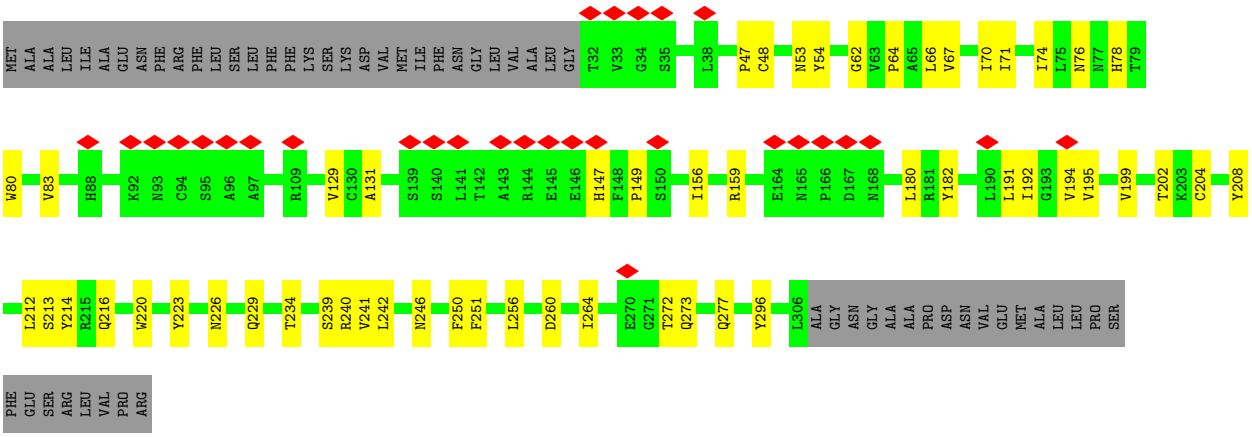
• Molecule 1: Calcium homeostasis modulator protein 2

Chain U:



• Molecule 1: Calcium homeostasis modulator protein 2

Chain V:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C11	Depositor
Number of particles used	71934	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 ($e^-/Å^2$)	54.4	Depositor
Minimum defocus (nm)	1000.0	Depositor
Maximum defocus (nm)	2500.0	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.041	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0097	Depositor
Map size (Å)	348.84, 348.84, 348.84	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.026, 1.026, 1.026	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.48	0/2063	0.54	0/2832
1	B	0.48	0/2063	0.54	0/2832
1	C	0.48	0/2063	0.54	0/2832
1	D	0.48	0/2063	0.54	0/2832
1	E	0.48	0/2063	0.54	0/2832
1	F	0.48	0/2063	0.54	0/2832
1	G	0.48	0/2063	0.54	0/2832
1	H	0.48	0/2063	0.53	0/2832
1	I	0.48	0/2063	0.54	0/2832
1	J	0.48	0/2063	0.54	0/2832
1	K	0.48	0/2063	0.54	0/2832
1	L	0.48	0/2063	0.54	0/2832
1	M	0.48	0/2063	0.54	0/2832
1	N	0.48	0/2063	0.54	0/2832
1	O	0.48	0/2063	0.54	0/2832
1	P	0.48	0/2063	0.54	0/2832
1	Q	0.48	0/2063	0.54	0/2832
1	R	0.48	0/2063	0.54	0/2832
1	S	0.48	0/2063	0.54	0/2832
1	T	0.48	0/2063	0.54	0/2832
1	U	0.48	0/2063	0.54	0/2832
1	V	0.48	0/2063	0.54	0/2832
All	All	0.48	0/45386	0.54	0/62304

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 (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	2009	0	1864	37	0
1	B	2009	0	1864	39	0
1	C	2009	0	1864	39	0
1	D	2009	0	1864	39	0
1	E	2009	0	1864	39	0
1	F	2009	0	1864	39	0
1	G	2009	0	1864	37	0
1	H	2009	0	1864	38	0
1	I	2009	0	1864	41	0
1	J	2009	0	1864	40	0
1	K	2009	0	1864	37	0
1	L	2009	0	1864	37	0
1	M	2009	0	1864	42	0
1	N	2009	0	1864	39	0
1	O	2009	0	1864	39	0
1	P	2009	0	1864	39	0
1	Q	2009	0	1864	38	0
1	R	2009	0	1864	39	0
1	S	2009	0	1864	38	0
1	T	2009	0	1864	37	0
1	U	2009	0	1864	37	0
1	V	2009	0	1864	39	0
All	All	44198	0	41008	695	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 8.

