Full wwPDB EM Validation Report ⓘ

Dec 18, 2022 – 10:47 am GMT

PDB ID	:	7ALW
EMDB ID	:	EMD-11820
Title	:	Nonameric cytoplasmic domain of SctV from Yersinia enterocolitica
Authors	:	Kuhlen, L.; Johnson, S.
Deposited on	:	2020-10-07
Resolution	:	3.70 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:

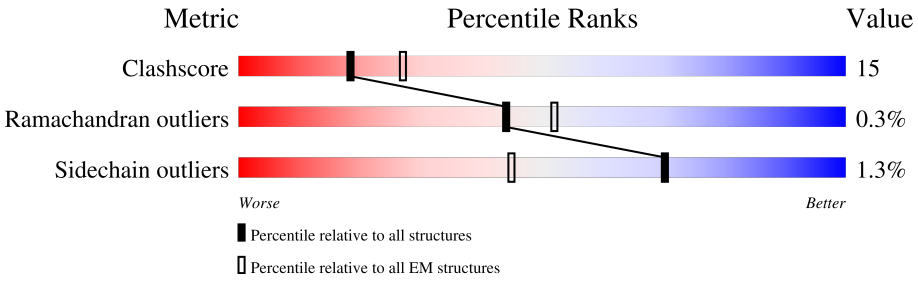
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.70 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	710	10% 31% 17% 52%
1	B	710	10% 31% 17% 52%
1	C	710	10% 31% 17% 52%
1	D	710	10% 31% 17% 52%
1	E	710	10% 31% 17% 52%
1	F	710	10% 32% 16% 52%
1	G	710	10% 31% 17% 52%
1	H	710	10% 31% 17% 52%

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Mol	Chain	Length	Quality of chain
1	I	710	10% 31% 17% 52%
1	J	710	10% 31% 17% 52%
1	K	710	10% 31% 17% 52%
1	L	710	10% 31% 17% 52%
1	M	710	10% 30% 18% 52%
1	N	710	10% 31% 17% 52%
1	O	710	10% 31% 17% 52%
1	P	710	10% 31% 17% 52%
1	Q	710	10% 31% 17% 52%
1	R	710	10% 32% 16% 52%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 50148 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 Low calcium response protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	B	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	C	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	D	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	E	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	F	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	G	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	H	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	I	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	J	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	K	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	L	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	M	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	N	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	O	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	P	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		
1	Q	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	344	Total	C	N	O	S	0	0
			2786	1776	469	532	9		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	ILE	LEU	conflict	UNP Q51875
A	705	GLU	-	expression tag	UNP Q51875
A	706	ASN	-	expression tag	UNP Q51875
A	707	LEU	-	expression tag	UNP Q51875
A	708	TYR	-	expression tag	UNP Q51875
A	709	PHE	-	expression tag	UNP Q51875
A	710	GLN	-	expression tag	UNP Q51875
B	38	ILE	LEU	conflict	UNP Q51875
B	705	GLU	-	expression tag	UNP Q51875
B	706	ASN	-	expression tag	UNP Q51875
B	707	LEU	-	expression tag	UNP Q51875
B	708	TYR	-	expression tag	UNP Q51875
B	709	PHE	-	expression tag	UNP Q51875
B	710	GLN	-	expression tag	UNP Q51875
C	38	ILE	LEU	conflict	UNP Q51875
C	705	GLU	-	expression tag	UNP Q51875
C	706	ASN	-	expression tag	UNP Q51875
C	707	LEU	-	expression tag	UNP Q51875
C	708	TYR	-	expression tag	UNP Q51875
C	709	PHE	-	expression tag	UNP Q51875
C	710	GLN	-	expression tag	UNP Q51875
D	38	ILE	LEU	conflict	UNP Q51875
D	705	GLU	-	expression tag	UNP Q51875
D	706	ASN	-	expression tag	UNP Q51875
D	707	LEU	-	expression tag	UNP Q51875
D	708	TYR	-	expression tag	UNP Q51875
D	709	PHE	-	expression tag	UNP Q51875
D	710	GLN	-	expression tag	UNP Q51875
E	38	ILE	LEU	conflict	UNP Q51875
E	705	GLU	-	expression tag	UNP Q51875
E	706	ASN	-	expression tag	UNP Q51875
E	707	LEU	-	expression tag	UNP Q51875
E	708	TYR	-	expression tag	UNP Q51875
E	709	PHE	-	expression tag	UNP Q51875
E	710	GLN	-	expression tag	UNP Q51875
F	38	ILE	LEU	conflict	UNP Q51875

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Chain	Residue	Modelled	Actual	Comment	Reference
F	705	GLU	-	expression tag	UNP Q51875
F	706	ASN	-	expression tag	UNP Q51875
F	707	LEU	-	expression tag	UNP Q51875
F	708	TYR	-	expression tag	UNP Q51875
F	709	PHE	-	expression tag	UNP Q51875
F	710	GLN	-	expression tag	UNP Q51875
G	38	ILE	LEU	conflict	UNP Q51875
G	705	GLU	-	expression tag	UNP Q51875
G	706	ASN	-	expression tag	UNP Q51875
G	707	LEU	-	expression tag	UNP Q51875
G	708	TYR	-	expression tag	UNP Q51875
G	709	PHE	-	expression tag	UNP Q51875
G	710	GLN	-	expression tag	UNP Q51875
H	38	ILE	LEU	conflict	UNP Q51875
H	705	GLU	-	expression tag	UNP Q51875
H	706	ASN	-	expression tag	UNP Q51875
H	707	LEU	-	expression tag	UNP Q51875
H	708	TYR	-	expression tag	UNP Q51875
H	709	PHE	-	expression tag	UNP Q51875
H	710	GLN	-	expression tag	UNP Q51875
I	38	ILE	LEU	conflict	UNP Q51875
I	705	GLU	-	expression tag	UNP Q51875
I	706	ASN	-	expression tag	UNP Q51875
I	707	LEU	-	expression tag	UNP Q51875
I	708	TYR	-	expression tag	UNP Q51875
I	709	PHE	-	expression tag	UNP Q51875
I	710	GLN	-	expression tag	UNP Q51875
J	38	ILE	LEU	conflict	UNP Q51875
J	705	GLU	-	expression tag	UNP Q51875
J	706	ASN	-	expression tag	UNP Q51875
J	707	LEU	-	expression tag	UNP Q51875
J	708	TYR	-	expression tag	UNP Q51875
J	709	PHE	-	expression tag	UNP Q51875
J	710	GLN	-	expression tag	UNP Q51875
K	38	ILE	LEU	conflict	UNP Q51875
K	705	GLU	-	expression tag	UNP Q51875
K	706	ASN	-	expression tag	UNP Q51875
K	707	LEU	-	expression tag	UNP Q51875
K	708	TYR	-	expression tag	UNP Q51875
K	709	PHE	-	expression tag	UNP Q51875
K	710	GLN	-	expression tag	UNP Q51875
L	38	ILE	LEU	conflict	UNP Q51875

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Chain	Residue	Modelled	Actual	Comment	Reference
L	705	GLU	-	expression tag	UNP Q51875
L	706	ASN	-	expression tag	UNP Q51875
L	707	LEU	-	expression tag	UNP Q51875
L	708	TYR	-	expression tag	UNP Q51875
L	709	PHE	-	expression tag	UNP Q51875
L	710	GLN	-	expression tag	UNP Q51875
M	38	ILE	LEU	conflict	UNP Q51875
M	705	GLU	-	expression tag	UNP Q51875
M	706	ASN	-	expression tag	UNP Q51875
M	707	LEU	-	expression tag	UNP Q51875
M	708	TYR	-	expression tag	UNP Q51875
M	709	PHE	-	expression tag	UNP Q51875
M	710	GLN	-	expression tag	UNP Q51875
N	38	ILE	LEU	conflict	UNP Q51875
N	705	GLU	-	expression tag	UNP Q51875
N	706	ASN	-	expression tag	UNP Q51875
N	707	LEU	-	expression tag	UNP Q51875
N	708	TYR	-	expression tag	UNP Q51875
N	709	PHE	-	expression tag	UNP Q51875
N	710	GLN	-	expression tag	UNP Q51875
O	38	ILE	LEU	conflict	UNP Q51875
O	705	GLU	-	expression tag	UNP Q51875
O	706	ASN	-	expression tag	UNP Q51875
O	707	LEU	-	expression tag	UNP Q51875
O	708	TYR	-	expression tag	UNP Q51875
O	709	PHE	-	expression tag	UNP Q51875
O	710	GLN	-	expression tag	UNP Q51875
P	38	ILE	LEU	conflict	UNP Q51875
P	705	GLU	-	expression tag	UNP Q51875
P	706	ASN	-	expression tag	UNP Q51875
P	707	LEU	-	expression tag	UNP Q51875
P	708	TYR	-	expression tag	UNP Q51875
P	709	PHE	-	expression tag	UNP Q51875
P	710	GLN	-	expression tag	UNP Q51875
Q	38	ILE	LEU	conflict	UNP Q51875
Q	705	GLU	-	expression tag	UNP Q51875
Q	706	ASN	-	expression tag	UNP Q51875
Q	707	LEU	-	expression tag	UNP Q51875
Q	708	TYR	-	expression tag	UNP Q51875
Q	709	PHE	-	expression tag	UNP Q51875
Q	710	GLN	-	expression tag	UNP Q51875
R	38	ILE	LEU	conflict	UNP Q51875

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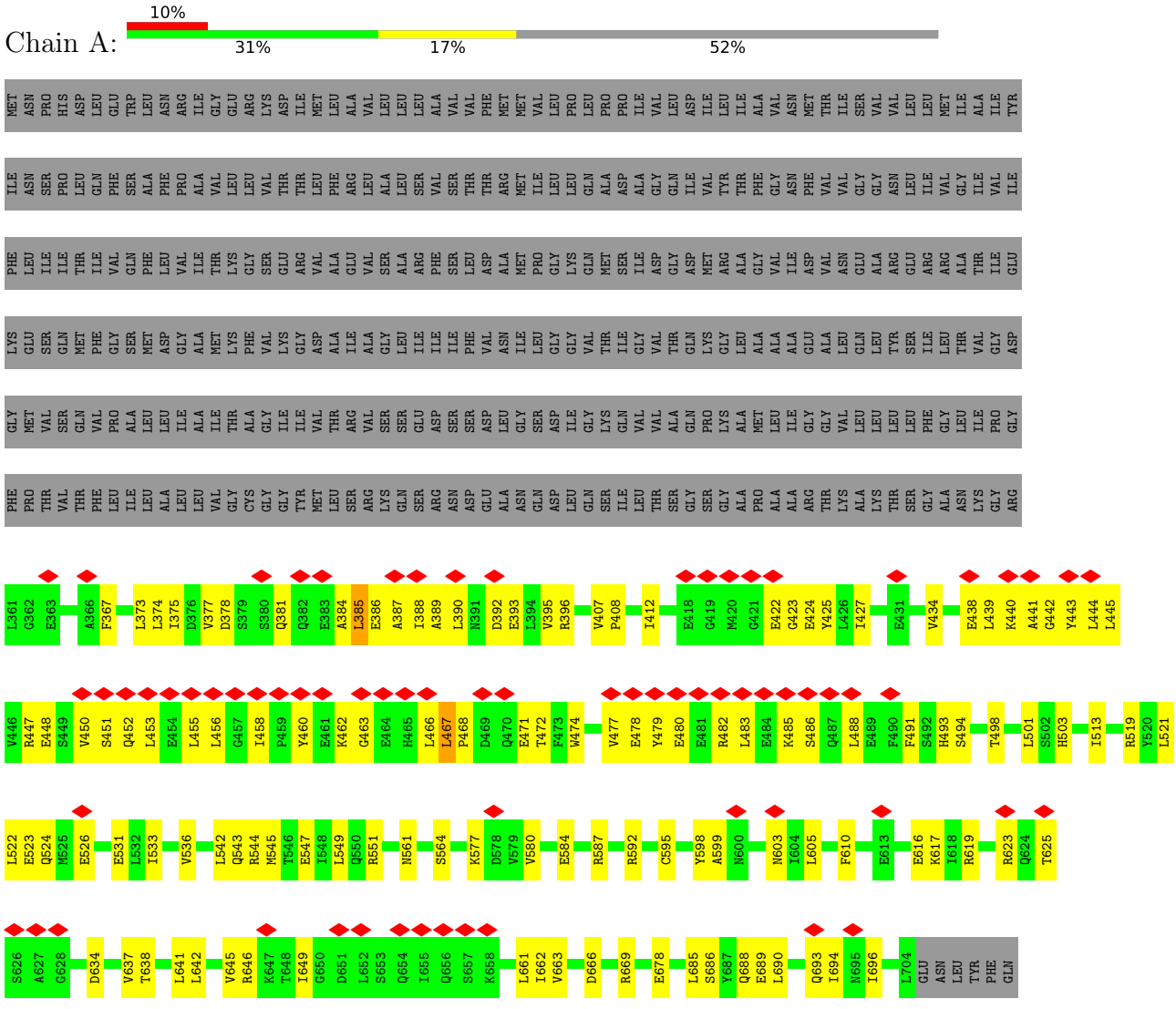
Chain	Residue	Modelled	Actual	Comment	Reference
R	705	GLU	-	expression tag	UNP Q51875
R	706	ASN	-	expression tag	UNP Q51875
R	707	LEU	-	expression tag	UNP Q51875
R	708	TYR	-	expression tag	UNP Q51875
R	709	PHE	-	expression tag	UNP Q51875
R	710	GLN	-	expression tag	UNP Q51875

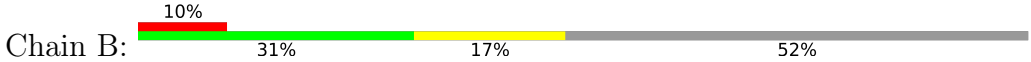
3 Residue-property plots (i)

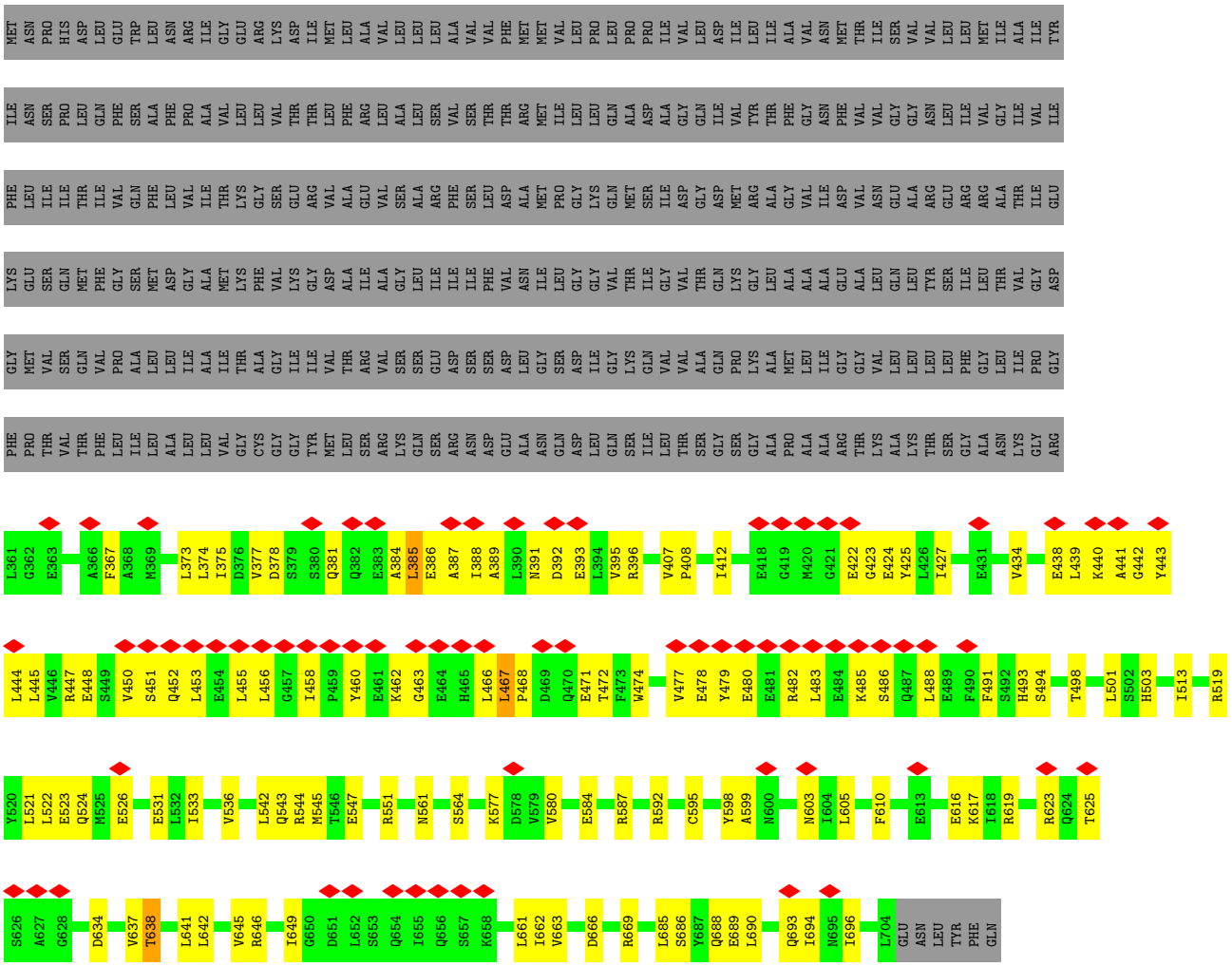
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