All (695) 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:L:204:CYS:O	1:L:208:TYR:HB2	1.78	0.84
1:C:204:CYS:O	1:C:208:TYR:HB2	1.78	0.84
1:M:204:CYS:O	1:M:208:TYR:HB2	1.78	0.84
1:D:204:CYS:O	1:D:208:TYR:HB2	1.78	0.84
1:G:204:CYS:O	1:G:208:TYR:HB2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:204:CYS:O	1:S:208:TYR:HB2	1.78	0.84
1:T:204:CYS:O	1:T:208:TYR:HB2	1.78	0.84
1:K:204:CYS:O	1:K:208:TYR:HB2	1.78	0.84
1:B:204:CYS:O	1:B:208:TYR:HB2	1.78	0.84
1:J:204:CYS:O	1:J:208:TYR:HB2	1.78	0.84
1:P:204:CYS:O	1:P:208:TYR:HB2	1.78	0.84
1:H:204:CYS:O	1:H:208:TYR:HB2	1.78	0.83
1:V:204:CYS:O	1:V:208:TYR:HB2	1.78	0.83
1:E:204:CYS:O	1:E:208:TYR:HB2	1.78	0.83
1:N:204:CYS:O	1:N:208:TYR:HB2	1.78	0.83
1:Q:204:CYS:O	1:Q:208:TYR:HB2	1.78	0.83
1:O:204:CYS:O	1:O:208:TYR:HB2	1.78	0.83
1:F:204:CYS:O	1:F:208:TYR:HB2	1.78	0.83
1:A:204:CYS:O	1:A:208:TYR:HB2	1.78	0.83
1:R:204:CYS:O	1:R:208:TYR:HB2	1.78	0.82
1:U:204:CYS:O	1:U:208:TYR:HB2	1.78	0.82
1:I:204:CYS:O	1:I:208:TYR:HB2	1.78	0.82
1:L:229:GLN:NE2	1:M:240:ARG:HH22	1.92	0.67
1:F:229:GLN:NE2	1:G:240:ARG:HH22	1.93	0.67
1:Q:229:GLN:NE2	1:R:240:ARG:HH22	1.93	0.67
1:E:229:GLN:NE2	1:F:240:ARG:HH22	1.93	0.67
1:A:229:GLN:NE2	1:B:240:ARG:HH22	1.92	0.66
1:P:229:GLN:NE2	1:Q:240:ARG:HH22	1.93	0.66
1:D:229:GLN:NE2	1:E:240:ARG:HH22	1.93	0.66
1:I:229:GLN:NE2	1:J:240:ARG:HH22	1.93	0.66
1:O:229:GLN:NE2	1:P:240:ARG:HH22	1.93	0.66
1:T:229:GLN:NE2	1:U:240:ARG:HH22	1.93	0.66
1:M:229:GLN:NE2	1:N:240:ARG:HH22	1.94	0.66
1:R:229:GLN:NE2	1:S:240:ARG:HH22	1.94	0.66
1:G:229:GLN:NE2	1:H:240:ARG:HH22	1.94	0.66
1:L:240:ARG:HH22	1:V:229:GLN:NE2	1.94	0.66
1:S:229:GLN:NE2	1:T:240:ARG:HH22	1.94	0.66
1:N:229:GLN:NE2	1:O:240:ARG:HH22	1.95	0.65
1:B:229:GLN:NE2	1:C:240:ARG:HH22	1.94	0.65
1:H:229:GLN:NE2	1:I:240:ARG:HH22	1.94	0.65
1:A:240:ARG:HH22	1:K:229:GLN:NE2	1.94	0.65
1:C:229:GLN:NE2	1:D:240:ARG:HH22	1.95	0.65
1:J:229:GLN:NE2	1:K:240:ARG:HH22	1.95	0.65
1:U:229:GLN:NE2	1:V:240:ARG:HH22	1.95	0.64
1:J:256:LEU:HB3	1:J:260:ASP:HB2	1.80	0.64
1:N:256:LEU:HB3	1:N:260:ASP:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:256:LEU:HB3	1:S:260:ASP:HB2	1.80	0.64
1:E:256:LEU:HB3	1:E:260:ASP:HB2	1.80	0.64
1:F:256:LEU:HB3	1:F:260:ASP:HB2	1.80	0.64
1:D:256:LEU:HB3	1:D:260:ASP:HB2	1.80	0.64
1:O:256:LEU:HB3	1:O:260:ASP:HB2	1.80	0.64
1:A:256:LEU:HB3	1:A:260:ASP:HB2	1.80	0.64
1:K:256:LEU:HB3	1:K:260:ASP:HB2	1.80	0.64
1:M:256:LEU:HB3	1:M:260:ASP:HB2	1.80	0.64
1:B:256:LEU:HB3	1:B:260:ASP:HB2	1.80	0.64
1:G:256:LEU:HB3	1:G:260:ASP:HB2	1.80	0.64
1:H:256:LEU:HB3	1:H:260:ASP:HB2	1.80	0.64
1:P:256:LEU:HB3	1:P:260:ASP:HB2	1.80	0.64
1:Q:256:LEU:HB3	1:Q:260:ASP:HB2	1.80	0.64
1:T:256:LEU:HB3	1:T:260:ASP:HB2	1.80	0.64
1:U:256:LEU:HB3	1:U:260:ASP:HB2	1.80	0.64
1:V:256:LEU:HB3	1:V:260:ASP:HB2	1.80	0.64
1:I:256:LEU:HB3	1:I:260:ASP:HB2	1.80	0.64
1:L:256:LEU:HB3	1:L:260:ASP:HB2	1.80	0.64
1:R:256:LEU:HB3	1:R:260:ASP:HB2	1.80	0.64
1:C:256:LEU:HB3	1:C:260:ASP:HB2	1.80	0.63
1:D:234:THR:HG23	1:E:251:PHE:CE2	2.34	0.63
1:J:234:THR:HG23	1:K:251:PHE:CE2	2.34	0.63
1:O:234:THR:HG23	1:P:251:PHE:CE2	2.34	0.63
1:H:234:THR:HG23	1:I:251:PHE:CE2	2.34	0.62
1:L:234:THR:HG23	1:M:251:PHE:CE2	2.35	0.62
1:P:234:THR:HG23	1:Q:251:PHE:CE2	2.35	0.62
1:U:234:THR:HG23	1:V:251:PHE:CE2	2.34	0.62
1:G:234:THR:HG23	1:H:251:PHE:CE2	2.35	0.62
1:A:251:PHE:CE2	1:K:234:THR:HG23	2.35	0.62
1:S:234:THR:HG23	1:T:251:PHE:CE2	2.34	0.62
1:E:234:THR:HG23	1:F:251:PHE:CE2	2.35	0.62
1:L:251:PHE:CE2	1:V:234:THR:HG23	2.35	0.62
1:R:234:THR:HG23	1:S:251:PHE:CE2	2.35	0.62
1:B:234:THR:HG23	1:C:251:PHE:CE2	2.35	0.61
1:T:234:THR:HG23	1:U:251:PHE:CE2	2.36	0.61
1:A:234:THR:HG23	1:B:251:PHE:CE2	2.35	0.61
1:M:234:THR:HG23	1:N:251:PHE:CE2	2.35	0.61
1:F:234:THR:HG23	1:G:251:PHE:CE2	2.35	0.61
1:I:234:THR:HG23	1:J:251:PHE:CE2	2.35	0.61
1:C:234:THR:HG23	1:D:251:PHE:CE2	2.36	0.60
1:Q:234:THR:HG23	1:R:251:PHE:CE2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:234:THR:HG23	1:O:251:PHE:CE2	2.36	0.60
1:L:226:ASN:OD1	1:M:239:SER:OG	2.20	0.59
1:N:80:TRP:HA	1:N:83:VAL:HG12	1.85	0.59
1:D:80:TRP:HA	1:D:83:VAL:HG12	1.85	0.59
1:O:80:TRP:HA	1:O:83:VAL:HG12	1.85	0.59
1:F:80:TRP:HA	1:F:83:VAL:HG12	1.85	0.59
1:G:80:TRP:HA	1:G:83:VAL:HG12	1.85	0.59
1:L:80:TRP:HA	1:L:83:VAL:HG12	1.85	0.59
1:L:239:SER:OG	1:V:226:ASN:OD1	2.21	0.59
1:C:80:TRP:HA	1:C:83:VAL:HG12	1.85	0.59
1:D:226:ASN:OD1	1:E:239:SER:OG	2.21	0.59
1:E:80:TRP:HA	1:E:83:VAL:HG12	1.85	0.59
1:M:80:TRP:HA	1:M:83:VAL:HG12	1.85	0.59
1:V:80:TRP:HA	1:V:83:VAL:HG12	1.85	0.59
1:A:226:ASN:OD1	1:B:239:SER:OG	2.20	0.59
1:G:76:ASN:OD1	1:G:78:HIS:ND1	2.36	0.59
1:M:226:ASN:OD1	1:N:239:SER:OG	2.21	0.59
1:O:76:ASN:OD1	1:O:78:HIS:ND1	2.36	0.59
1:D:213:SER:OG	1:D:214:TYR:N	2.36	0.59
1:F:76:ASN:OD1	1:F:78:HIS:ND1	2.36	0.59
1:P:213:SER:OG	1:P:214:TYR:N	2.36	0.59
1:S:213:SER:OG	1:S:214:TYR:N	2.36	0.59
1:B:226:ASN:OD1	1:C:239:SER:OG	2.21	0.58
1:H:80:TRP:HA	1:H:83:VAL:HG12	1.85	0.58
1:H:213:SER:OG	1:H:214:TYR:N	2.36	0.58
1:K:213:SER:OG	1:K:214:TYR:N	2.36	0.58
1:P:80:TRP:HA	1:P:83:VAL:HG12	1.85	0.58
1:B:213:SER:OG	1:B:214:TYR:N	2.36	0.58
1:C:226:ASN:OD1	1:D:239:SER:OG	2.21	0.58
1:E:226:ASN:OD1	1:F:239:SER:OG	2.21	0.58
1:L:213:SER:OG	1:L:214:TYR:N	2.36	0.58
1:M:213:SER:OG	1:M:214:TYR:N	2.36	0.58
1:N:76:ASN:OD1	1:N:78:HIS:ND1	2.36	0.58
1:U:213:SER:OG	1:U:214:TYR:N	2.36	0.58
1:A:76:ASN:OD1	1:A:78:HIS:ND1	2.36	0.58
1:J:213:SER:OG	1:J:214:TYR:N	2.36	0.58
1:O:213:SER:OG	1:O:214:TYR:N	2.36	0.58
1:B:76:ASN:OD1	1:B:78:HIS:ND1	2.36	0.58
1:B:80:TRP:HA	1:B:83:VAL:HG12	1.85	0.58
1:G:213:SER:OG	1:G:214:TYR:N	2.36	0.58
1:K:76:ASN:OD1	1:K:78:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:226:ASN:OD1	1:R:239:SER:OG	2.21	0.58
1:U:226:ASN:OD1	1:V:239:SER:OG	2.21	0.58
1:F:226:ASN:OD1	1:G:239:SER:OG	2.21	0.58
1:Q:80:TRP:HA	1:Q:83:VAL:HG12	1.85	0.58
1:T:226:ASN:OD1	1:U:239:SER:OG	2.21	0.58
1:I:226:ASN:OD1	1:J:239:SER:OG	2.21	0.58
1:R:213:SER:OG	1:R:214:TYR:N	2.36	0.58
1:U:80:TRP:HA	1:U:83:VAL:HG12	1.85	0.58
1:C:76:ASN:OD1	1:C:78:HIS:ND1	2.36	0.58
1:N:226:ASN:OD1	1:O:239:SER:OG	2.21	0.58
1:T:76:ASN:OD1	1:T:78:HIS:ND1	2.36	0.58
1:O:226:ASN:OD1	1:P:239:SER:OG	2.21	0.58
1:P:76:ASN:OD1	1:P:78:HIS:ND1	2.36	0.58
1:Q:76:ASN:OD1	1:Q:78:HIS:ND1	2.36	0.58
1:U:76:ASN:OD1	1:U:78:HIS:ND1	2.36	0.58
1:A:239:SER:OG	1:K:226:ASN:OD1	2.21	0.58
1:F:213:SER:OG	1:F:214:TYR:N	2.36	0.58
1:Q:213:SER:OG	1:Q:214:TYR:N	2.36	0.58
1:R:76:ASN:OD1	1:R:78:HIS:ND1	2.36	0.58
1:A:80:TRP:HA	1:A:83:VAL:HG12	1.85	0.58
1:I:76:ASN:OD1	1:I:78:HIS:ND1	2.36	0.58
1:J:76:ASN:OD1	1:J:78:HIS:ND1	2.36	0.58
1:P:226:ASN:OD1	1:Q:239:SER:OG	2.21	0.58
1:R:80:TRP:HA	1:R:83:VAL:HG12	1.85	0.58
1:S:76:ASN:OD1	1:S:78:HIS:ND1	2.36	0.58
1:V:76:ASN:OD1	1:V:78:HIS:ND1	2.36	0.58
1:V:213:SER:OG	1:V:214:TYR:N	2.36	0.58
1:A:213:SER:OG	1:A:214:TYR:N	2.36	0.57
1:D:76:ASN:OD1	1:D:78:HIS:ND1	2.36	0.57
1:E:213:SER:OG	1:E:214:TYR:N	2.36	0.57
1:J:226:ASN:OD1	1:K:239:SER:OG	2.21	0.57
1:N:213:SER:OG	1:N:214:TYR:N	2.36	0.57
1:R:226:ASN:OD1	1:S:239:SER:OG	2.21	0.57
1:S:80:TRP:HA	1:S:83:VAL:HG12	1.85	0.57
1:T:80:TRP:HA	1:T:83:VAL:HG12	1.84	0.57
1:H:76:ASN:OD1	1:H:78:HIS:ND1	2.36	0.57
1:G:226:ASN:OD1	1:H:239:SER:OG	2.21	0.57
1:H:226:ASN:OD1	1:I:239:SER:OG	2.21	0.57
1:I:80:TRP:HA	1:I:83:VAL:HG12	1.85	0.57
1:J:80:TRP:HA	1:J:83:VAL:HG12	1.85	0.57
1:K:80:TRP:HA	1:K:83:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:76:ASN:OD1	1:L:78:HIS:ND1	2.36	0.57
1:T:213:SER:OG	1:T:214:TYR:N	2.36	0.57
1:E:76:ASN:OD1	1:E:78:HIS:ND1	2.36	0.57
1:I:213:SER:OG	1:I:214:TYR:N	2.36	0.57
1:C:213:SER:OG	1:C:214:TYR:N	2.36	0.57
1:S:226:ASN:OD1	1:T:239:SER:OG	2.21	0.57
1:E:223:TYR:OH	1:F:246:ASN:ND2	2.38	0.57
1:P:223:TYR:OH	1:Q:246:ASN:ND2	2.38	0.57
1:M:76:ASN:OD1	1:M:78:HIS:ND1	2.36	0.56
1:L:223:TYR:OH	1:M:246:ASN:ND2	2.38	0.56
1:H:223:TYR:OH	1:I:246:ASN:ND2	2.39	0.56
1:M:223:TYR:OH	1:N:246:ASN:ND2	2.39	0.55
1:G:223:TYR:OH	1:H:246:ASN:ND2	2.39	0.55
1:R:223:TYR:OH	1:S:246:ASN:ND2	2.39	0.55
1:O:223:TYR:OH	1:P:246:ASN:ND2	2.38	0.55
1:A:223:TYR:OH	1:B:246:ASN:ND2	2.38	0.55
1:D:223:TYR:OH	1:E:246:ASN:ND2	2.38	0.55
1:I:223:TYR:OH	1:J:246:ASN:ND2	2.39	0.55
1:A:246:ASN:ND2	1:K:223:TYR:OH	2.39	0.55
1:L:246:ASN:ND2	1:V:223:TYR:OH	2.39	0.55