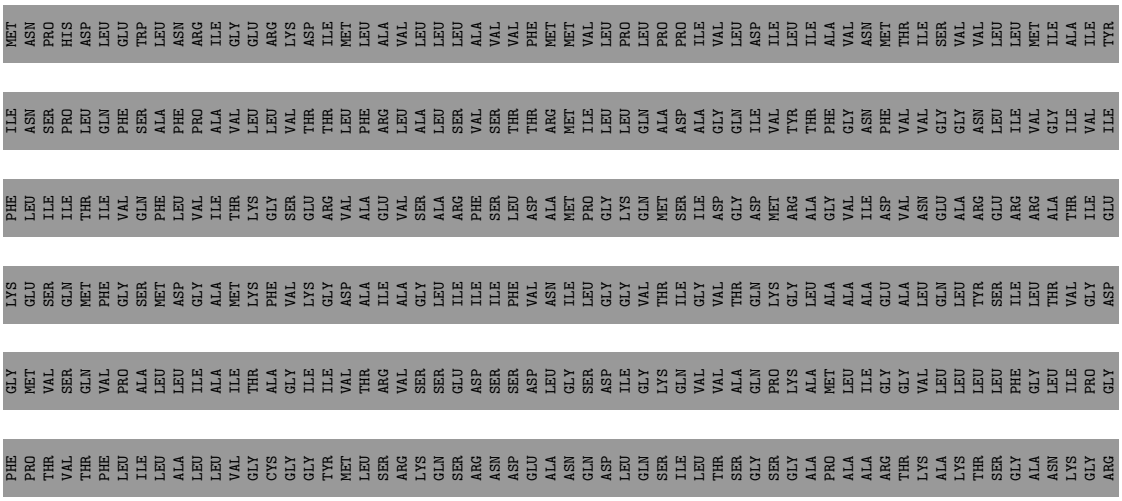
• Molecule 1: Low calcium response protein

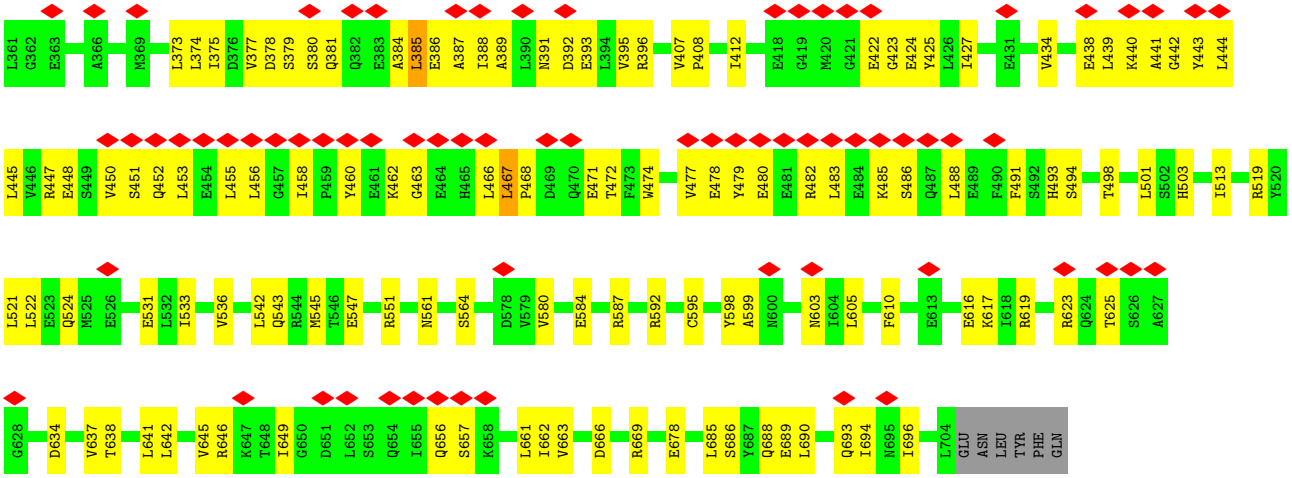




• Molecule 1: Low calcium response protein

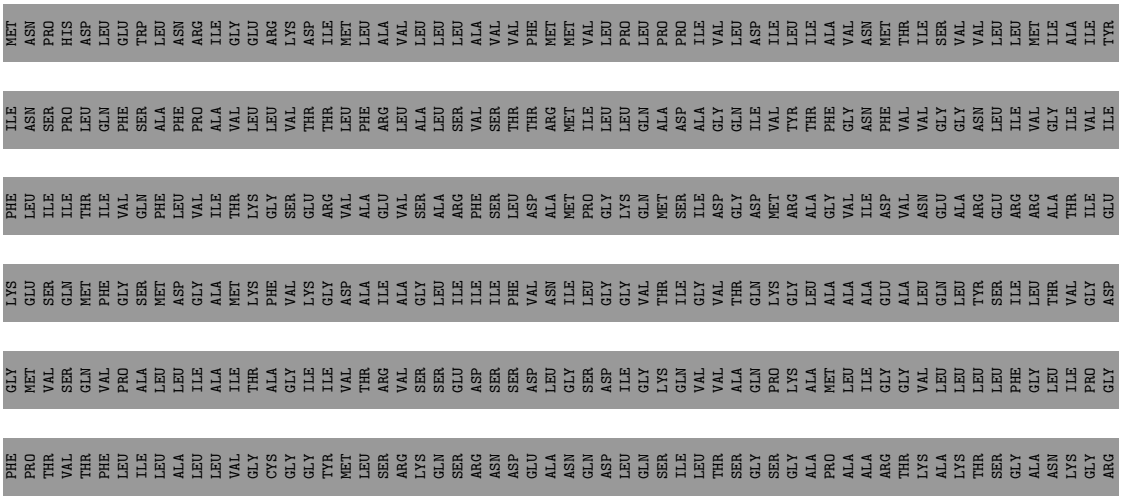
Chain C:

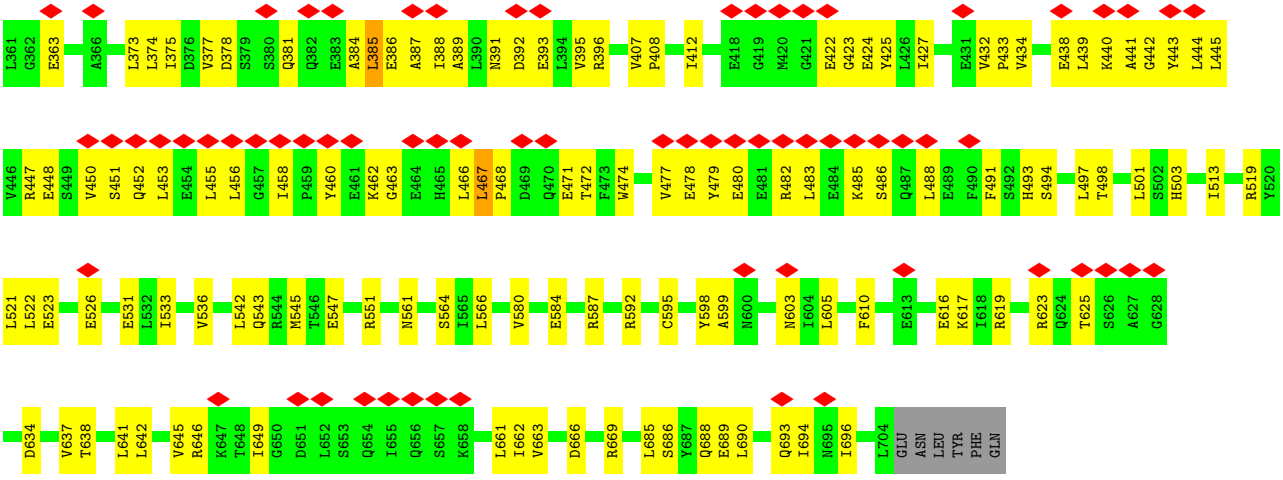




• Molecule 1: Low calcium response protein

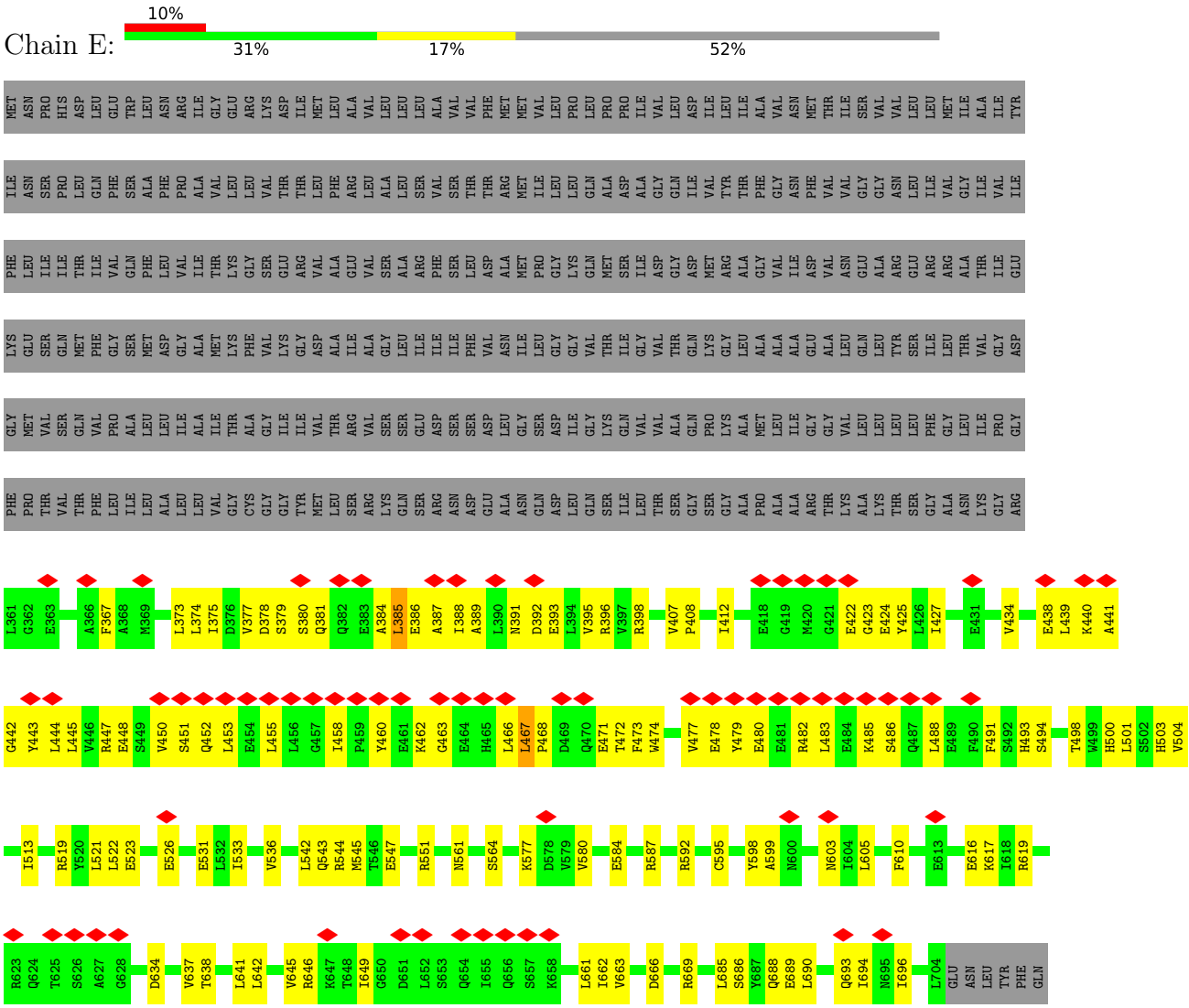
Chain D:





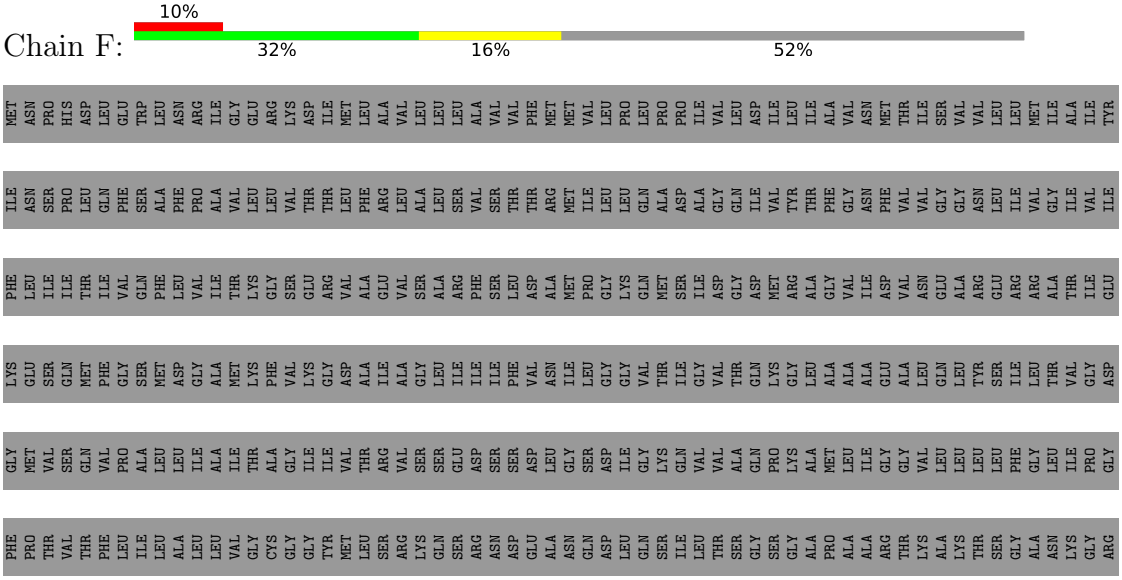
• Molecule 1: Low calcium response protein

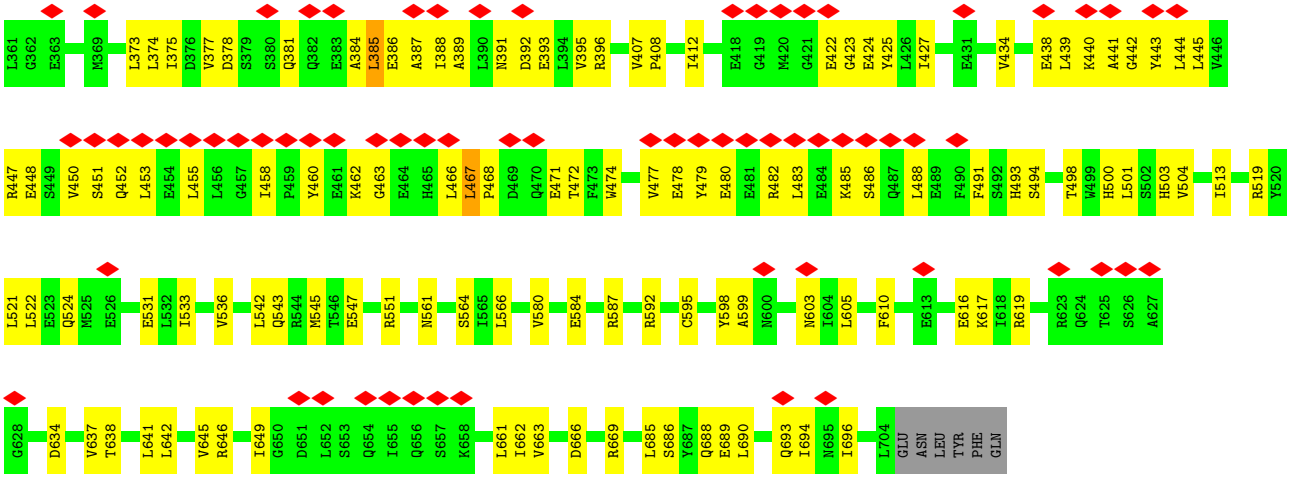
Chain E:



• Molecule 1: Low calcium response protein

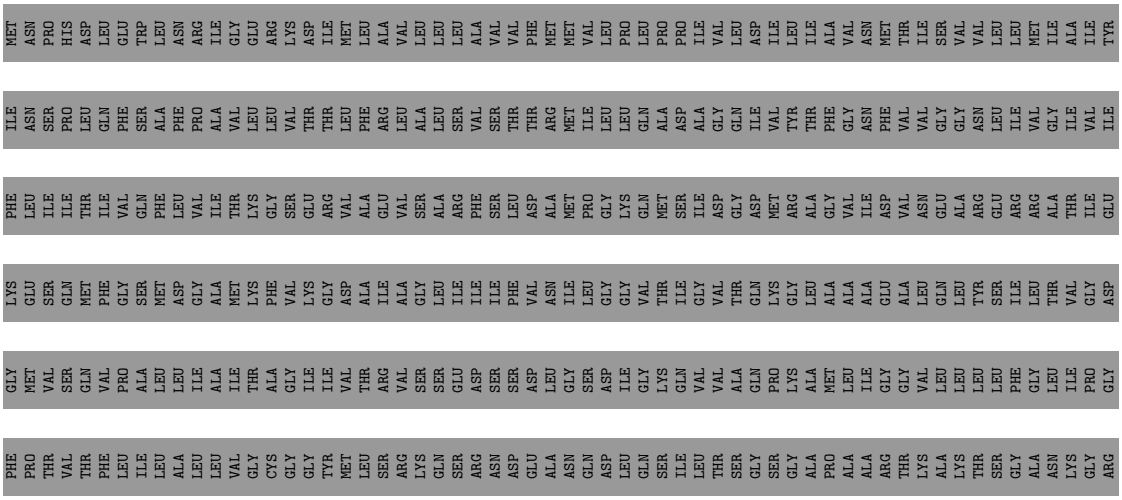
Chain F:

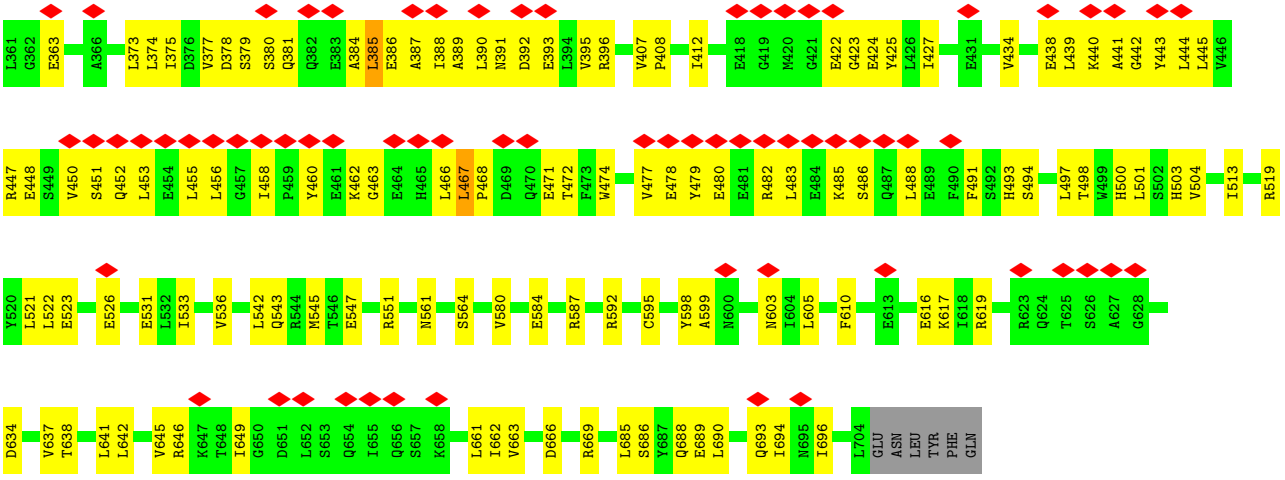




• Molecule 1: Low calcium response protein

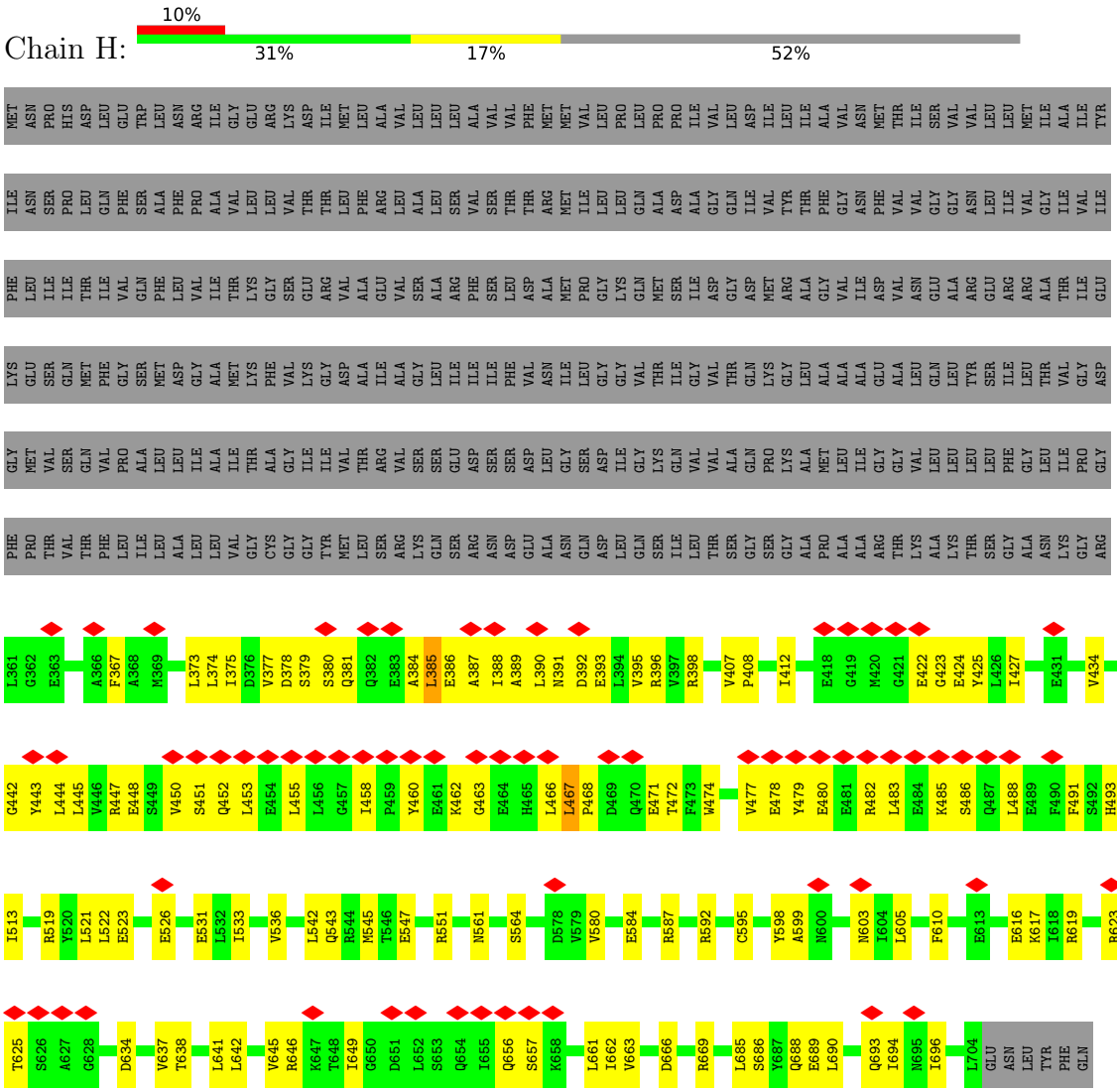
Chain G:





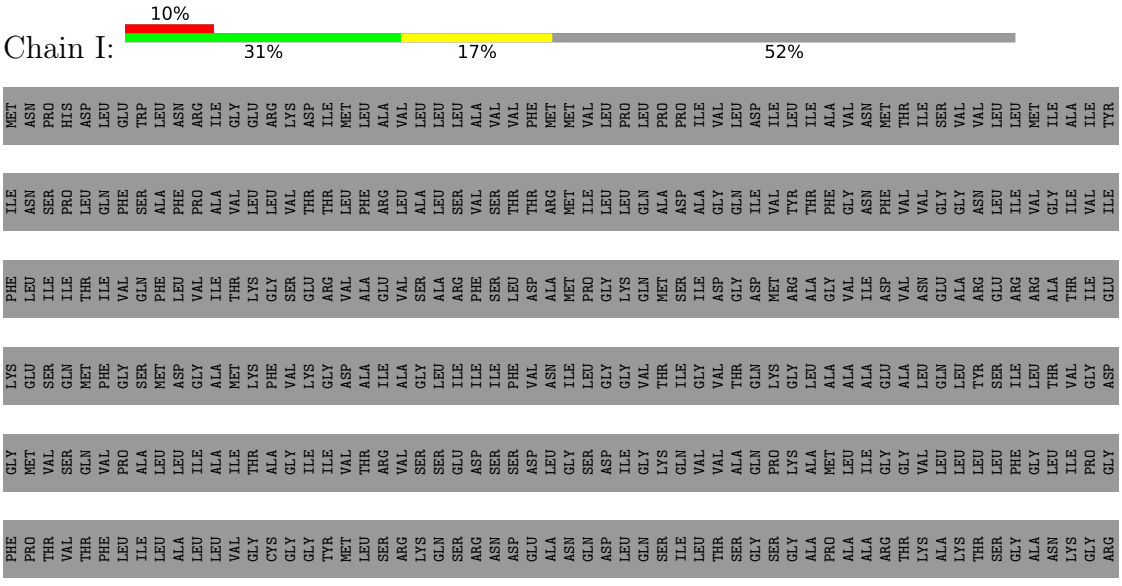
• Molecule 1: Low calcium response protein

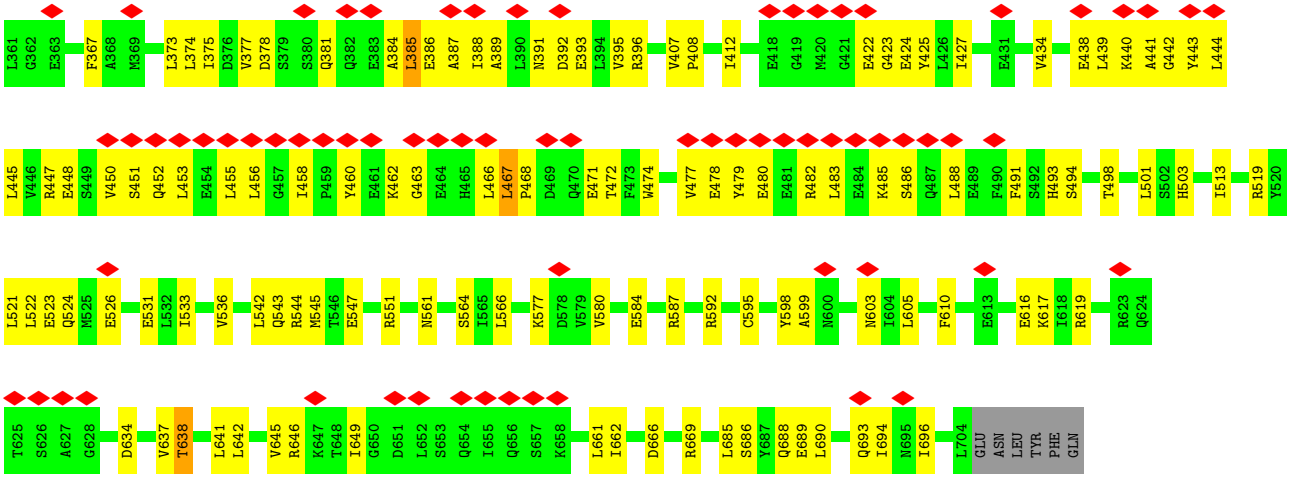
Chain H:



• Molecule 1: Low calcium response protein

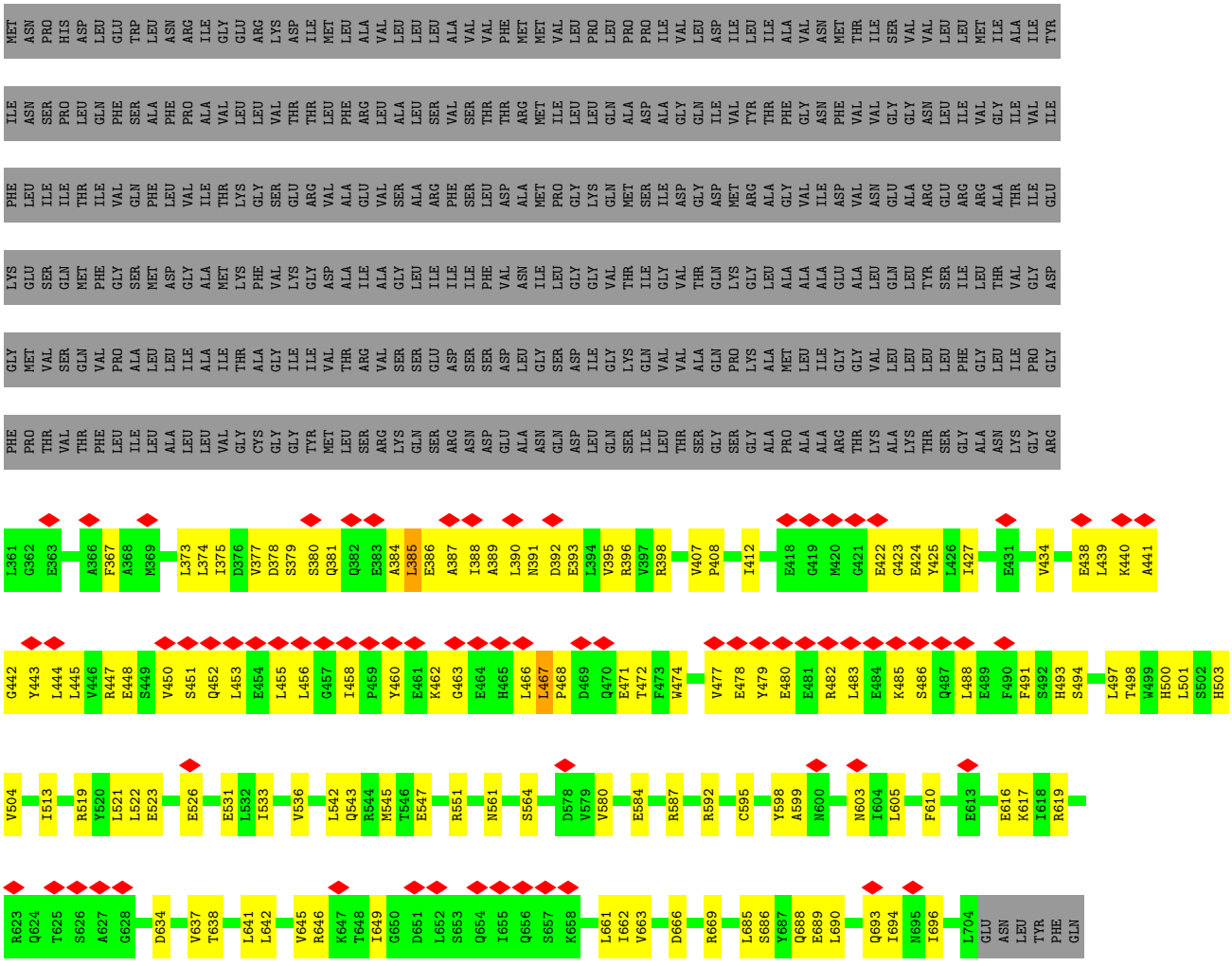
Chain I:





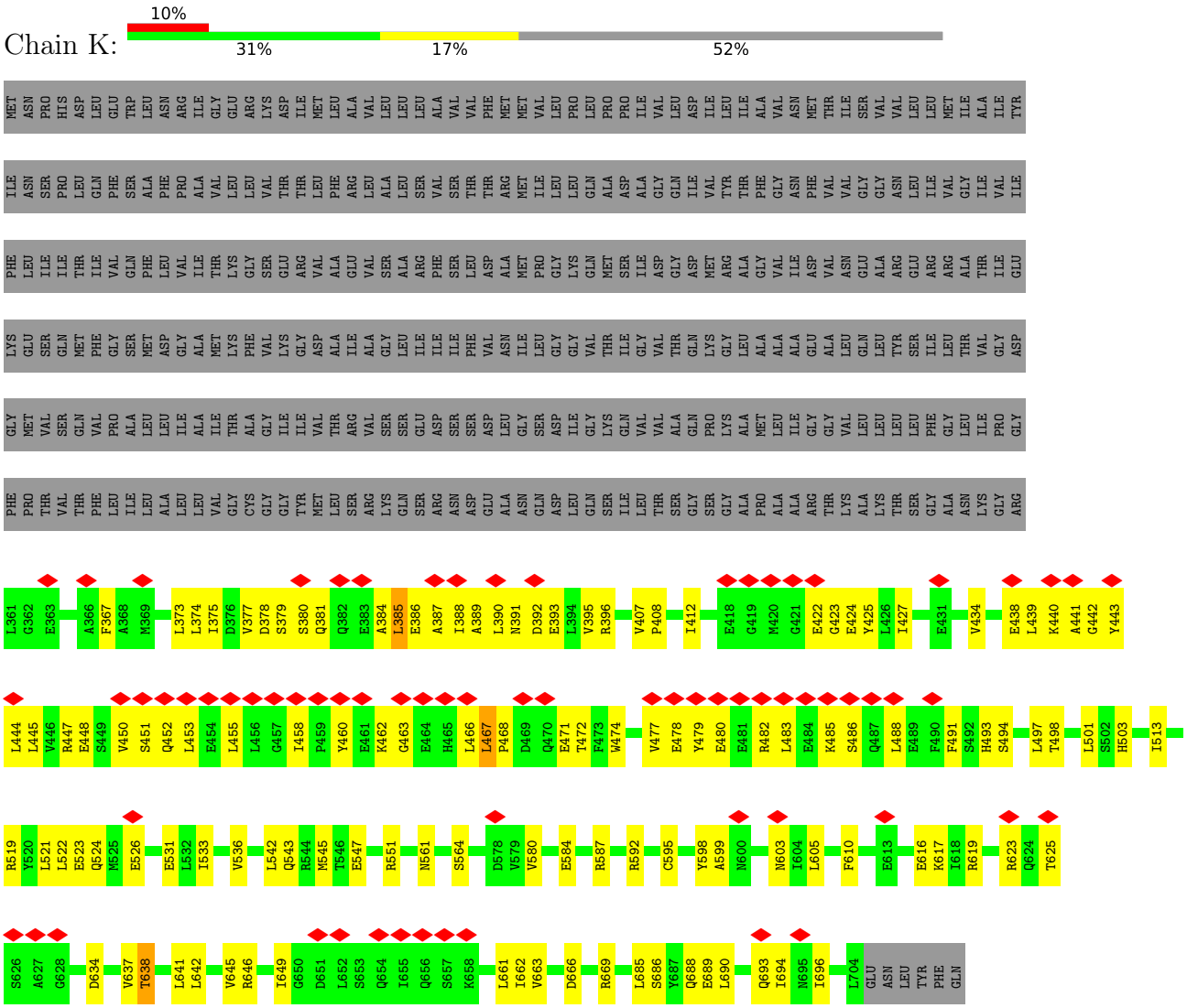
• Molecule 1: Low calcium response protein

Chain J:



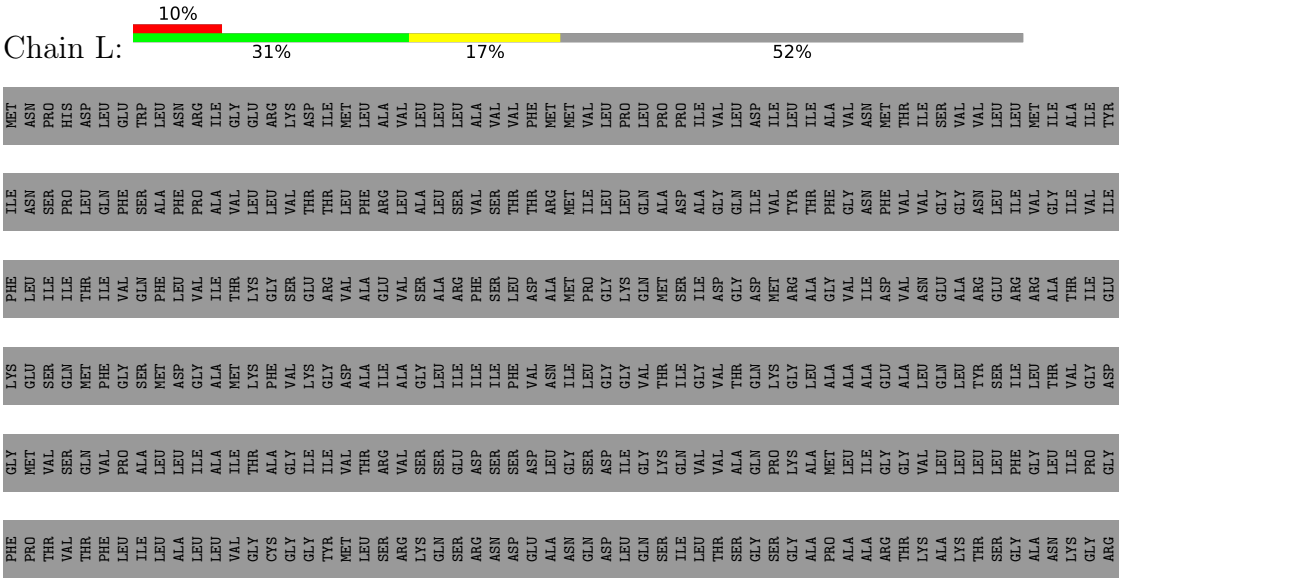
• Molecule 1: Low calcium response protein