1:N:223:TYR:OH	1:O:246:ASN:ND2	2.40	0.55
1:U:223:TYR:OH	1:V:246:ASN:ND2	2.40	0.54
1:C:223:TYR:OH	1:D:246:ASN:ND2	2.40	0.54
1:Q:223:TYR:OH	1:R:246:ASN:ND2	2.39	0.54
1:S:223:TYR:OH	1:T:246:ASN:ND2	2.39	0.54
1:B:223:TYR:OH	1:C:246:ASN:ND2	2.39	0.54
1:T:223:TYR:OH	1:U:246:ASN:ND2	2.39	0.54
1:F:223:TYR:OH	1:G:246:ASN:ND2	2.39	0.54
1:F:212:LEU:HD12	1:F:216:GLN:HB3	1.90	0.53
1:G:212:LEU:HD12	1:G:216:GLN:HB3	1.90	0.53
1:N:212:LEU:HD12	1:N:216:GLN:HB3	1.90	0.53
1:P:212:LEU:HD12	1:P:216:GLN:HB3	1.90	0.53
1:A:212:LEU:HD12	1:A:216:GLN:HB3	1.90	0.53
1:M:212:LEU:HD12	1:M:216:GLN:HB3	1.90	0.53
1:O:212:LEU:HD12	1:O:216:GLN:HB3	1.90	0.53
1:J:223:TYR:OH	1:K:246:ASN:ND2	2.40	0.53
1:E:212:LEU:HD12	1:E:216:GLN:HB3	1.90	0.53
1:J:212:LEU:HD12	1:J:216:GLN:HB3	1.90	0.53
1:T:212:LEU:HD12	1:T:216:GLN:HB3	1.90	0.53
1:D:212:LEU:HD12	1:D:216:GLN:HB3	1.91	0.52
1:S:212:LEU:HD12	1:S:216:GLN:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:212:LEU:HD12	1:U:216:GLN:HB3	1.91	0.52
1:J:54:TYR:HA	1:J:131:ALA:HA	1.92	0.52
1:A:54:TYR:HA	1:A:131:ALA:HA	1.92	0.52
1:H:212:LEU:HD12	1:H:216:GLN:HB3	1.90	0.52
1:S:54:TYR:HA	1:S:131:ALA:HA	1.92	0.52
1:V:54:TYR:HA	1:V:131:ALA:HA	1.92	0.52
1:B:220:TRP:NE1	1:B:296:TYR:O	2.41	0.52
1:V:212:LEU:HD12	1:V:216:GLN:HB3	1.90	0.52
1:L:212:LEU:HD12	1:L:216:GLN:HB3	1.90	0.52
1:C:54:TYR:HA	1:C:131:ALA:HA	1.92	0.52
1:C:212:LEU:HD12	1:C:216:GLN:HB3	1.90	0.52
1:I:212:LEU:HD12	1:I:216:GLN:HB3	1.90	0.52
1:K:212:LEU:HD12	1:K:216:GLN:HB3	1.91	0.52
1:M:54:TYR:HA	1:M:131:ALA:HA	1.92	0.52
1:O:220:TRP:NE1	1:O:296:TYR:O	2.41	0.52
1:Q:212:LEU:HD12	1:Q:216:GLN:HB3	1.90	0.52
1:B:212:LEU:HD12	1:B:216:GLN:HB3	1.90	0.52
1:D:54:TYR:HA	1:D:131:ALA:HA	1.92	0.52
1:U:54:TYR:HA	1:U:131:ALA:HA	1.92	0.52
1:E:220:TRP:NE1	1:E:296:TYR:O	2.41	0.52
1:Q:54:TYR:HA	1:Q:131:ALA:HA	1.92	0.52
1:R:212:LEU:HD12	1:R:216:GLN:HB3	1.91	0.52
1:H:54:TYR:HA	1:H:131:ALA:HA	1.92	0.51
1:T:54:TYR:HA	1:T:131:ALA:HA	1.92	0.51
1:B:54:TYR:HA	1:B:131:ALA:HA	1.92	0.51
1:Q:272:THR:OG1	1:Q:273:GLN:N	2.44	0.51
1:T:220:TRP:NE1	1:T:296:TYR:O	2.41	0.51
1:I:272:THR:OG1	1:I:273:GLN:N	2.44	0.51
1:O:54:TYR:HA	1:O:131:ALA:HA	1.92	0.51
1:S:272:THR:OG1	1:S:273:GLN:N	2.44	0.51
1:G:272:THR:OG1	1:G:273:GLN:N	2.44	0.51
1:L:54:TYR:HA	1:L:131:ALA:HA	1.92	0.51
1:M:277:GLN:HG2	1:N:250:PHE:HE1	1.76	0.51
1:R:220:TRP:NE1	1:R:296:TYR:O	2.41	0.51
1:F:54:TYR:HA	1:F:131:ALA:HA	1.92	0.51
1:J:272:THR:OG1	1:J:273:GLN:N	2.44	0.51
1:E:54:TYR:HA	1:E:131:ALA:HA	1.92	0.51
1:F:277:GLN:HG2	1:G:250:PHE:HE1	1.76	0.51
1:K:272:THR:OG1	1:K:273:GLN:N	2.44	0.51
1:P:272:THR:OG1	1:P:273:GLN:N	2.44	0.51
1:H:272:THR:OG1	1:H:273:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:54:TYR:HA	1:I:131:ALA:HA	1.92	0.51
1:N:277:GLN:HG2	1:O:250:PHE:HE1	1.76	0.51
1:O:272:THR:OG1	1:O:273:GLN:N	2.44	0.51
1:R:272:THR:OG1	1:R:273:GLN:N	2.44	0.51
1:V:220:TRP:NE1	1:V:296:TYR:O	2.41	0.51
1:M:220:TRP:NE1	1:M:296:TYR:O	2.41	0.51
1:R:54:TYR:HA	1:R:131:ALA:HA	1.92	0.51
1:C:129:VAL:HG23	1:C:180:LEU:HD23	1.93	0.51
1:E:277:GLN:HG2	1:F:250:PHE:HE1	1.76	0.51
1:N:129:VAL:HG23	1:N:180:LEU:HD23	1.93	0.51
1:V:129:VAL:HG23	1:V:180:LEU:HD23	1.93	0.51
1:C:277:GLN:HG2	1:D:250:PHE:HE1	1.76	0.50
1:D:129:VAL:HG23	1:D:180:LEU:HD23	1.94	0.50
1:K:54:TYR:HA	1:K:131:ALA:HA	1.92	0.50
1:M:129:VAL:HG23	1:M:180:LEU:HD23	1.93	0.50
1:F:129:VAL:HG23	1:F:180:LEU:HD23	1.94	0.50
1:G:54:TYR:HA	1:G:131:ALA:HA	1.92	0.50
1:T:272:THR:OG1	1:T:273:GLN:N	2.44	0.50
1:F:272:THR:OG1	1:F:273:GLN:N	2.44	0.50
1:O:129:VAL:HG23	1:O:180:LEU:HD23	1.93	0.50
1:U:129:VAL:HG23	1:U:180:LEU:HD23	1.94	0.50
1:B:129:VAL:HG23	1:B:180:LEU:HD23	1.94	0.50
1:G:129:VAL:HG23	1:G:180:LEU:HD23	1.94	0.50
1:L:129:VAL:HG23	1:L:180:LEU:HD23	1.94	0.50
1:U:272:THR:OG1	1:U:273:GLN:N	2.44	0.50
1:A:272:THR:OG1	1:A:273:GLN:N	2.44	0.50
1:D:272:THR:OG1	1:D:273:GLN:N	2.44	0.50
1:E:129:VAL:HG23	1:E:180:LEU:HD23	1.94	0.50
1:I:277:GLN:HG2	1:J:250:PHE:HE1	1.76	0.50
1:M:272:THR:OG1	1:M:273:GLN:N	2.44	0.50
1:N:220:TRP:NE1	1:N:296:TYR:O	2.41	0.50
1:P:277:GLN:HG2	1:Q:250:PHE:HE1	1.76	0.50
1:Q:277:GLN:HG2	1:R:250:PHE:HE1	1.76	0.50
1:I:220:TRP:NE1	1:I:296:TYR:O	2.41	0.50
1:T:182:TYR:HB2	1:U:47:PRO:HB3	1.94	0.50
1:A:129:VAL:HG23	1:A:180:LEU:HD23	1.94	0.50
1:B:277:GLN:HG2	1:C:250:PHE:HE1	1.76	0.50
1:L:277:GLN:HG2	1:M:250:PHE:HE1	1.76	0.50
1:N:54:TYR:HA	1:N:131:ALA:HA	1.92	0.50
1:I:182:TYR:HB2	1:J:47:PRO:HB3	1.94	0.50
1:J:220:TRP:NE1	1:J:296:TYR:O	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:129:VAL:HG23	1:K:180:LEU:HD23	1.93	0.50
1:L:250:PHE:HE1	1:V:277:GLN:HG2	1.76	0.50
1:P:54:TYR:HA	1:P:131:ALA:HA	1.92	0.50
1:H:129:VAL:HG23	1:H:180:LEU:HD23	1.93	0.49
1:H:277:GLN:HG2	1:I:250:PHE:HE1	1.77	0.49
1:P:129:VAL:HG23	1:P:180:LEU:HD23	1.94	0.49
1:R:182:TYR:HB2	1:S:47:PRO:HB3	1.94	0.49
1:G:277:GLN:HG2	1:H:250:PHE:HE1	1.77	0.49
1:Q:129:VAL:HG23	1:Q:180:LEU:HD23	1.93	0.49
1:S:129:VAL:HG23	1:S:180:LEU:HD23	1.93	0.49
1:C:272:THR:OG1	1:C:273:GLN:N	2.44	0.49
1:D:277:GLN:HG2	1:E:250:PHE:HE1	1.77	0.49
1:G:220:TRP:NE1	1:G:296:TYR:O	2.41	0.49
1:H:220:TRP:NE1	1:H:296:TYR:O	2.41	0.49
1:J:129:VAL:HG23	1:J:180:LEU:HD23	1.93	0.49
1:O:277:GLN:HG2	1:P:250:PHE:HE1	1.77	0.49
1:T:129:VAL:HG23	1:T:180:LEU:HD23	1.94	0.49
1:A:277:GLN:HG2	1:B:250:PHE:HE1	1.76	0.49
1:D:220:TRP:NE1	1:D:296:TYR:O	2.41	0.49
1:I:129:VAL:HG23	1:I:180:LEU:HD23	1.93	0.49
1:N:272:THR:OG1	1:N:273:GLN:N	2.44	0.49
1:R:129:VAL:HG23	1:R:180:LEU:HD23	1.94	0.49
1:R:277:GLN:HG2	1:S:250:PHE:HE1	1.77	0.49
1:P:220:TRP:NE1	1:P:296:TYR:O	2.41	0.49
1:V:272:THR:OG1	1:V:273:GLN:N	2.44	0.49
1:C:182:TYR:HB2	1:D:47:PRO:HB3	1.94	0.49
1:I:62:GLY:O	1:I:66:LEU:N	2.45	0.49
1:H:147:HIS:O	1:O:149:PRO:HG3	2.13	0.49
1:L:272:THR:OG1	1:L:273:GLN:N	2.44	0.49
1:N:182:TYR:HB2	1:O:47:PRO:HB3	1.94	0.49
1:T:62:GLY:O	1:T:66:LEU:N	2.45	0.49
1:T:277:GLN:HG2	1:U:250:PHE:HE1	1.76	0.49
1:A:250:PHE:HE1	1:K:277:GLN:HG2	1.77	0.48
1:U:220:TRP:NE1	1:U:296:TYR:O	2.41	0.48
1:G:182:TYR:HB2	1:H:47:PRO:HB3	1.94	0.48
1:J:182:TYR:HB2	1:K:47:PRO:HB3	1.95	0.48
1:S:277:GLN:HG2	1:T:250:PHE:HE1	1.77	0.48
1:U:277:GLN:HG2	1:V:250:PHE:HE1	1.78	0.48
1:A:47:PRO:HB3	1:K:182:TYR:HB2	1.96	0.48
1:A:182:TYR:HB2	1:B:47:PRO:HB3	1.95	0.48
1:U:182:TYR:HB2	1:V:47:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:THR:OG1	1:B:273:GLN:N	2.44	0.48
1:R:62:GLY:O	1:R:66:LEU:N	2.45	0.48
1:Q:182:TYR:HB2	1:R:47:PRO:HB3	1.96	0.48
1:S:220:TRP:NE1	1:S:296:TYR:O	2.41	0.48
1:B:48:CYS:HB3	1:B:159:ARG:HA	1.96	0.47
1:B:182:TYR:HB2	1:C:47:PRO:HB3	1.96	0.47
1:C:48:CYS:HB3	1:C:159:ARG:HA	1.96	0.47
1:L:48:CYS:HB3	1:L:159:ARG:HA	1.96	0.47
1:T:48:CYS:HB3	1:T:159:ARG:HA	1.96	0.47
1:V:48:CYS:HB3	1:V:159:ARG:HA	1.96	0.47
1:K:48:CYS:HB3	1:K:159:ARG:HA	1.97	0.47
1:A:220:TRP:NE1	1:A:296:TYR:O	2.41	0.47
1:L:47:PRO:HB3	1:V:182:TYR:HB2	1.96	0.47
1:S:48:CYS:HB3	1:S:159:ARG:HA	1.96	0.47
1:E:272:THR:OG1	1:E:273:GLN:N	2.44	0.47
1:J:48:CYS:HB3	1:J:159:ARG:HA	1.96	0.47
1:P:62:GLY:O	1:P:66:LEU:N	2.45	0.47
1:U:48:CYS:HB3	1:U:159:ARG:HA	1.96	0.47
1:A:48:CYS:HB3	1:A:159:ARG:HA	1.96	0.47
1:D:48:CYS:HB3	1:D:159:ARG:HA	1.96	0.47
1:E:48:CYS:HB3	1:E:159:ARG:HA	1.96	0.47
1:L:182:TYR:HB2	1:M:47:PRO:HB3	1.95	0.47
1:R:48:CYS:HB3	1:R:159:ARG:HA	1.96	0.47
1:D:62:GLY:O	1:D:66:LEU:N	2.45	0.47
1:D:149:PRO:HG3	1:S:147:HIS:O	2.14	0.47
1:L:62:GLY:O	1:L:66:LEU:N	2.45	0.47
1:M:182:TYR:HB2	1:N:47:PRO:HB3	1.96	0.47
1:N:48:CYS:HB3	1:N:159:ARG:HA	1.96	0.47
1:S:182:TYR:HB2	1:T:47:PRO:HB3	1.96	0.47
1:A:62:GLY:O	1:A:66:LEU:N	2.45	0.47
1:C:62:GLY:O	1:C:66:LEU:N	2.45	0.47
1:C:220:TRP:NE1	1:C:296:TYR:O	2.41	0.47
1:F:182:TYR:HB2	1:G:47:PRO:HB3	1.96	0.47
1:I:48:CYS:HB3	1:I:159:ARG:HA	1.96	0.47
1:M:48:CYS:HB3	1:M:159:ARG:HA	1.96	0.47
1:M:62:GLY:O	1:M:66:LEU:N	2.45	0.47
1:Q:220:TRP:NE1	1:Q:296:TYR:O	2.41	0.47
1:J:277:GLN:HG2	1:K:250:PHE:HE1	1.78	0.47
1:D:182:TYR:HB2	1:E:47:PRO:HB3	1.96	0.47
1:E:182:TYR:HB2	1:F:47:PRO:HB3	1.96	0.47
1:O:182:TYR:HB2	1:P:47:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:182:TYR:HB2	1:Q:47:PRO:HB3	1.96	0.47
1:Q:48:CYS:HB3	1:Q:159:ARG:HA	1.96	0.47
1:E:62:GLY:O	1:E:66:LEU:N	2.45	0.46
1:F:48:CYS:HB3	1:F:159:ARG:HA	1.97	0.46
1:G:48:CYS:HB3	1:G:159:ARG:HA	1.97	0.46