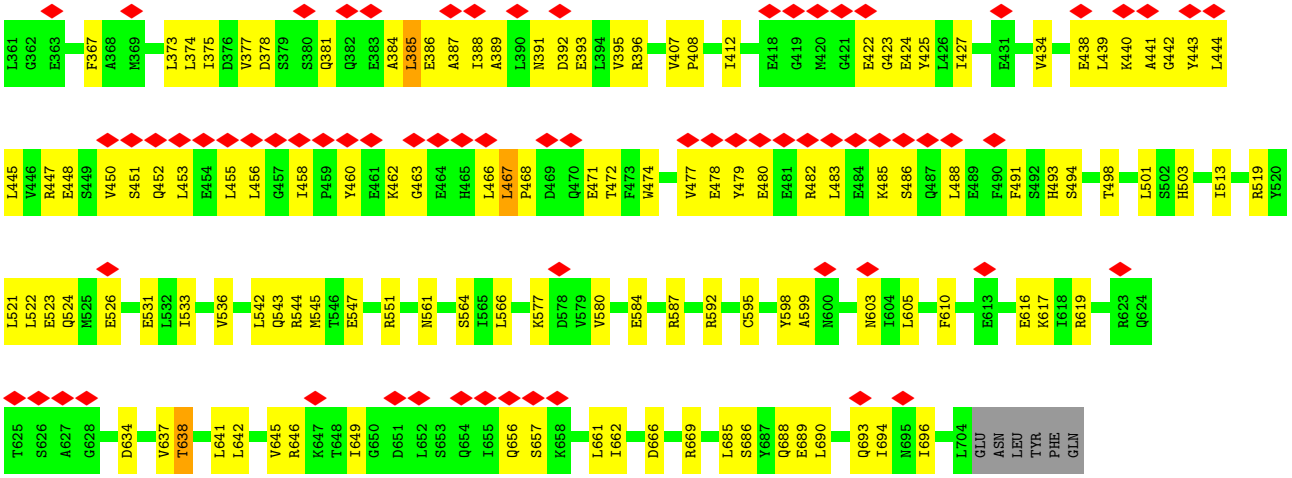
Chain K:



• Molecule 1: Low calcium response protein

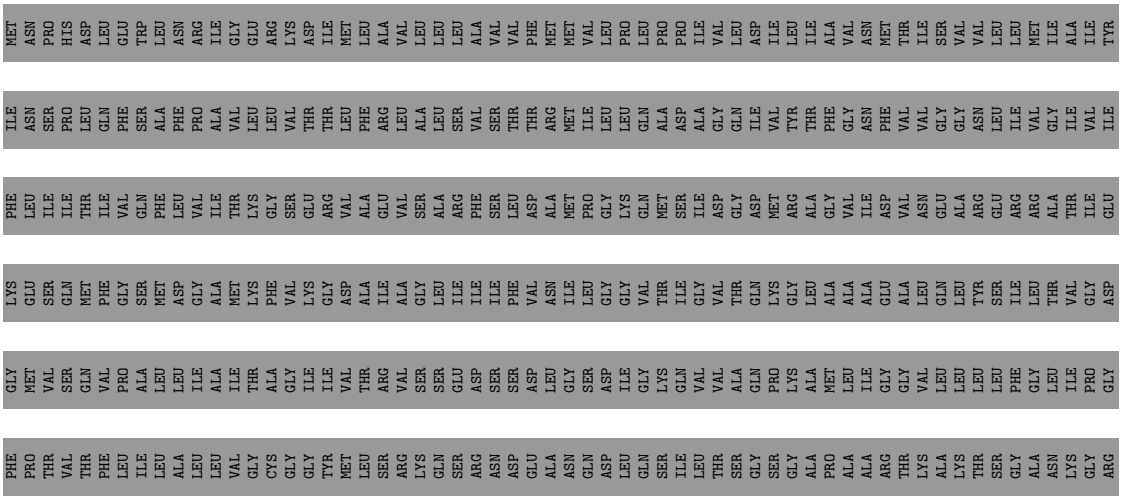
Chain L:

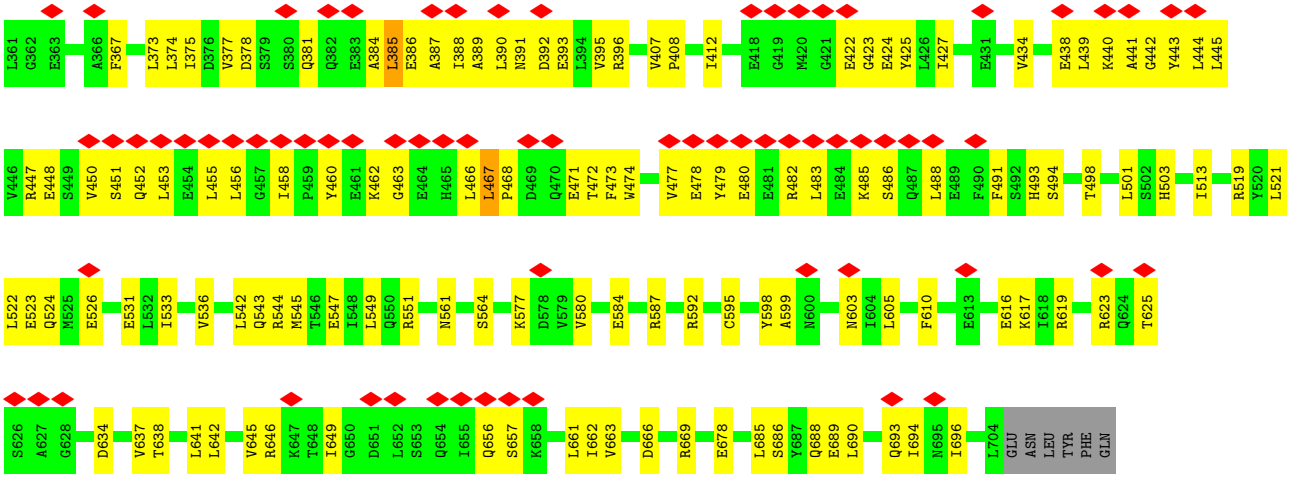




• Molecule 1: Low calcium response protein

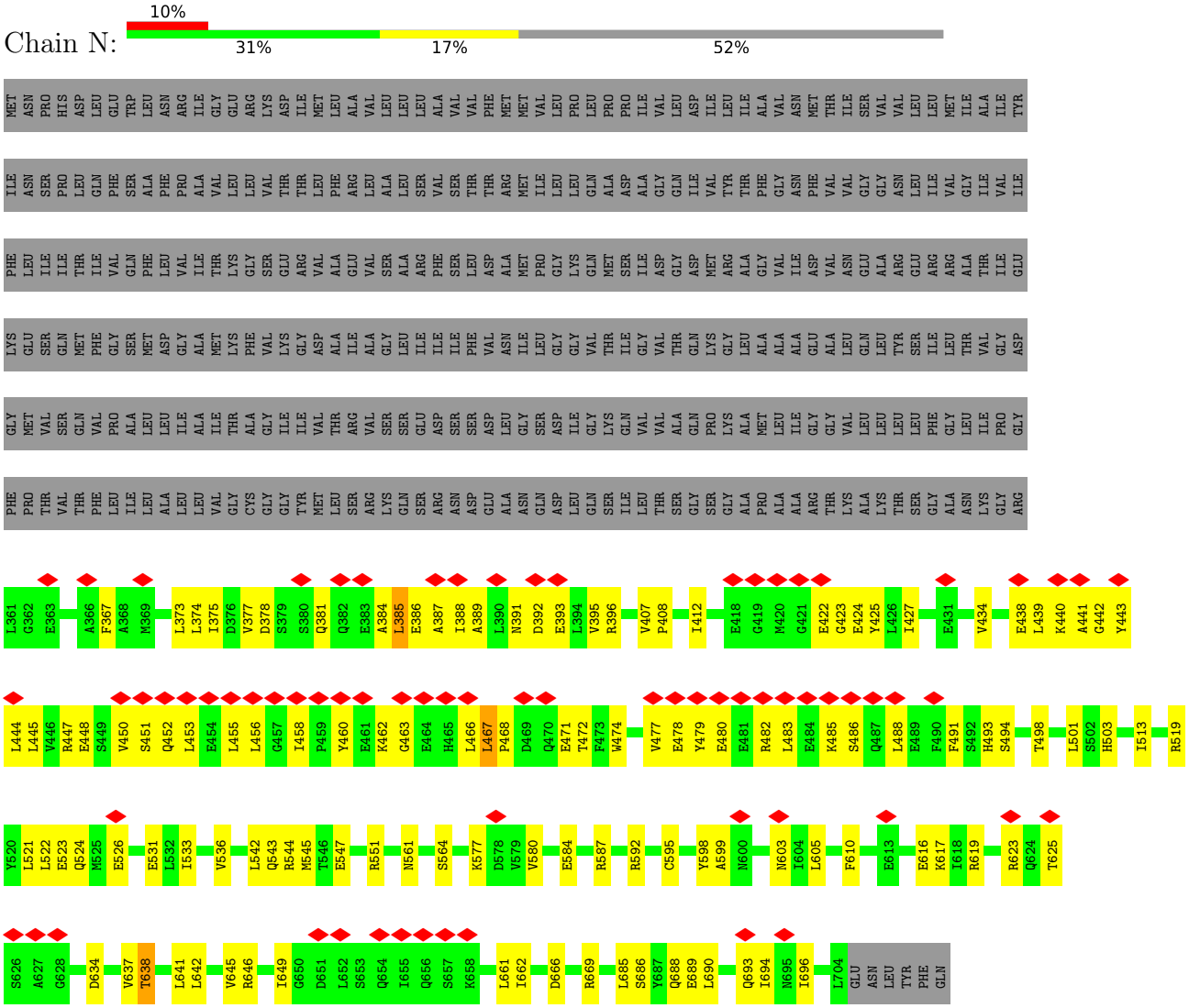
Chain M:





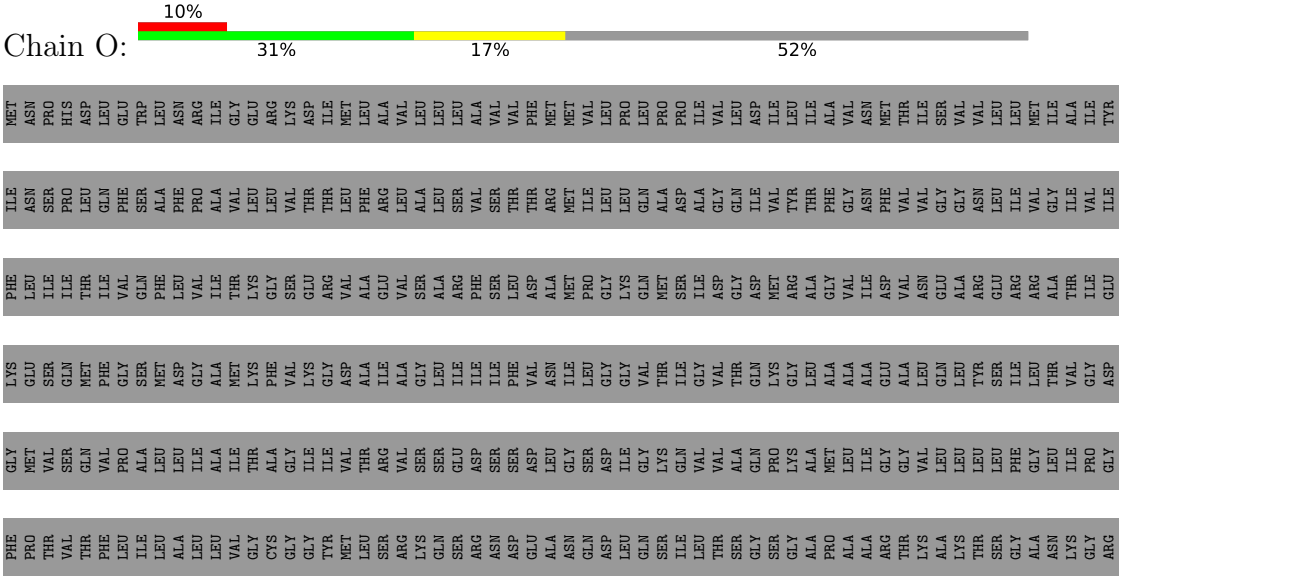
• Molecule 1: Low calcium response protein

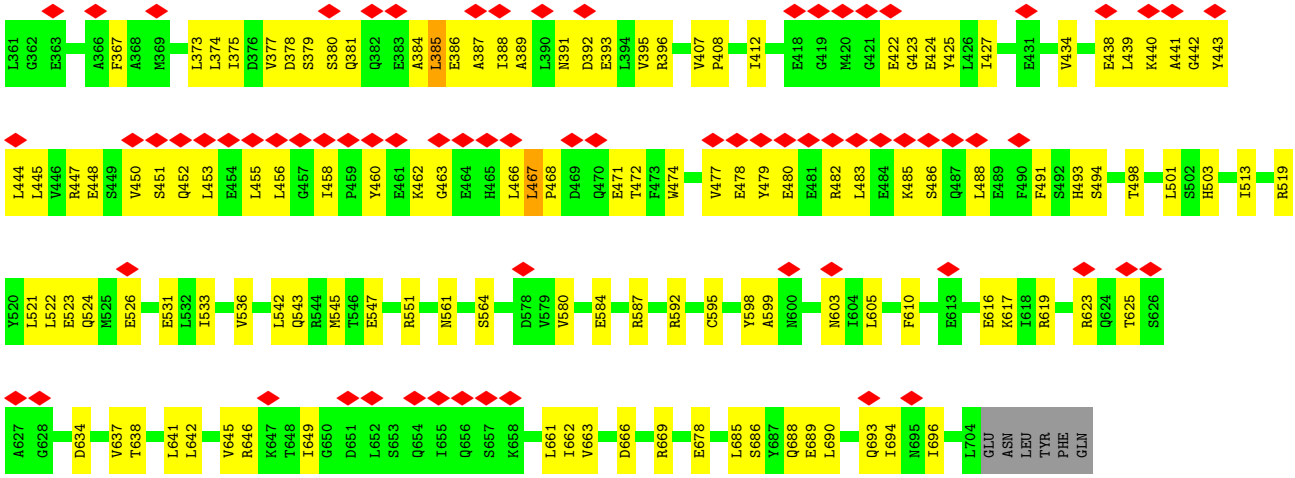
Chain N:



• Molecule 1: Low calcium response protein

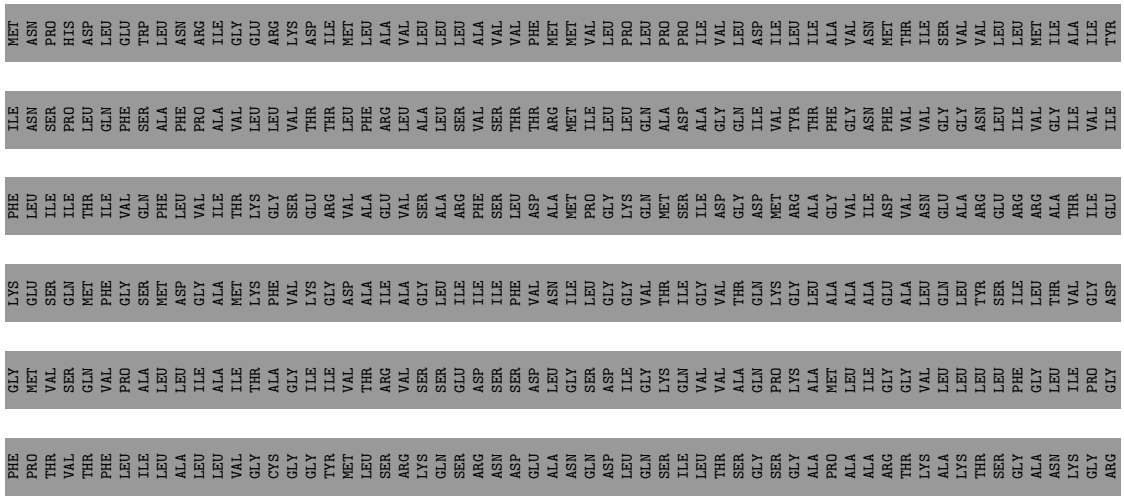
Chain O:

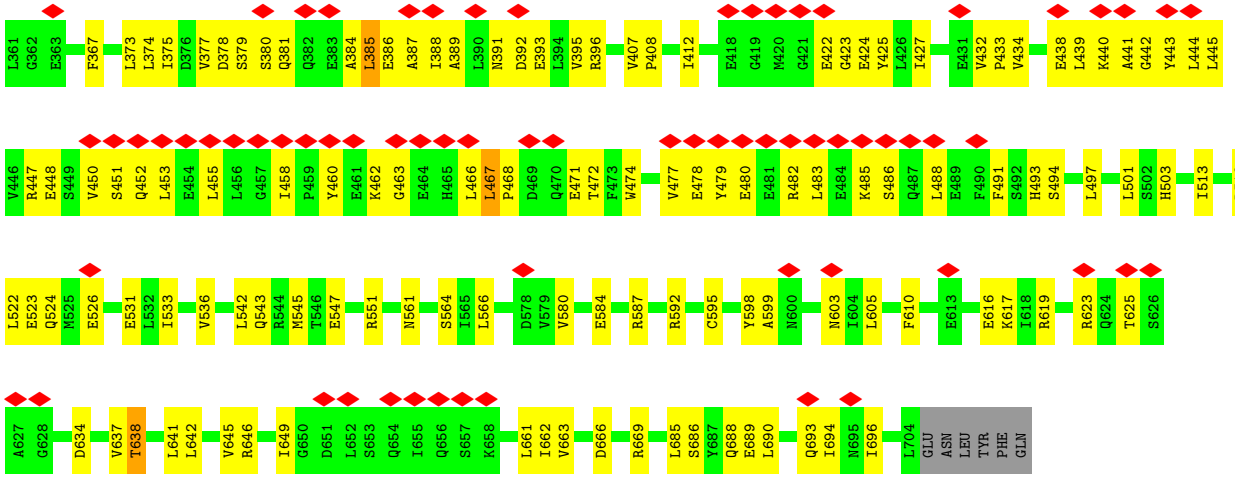




• Molecule 1: Low calcium response protein

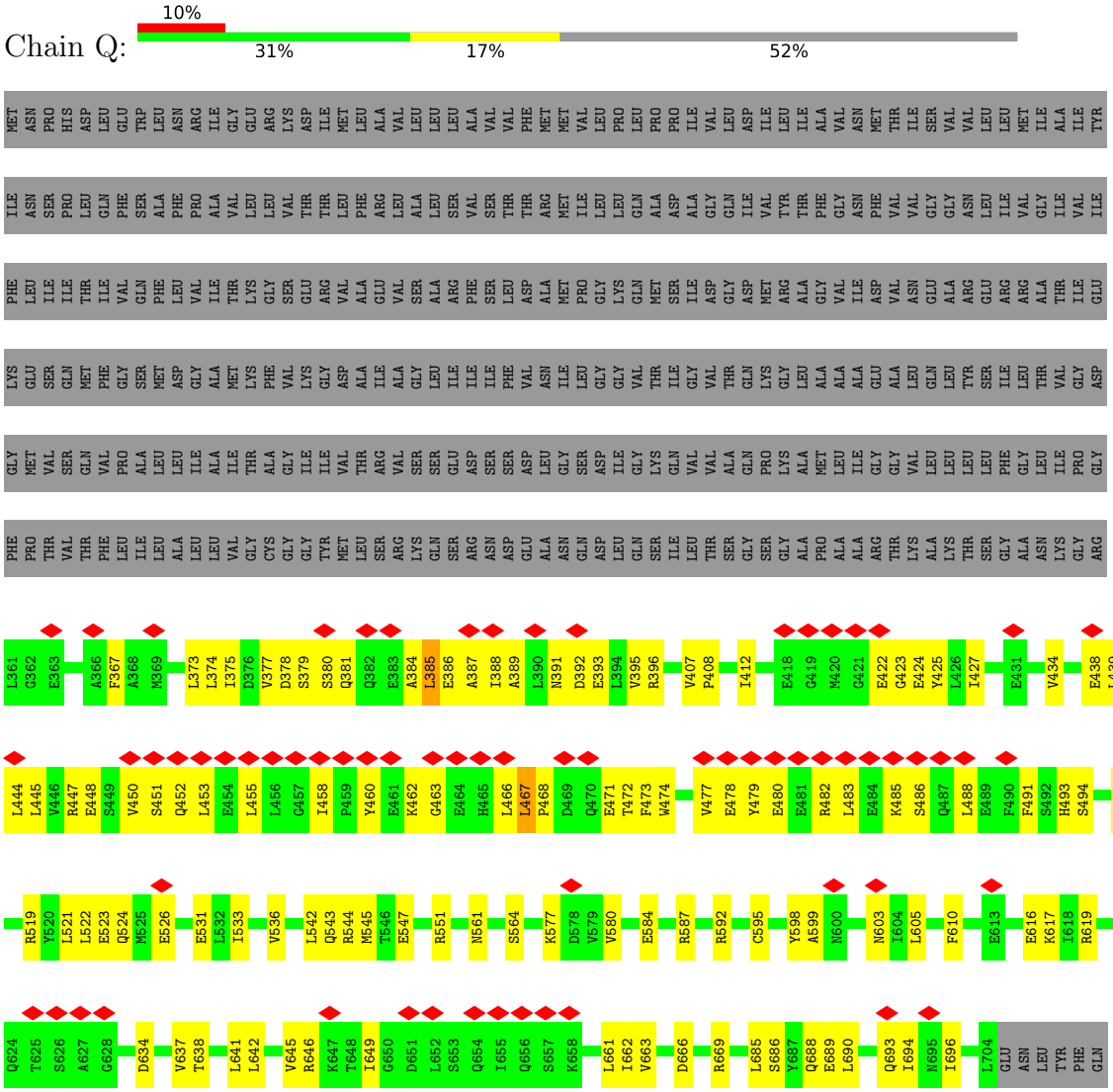
Chain P:





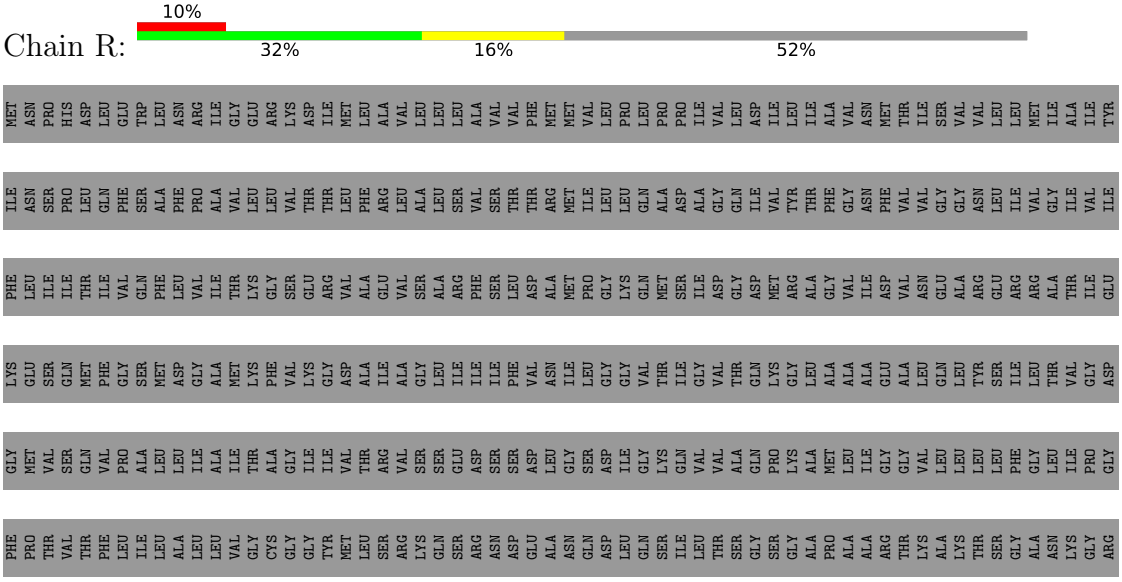
• Molecule 1: Low calcium response protein

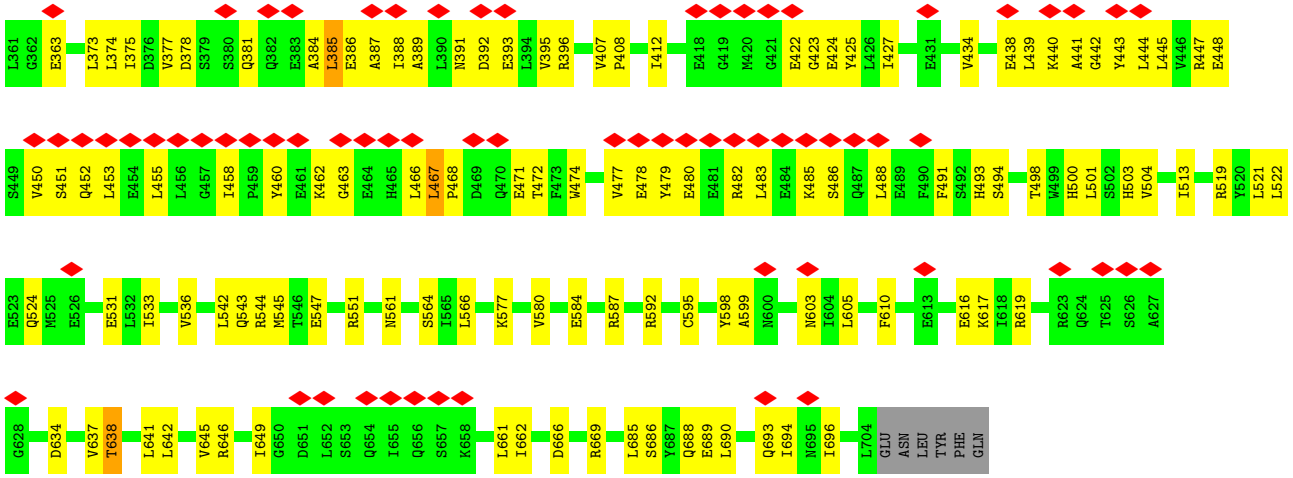
Chain Q:



• Molecule 1: Low calcium response protein

Chain R:




L361 G362 E363 L373 L374 I375 D376 V377 D378 S379 S380 Q381 Q382 E383 A384 L385 E386 A387 I388 A389 L390 N391 D392 E393 L394 V395 R396 V407 P408 I412 E418 G419 M420 G421 E422 G423 E424 Y425 L426 I427 E431 V434 E438 L439 K440 A441 G442 Y443 L444 L445 V446 R447 E448
S449 V450 S451 Q452 L453 E454 L455 L456 G457 I458 P459 Y460 E461 K462 G463 E464 H465 L466 I467 P468 D469 Q470 E471 T472 F473 W474 V477 E478 Y479 E480 E481 R482 L483 E484 K485 S486 Q487 L488 E489 F490 F491 S492 H493 S494 T498 W499 H500 L501 S502 H503 V504 I513 R519 Y520 L521 L522
E523 Q524 M525 E526 E531 L532 I533 V536 L542 Q543 R544 M545 T546 E547 R551 N561 S564 I565 L566 K577 V580 E584 R587 R592 C595 Y598 A599 N600 N603 I604 L605 F610 E613 E616 K617 I618 R619 R623 Q624 T625 S626 A627
G628 D634 V637 T638 L641 L642 V645 R646 I649 G650 D651 L652 S653 Q654 I655 Q656 S657 K658 L661 I662 D666 R669 L685 S686 Y687 Q688 E689 L690 Q693 I694 N695 I696 L704 GLU ASN LEU TYR PHE GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D9	Depositor
Number of particles used	15913	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 ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.047	Depositor
Minimum map value	-0.025	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0112	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	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	0.49	0/2834	0.55	0/3833
1	B	0.49	0/2834	0.55	0/3833
1	C	0.49	0/2834	0.55	0/3833
1	D	0.49	0/2834	0.55	0/3833
1	E	0.49	0/2834	0.55	0/3833
1	F	0.49	0/2834	0.55	0/3833
1	G	0.49	0/2834	0.55	0/3833
1	H	0.49	0/2834	0.55	0/3833
1	I	0.49	0/2834	0.55	0/3833
1	J	0.49	0/2834	0.55	0/3833
1	K	0.49	0/2834	0.55	0/3833
1	L	0.49	0/2834	0.55	0/3833
1	M	0.49	0/2834	0.55	0/3833
1	N	0.49	0/2834	0.55	0/3833
1	O	0.49	0/2834	0.55	0/3833
1	P	0.49	0/2834	0.55	0/3833
1	Q	0.49	0/2834	0.55	0/3833
1	R	0.49	0/2834	0.55	0/3833
All	All	0.49	0/51012	0.55	0/68994

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	A	0	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	4
1	G	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	4
1	I	0	4
1	J	0	4
1	K	0	4
1	L	0	4
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	4
1	Q	0	4
1	R	0	4
All	All	0	72

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (72) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	385	LEU	Peptide
1	A	388	ILE	Peptide
1	A	458	ILE	Peptide
1	A	467	LEU	Peptide
1	B	385	LEU	Peptide
1	B	388	ILE	Peptide
1	B	458	ILE	Peptide
1	B	467	LEU	Peptide
1	C	385	LEU	Peptide
1	C	388	ILE	Peptide
1	C	458	ILE	Peptide
1	C	467	LEU	Peptide
1	D	385	LEU	Peptide
1	D	388	ILE	Peptide
1	D	458	ILE	Peptide
1	D	467	LEU	Peptide
1	E	385	LEU	Peptide
1	E	388	ILE	Peptide
1	E	458	ILE	Peptide
1	E	467	LEU	Peptide
1	F	385	LEU	Peptide
1	F	388	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	F	458	ILE	Peptide
1	F	467	LEU	Peptide
1	G	385	LEU	Peptide
1	G	388	ILE	Peptide
1	G	458	ILE	Peptide
1	G	467	LEU	Peptide
1	H	385	LEU	Peptide
1	H	388	ILE	Peptide
1	H	458	ILE	Peptide
1	H	467	LEU	Peptide
1	I	385	LEU	Peptide
1	I	388	ILE	Peptide
1	I	458	ILE	Peptide
1	I	467	LEU	Peptide
1	J	385	LEU	Peptide
1	J	388	ILE	Peptide
1	J	458	ILE	Peptide
1	J	467	LEU	Peptide
1	K	385	LEU	Peptide
1	K	388	ILE	Peptide
1	K	458	ILE	Peptide
1	K	467	LEU	Peptide
1	L	385	LEU	Peptide
1	L	388	ILE	Peptide
1	L	458	ILE	Peptide
1	L	467	LEU	Peptide
1	M	385	LEU	Peptide
1	M	388	ILE	Peptide
1	M	458	ILE	Peptide
1	M	467	LEU	Peptide
1	N	385	LEU	Peptide
1	N	388	ILE	Peptide
1	N	458	ILE	Peptide
1	N	467	LEU	Peptide
1	O	385	LEU	Peptide
1	O	388	ILE	Peptide
1	O	458	ILE	Peptide
1	O	467	LEU	Peptide
1	P	385	LEU	Peptide
1	P	388	ILE	Peptide
1	P	458	ILE	Peptide
1	P	467	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	Q	385	LEU	Peptide
1	Q	388	ILE	Peptide
1	Q	458	ILE	Peptide
1	Q	467	LEU	Peptide
1	R	385	LEU	Peptide
1	R	388	ILE	Peptide
1	R	458	ILE	Peptide
1	R	467	LEU	Peptide

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	2786	0	2799	84	0
1	B	2786	0	2799	85	0
1	C	2786	0	2799	83	0
1	D	2786	0	2799	82	0
1	E	2786	0	2799	84	0
1	F	2786	0	2799	76	0
1	G	2786	0	2799	85	0
1	H	2786	0	2799	84	0
1	I	2786	0	2799	84	0
1	J	2786	0	2799	86	0
1	K	2786	0	2799	83	0
1	L	2786	0	2799	85	0
1	M	2786	0	2799	86	0
1	N	2786	0	2799	84	0
1	O	2786	0	2799	84	0
1	P	2786	0	2799	84	0
1	Q	2786	0	2799	84	0
1	R	2786	0	2799	79	0
All	All	50148	0	50382	1466	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 15.

All (1466) 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:F:385:LEU:O	1:F:387:ALA:N	2.15	0.80
1:R:385:LEU:O	1:R:387:ALA:N	2.15	0.80
1:E:385:LEU:O	1:E:387:ALA:N	2.15	0.80
1:Q:385:LEU:O	1:Q:387:ALA:N	2.15	0.80
1:G:385:LEU:O	1:G:387:ALA:N	2.15	0.80
1:J:385:LEU:O	1:J:387:ALA:N	2.15	0.80
1:D:385:LEU:O	1:D:387:ALA:N	2.15	0.79
1:P:385:LEU:O	1:P:387:ALA:N	2.15	0.79
1:H:385:LEU:O	1:H:387:ALA:N	2.15	0.79
1:K:385:LEU:O	1:K:387:ALA:N	2.15	0.79
1:A:385:LEU:O	1:A:387:ALA:N	2.15	0.79
1:M:385:LEU:O	1:M:387:ALA:N	2.15	0.79
1:O:385:LEU:O	1:O:387:ALA:N	2.15	0.79
1:C:385:LEU:O	1:C:387:ALA:N	2.15	0.79
1:I:385:LEU:O	1:I:387:ALA:N	2.15	0.78
1:L:385:LEU:O	1:L:387:ALA:N	2.15	0.78
1:B:385:LEU:O	1:B:387:ALA:N	2.15	0.78
1:N:385:LEU:O	1:N:387:ALA:N	2.15	0.78
1:G:519:ARG:HG2	1:H:531:GLU:HG2	1.68	0.76
1:D:519:ARG:HG2	1:E:531:GLU:HG2	1.69	0.75
1:J:531:GLU:HG2	1:R:519:ARG:HG2	1.71	0.73
1:J:519:ARG:HG2	1:K:531:GLU:HG2	1.72	0.72
1:K:519:ARG:HG2	1:L:531:GLU:HG2	1.72	0.72
1:A:531:GLU:HG2	1:I:519:ARG:HG2	1.72	0.72
1:E:519:ARG:HG2	1:F:531:GLU:HG2	1.72	0.72
1:L:444:LEU:HD13	1:L:477:VAL:HG11	1.72	0.72
1:M:519:ARG:HG2	1:N:531:GLU:HG2	1.72	0.72
1:A:519:ARG:HG2	1:B:531:GLU:HG2	1.72	0.71
1:H:519:ARG:HG2	1:I:531:GLU:HG2	1.72	0.71
1:I:444:LEU:HD13	1:I:477:VAL:HG11	1.72	0.71
1:L:519:ARG:HG2	1:M:531:GLU:HG2	1.72	0.71
1:F:444:LEU:HD13	1:F:477:VAL:HG11	1.72	0.71
1:R:444:LEU:HD13	1:R:477:VAL:HG11	1.72	0.71
1:H:444:LEU:HD13	1:H:477:VAL:HG11	1.72	0.71
1:N:519:ARG:HG2	1:O:531:GLU:HG2	1.72	0.71
1:K:444:LEU:HD13	1:K:477:VAL:HG11	1.72	0.71
1:P:519:ARG:HG2	1:Q:531:GLU:HG2	1.71	0.71
1:B:519:ARG:HG2	1:C:531:GLU:HG2	1.72	0.71
1:J:444:LEU:HD13	1:J:477:VAL:HG11	1.72	0.71
1:G:444:LEU:HD13	1:G:477:VAL:HG11	1.72	0.71
1:B:444:LEU:HD13	1:B:477:VAL:HG11	1.72	0.70
1:N:444:LEU:HD13	1:N:477:VAL:HG11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:519:ARG:HG2	1:P:531:GLU:HG2	1.73	0.70
1:P:444:LEU:HD13	1:P:477:VAL:HG11	1.72	0.70
1:D:444:LEU:HD13	1:D:477:VAL:HG11	1.72	0.70
1:M:444:LEU:HD13	1:M:477:VAL:HG11	1.72	0.70
1:A:444:LEU:HD13	1:A:477:VAL:HG11	1.72	0.69
1:C:444:LEU:HD13	1:C:477:VAL:HG11	1.72	0.69
1:O:444:LEU:HD13	1:O:477:VAL:HG11	1.72	0.69
1:D:407:VAL:HG22	1:D:513:ILE:HD11	1.74	0.69
1:E:444:LEU:HD13	1:E:477:VAL:HG11	1.72	0.69
1:N:407:VAL:HG22	1:N:513:ILE:HD11	1.74	0.69
1:A:407:VAL:HG22	1:A:513:ILE:HD11	1.74	0.69
1:B:407:VAL:HG22	1:B:513:ILE:HD11	1.74	0.69
1:M:407:VAL:HG22	1:M:513:ILE:HD11	1.74	0.69
1:P:407:VAL:HG22	1:P:513:ILE:HD11	1.74	0.69
1:Q:444:LEU:HD13	1:Q:477:VAL:HG11	1.72	0.69
1:J:407:VAL:HG22	1:J:513:ILE:HD11	1.74	0.68
1:E:378:ASP:OD2	1:E:424:GLU:N	2.27	0.68
1:G:407:VAL:HG22	1:G:513:ILE:HD11	1.74	0.68
1:K:407:VAL:HG22	1:K:513:ILE:HD11	1.74	0.68
1:C:407:VAL:HG22	1:C:513:ILE:HD11	1.74	0.68
1:Q:378:ASP:OD2	1:Q:424:GLU:N	2.27	0.68
1:D:378:ASP:OD2	1:D:424:GLU:N	2.27	0.68
1:H:407:VAL:HG22	1:H:513:ILE:HD11	1.74	0.68
1:O:407:VAL:HG22	1:O:513:ILE:HD11	1.74	0.68
1:P:378:ASP:OD2	1:P:424:GLU:N	2.27	0.68
1:R:407:VAL:HG22	1:R:513:ILE:HD11	1.74	0.68
1:F:378:ASP:OD2	1:F:424:GLU:N	2.27	0.68
1:F:407:VAL:HG22	1:F:513:ILE:HD11	1.74	0.68
1:Q:519:ARG:HG2	1:R:531:GLU:HG2	1.75	0.68
1:G:688:GLN:N	1:G:688:GLN:OE1	2.28	0.67
1:J:688:GLN:N	1:J:688:GLN:OE1	2.28	0.67
1:K:447:ARG:NH2	1:K:472:THR:OG1	2.21	0.67
1:Q:407:VAL:HG22	1:Q:513:ILE:HD11	1.74	0.67
1:A:688:GLN:N	1:A:688:GLN:OE1	2.28	0.67
1:I:407:VAL:HG22	1:I:513:ILE:HD11	1.74	0.67
1:Q:447:ARG:NH2	1:Q:472:THR:OG1	2.21	0.67
1:E:688:GLN:N	1:E:688:GLN:OE1	2.28	0.67
1:L:407:VAL:HG22	1:L:513:ILE:HD11	1.74	0.67
1:L:447:ARG:NH2	1:L:472:THR:OG1	2.21	0.67
1:M:688:GLN:N	1:M:688:GLN:OE1	2.28	0.67
1:Q:688:GLN:N	1:Q:688:GLN:OE1	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:407:VAL:HG22	1:E:513:ILE:HD11	1.74	0.67
1:H:447:ARG:NH2	1:H:472:THR:OG1	2.21	0.67
1:H:688:GLN:N	1:H:688:GLN:OE1	2.28	0.67
1:L:688:GLN:N	1:L:688:GLN:OE1	2.28	0.67
1:E:447:ARG:NH2	1:E:472:THR:OG1	2.21	0.67
1:K:688:GLN:OE1	1:K:688:GLN:N	2.28	0.67
1:N:378:ASP:OD2	1:N:424:GLU:N	2.27	0.67
1:I:447:ARG:NH2	1:I:472:THR:OG1	2.21	0.67
1:I:688:GLN:OE1	1:I:688:GLN:N	2.28	0.67
1:P:688:GLN:OE1	1:P:688:GLN:N	2.28	0.67
1:R:688:GLN:N	1:R:688:GLN:OE1	2.28	0.67
1:B:378:ASP:OD2	1:B:424:GLU:N	2.27	0.67
1:C:688:GLN:N	1:C:688:GLN:OE1	2.28	0.67
1:D:688:GLN:OE1	1:D:688:GLN:N	2.28	0.67
1:E:599:ALA:HB2	1:E:605:LEU:HD13	1.77	0.67
1:F:688:GLN:OE1	1:F:688:GLN:N	2.28	0.67
1:M:378:ASP:OD2	1:M:424:GLU:N	2.27	0.67
1:O:688:GLN:N	1:O:688:GLN:OE1	2.28	0.67
1:Q:599:ALA:HB2	1:Q:605:LEU:HD13	1.77	0.67
1:C:599:ALA:HB2	1:C:605:LEU:HD13	1.77	0.66
1:K:478:GLU:N	1:K:478:GLU:OE1	2.28	0.66
1:O:599:ALA:HB2	1:O:605:LEU:HD13	1.77	0.66
1:R:543:GLN:NE2	1:R:547:GLU:OE1	2.28	0.66
1:R:599:ALA:HB2	1:R:605:LEU:HD13	1.77	0.66
1:A:378:ASP:OD2	1:A:424:GLU:N	2.27	0.66
1:F:543:GLN:NE2	1:F:547:GLU:OE1	2.28	0.66
1:F:599:ALA:HB2	1:F:605:LEU:HD13	1.77	0.66
1:H:478:GLU:N	1:H:478:GLU:OE1	2.28	0.66
1:P:599:ALA:HB2	1:P:605:LEU:HD13	1.77	0.66
1:D:599:ALA:HB2	1:D:605:LEU:HD13	1.77	0.66
1:H:378:ASP:OD2	1:H:424:GLU:N	2.27	0.66
1:H:543:GLN:NE2	1:H:547:GLU:OE1	2.28	0.66
1:K:378:ASP:OD2	1:K:424:GLU:N	2.27	0.66
1:K:543:GLN:NE2	1:K:547:GLU:OE1	2.28	0.66
1:E:543:GLN:NE2	1:E:547:GLU:OE1	2.28	0.66
1:J:447:ARG:NH2	1:J:472:THR:OG1	2.21	0.66
1:N:688:GLN:OE1	1:N:688:GLN:N	2.28	0.66
1:O:378:ASP:OD2	1:O:424:GLU:N	2.27	0.66
1:Q:543:GLN:NE2	1:Q:547:GLU:OE1	2.28	0.66
1:G:543:GLN:NE2	1:G:547:GLU:OE1	2.28	0.66
1:I:478:GLU:OE1	1:I:478:GLU:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:543:GLN:NE2	1:J:547:GLU:OE1	2.28	0.66
1:B:688:GLN:N	1:B:688:GLN:OE1	2.28	0.66
1:C:378:ASP:OD2	1:C:424:GLU:N	2.27	0.66
1:G:447:ARG:NH2	1:G:472:THR:OG1	2.21	0.66
1:J:478:GLU:N	1:J:478:GLU:OE1	2.28	0.66
1:M:447:ARG:NH2	1:M:472:THR:OG1	2.21	0.66
1:G:478:GLU:OE1	1:G:478:GLU:N	2.29	0.66
1:L:478:GLU:OE1	1:L:478:GLU:N	2.29	0.66
1:R:392:ASP:HA	1:R:395:VAL:HG12	1.78	0.66
1:B:478:GLU:OE1	1:B:478:GLU:N	2.28	0.66
1:F:392:ASP:HA	1:F:395:VAL:HG12	1.78	0.66
1:N:478:GLU:OE1	1:N:478:GLU:N	2.29	0.66
1:L:378:ASP:OD2	1:L:424:GLU:N	2.27	0.66
1:A:447:ARG:NH2	1:A:472:THR:OG1	2.21	0.65
1:B:543:GLN:NE2	1:B:547:GLU:OE1	2.28	0.65
1:B:599:ALA:HB2	1:B:605:LEU:HD13	1.77	0.65
1:C:543:GLN:NE2	1:C:547:GLU:OE1	2.28	0.65
1:J:599:ALA:HB2	1:J:605:LEU:HD13	1.77	0.65
1:O:543:GLN:NE2	1:O:547:GLU:OE1	2.28	0.65
1:G:599:ALA:HB2	1:G:605:LEU:HD13	1.77	0.65
1:I:378:ASP:OD2	1:I:424:GLU:N	2.27	0.65
1:N:543:GLN:NE2	1:N:547:GLU:OE1	2.28	0.65
1:N:599:ALA:HB2	1:N:605:LEU:HD13	1.77	0.65
1:P:543:GLN:NE2	1:P:547:GLU:OE1	2.28	0.65
1:C:478:GLU:OE1	1:C:478:GLU:N	2.28	0.65
1:D:543:GLN:NE2	1:D:547:GLU:OE1	2.28	0.65
1:O:478:GLU:OE1	1:O:478:GLU:N	2.28	0.65
1:H:392:ASP:HA	1:H:395:VAL:HG12	1.78	0.65
1:B:392:ASP:HA	1:B:395:VAL:HG12	1.78	0.65
1:F:445:LEU:HG	1:F:474:TRP:HB3	1.79	0.65
1:G:445:LEU:HG	1:G:474:TRP:HB3	1.79	0.65
1:J:445:LEU:HG	1:J:474:TRP:HB3	1.79	0.65
1:K:392:ASP:HA	1:K:395:VAL:HG12	1.78	0.65
1:R:445:LEU:HG	1:R:474:TRP:HB3	1.79	0.65
1:A:599:ALA:HB2	1:A:605:LEU:HD13	1.77	0.65
1:E:445:LEU:HG	1:E:474:TRP:HB3	1.79	0.65
1:I:543:GLN:NE2	1:I:547:GLU:OE1	2.28	0.65
1:L:543:GLN:NE2	1:L:547:GLU:OE1	2.28	0.65
1:M:599:ALA:HB2	1:M:605:LEU:HD13	1.77	0.65
1:N:392:ASP:HA	1:N:395:VAL:HG12	1.78	0.65
1:Q:392:ASP:HA	1:Q:395:VAL:HG12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:445:LEU:HG	1:Q:474:TRP:HB3	1.79	0.65
1:R:378:ASP:OD2	1:R:424:GLU:N	2.27	0.65
1:D:445:LEU:HG	1:D:474:TRP:HB3	1.79	0.65
1:J:392:ASP:HA	1:J:395:VAL:HG12	1.78	0.65
1:K:445:LEU:HG	1:K:474:TRP:HB3	1.79	0.65
1:A:478:GLU:N	1:A:478:GLU:OE1	2.28	0.65
1:C:445:LEU:HG	1:C:474:TRP:HB3	1.79	0.65
1:E:392:ASP:HA	1:E:395:VAL:HG12	1.78	0.65
1:G:378:ASP:OD2	1:G:424:GLU:N	2.27	0.65
1:G:392:ASP:HA	1:G:395:VAL:HG12	1.78	0.65
1:I:599:ALA:HB2	1:I:605:LEU:HD13	1.77	0.65
1:J:378:ASP:OD2	1:J:424:GLU:N	2.27	0.65
1:P:445:LEU:HG	1:P:474:TRP:HB3	1.79	0.65
1:A:543:GLN:NE2	1:A:547:GLU:OE1	2.28	0.65
1:D:392:ASP:HA	1:D:395:VAL:HG12	1.78	0.65
1:H:445:LEU:HG	1:H:474:TRP:HB3	1.79	0.65
1:O:392:ASP:HA	1:O:395:VAL:HG12	1.78	0.65
1:Q:662:ILE:HD13	1:Q:690:LEU:HD11	1.79	0.65
1:R:447:ARG:NH2	1:R:472:THR:OG1	2.21	0.65
1:E:662:ILE:HD13	1:E:690:LEU:HD11	1.79	0.64
1:K:599:ALA:HB2	1:K:605:LEU:HD13	1.77	0.64
1:L:599:ALA:HB2	1:L:605:LEU:HD13	1.77	0.64
1:M:392:ASP:HA	1:M:395:VAL:HG12	1.78	0.64
1:M:478:GLU:OE1	1:M:478:GLU:N	2.28	0.64
1:M:543:GLN:NE2	1:M:547:GLU:OE1	2.28	0.64
1:O:445:LEU:HG	1:O:474:TRP:HB3	1.79	0.64
1:P:392:ASP:HA	1:P:395:VAL:HG12	1.78	0.64
1:R:478:GLU:N	1:R:478:GLU:OE1	2.28	0.64
1:A:392:ASP:HA	1:A:395:VAL:HG12	1.78	0.64
1:C:392:ASP:HA	1:C:395:VAL:HG12	1.78	0.64
1:F:478:GLU:N	1:F:478:GLU:OE1	2.28	0.64
1:H:599:ALA:HB2	1:H:605:LEU:HD13	1.77	0.64
1:D:478:GLU:OE1	1:D:478:GLU:N	2.28	0.64
1:N:447:ARG:NH2	1:N:472:THR:OG1	2.21	0.64
1:P:662:ILE:HD13	1:P:690:LEU:HD11	1.79	0.64
1:D:662:ILE:HD13	1:D:690:LEU:HD11	1.79	0.64
1:P:478:GLU:OE1	1:P:478:GLU:N	2.28	0.64
1:F:447:ARG:NH2	1:F:472:THR:OG1	2.21	0.64
1:L:445:LEU:HG	1:L:474:TRP:HB3	1.79	0.64
1:B:445:LEU:HG	1:B:474:TRP:HB3	1.79	0.64
1:I:392:ASP:HA	1:I:395:VAL:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:445:LEU:HG	1:I:474:TRP:HB3	1.79	0.64
1:N:445:LEU:HG	1:N:474:TRP:HB3	1.79	0.64
1:B:447:ARG:NH2	1:B:472:THR:OG1	2.21	0.64
1:L:392:ASP:HA	1:L:395:VAL:HG12	1.78	0.64
1:E:478:GLU:N	1:E:478:GLU:OE1	2.28	0.64
1:F:662:ILE:HD13	1:F:690:LEU:HD11	1.79	0.64
1:O:447:ARG:NH2	1:O:472:THR:OG1	2.21	0.64
1:A:662:ILE:HD13	1:A:690:LEU:HD11	1.79	0.64
1:C:662:ILE:HD13	1:C:690:LEU:HD11	1.79	0.64
1:G:662:ILE:HD13	1:G:690:LEU:HD11	1.79	0.64
1:M:662:ILE:HD13	1:M:690:LEU:HD11	1.79	0.64
1:O:662:ILE:HD13	1:O:690:LEU:HD11	1.79	0.64
1:R:662:ILE:HD13	1:R:690:LEU:HD11	1.79	0.64
1:F:377:VAL:HG12	1:F:425:TYR:HB2	1.81	0.64
1:J:662:ILE:HD13	1:J:690:LEU:HD11	1.79	0.64
1:Q:478:GLU:OE1	1:Q:478:GLU:N	2.28	0.64
1:R:377:VAL:HG12	1:R:425:TYR:HB2	1.80	0.64
1:C:447:ARG:NH2	1:C:472:THR:OG1	2.21	0.63
1:E:377:VAL:HG12	1:E:425:TYR:HB2	1.80	0.63
1:H:662:ILE:HD13	1:H:690:LEU:HD11	1.79	0.63
1:K:662:ILE:HD13	1:K:690:LEU:HD11	1.79	0.63
1:M:445:LEU:HG	1:M:474:TRP:HB3	1.79	0.63
1:Q:377:VAL:HG12	1:Q:425:TYR:HB2	1.81	0.63
1:F:519:ARG:HG2	1:G:531:GLU:HG2	1.80	0.63