1:H:48:CYS:HB3	1:H:159:ARG:HA	1.96	0.46
1:M:53:ASN:N	1:M:53:ASN:OD1	2.48	0.46
1:O:48:CYS:HB3	1:O:159:ARG:HA	1.96	0.46
1:P:48:CYS:HB3	1:P:159:ARG:HA	1.96	0.46
1:H:149:PRO:HG3	1:O:147:HIS:O	2.16	0.46
1:V:62:GLY:O	1:V:66:LEU:N	2.45	0.46
1:H:182:TYR:HB2	1:I:47:PRO:HB3	1.96	0.46
1:K:53:ASN:OD1	1:K:53:ASN:N	2.48	0.46
1:R:53:ASN:OD1	1:R:53:ASN:N	2.49	0.46
1:H:53:ASN:OD1	1:H:53:ASN:N	2.49	0.46
1:J:149:PRO:HG3	1:M:147:HIS:O	2.15	0.46
1:L:53:ASN:OD1	1:L:53:ASN:N	2.49	0.46
1:N:53:ASN:OD1	1:N:53:ASN:N	2.49	0.46
1:N:62:GLY:O	1:N:66:LEU:N	2.45	0.46
1:A:53:ASN:OD1	1:A:53:ASN:N	2.49	0.46
1:B:62:GLY:O	1:B:66:LEU:N	2.45	0.46
1:B:53:ASN:OD1	1:B:53:ASN:N	2.49	0.46
1:C:53:ASN:N	1:C:53:ASN:OD1	2.49	0.46
1:V:53:ASN:N	1:V:53:ASN:OD1	2.49	0.46
1:J:147:HIS:O	1:M:149:PRO:HG3	2.15	0.46
1:D:53:ASN:OD1	1:D:53:ASN:N	2.49	0.46
1:F:62:GLY:O	1:F:66:LEU:N	2.45	0.46
1:J:62:GLY:O	1:J:66:LEU:N	2.45	0.46
1:S:53:ASN:OD1	1:S:53:ASN:N	2.48	0.46
1:J:67:VAL:HA	1:J:70:ILE:HG22	1.99	0.45
1:Q:67:VAL:HA	1:Q:70:ILE:HG22	1.99	0.45
1:U:53:ASN:OD1	1:U:53:ASN:N	2.48	0.45
1:K:67:VAL:HA	1:K:70:ILE:HG22	1.99	0.45
1:P:67:VAL:HA	1:P:70:ILE:HG22	1.99	0.45
1:I:53:ASN:OD1	1:I:53:ASN:N	2.49	0.45
1:U:62:GLY:O	1:U:66:LEU:N	2.45	0.45
1:D:147:HIS:O	1:S:149:PRO:HG3	2.16	0.45
1:L:220:TRP:NE1	1:L:296:TYR:O	2.41	0.45
1:O:53:ASN:N	1:O:53:ASN:OD1	2.48	0.45
1:O:67:VAL:HA	1:O:70:ILE:HG22	1.98	0.45
1:F:220:TRP:NE1	1:F:296:TYR:O	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:53:ASN:OD1	1:P:53:ASN:N	2.49	0.45
1:R:67:VAL:HA	1:R:70:ILE:HG22	1.99	0.45
1:V:67:VAL:HA	1:V:70:ILE:HG22	1.99	0.45
1:A:67:VAL:HA	1:A:70:ILE:HG22	1.99	0.45
1:I:67:VAL:HA	1:I:70:ILE:HG22	1.99	0.45
1:P:180:LEU:HD12	1:P:180:LEU:HA	1.86	0.45
1:U:67:VAL:HA	1:U:70:ILE:HG22	1.99	0.45
1:E:53:ASN:OD1	1:E:53:ASN:N	2.49	0.45
1:P:199:VAL:HA	1:P:202:THR:HG22	1.99	0.45
1:B:199:VAL:HA	1:B:202:THR:HG22	1.99	0.45
1:L:67:VAL:HA	1:L:70:ILE:HG22	1.99	0.45
1:M:67:VAL:HA	1:M:70:ILE:HG22	1.99	0.45
1:O:62:GLY:O	1:O:66:LEU:N	2.45	0.45
1:Q:53:ASN:OD1	1:Q:53:ASN:N	2.49	0.45
1:A:199:VAL:HA	1:A:202:THR:HG22	1.99	0.45
1:B:147:HIS:O	1:U:149:PRO:HG3	2.16	0.45
1:N:67:VAL:HA	1:N:70:ILE:HG22	1.99	0.45
1:O:199:VAL:HA	1:O:202:THR:HG22	1.99	0.45
1:B:149:PRO:HG3	1:U:147:HIS:O	2.16	0.45
1:H:62:GLY:O	1:H:66:LEU:N	2.45	0.45
1:K:147:HIS:O	1:L:149:PRO:HG3	2.16	0.45
1:Q:199:VAL:HA	1:Q:202:THR:HG22	1.99	0.45
1:T:67:VAL:HA	1:T:70:ILE:HG22	1.99	0.45
1:C:199:VAL:HA	1:C:202:THR:HG22	1.99	0.44
1:N:199:VAL:HA	1:N:202:THR:HG22	1.99	0.44
1:S:180:LEU:HD12	1:S:180:LEU:HA	1.86	0.44
1:T:53:ASN:N	1:T:53:ASN:OD1	2.49	0.44
1:K:149:PRO:HG3	1:L:147:HIS:O	2.17	0.44
1:A:149:PRO:HG3	1:V:147:HIS:O	2.16	0.44
1:B:67:VAL:HA	1:B:70:ILE:HG22	1.99	0.44
1:G:199:VAL:HA	1:G:202:THR:HG22	1.99	0.44
1:R:199:VAL:HA	1:R:202:THR:HG22	1.99	0.44
1:S:67:VAL:HA	1:S:70:ILE:HG22	1.99	0.44
1:H:67:VAL:HA	1:H:70:ILE:HG22	1.99	0.44
1:H:199:VAL:HA	1:H:202:THR:HG22	1.99	0.44
1:I:147:HIS:O	1:N:149:PRO:HG3	2.17	0.44
1:J:53:ASN:OD1	1:J:53:ASN:N	2.48	0.44
1:K:199:VAL:HA	1:K:202:THR:HG22	1.99	0.44
1:U:199:VAL:HA	1:U:202:THR:HG22	1.99	0.44
1:D:199:VAL:HA	1:D:202:THR:HG22	1.99	0.44
1:V:199:VAL:HA	1:V:202:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:199:VAL:HA	1:F:202:THR:HG22	1.99	0.44
1:G:62:GLY:O	1:G:66:LEU:N	2.45	0.44
1:A:241:VAL:HG22	1:A:264:ILE:HD13	2.00	0.44
1:C:241:VAL:HG22	1:C:264:ILE:HD13	2.00	0.44
1:M:199:VAL:HA	1:M:202:THR:HG22	1.99	0.44
1:S:62:GLY:O	1:S:66:LEU:N	2.45	0.44
1:T:199:VAL:HA	1:T:202:THR:HG22	1.99	0.44
1:U:241:VAL:HG22	1:U:264:ILE:HD13	2.00	0.44
1:C:67:VAL:HA	1:C:70:ILE:HG22	1.99	0.44
1:D:241:VAL:HG22	1:D:264:ILE:HD13	2.00	0.44
1:E:241:VAL:HG22	1:E:264:ILE:HD13	2.00	0.44
1:G:67:VAL:HA	1:G:70:ILE:HG22	1.98	0.44
1:I:199:VAL:HA	1:I:202:THR:HG22	1.99	0.44
1:K:241:VAL:HG22	1:K:264:ILE:HD13	2.00	0.44
1:L:241:VAL:HG22	1:L:264:ILE:HD13	2.00	0.44
1:M:241:VAL:HG22	1:M:264:ILE:HD13	2.00	0.44
1:F:241:VAL:HG22	1:F:264:ILE:HD13	2.00	0.44
1:J:199:VAL:HA	1:J:202:THR:HG22	1.99	0.44
1:K:220:TRP:NE1	1:K:296:TYR:O	2.41	0.44
1:S:199:VAL:HA	1:S:202:THR:HG22	1.99	0.44
1:T:241:VAL:HG22	1:T:264:ILE:HD13	2.00	0.44
1:F:67:VAL:HA	1:F:70:ILE:HG22	1.99	0.43
1:L:199:VAL:HA	1:L:202:THR:HG22	1.99	0.43
1:N:241:VAL:HG22	1:N:264:ILE:HD13	2.00	0.43
1:O:241:VAL:HG22	1:O:264:ILE:HD13	2.00	0.43
1:B:241:VAL:HG22	1:B:264:ILE:HD13	2.00	0.43
1:E:199:VAL:HA	1:E:202:THR:HG22	1.99	0.43
1:G:147:HIS:O	1:P:149:PRO:HG3	2.18	0.43
1:A:147:HIS:O	1:V:149:PRO:HG3	2.17	0.43
1:D:67:VAL:HA	1:D:70:ILE:HG22	1.99	0.43
1:E:67:VAL:HA	1:E:70:ILE:HG22	1.99	0.43
1:F:53:ASN:OD1	1:F:53:ASN:N	2.49	0.43
1:N:71:ILE:HA	1:N:74:ILE:HB	2.01	0.43
1:P:71:ILE:HA	1:P:74:ILE:HB	2.01	0.43
1:Q:71:ILE:HA	1:Q:74:ILE:HB	2.01	0.43
1:R:71:ILE:HA	1:R:74:ILE:HB	2.01	0.43
1:V:241:VAL:HG22	1:V:264:ILE:HD13	2.00	0.43
1:J:241:VAL:HG22	1:J:264:ILE:HD13	2.00	0.43
1:K:62:GLY:O	1:K:66:LEU:N	2.45	0.43
1:M:71:ILE:HA	1:M:74:ILE:HB	2.01	0.43
1:O:71:ILE:HA	1:O:74:ILE:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:241:VAL:HG22	1:S:264:ILE:HD13	2.00	0.43
1:G:64:PRO:HA	1:G:67:VAL:HG12	2.01	0.43
1:G:241:VAL:HG22	1:G:264:ILE:HD13	2.00	0.43
1:J:273:GLN:HE21	1:J:277:GLN:NE2	2.17	0.43
1:F:64:PRO:HA	1:F:67:VAL:HG12	2.01	0.43
1:H:64:PRO:HA	1:H:67:VAL:HG12	2.01	0.43
1:H:241:VAL:HG22	1:H:264:ILE:HD13	2.00	0.43
1:P:241:VAL:HG22	1:P:264:ILE:HD13	2.00	0.43
1:Q:241:VAL:HG22	1:Q:264:ILE:HD13	2.00	0.43
1:Q:273:GLN:HE21	1:Q:277:GLN:NE2	2.17	0.43
1:R:241:VAL:HG22	1:R:264:ILE:HD13	2.00	0.43
1:S:71:ILE:HA	1:S:74:ILE:HB	2.01	0.43
1:C:64:PRO:HA	1:C:67:VAL:HG12	2.01	0.43
1:C:273:GLN:HE21	1:C:277:GLN:NE2	2.17	0.43
1:D:64:PRO:HA	1:D:67:VAL:HG12	2.01	0.43
1:E:64:PRO:HA	1:E:67:VAL:HG12	2.01	0.43
1:F:273:GLN:HE21	1:F:277:GLN:NE2	2.17	0.43
1:I:149:PRO:HG3	1:N:147:HIS:O	2.18	0.43
1:I:241:VAL:HG22	1:I:264:ILE:HD13	2.00	0.43
1:L:71:ILE:HA	1:L:74:ILE:HB	2.01	0.43
1:L:273:GLN:HE21	1:L:277:GLN:NE2	2.17	0.43
1:P:64:PRO:HA	1:P:67:VAL:HG12	2.01	0.43
1:Q:64:PRO:HA	1:Q:67:VAL:HG12	2.01	0.43
1:I:64:PRO:HA	1:I:67:VAL:HG12	2.01	0.43
1:R:273:GLN:HE21	1:R:277:GLN:NE2	2.17	0.43
1:B:71:ILE:HA	1:B:74:ILE:HB	2.01	0.43
1:B:273:GLN:HE21	1:B:277:GLN:NE2	2.17	0.43
1:G:273:GLN:HE21	1:G:277:GLN:NE2	2.17	0.43
1:K:273:GLN:HE21	1:K:277:GLN:NE2	2.17	0.43
1:O:64:PRO:HA	1:O:67:VAL:HG12	2.01	0.43
1:V:273:GLN:HE21	1:V:277:GLN:NE2	2.17	0.43
1:A:71:ILE:HA	1:A:74:ILE:HB	2.01	0.43
1:A:180:LEU:HD12	1:A:180:LEU:HA	1.86	0.43
1:C:71:ILE:HA	1:C:74:ILE:HB	2.01	0.43
1:I:180:LEU:HD12	1:I:180:LEU:HA	1.87	0.43
1:M:64:PRO:HA	1:M:67:VAL:HG12	2.01	0.43
1:N:64:PRO:HA	1:N:67:VAL:HG12	2.01	0.43
1:R:64:PRO:HA	1:R:67:VAL:HG12	2.01	0.43
1:I:230:LEU:HD23	1:I:230:LEU:HA	1.90	0.42
1:J:64:PRO:HA	1:J:67:VAL:HG12	2.01	0.42
1:L:191:LEU:HA	1:L:194:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:180:LEU:HD12	1:M:180:LEU:HA	1.87	0.42
1:N:273:GLN:HE21	1:N:277:GLN:NE2	2.17	0.42
1:Q:62:GLY:O	1:Q:66:LEU:N	2.45	0.42
1:B:64:PRO:HA	1:B:67:VAL:HG12	2.01	0.42
1:D:191:LEU:HA	1:D:194:VAL:HG12	2.01	0.42
1:E:191:LEU:HA	1:E:194:VAL:HG12	2.01	0.42
1:F:147:HIS:O	1:Q:149:PRO:HG3	2.19	0.42
1:H:192:ILE:HA	1:H:195:VAL:HG12	2.02	0.42
1:K:71:ILE:HA	1:K:74:ILE:HB	2.01	0.42
1:K:192:ILE:HA	1:K:195:VAL:HG12	2.02	0.42
1:L:64:PRO:HA	1:L:67:VAL:HG12	2.01	0.42
1:M:191:LEU:HA	1:M:194:VAL:HG12	2.02	0.42
1:P:273:GLN:HE21	1:P:277:GLN:NE2	2.17	0.42
1:S:192:ILE:HA	1:S:195:VAL:HG12	2.01	0.42
1:T:71:ILE:HA	1:T:74:ILE:HB	2.01	0.42
1:V:64:PRO:HA	1:V:67:VAL:HG12	2.01	0.42
1:A:192:ILE:HA	1:A:195:VAL:HG12	2.02	0.42
1:C:149:PRO:HG3	1:T:147:HIS:O	2.18	0.42
1:D:71:ILE:HA	1:D:74:ILE:HB	2.01	0.42
1:D:273:GLN:HE21	1:D:277:GLN:NE2	2.17	0.42
1:E:149:PRO:HG3	1:R:147:HIS:O	2.19	0.42
1:G:192:ILE:HA	1:G:195:VAL:HG12	2.02	0.42
1:I:273:GLN:HE21	1:I:277:GLN:NE2	2.17	0.42
1:M:74:ILE:HD13	1:M:74:ILE:HA	1.93	0.42
1:M:273:GLN:HE21	1:M:277:GLN:NE2	2.17	0.42
1:N:191:LEU:HA	1:N:194:VAL:HG12	2.02	0.42
1:T:64:PRO:HA	1:T:67:VAL:HG12	2.01	0.42
1:T:192:ILE:HA	1:T:195:VAL:HG12	2.02	0.42
1:V:191:LEU:HA	1:V:194:VAL:HG12	2.01	0.42
1:B:192:ILE:HA	1:B:195:VAL:HG12	2.02	0.42
1:C:191:LEU:HA	1:C:194:VAL:HG12	2.01	0.42
1:E:71:ILE:HA	1:E:74:ILE:HB	2.01	0.42
1:H:71:ILE:HA	1:H:74:ILE:HB	2.01	0.42
1:J:71:ILE:HA	1:J:74:ILE:HB	2.00	0.42
1:J:273:GLN:HE21	1:J:277:GLN:HE22	1.68	0.42
1:M:149:PRO:O	1:M:153:ALA:N	2.51	0.42
1:O:273:GLN:HE21	1:O:277:GLN:HE22	1.68	0.42
1:S:64:PRO:HA	1:S:67:VAL:HG12	2.01	0.42
1:U:64:PRO:HA	1:U:67:VAL:HG12	2.01	0.42
1:C:147:HIS:O	1:T:149:PRO:HG3	2.19	0.42
1:C:192:ILE:HA	1:C:195:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:PRO:O	1:D:153:ALA:N	2.51	0.42
1:F:149:PRO:HG3	1:Q:147:HIS:O	2.20	0.42
1:F:191:LEU:HA	1:F:194:VAL:HG12	2.01	0.42
1:G:71:ILE:HA	1:G:74:ILE:HB	2.01	0.42
1:I:71:ILE:HA	1:I:74:ILE:HB	2.01	0.42
1:I:192:ILE:HA	1:I:195:VAL:HG12	2.02	0.42
1:Q:273:GLN:HE21	1:Q:277:GLN:HE22	1.68	0.42
1:R:192:ILE:HA	1:R:195:VAL:HG12	2.02	0.42
1:U:273:GLN:HE21	1:U:277:GLN:NE2	2.17	0.42
1:V:71:ILE:HA	1:V:74:ILE:HB	2.01	0.42
1:V:192:ILE:HA	1:V:195:VAL:HG12	2.02	0.42
1:A:64:PRO:HA	1:A:67:VAL:HG12	2.01	0.42
1:B:191:LEU:HA	1:B:194:VAL:HG12	2.01	0.42
1:E:147:HIS:O	1:R:149:PRO:HG3	2.20	0.42
1:F:71:ILE:HA	1:F:74:ILE:HB	2.01	0.42
1:F:192:ILE:HA	1:F:195:VAL:HG12	2.02	0.42
1:F:273:GLN:HE21	1:F:277:GLN:HE22	1.68	0.42
1:H:273:GLN:HE21	1:H:277:GLN:HE22	1.68	0.42
1:J:192:ILE:HA	1:J:195:VAL:HG12	2.02	0.42
1:K:64:PRO:HA	1:K:67:VAL:HG12	2.01	0.42
1:O:191:LEU:HA	1:O:194:VAL:HG12	2.01	0.42
1:Q:192:ILE:HA	1:Q:195:VAL:HG12	2.02	0.42
1:S:273:GLN:HE21	1:S:277:GLN:HE22	1.68	0.42
1:T:273:GLN:HE21	1:T:277:GLN:NE2	2.17	0.42
1:U:191:LEU:HA	1:U:194:VAL:HG12	2.02	0.42
1:U:192:ILE:HA	1:U:195:VAL:HG12	2.02	0.42
1:A:273:GLN:HE21	1:A:277:GLN:NE2	2.17	0.42
1:D:74:ILE:HD13	1:D:74:ILE:HA	1.93	0.42
1:D:192:ILE:HA	1:D:195:VAL:HG12	2.01	0.42
1:G:149:PRO:HG3	1:P:147:HIS:O	2.20	0.42
1:O:192:ILE:HA	1:O:195:VAL:HG12	2.02	0.42
1:P:192:ILE:HA	1:P:195:VAL:HG12	2.02	0.42
1:Q:180:LEU:HD12	1:Q:180:LEU:HA	1.87	0.42
1:R:230:LEU:HD23	1:R:230:LEU:HA	1.90	0.42
1:T:191:LEU:HA	1:T:194:VAL:HG12	2.01	0.42
1:E:273:GLN:HE21	1:E:277:GLN:NE2	2.17	0.42
1:I:273:GLN:HE21	1:I:277:GLN:HE22	1.68	0.42
1:K:273:GLN:HE21	1:K:277:GLN:HE22	1.68	0.42
1:N:273:GLN:HE21	1:N:277:GLN:HE22	1.68	0.42
1:R:273:GLN:HE21	1:R:277:GLN:HE22	1.68	0.42
1:A:273:GLN:HE21	1:A:277:GLN:HE22	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ILE:HA	1:E:195:VAL:HG12	2.02	0.42
1:F:180:LEU:HD12	1:F:180:LEU:HA	1.86	0.42
1:G:191:LEU:HA	1:G:194:VAL:HG12	2.01	0.42
1:G:273:GLN:HE21	1:G:277:GLN:HE22	1.68	0.42
1:L:192:ILE:HA	1:L:195:VAL:HG12	2.02	0.42
1:P:273:GLN:HE21	1:P:277:GLN:HE22	1.68	0.42
1:S:273:GLN:HE21	1:S:277:GLN:NE2	2.17	0.42
1:T:273:GLN:HE21	1:T:277:GLN:HE22	1.68	0.42
1:V:242:LEU:HD12	1:V:242:LEU:HA	1.92	0.42
1:A:191:LEU:HA	1:A:194:VAL:HG12	2.01	0.42
1:C:74:ILE:HD13	1:C:74:ILE:HA	1.93	0.42
1:E:273:GLN:HE21	1:E:277:GLN:HE22	1.68	0.42
1:G:53:ASN:OD1	1:G:53:ASN:N	2.49	0.42
1:M:273:GLN:HE21	1:M:277:GLN:HE22	1.68	0.42
1:N:192:ILE:HA	1:N:195:VAL:HG12	2.01	0.42
1:U:71:ILE:HA	1:U:74:ILE:HB	2.01	0.42
1:B:156:ILE:HD12	1:B:156:ILE:HA	1.95	0.41
1:H:273:GLN:HE21	1:H:277:GLN:NE2	2.17	0.41
1:M:192:ILE:HA	1:M:195:VAL:HG12	2.02	0.41
1:O:273:GLN:HE21	1:O:277:GLN:NE2	2.17	0.41
1:P:70:ILE:HD12	1:P:70:ILE:HA	1.95	0.41
1:P:191:LEU:HA	1:P:194:VAL:HG12	2.01	0.41
1:P:242:LEU:HD12	1:P:242:LEU:HA	1.92	0.41
1:R:74:ILE:HD13	1:R:74:ILE:HA	1.93	0.41
1:F:230:LEU:HD23	1:F:230:LEU:HA	1.90	0.41
1:S:191:LEU:HA	1:S:194:VAL:HG12	2.01	0.41
1:B:273:GLN:HE21	1:B:277:GLN:HE22	1.68	0.41
1:D:273:GLN:HE21	1:D:277:GLN:HE22	1.68	0.41
1:H:191:LEU:HA	1:H:194:VAL:HG12	2.01	0.41
1:Q:191:LEU:HA	1:Q:194:VAL:HG12	2.01	0.41
1:V:156:ILE:HD12	1:V:156:ILE:HA	1.95	0.41
1:K:132:LEU:HD23	1:K:132:LEU:HA	1.87	0.41
1:K:191:LEU:HA	1:K:194:VAL:HG12	2.01	0.41
1:R:149:PRO:O	1:R:153:ALA:N	2.51	0.41
1:R:191:LEU:HA	1:R:194:VAL:HG12	2.01	0.41
1:U:273:GLN:HE21	1:U:277:GLN:HE22	1.68	0.41
1:V:74:ILE:HD13	1:V:74:ILE:HA	1.93	0.41
1:V:273:GLN:HE21	1:V:277:GLN:HE22	1.68	0.41
1:C:273:GLN:HE21	1:C:277:GLN:HE22	1.68	0.41
1:I:149:PRO:O	1:I:153:ALA:N	2.51	0.41
1:L:273:GLN:HE21	1:L:277:GLN:HE22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:242:LEU:HD12	1:O:242:LEU:HA	1.92	0.41
1:I:191:LEU:HA	1:I:194:VAL:HG12	2.01	0.41
1:J:191:LEU:HA	1:J:194:VAL:HG12	2.01	0.41
1:N:149:PRO:O	1:N:153:ALA:N	2.51	0.41
1:U:133:SER:OG	1:U:157:LEU:O	2.36	0.41
1:I:70:ILE:HD12	1:I:70:ILE:HA	1.95	0.41
1:J:149:PRO:O	1:J:153:ALA:N	2.51	0.41
1:B:242:LEU:HD12	1:B:242:LEU:HA	1.92	0.41
1:C:242:LEU:HD12	1:C:242:LEU:HA	1.92	0.41
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.87	0.41
1:E:149:PRO:O	1:E:153:ALA:N	2.51	0.41
1:H:155:GLU:O	1:H:159:ARG:NH2	2.51	0.41
1:I:155:GLU:O	1:I:159:ARG:NH2	2.51	0.41
1:J:132:LEU:HD23	1:J:132:LEU:HA	1.87	0.41
1:M:132:LEU:HD23	1:M:132:LEU:HA	1.87	0.41
1:S:149:PRO:O	1:S:153:ALA:N	2.51	0.41
1:T:133:SER:OG	1:T:157:LEU:O	2.36	0.41
1:B:74:ILE:HD13	1:B:74:ILE:HA	1.93	0.41
1:G:155:GLU:O	1:G:159:ARG:NH2	2.51	0.41
1:H:74:ILE:HD13	1:H:74:ILE:HA	1.93	0.41
1:M:242:LEU:HD12	1:M:242:LEU:HA	1.92	0.41
1:E:74:ILE:HD13	1:E:74:ILE:HA	1.93	0.40
1:E:156:ILE:HD12	1:E:156:ILE:HA	1.95	0.40
1:L:156:ILE:HD12	1:L:156:ILE:HA	1.95	0.40
1:N:74:ILE:HD13	1:N:74:ILE:HA	1.93	0.40
1:C:156:ILE:HD12	1:C:156:ILE:HA	1.95	0.40
1:J:74:ILE:HD13	1:J:74:ILE:HA	1.93	0.40
1:J:155:GLU:O	1:J:159:ARG:NH2	2.51	0.40
1:M:156:ILE:HD12	1:M:156:ILE:HA	1.95	0.40
1:O:230:LEU:HD23	1:O:230:LEU:HA	1.90	0.40
1:N:180:LEU:HD12	1:N:180:LEU:HA	1.86	0.40
1:Q:149:PRO:O	1:Q:153:ALA:N	2.51	0.40
1:F:242:LEU:HD12	1:F:242:LEU:HA	1.92	0.40
1:O:149:PRO:O	1:O:153:ALA:N	2.51	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	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	B	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	C	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	D	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	E	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	F	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	G	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	H	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	I	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	J	273/331 (82%)	263 (96%)	10 (4%)	0	100	100
1	K	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	L	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	M	273/331 (82%)	263 (96%)	10 (4%)	0	100	100
1	N	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	O	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	P	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	Q	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	R	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	S	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	T	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	U	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
1	V	273/331 (82%)	262 (96%)	11 (4%)	0	100	100
All	All	6006/7282 (82%)	5766 (96%)	240 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	175/278 (63%)	175 (100%)	0	100	100
1	B	175/278 (63%)	175 (100%)	0	100	100
1	C	175/278 (63%)	175 (100%)	0	100	100
1	D	175/278 (63%)	175 (100%)	0	100	100
1	E	175/278 (63%)	175 (100%)	0	100	100
1	F	175/278 (63%)	175 (100%)	0	100	100
1	G	175/278 (63%)	175 (100%)	0	100	100
1	H	175/278 (63%)	175 (100%)	0	100	100
1	I	175/278 (63%)	175 (100%)	0	100	100
1	J	175/278 (63%)	175 (100%)	0	100	100
1	K	175/278 (63%)	175 (100%)	0	100	100
1	L	175/278 (63%)	175 (100%)	0	100	100
1	M	175/278 (63%)	175 (100%)	0	100	100
1	N	175/278 (63%)	175 (100%)	0	100	100
1	O	175/278 (63%)	175 (100%)	0	100	100
1	P	175/278 (63%)	175 (100%)	0	100	100
1	Q	175/278 (63%)	175 (100%)	0	100	100
1	R	175/278 (63%)	175 (100%)	0	100	100
1	S	175/278 (63%)	175 (100%)	0	100	100
1	T	175/278 (63%)	175 (100%)	0	100	100
1	U	175/278 (63%)	175 (100%)	0	100	100
1	V	175/278 (63%)	175 (100%)	0	100	100
All	All	3850/6116 (63%)	3850 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	246	ASN
1	A	273	GLN
1	A	279	ASN
1	B	229	GLN
1	B	246	ASN
1	B	273	GLN
1	B	279	ASN
1	C	229	GLN
1	C	246	ASN
1	C	273	GLN
1	C	279	ASN
1	D	229	GLN
1	D	246	ASN
1	D	273	GLN
1	D	279	ASN
1	E	229	GLN
1	E	246	ASN
1	E	273	GLN
1	E	279	ASN
1	F	229	GLN
1	F	246	ASN
1	F	273	GLN
1	F	279	ASN
1	G	229	GLN
1	G	246	ASN
1	G	273	GLN
1	G	279	ASN
1	H	229	GLN
1	H	246	ASN
1	H	273	GLN
1	H	279	ASN
1	I	229	GLN
1	I	246	ASN
1	I	273	GLN
1	I	279	ASN
1	J	229	GLN
1	J	246	ASN
1	J	273	GLN
1	J	279	ASN
1	K	229	GLN
1	K	246	ASN
1	K	273	GLN