1:G:561:ASN:ND2	1:G:564:SER:OG	2.32	0.63
1:J:561:ASN:ND2	1:J:564:SER:OG	2.32	0.63
1:A:445:LEU:HG	1:A:474:TRP:HB3	1.79	0.63
1:E:561:ASN:ND2	1:E:564:SER:OG	2.32	0.63
1:J:377:VAL:HG12	1:J:425:TYR:HB2	1.81	0.63
1:N:377:VAL:HG12	1:N:425:TYR:HB2	1.80	0.63
1:Q:561:ASN:ND2	1:Q:564:SER:OG	2.32	0.63
1:B:377:VAL:HG12	1:B:425:TYR:HB2	1.81	0.63
1:C:561:ASN:ND2	1:C:564:SER:OG	2.32	0.63
1:G:377:VAL:HG12	1:G:425:TYR:HB2	1.81	0.63
1:B:561:ASN:ND2	1:B:564:SER:OG	2.32	0.63
1:H:561:ASN:ND2	1:H:564:SER:OG	2.32	0.63
1:K:561:ASN:ND2	1:K:564:SER:OG	2.32	0.63
1:I:377:VAL:HG12	1:I:425:TYR:HB2	1.80	0.63
1:I:561:ASN:ND2	1:I:564:SER:OG	2.32	0.63
1:L:561:ASN:ND2	1:L:564:SER:OG	2.32	0.63
1:N:561:ASN:ND2	1:N:564:SER:OG	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:377:VAL:HG12	1:O:425:TYR:HB2	1.81	0.63
1:O:561:ASN:ND2	1:O:564:SER:OG	2.32	0.63
1:B:662:ILE:HD13	1:B:690:LEU:HD11	1.79	0.62
1:C:377:VAL:HG12	1:C:425:TYR:HB2	1.80	0.62
1:D:377:VAL:HG12	1:D:425:TYR:HB2	1.80	0.62
1:L:377:VAL:HG12	1:L:425:TYR:HB2	1.80	0.62
1:N:662:ILE:HD13	1:N:690:LEU:HD11	1.79	0.62
1:B:412:ILE:HD13	1:B:501:LEU:HD11	1.81	0.62
1:N:412:ILE:HD13	1:N:501:LEU:HD11	1.81	0.62
1:P:377:VAL:HG12	1:P:425:TYR:HB2	1.80	0.62
1:P:447:ARG:NH2	1:P:472:THR:OG1	2.21	0.62
1:R:561:ASN:ND2	1:R:564:SER:OG	2.32	0.62
1:A:412:ILE:HD13	1:A:501:LEU:HD11	1.81	0.62
1:B:423:GLY:O	1:B:439:LEU:N	2.33	0.62
1:E:423:GLY:O	1:E:439:LEU:N	2.33	0.62
1:N:423:GLY:O	1:N:439:LEU:N	2.33	0.62
1:R:412:ILE:HD13	1:R:501:LEU:HD11	1.81	0.62
1:D:447:ARG:NH2	1:D:472:THR:OG1	2.21	0.62
1:F:412:ILE:HD13	1:F:501:LEU:HD11	1.81	0.62
1:F:561:ASN:ND2	1:F:564:SER:OG	2.32	0.62
1:H:377:VAL:HG12	1:H:425:TYR:HB2	1.80	0.62
1:M:412:ILE:HD13	1:M:501:LEU:HD11	1.81	0.62
1:O:412:ILE:HD13	1:O:501:LEU:HD11	1.81	0.62
1:Q:423:GLY:O	1:Q:439:LEU:N	2.33	0.62
1:C:412:ILE:HD13	1:C:501:LEU:HD11	1.81	0.62
1:I:412:ILE:HD13	1:I:501:LEU:HD11	1.81	0.62
1:I:662:ILE:HD13	1:I:690:LEU:HD11	1.79	0.62
1:K:377:VAL:HG12	1:K:425:TYR:HB2	1.80	0.62
1:L:412:ILE:HD13	1:L:501:LEU:HD11	1.81	0.62
1:M:561:ASN:ND2	1:M:564:SER:OG	2.32	0.62
1:D:423:GLY:O	1:D:439:LEU:N	2.33	0.62
1:D:561:ASN:ND2	1:D:564:SER:OG	2.32	0.62
1:F:455:LEU:HB3	1:F:462:LYS:HE2	1.82	0.62
1:G:686:SER:HB2	1:G:689:GLU:HG3	1.82	0.62
1:I:423:GLY:O	1:I:439:LEU:N	2.33	0.62
1:J:686:SER:HB2	1:J:689:GLU:HG3	1.82	0.62
1:O:455:LEU:HB3	1:O:462:LYS:HE2	1.82	0.62
1:P:423:GLY:O	1:P:439:LEU:N	2.33	0.62
1:A:561:ASN:ND2	1:A:564:SER:OG	2.32	0.62
1:B:455:LEU:HB3	1:B:462:LYS:HE2	1.82	0.62
1:C:455:LEU:HB3	1:C:462:LYS:HE2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:ARG:HG2	1:D:531:GLU:HG2	1.80	0.62
1:E:686:SER:HB2	1:E:689:GLU:HG3	1.82	0.62
1:G:423:GLY:O	1:G:439:LEU:N	2.33	0.62
1:J:423:GLY:O	1:J:439:LEU:N	2.33	0.62
1:L:662:ILE:HD13	1:L:690:LEU:HD11	1.79	0.62
1:N:455:LEU:HB3	1:N:462:LYS:HE2	1.82	0.62
1:P:412:ILE:HD13	1:P:501:LEU:HD11	1.81	0.62
1:P:455:LEU:HB3	1:P:462:LYS:HE2	1.82	0.62
1:Q:686:SER:HB2	1:Q:689:GLU:HG3	1.82	0.62
1:R:455:LEU:HB3	1:R:462:LYS:HE2	1.82	0.62
1:D:412:ILE:HD13	1:D:501:LEU:HD11	1.81	0.62
1:H:455:LEU:HB3	1:H:462:LYS:HE2	1.82	0.62
1:J:412:ILE:HD13	1:J:501:LEU:HD11	1.81	0.62
1:J:455:LEU:HB3	1:J:462:LYS:HE2	1.82	0.62
1:K:455:LEU:HB3	1:K:462:LYS:HE2	1.82	0.62
1:L:423:GLY:O	1:L:439:LEU:N	2.33	0.62
1:P:561:ASN:ND2	1:P:564:SER:OG	2.32	0.62
1:A:423:GLY:O	1:A:439:LEU:N	2.33	0.61
1:D:455:LEU:HB3	1:D:462:LYS:HE2	1.82	0.61
1:G:412:ILE:HD13	1:G:501:LEU:HD11	1.81	0.61
1:G:455:LEU:HB3	1:G:462:LYS:HE2	1.82	0.61
1:L:686:SER:HB2	1:L:689:GLU:HG3	1.82	0.61
1:M:423:GLY:O	1:M:439:LEU:N	2.33	0.61
1:A:455:LEU:HB3	1:A:462:LYS:HE2	1.82	0.61
1:I:686:SER:HB2	1:I:689:GLU:HG3	1.82	0.61
1:M:455:LEU:HB3	1:M:462:LYS:HE2	1.82	0.61
1:P:686:SER:HB2	1:P:689:GLU:HG3	1.82	0.61
1:A:686:SER:HB2	1:A:689:GLU:HG3	1.82	0.61
1:E:455:LEU:HB3	1:E:462:LYS:HE2	1.82	0.61
1:H:412:ILE:HD13	1:H:501:LEU:HD11	1.81	0.61
1:K:412:ILE:HD13	1:K:501:LEU:HD11	1.81	0.61
1:M:686:SER:HB2	1:M:689:GLU:HG3	1.82	0.61
1:Q:455:LEU:HB3	1:Q:462:LYS:HE2	1.82	0.61
1:C:423:GLY:O	1:C:439:LEU:N	2.33	0.61
1:A:377:VAL:HG12	1:A:425:TYR:HB2	1.80	0.61
1:D:686:SER:HB2	1:D:689:GLU:HG3	1.82	0.61
1:L:455:LEU:HB3	1:L:462:LYS:HE2	1.82	0.61
1:O:423:GLY:O	1:O:439:LEU:N	2.33	0.61
1:I:455:LEU:HB3	1:I:462:LYS:HE2	1.82	0.61
1:N:686:SER:HB2	1:N:689:GLU:HG3	1.82	0.61
1:B:686:SER:HB2	1:B:689:GLU:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:377:VAL:HG12	1:M:425:TYR:HB2	1.80	0.61
1:B:381:GLN:NE2	1:B:422:GLU:OE2	2.34	0.61
1:K:423:GLY:O	1:K:439:LEU:N	2.33	0.61
1:M:381:GLN:NE2	1:M:422:GLU:OE2	2.34	0.61
1:Q:412:ILE:HD13	1:Q:501:LEU:HD11	1.81	0.61
1:A:381:GLN:NE2	1:A:422:GLU:OE2	2.34	0.61
1:E:412:ILE:HD13	1:E:501:LEU:HD11	1.81	0.61
1:H:423:GLY:O	1:H:439:LEU:N	2.33	0.61
1:C:686:SER:HB2	1:C:689:GLU:HG3	1.82	0.61
1:I:381:GLN:NE2	1:I:422:GLU:OE2	2.34	0.61
1:L:381:GLN:NE2	1:L:422:GLU:OE2	2.34	0.61
1:N:381:GLN:NE2	1:N:422:GLU:OE2	2.34	0.61
1:O:686:SER:HB2	1:O:689:GLU:HG3	1.82	0.61
1:C:381:GLN:NE2	1:C:422:GLU:OE2	2.34	0.60
1:K:381:GLN:NE2	1:K:422:GLU:OE2	2.34	0.60
1:O:381:GLN:NE2	1:O:422:GLU:OE2	2.34	0.60
1:H:381:GLN:NE2	1:H:422:GLU:OE2	2.34	0.60
1:H:686:SER:HB2	1:H:689:GLU:HG3	1.82	0.60
1:R:686:SER:HB2	1:R:689:GLU:HG3	1.82	0.60
1:F:423:GLY:O	1:F:439:LEU:N	2.33	0.60
1:K:686:SER:HB2	1:K:689:GLU:HG3	1.82	0.60
1:F:686:SER:HB2	1:F:689:GLU:HG3	1.82	0.60
1:G:381:GLN:NE2	1:G:422:GLU:OE2	2.34	0.60
1:J:381:GLN:NE2	1:J:422:GLU:OE2	2.34	0.60
1:R:423:GLY:O	1:R:439:LEU:N	2.33	0.60
1:E:381:GLN:NE2	1:E:422:GLU:OE2	2.34	0.60
1:Q:381:GLN:NE2	1:Q:422:GLU:OE2	2.34	0.60
1:D:381:GLN:NE2	1:D:422:GLU:OE2	2.34	0.59
1:F:381:GLN:NE2	1:F:422:GLU:OE2	2.34	0.59
1:R:381:GLN:NE2	1:R:422:GLU:OE2	2.34	0.59
1:P:381:GLN:NE2	1:P:422:GLU:OE2	2.34	0.59
1:P:467:LEU:HG	1:P:468:PRO:HD2	1.85	0.59
1:R:467:LEU:HG	1:R:468:PRO:HD2	1.85	0.59
1:F:467:LEU:HG	1:F:468:PRO:HD2	1.85	0.58
1:G:467:LEU:HG	1:G:468:PRO:HD2	1.85	0.58
1:D:467:LEU:HG	1:D:468:PRO:HD2	1.85	0.58
1:J:467:LEU:HG	1:J:468:PRO:HD2	1.85	0.58
1:E:467:LEU:HG	1:E:468:PRO:HD2	1.85	0.58
1:Q:467:LEU:HG	1:Q:468:PRO:HD2	1.85	0.58
1:J:482:ARG:HA	1:J:485:LYS:HD2	1.86	0.58
1:K:467:LEU:HG	1:K:468:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:ASP:HB3	1:C:637:VAL:HG23	1.86	0.58
1:F:482:ARG:HA	1:F:485:LYS:HD2	1.86	0.58
1:G:482:ARG:HA	1:G:485:LYS:HD2	1.86	0.58
1:H:467:LEU:HG	1:H:468:PRO:HD2	1.85	0.58
1:R:482:ARG:HA	1:R:485:LYS:HD2	1.86	0.58
1:C:467:LEU:HG	1:C:468:PRO:HD2	1.85	0.58
1:O:634:ASP:HB3	1:O:637:VAL:HG23	1.86	0.58
1:B:451:SER:OG	1:B:471:GLU:O	2.21	0.58
1:N:451:SER:OG	1:N:471:GLU:O	2.21	0.58
1:O:467:LEU:HG	1:O:468:PRO:HD2	1.85	0.58
1:H:482:ARG:HA	1:H:485:LYS:HD2	1.85	0.58
1:K:482:ARG:HA	1:K:485:LYS:HD2	1.86	0.58
1:E:482:ARG:HA	1:E:485:LYS:HD2	1.86	0.57
1:F:441:ALA:O	1:F:493:HIS:NE2	2.37	0.57
1:Q:482:ARG:HA	1:Q:485:LYS:HD2	1.86	0.57
1:R:441:ALA:O	1:R:493:HIS:NE2	2.37	0.57
1:A:467:LEU:HG	1:A:468:PRO:HD2	1.85	0.57
1:H:634:ASP:HB3	1:H:637:VAL:HG23	1.86	0.57
1:K:634:ASP:HB3	1:K:637:VAL:HG23	1.86	0.57
1:B:482:ARG:HA	1:B:485:LYS:HD2	1.86	0.57
1:C:451:SER:OG	1:C:471:GLU:O	2.21	0.57
1:M:467:LEU:HG	1:M:468:PRO:HD2	1.85	0.57
1:E:634:ASP:HB3	1:E:637:VAL:HG23	1.86	0.57
1:N:482:ARG:HA	1:N:485:LYS:HD2	1.86	0.57
1:O:451:SER:OG	1:O:471:GLU:O	2.21	0.57
1:Q:634:ASP:HB3	1:Q:637:VAL:HG23	1.86	0.57
1:A:482:ARG:HA	1:A:485:LYS:HD2	1.86	0.57
1:D:441:ALA:O	1:D:493:HIS:NE2	2.37	0.57
1:J:634:ASP:HB3	1:J:637:VAL:HG23	1.86	0.57
1:D:482:ARG:HA	1:D:485:LYS:HD2	1.86	0.57
1:G:634:ASP:HB3	1:G:637:VAL:HG23	1.86	0.57
1:M:451:SER:OG	1:M:471:GLU:O	2.21	0.57
1:M:482:ARG:HA	1:M:485:LYS:HD2	1.86	0.57
1:P:441:ALA:O	1:P:493:HIS:NE2	2.37	0.57
1:P:482:ARG:HA	1:P:485:LYS:HD2	1.86	0.57
1:A:451:SER:OG	1:A:471:GLU:O	2.21	0.57
1:C:482:ARG:HA	1:C:485:LYS:HD2	1.86	0.57
1:I:467:LEU:HG	1:I:468:PRO:HD2	1.85	0.57
1:M:634:ASP:HB3	1:M:637:VAL:HG23	1.86	0.57
1:O:482:ARG:HA	1:O:485:LYS:HD2	1.86	0.57
1:A:634:ASP:HB3	1:A:637:VAL:HG23	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:467:LEU:HG	1:L:468:PRO:HD2	1.85	0.57
1:L:482:ARG:HA	1:L:485:LYS:HD2	1.86	0.57
1:D:451:SER:OG	1:D:471:GLU:O	2.21	0.57
1:F:533:ILE:HA	1:F:536:VAL:HG12	1.87	0.57
1:F:634:ASP:HB3	1:F:637:VAL:HG23	1.86	0.57
1:I:634:ASP:HB3	1:I:637:VAL:HG23	1.86	0.57
1:L:634:ASP:HB3	1:L:637:VAL:HG23	1.86	0.57
1:N:467:LEU:HG	1:N:468:PRO:HD2	1.85	0.57
1:P:451:SER:OG	1:P:471:GLU:O	2.21	0.57
1:B:467:LEU:HG	1:B:468:PRO:HD2	1.85	0.56
1:B:533:ILE:HA	1:B:536:VAL:HG12	1.87	0.56
1:I:441:ALA:O	1:I:493:HIS:NE2	2.37	0.56
1:L:441:ALA:O	1:L:493:HIS:NE2	2.37	0.56
1:N:533:ILE:HA	1:N:536:VAL:HG12	1.87	0.56
1:O:533:ILE:HA	1:O:536:VAL:HG12	1.87	0.56
1:R:634:ASP:HB3	1:R:637:VAL:HG23	1.86	0.56
1:B:441:ALA:O	1:B:493:HIS:NE2	2.37	0.56
1:G:441:ALA:O	1:G:493:HIS:NE2	2.37	0.56
1:I:482:ARG:HA	1:I:485:LYS:HD2	1.86	0.56
1:J:441:ALA:O	1:J:493:HIS:NE2	2.37	0.56
1:N:441:ALA:O	1:N:493:HIS:NE2	2.37	0.56
1:R:533:ILE:HA	1:R:536:VAL:HG12	1.87	0.56
1:C:533:ILE:HA	1:C:536:VAL:HG12	1.87	0.56
1:D:666:ASP:OD1	1:D:666:ASP:N	2.39	0.56
1:E:451:SER:OG	1:E:471:GLU:O	2.21	0.56
1:P:666:ASP:OD1	1:P:666:ASP:N	2.39	0.56
1:E:666:ASP:N	1:E:666:ASP:OD1	2.39	0.56
1:N:634:ASP:HB3	1:N:637:VAL:HG23	1.86	0.56
1:P:634:ASP:HB3	1:P:637:VAL:HG23	1.86	0.56
1:B:634:ASP:HB3	1:B:637:VAL:HG23	1.86	0.56
1:J:533:ILE:HA	1:J:536:VAL:HG12	1.87	0.56
1:L:533:ILE:HA	1:L:536:VAL:HG12	1.87	0.56
1:Q:451:SER:OG	1:Q:471:GLU:O	2.21	0.56
1:Q:666:ASP:OD1	1:Q:666:ASP:N	2.39	0.56
1:B:666:ASP:OD1	1:B:666:ASP:N	2.39	0.56
1:D:634:ASP:HB3	1:D:637:VAL:HG23	1.86	0.56
1:G:533:ILE:HA	1:G:536:VAL:HG12	1.87	0.56
1:I:533:ILE:HA	1:I:536:VAL:HG12	1.88	0.56
1:N:666:ASP:OD1	1:N:666:ASP:N	2.39	0.56
1:E:441:ALA:O	1:E:493:HIS:NE2	2.37	0.56
1:H:533:ILE:HA	1:H:536:VAL:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:451:SER:OG	1:I:471:GLU:O	2.21	0.56
1:P:533:ILE:HA	1:P:536:VAL:HG12	1.87	0.56
1:Q:441:ALA:O	1:Q:493:HIS:NE2	2.37	0.56
1:A:533:ILE:HA	1:A:536:VAL:HG12	1.87	0.55
1:E:533:ILE:HA	1:E:536:VAL:HG12	1.87	0.55
1:F:666:ASP:OD1	1:F:666:ASP:N	2.39	0.55
1:K:533:ILE:HA	1:K:536:VAL:HG12	1.87	0.55
1:L:451:SER:OG	1:L:471:GLU:O	2.21	0.55
1:R:666:ASP:OD1	1:R:666:ASP:N	2.39	0.55
1:D:533:ILE:HA	1:D:536:VAL:HG12	1.87	0.55
1:H:451:SER:OG	1:H:471:GLU:O	2.21	0.55