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Mol	Chain	Res	Type
1	K	279	ASN
1	L	229	GLN
1	L	246	ASN
1	L	273	GLN
1	L	279	ASN
1	M	229	GLN
1	M	246	ASN
1	M	273	GLN
1	M	279	ASN
1	N	229	GLN
1	N	246	ASN
1	N	273	GLN
1	N	279	ASN
1	O	229	GLN
1	O	246	ASN
1	O	273	GLN
1	O	279	ASN
1	P	229	GLN
1	P	246	ASN
1	P	273	GLN
1	P	279	ASN
1	Q	229	GLN
1	Q	246	ASN
1	Q	273	GLN
1	Q	279	ASN
1	R	229	GLN
1	R	246	ASN
1	R	273	GLN
1	R	279	ASN
1	S	229	GLN
1	S	246	ASN
1	S	273	GLN
1	S	279	ASN
1	T	229	GLN
1	T	246	ASN
1	T	273	GLN
1	T	279	ASN
1	U	229	GLN
1	U	246	ASN
1	U	273	GLN
1	U	279	ASN
1	V	229	GLN

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Mol	Chain	Res	Type
1	V	246	ASN
1	V	273	GLN
1	V	279	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)

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.

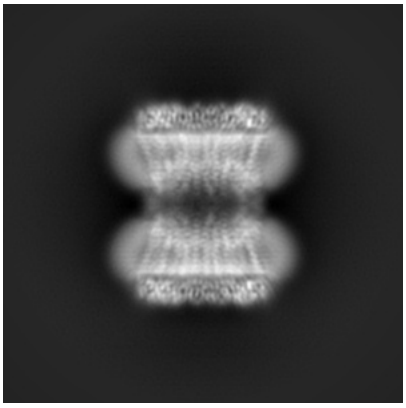
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-20790. These allow visual inspection of the internal detail of the map and identification of artifacts.

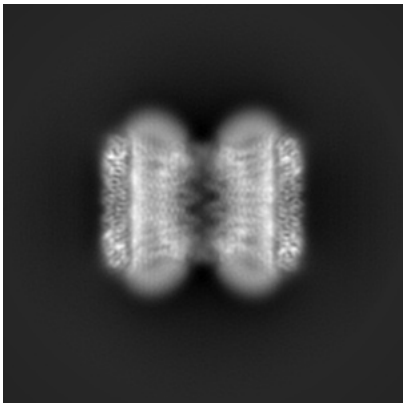
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

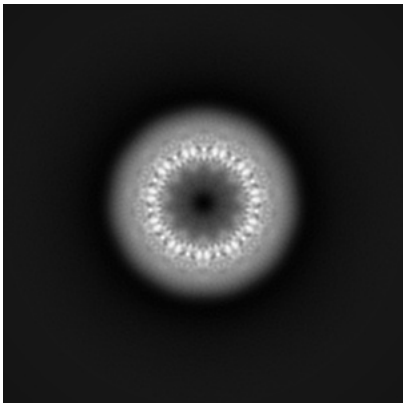
6.1.1 Primary map



X



Y

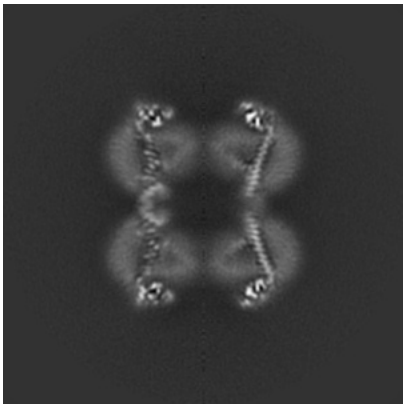


Z

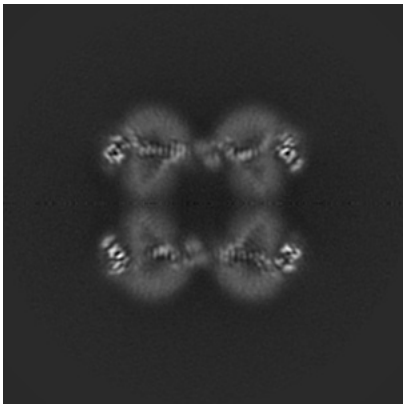
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

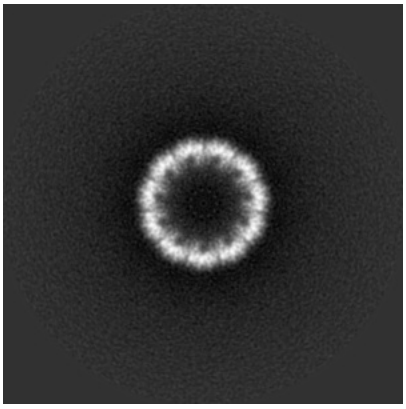
6.2.1 Primary map



X Index: 170



Y Index: 170

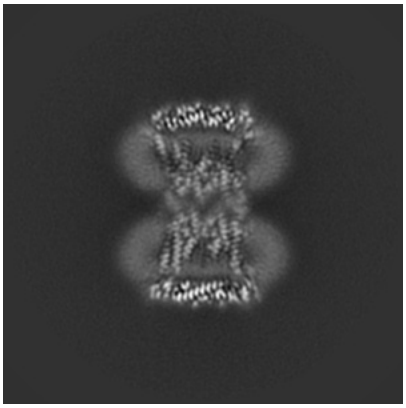


Z Index: 170

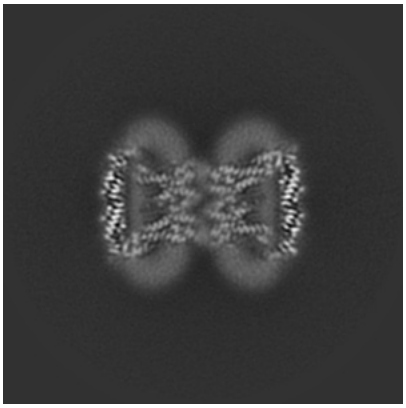
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

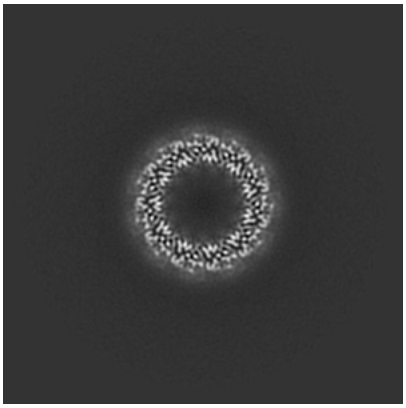
6.3.1 Primary map



X Index: 209



Y Index: 132

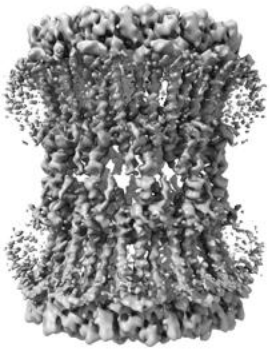


Z Index: 241

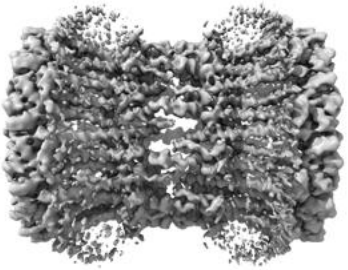
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

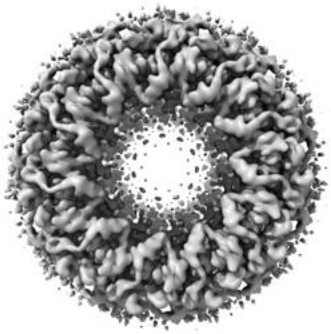
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0097. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

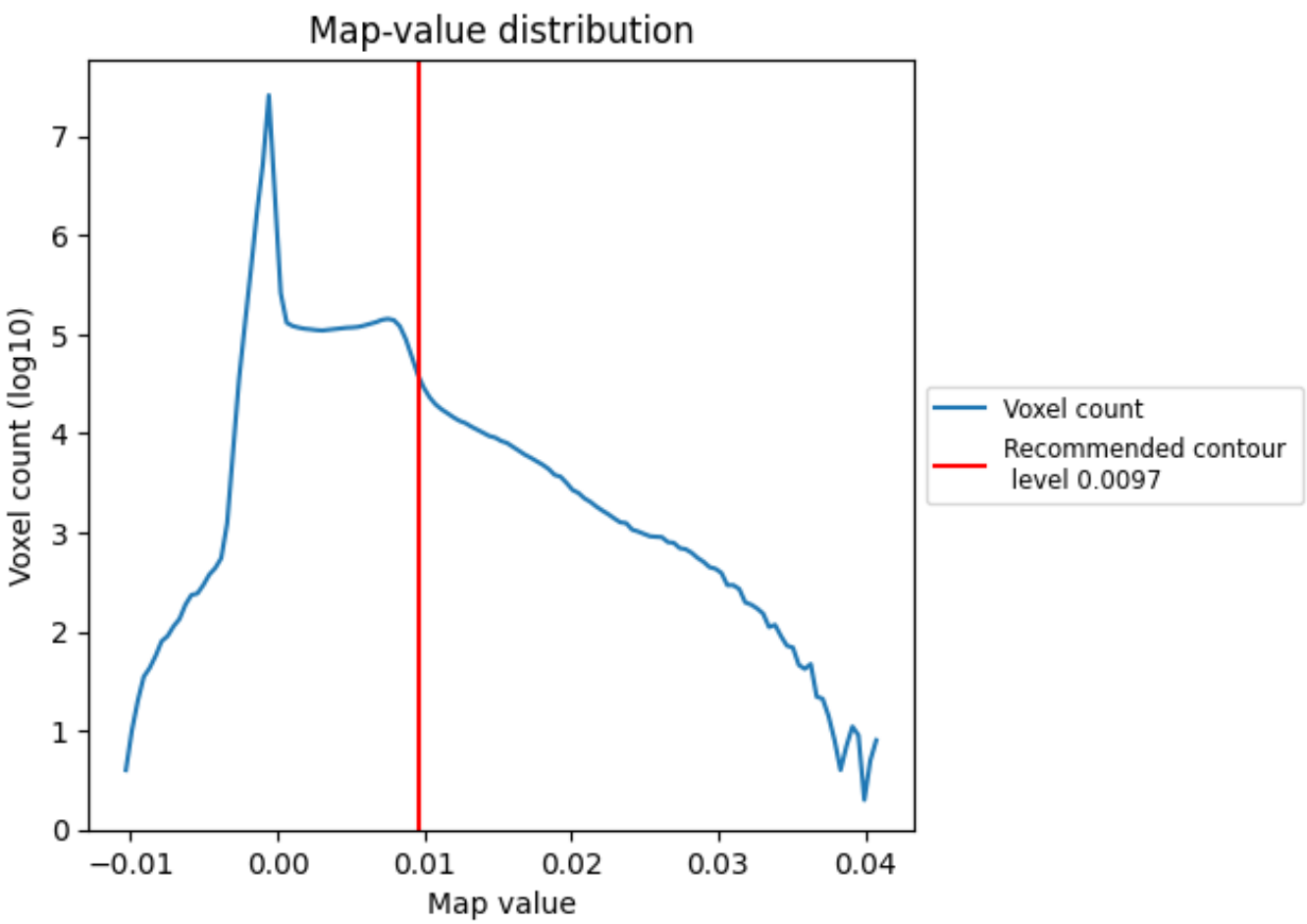
6.5 Mask visualisation (i)

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

7 Map analysis (i)

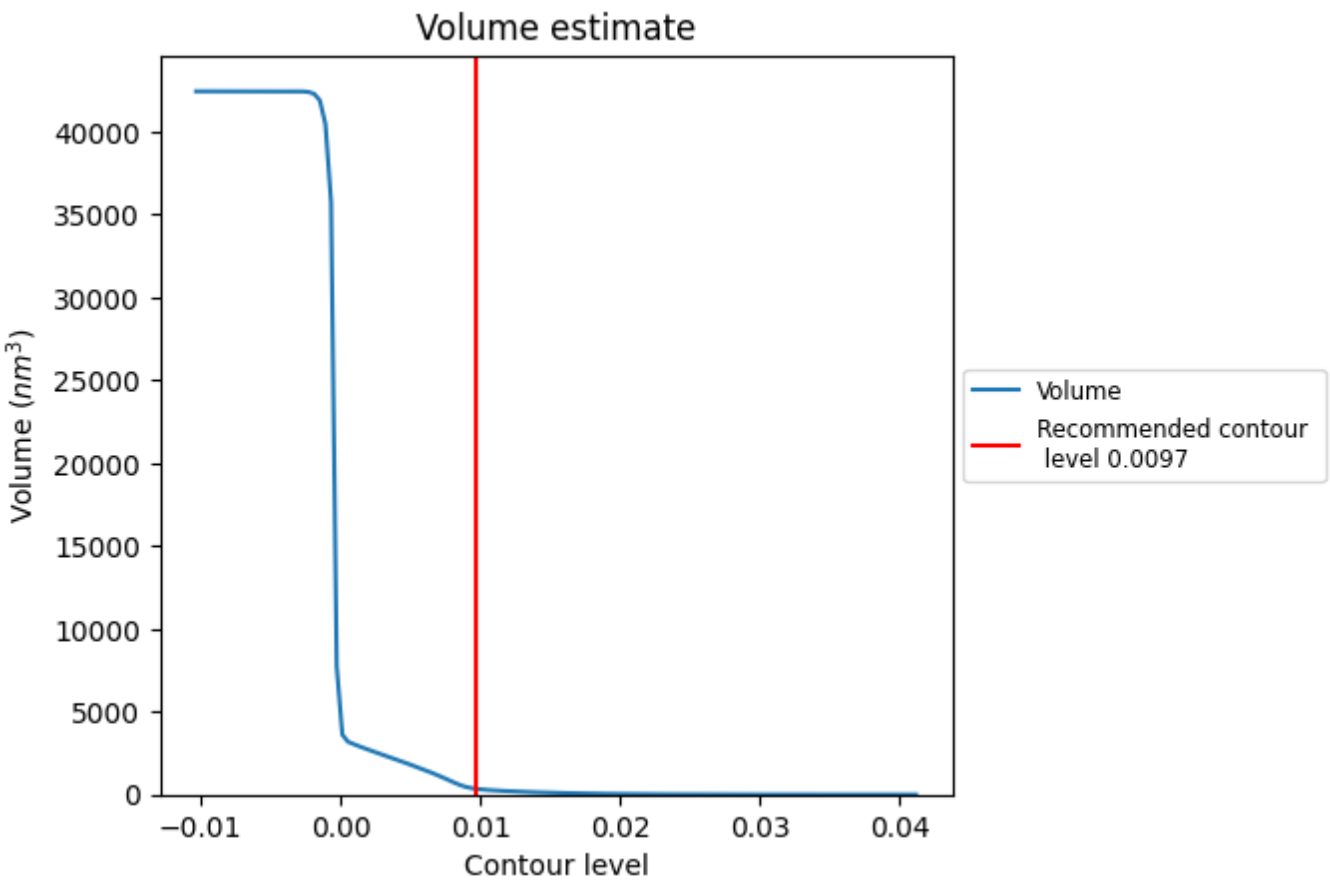
This section contains the results of statistical analysis of the map.

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.

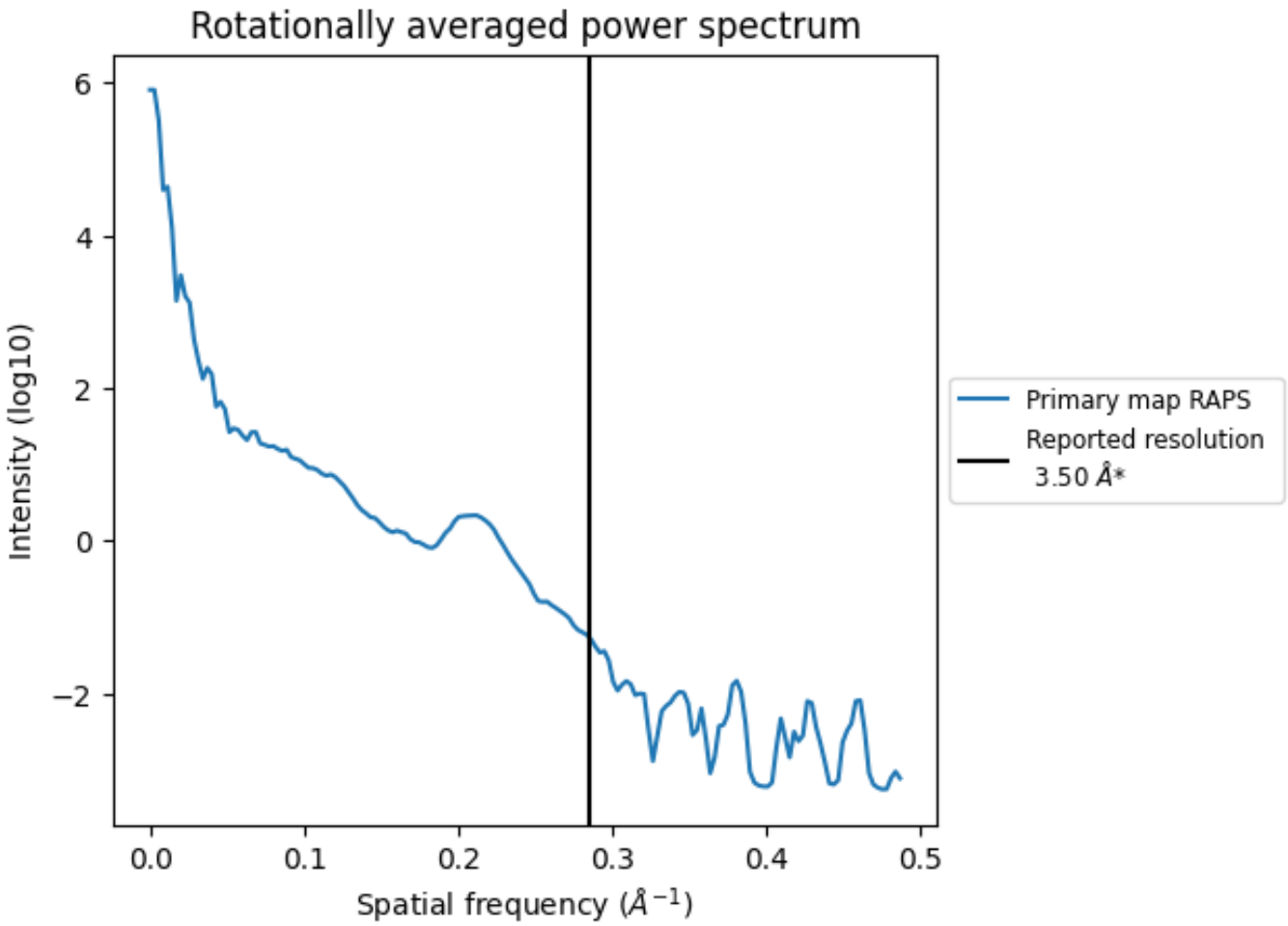
7.2 Volume estimate (i)



The volume at the recommended contour level is 348 nm^3; this corresponds to an approximate mass of 315 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 (i)



*Reported resolution corresponds to spatial frequency of 0.286 Å^{-1}

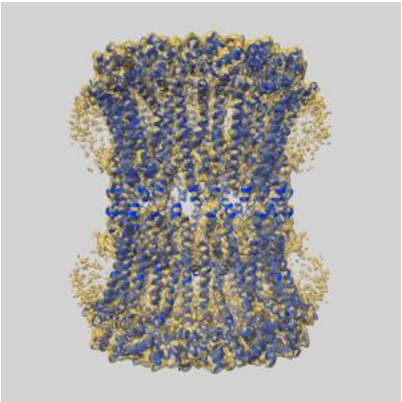
8 Fourier-Shell correlation (i)

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

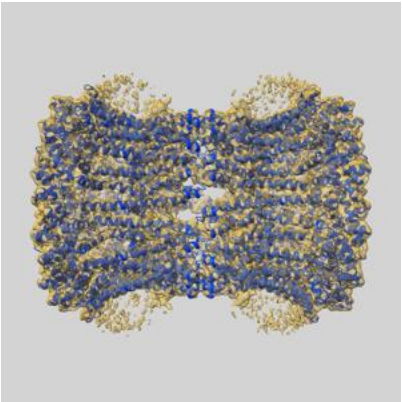
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-20790 and PDB model 6UIX. Per-residue inclusion information can be found in section 3 on page 10.

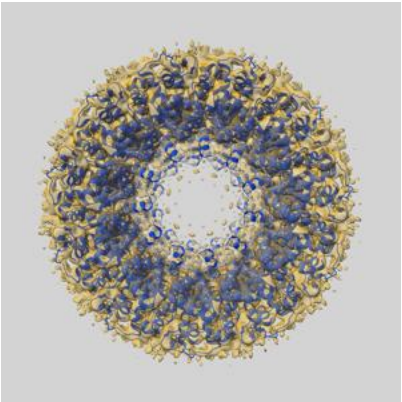
9.1 Map-model overlay (i)



X



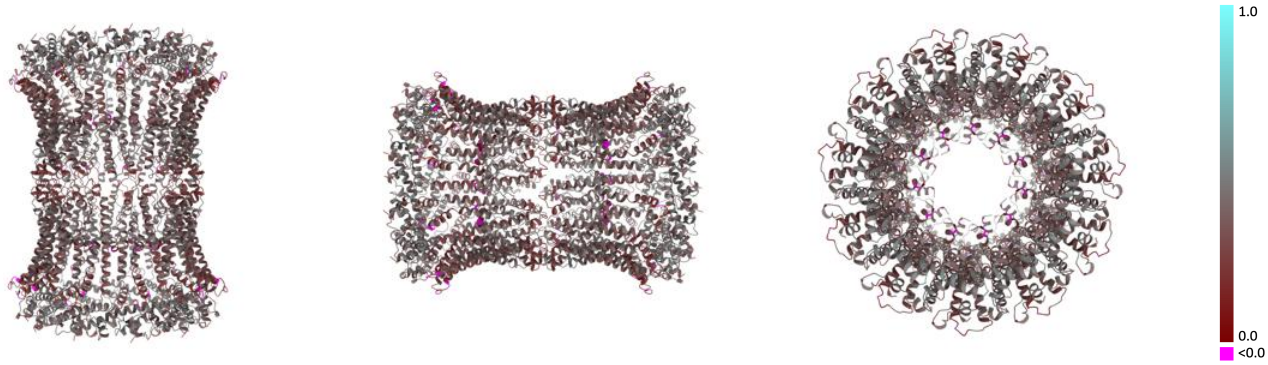
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0097 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.

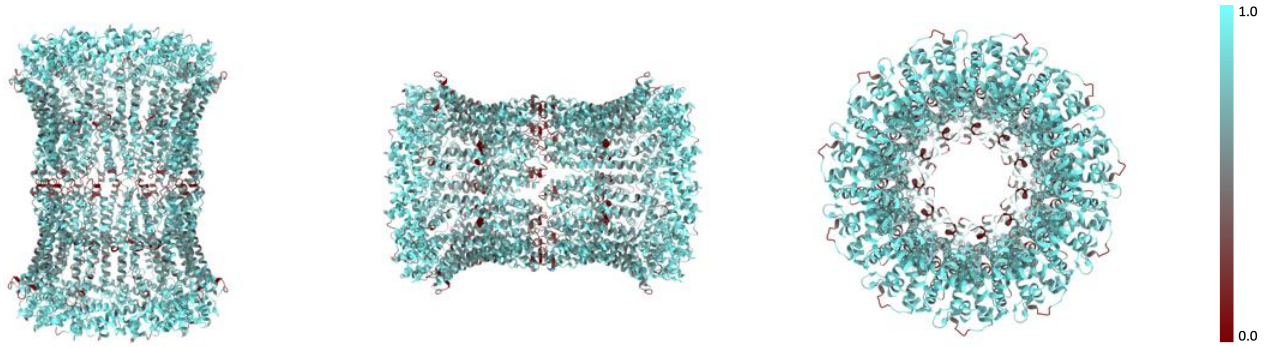
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

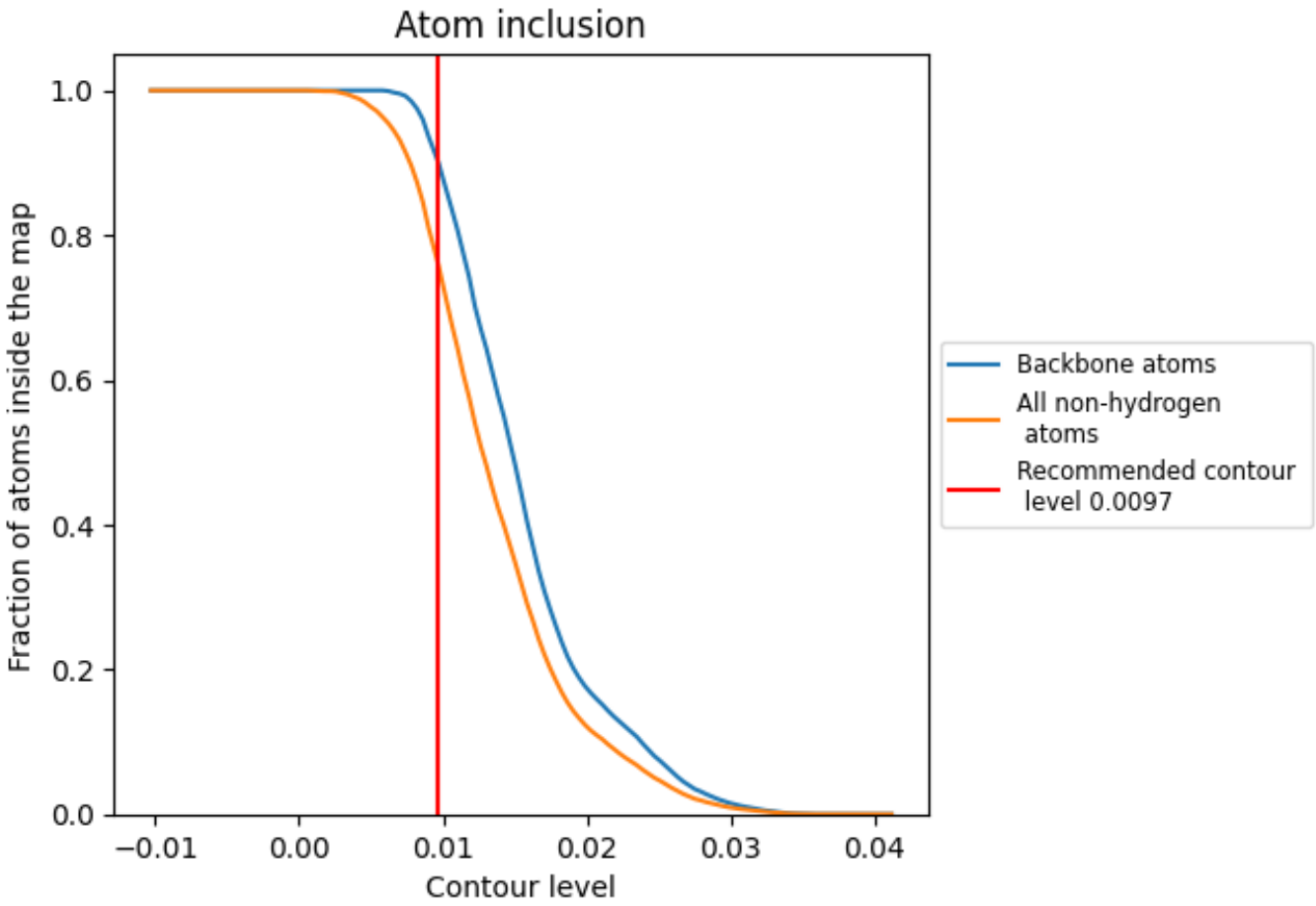
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0097).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0097) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7570	0.3820
A	0.7697	0.3890
B	0.7661	0.3890
C	0.7671	0.3900
D	0.7666	0.3880
E	0.7671	0.3880
F	0.7681	0.3890
G	0.7692	0.3890
H	0.7676	0.3870
I	0.7661	0.3870
J	0.7661	0.3870
K	0.7666	0.3870
L	0.7487	0.3760
M	0.7477	0.3750
N	0.7451	0.3760
O	0.7457	0.3750
P	0.7441	0.3770
Q	0.7457	0.3750
R	0.7472	0.3740
S	0.7482	0.3750
T	0.7482	0.3740
U	0.7457	0.3740
V	0.7477	0.3740