1:M:533:ILE:HA	1:M:536:VAL:HG12	1.87	0.55
1:Q:533:ILE:HA	1:Q:536:VAL:HG12	1.87	0.55
1:A:666:ASP:OD1	1:A:666:ASP:N	2.39	0.55
1:K:451:SER:OG	1:K:471:GLU:O	2.21	0.55
1:M:666:ASP:N	1:M:666:ASP:OD1	2.39	0.55
1:A:441:ALA:O	1:A:493:HIS:NE2	2.37	0.55
1:G:666:ASP:OD1	1:G:666:ASP:N	2.39	0.55
1:J:666:ASP:N	1:J:666:ASP:OD1	2.39	0.55
1:F:451:SER:OG	1:F:471:GLU:O	2.21	0.55
1:M:441:ALA:O	1:M:493:HIS:NE2	2.37	0.55
1:I:666:ASP:OD1	1:I:666:ASP:N	2.39	0.55
1:L:666:ASP:OD1	1:L:666:ASP:N	2.39	0.55
1:G:451:SER:OG	1:G:471:GLU:O	2.21	0.55
1:J:451:SER:OG	1:J:471:GLU:O	2.21	0.55
1:K:666:ASP:OD1	1:K:666:ASP:N	2.39	0.55
1:H:666:ASP:N	1:H:666:ASP:OD1	2.39	0.55
1:K:381:GLN:HA	1:K:384:ALA:HB3	1.90	0.54
1:R:451:SER:OG	1:R:471:GLU:O	2.21	0.54
1:F:381:GLN:HA	1:F:384:ALA:HB3	1.90	0.54
1:H:381:GLN:HA	1:H:384:ALA:HB3	1.90	0.54
1:J:443:TYR:OH	1:J:445:LEU:HD13	2.08	0.54
1:A:443:TYR:OH	1:A:445:LEU:HD13	2.08	0.54
1:E:381:GLN:HA	1:E:384:ALA:HB3	1.90	0.54
1:G:443:TYR:OH	1:G:445:LEU:HD13	2.08	0.54
1:H:443:TYR:OH	1:H:445:LEU:HD13	2.08	0.54
1:K:443:TYR:OH	1:K:445:LEU:HD13	2.08	0.54
1:L:443:TYR:OH	1:L:445:LEU:HD13	2.08	0.54
1:M:443:TYR:OH	1:M:445:LEU:HD13	2.08	0.54
1:Q:381:GLN:HA	1:Q:384:ALA:HB3	1.90	0.54
1:I:381:GLN:HA	1:I:384:ALA:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:381:GLN:HA	1:R:384:ALA:HB3	1.90	0.54
1:G:617:LYS:HD2	1:G:641:LEU:HD21	1.90	0.54
1:H:441:ALA:O	1:H:493:HIS:NE2	2.37	0.54
1:H:617:LYS:HD2	1:H:641:LEU:HD21	1.90	0.54
1:I:443:TYR:OH	1:I:445:LEU:HD13	2.08	0.54
1:J:381:GLN:HA	1:J:384:ALA:HB3	1.90	0.54
1:J:617:LYS:HD2	1:J:641:LEU:HD21	1.90	0.54
1:K:617:LYS:HD2	1:K:641:LEU:HD21	1.90	0.54
1:L:381:GLN:HA	1:L:384:ALA:HB3	1.90	0.54
1:M:381:GLN:HA	1:M:384:ALA:HB3	1.90	0.54
1:N:443:TYR:OH	1:N:445:LEU:HD13	2.08	0.54
1:A:381:GLN:HA	1:A:384:ALA:HB3	1.90	0.54
1:B:443:TYR:OH	1:B:445:LEU:HD13	2.08	0.54
1:F:443:TYR:OH	1:F:445:LEU:HD13	2.08	0.54
1:G:381:GLN:HA	1:G:384:ALA:HB3	1.90	0.54
1:R:443:TYR:OH	1:R:445:LEU:HD13	2.08	0.54
1:K:441:ALA:O	1:K:493:HIS:NE2	2.37	0.54
1:C:381:GLN:HA	1:C:384:ALA:HB3	1.90	0.54
1:F:617:LYS:HD2	1:F:641:LEU:HD21	1.90	0.54
1:A:642:LEU:HG	1:A:646:ARG:HH12	1.73	0.54
1:B:381:GLN:HA	1:B:384:ALA:HB3	1.90	0.54
1:C:642:LEU:HG	1:C:646:ARG:HH12	1.73	0.54
1:D:381:GLN:HA	1:D:384:ALA:HB3	1.90	0.54
1:D:642:LEU:HG	1:D:646:ARG:HH12	1.73	0.54
1:L:617:LYS:HD2	1:L:641:LEU:HD21	1.90	0.54
1:M:551:ARG:HH11	1:M:669:ARG:HH12	1.56	0.54
1:M:642:LEU:HG	1:M:646:ARG:HH12	1.73	0.54
1:N:381:GLN:HA	1:N:384:ALA:HB3	1.90	0.54
1:O:381:GLN:HA	1:O:384:ALA:HB3	1.90	0.54
1:P:381:GLN:HA	1:P:384:ALA:HB3	1.90	0.54
1:P:642:LEU:HG	1:P:646:ARG:HH12	1.73	0.54
1:A:551:ARG:HH11	1:A:669:ARG:HH12	1.56	0.53
1:E:551:ARG:HH11	1:E:669:ARG:HH12	1.56	0.53
1:H:551:ARG:HH11	1:H:669:ARG:HH12	1.56	0.53
1:I:617:LYS:HD2	1:I:641:LEU:HD21	1.90	0.53
1:K:551:ARG:HH11	1:K:669:ARG:HH12	1.56	0.53
1:Q:551:ARG:HH11	1:Q:669:ARG:HH12	1.56	0.53
1:R:617:LYS:HD2	1:R:641:LEU:HD21	1.90	0.53
1:E:443:TYR:OH	1:E:445:LEU:HD13	2.08	0.53
1:G:551:ARG:HH11	1:G:669:ARG:HH12	1.56	0.53
1:J:551:ARG:HH11	1:J:669:ARG:HH12	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:642:LEU:HG	1:O:646:ARG:HH12	1.73	0.53
1:O:392:ASP:O	1:O:396:ARG:NH1	2.42	0.53
1:Q:443:TYR:OH	1:Q:445:LEU:HD13	2.08	0.53
1:Q:642:LEU:HG	1:Q:646:ARG:HH12	1.73	0.53
1:B:551:ARG:HH11	1:B:669:ARG:HH12	1.56	0.53
1:E:392:ASP:O	1:E:396:ARG:NH1	2.42	0.53
1:E:393:GLU:HG2	1:E:494:SER:HB3	1.91	0.53
1:F:393:GLU:HG2	1:F:494:SER:HB3	1.91	0.53
1:O:443:TYR:OH	1:O:445:LEU:HD13	2.08	0.53
1:Q:392:ASP:O	1:Q:396:ARG:NH1	2.42	0.53
1:R:393:GLU:HG2	1:R:494:SER:HB3	1.91	0.53
1:C:392:ASP:O	1:C:396:ARG:NH1	2.42	0.53
1:E:642:LEU:HG	1:E:646:ARG:HH12	1.74	0.53
1:J:393:GLU:HG2	1:J:494:SER:HB3	1.91	0.53
1:L:392:ASP:O	1:L:396:ARG:NH1	2.42	0.53
1:N:551:ARG:HH11	1:N:669:ARG:HH12	1.56	0.53
1:P:392:ASP:O	1:P:396:ARG:NH1	2.42	0.53
1:Q:393:GLU:HG2	1:Q:494:SER:HB3	1.91	0.53
1:C:443:TYR:OH	1:C:445:LEU:HD13	2.08	0.53
1:D:392:ASP:O	1:D:396:ARG:NH1	2.42	0.53
1:E:617:LYS:HD2	1:E:641:LEU:HD21	1.90	0.53
1:I:392:ASP:O	1:I:396:ARG:NH1	2.42	0.53
1:L:642:LEU:HG	1:L:646:ARG:HH12	1.73	0.53
1:A:392:ASP:O	1:A:396:ARG:NH1	2.42	0.53
1:C:441:ALA:O	1:C:493:HIS:NE2	2.37	0.53
1:G:393:GLU:HG2	1:G:494:SER:HB3	1.91	0.53
1:B:642:LEU:HG	1:B:646:ARG:HH12	1.74	0.53
1:D:393:GLU:HG2	1:D:494:SER:HB3	1.91	0.53
1:D:551:ARG:HH11	1:D:669:ARG:HH12	1.56	0.53
1:I:642:LEU:HG	1:I:646:ARG:HH12	1.74	0.53
1:M:392:ASP:O	1:M:396:ARG:NH1	2.42	0.53
1:M:617:LYS:HD2	1:M:641:LEU:HD21	1.90	0.53
1:P:393:GLU:HG2	1:P:494:SER:HB3	1.91	0.53
1:P:551:ARG:HH11	1:P:669:ARG:HH12	1.56	0.53
1:Q:617:LYS:HD2	1:Q:641:LEU:HD21	1.90	0.53
1:R:642:LEU:HG	1:R:646:ARG:HH12	1.73	0.53
1:A:617:LYS:HD2	1:A:641:LEU:HD21	1.90	0.53
1:F:642:LEU:HG	1:F:646:ARG:HH12	1.73	0.53
1:N:642:LEU:HG	1:N:646:ARG:HH12	1.73	0.53
1:F:392:ASP:O	1:F:396:ARG:NH1	2.42	0.53
1:G:642:LEU:HG	1:G:646:ARG:HH12	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:642:LEU:HG	1:J:646:ARG:HH12	1.73	0.53
1:K:642:LEU:HG	1:K:646:ARG:HH12	1.73	0.53
1:O:441:ALA:O	1:O:493:HIS:NE2	2.37	0.53
1:R:392:ASP:O	1:R:396:ARG:NH1	2.42	0.52
1:D:443:TYR:OH	1:D:445:LEU:HD13	2.08	0.52
1:F:551:ARG:HH11	1:F:669:ARG:HH12	1.56	0.52
1:H:392:ASP:O	1:H:396:ARG:NH1	2.42	0.52
1:P:443:TYR:OH	1:P:445:LEU:HD13	2.08	0.52
1:R:551:ARG:HH11	1:R:669:ARG:HH12	1.56	0.52
1:H:642:LEU:HG	1:H:646:ARG:HH12	1.73	0.52
1:K:392:ASP:O	1:K:396:ARG:NH1	2.42	0.52
1:B:392:ASP:O	1:B:396:ARG:NH1	2.42	0.52
1:K:393:GLU:HG2	1:K:494:SER:HB3	1.91	0.52
1:N:519:ARG:HD3	1:N:542:LEU:HD11	1.92	0.52
1:B:519:ARG:HD3	1:B:542:LEU:HD11	1.92	0.52
1:C:393:GLU:HG2	1:C:494:SER:HB3	1.91	0.52
1:H:393:GLU:HG2	1:H:494:SER:HB3	1.91	0.52
1:L:551:ARG:HH11	1:L:669:ARG:HH12	1.56	0.52
1:N:392:ASP:O	1:N:396:ARG:NH1	2.42	0.52
1:N:617:LYS:HD2	1:N:641:LEU:HD21	1.90	0.52
1:J:392:ASP:O	1:J:396:ARG:NH1	2.42	0.52
1:O:393:GLU:HG2	1:O:494:SER:HB3	1.91	0.52
1:P:617:LYS:HD2	1:P:641:LEU:HD21	1.90	0.52
1:G:392:ASP:O	1:G:396:ARG:NH1	2.42	0.52
1:O:617:LYS:HD2	1:O:641:LEU:HD21	1.90	0.52
1:A:393:GLU:HG2	1:A:494:SER:HB3	1.91	0.52
1:B:393:GLU:HG2	1:B:494:SER:HB3	1.91	0.52
1:B:617:LYS:HD2	1:B:641:LEU:HD21	1.90	0.52
1:D:617:LYS:HD2	1:D:641:LEU:HD21	1.90	0.52
1:I:551:ARG:HH11	1:I:669:ARG:HH12	1.56	0.52
1:I:645:VAL:HG13	1:I:649:ILE:HD12	1.92	0.52
1:K:645:VAL:HG13	1:K:649:ILE:HD12	1.92	0.52
1:L:645:VAL:HG13	1:L:649:ILE:HD12	1.92	0.52
1:N:393:GLU:HG2	1:N:494:SER:HB3	1.91	0.52
1:O:519:ARG:HD3	1:O:542:LEU:HD11	1.91	0.52
1:C:617:LYS:HD2	1:C:641:LEU:HD21	1.90	0.52
1:G:645:VAL:HG13	1:G:649:ILE:HD12	1.92	0.52
1:H:645:VAL:HG13	1:H:649:ILE:HD12	1.92	0.52
1:I:393:GLU:HG2	1:I:494:SER:HB3	1.91	0.52
1:J:645:VAL:HG13	1:J:649:ILE:HD12	1.92	0.52
1:M:393:GLU:HG2	1:M:494:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:645:VAL:HG13	1:M:649:ILE:HD12	1.92	0.52
1:A:645:VAL:HG13	1:A:649:ILE:HD12	1.92	0.51
1:L:393:GLU:HG2	1:L:494:SER:HB3	1.91	0.51
1:E:645:VAL:HG13	1:E:649:ILE:HD12	1.92	0.51
1:F:645:VAL:HG13	1:F:649:ILE:HD12	1.92	0.51
1:J:519:ARG:HD3	1:J:542:LEU:HD11	1.92	0.51
1:C:519:ARG:HD3	1:C:542:LEU:HD11	1.92	0.51
1:D:519:ARG:HD3	1:D:542:LEU:HD11	1.92	0.51
1:G:519:ARG:HD3	1:G:542:LEU:HD11	1.92	0.51
1:R:645:VAL:HG13	1:R:649:ILE:HD12	1.92	0.51
1:B:645:VAL:HG13	1:B:649:ILE:HD12	1.92	0.51
1:C:551:ARG:HH11	1:C:669:ARG:HH12	1.56	0.51
1:D:580:VAL:O	1:D:584:GLU:HG2	2.10	0.51
1:H:519:ARG:HD3	1:H:542:LEU:HD11	1.92	0.51
1:L:580:VAL:O	1:L:584:GLU:HG2	2.10	0.51
1:N:645:VAL:HG13	1:N:649:ILE:HD12	1.92	0.51
1:O:666:ASP:N	1:O:666:ASP:OD1	2.39	0.51
1:Q:645:VAL:HG13	1:Q:649:ILE:HD12	1.92	0.51
1:R:519:ARG:HD3	1:R:542:LEU:HD11	1.92	0.51
1:C:580:VAL:O	1:C:584:GLU:HG2	2.10	0.51
1:C:666:ASP:N	1:C:666:ASP:OD1	2.39	0.51
1:D:645:VAL:HG13	1:D:649:ILE:HD12	1.92	0.51
1:E:519:ARG:HD3	1:E:542:LEU:HD11	1.92	0.51
1:G:580:VAL:O	1:G:584:GLU:HG2	2.10	0.51
1:H:580:VAL:O	1:H:584:GLU:HG2	2.10	0.51
1:I:580:VAL:O	1:I:584:GLU:HG2	2.10	0.51
1:J:580:VAL:O	1:J:584:GLU:HG2	2.10	0.51
1:K:519:ARG:HD3	1:K:542:LEU:HD11	1.92	0.51
1:O:580:VAL:O	1:O:584:GLU:HG2	2.10	0.51
1:P:645:VAL:HG13	1:P:649:ILE:HD12	1.92	0.51
1:Q:519:ARG:HD3	1:Q:542:LEU:HD11	1.92	0.51
1:F:519:ARG:HD3	1:F:542:LEU:HD11	1.92	0.51
1:K:580:VAL:O	1:K:584:GLU:HG2	2.10	0.51
1:O:551:ARG:HH11	1:O:669:ARG:HH12	1.56	0.51
1:P:519:ARG:HD3	1:P:542:LEU:HD11	1.92	0.51
1:P:580:VAL:O	1:P:584:GLU:HG2	2.10	0.51
1:A:519:ARG:HD3	1:A:542:LEU:HD11	1.92	0.51
1:R:580:VAL:O	1:R:584:GLU:HG2	2.10	0.51
1:I:519:ARG:HD3	1:I:542:LEU:HD11	1.92	0.51
1:L:519:ARG:HD3	1:L:542:LEU:HD11	1.92	0.51
1:M:519:ARG:HD3	1:M:542:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:580:VAL:O	1:Q:584:GLU:HG2	2.10	0.51
1:C:645:VAL:HG13	1:C:649:ILE:HD12	1.92	0.50
1:E:580:VAL:O	1:E:584:GLU:HG2	2.10	0.50
1:H:373:LEU:HD23	1:H:374:LEU:N	2.26	0.50
1:O:645:VAL:HG13	1:O:649:ILE:HD12	1.92	0.50
1:A:580:VAL:O	1:A:584:GLU:HG2	2.10	0.50
1:C:373:LEU:HD23	1:C:374:LEU:N	2.26	0.50
1:D:373:LEU:HD23	1:D:374:LEU:N	2.26	0.50
1:F:580:VAL:O	1:F:584:GLU:HG2	2.10	0.50
1:G:373:LEU:HD23	1:G:374:LEU:N	2.26	0.50
1:J:373:LEU:HD23	1:J:374:LEU:N	2.26	0.50
1:K:373:LEU:HD23	1:K:374:LEU:N	2.26	0.50
1:M:580:VAL:O	1:M:584:GLU:HG2	2.10	0.50
1:N:580:VAL:O	1:N:584:GLU:HG2	2.10	0.50
1:O:373:LEU:HD23	1:O:374:LEU:N	2.26	0.50
1:P:373:LEU:HD23	1:P:374:LEU:N	2.26	0.50
1:B:580:VAL:O	1:B:584:GLU:HG2	2.10	0.50
1:E:616:GLU:OE1	1:E:619:ARG:NH2	2.45	0.50
1:Q:616:GLU:OE1	1:Q:619:ARG:NH2	2.45	0.50
1:R:616:GLU:OE1	1:R:619:ARG:NH2	2.45	0.50
1:F:616:GLU:OE1	1:F:619:ARG:NH2	2.45	0.50
1:Q:595:CYS:HB2	1:Q:694:ILE:HD11	1.94	0.50
1:D:595:CYS:HB2	1:D:694:ILE:HD11	1.94	0.50
1:D:616:GLU:OE1	1:D:619:ARG:NH2	2.45	0.50
1:E:595:CYS:HB2	1:E:694:ILE:HD11	1.94	0.50
1:H:616:GLU:OE1	1:H:619:ARG:NH2	2.45	0.50
1:N:595:CYS:HB2	1:N:694:ILE:HD11	1.94	0.50
1:E:373:LEU:HD23	1:E:374:LEU:N	2.26	0.50
1:F:595:CYS:HB2	1:F:694:ILE:HD11	1.94	0.50
1:I:595:CYS:HB2	1:I:694:ILE:HD11	1.94	0.50
1:K:616:GLU:OE1	1:K:619:ARG:NH2	2.45	0.50
1:L:373:LEU:HD23	1:L:374:LEU:N	2.26	0.50
1:M:595:CYS:HB2	1:M:694:ILE:HD11	1.94	0.50
1:P:595:CYS:HB2	1:P:694:ILE:HD11	1.94	0.50
1:Q:373:LEU:HD23	1:Q:374:LEU:N	2.26	0.50
1:R:595:CYS:HB2	1:R:694:ILE:HD11	1.94	0.50
1:B:595:CYS:HB2	1:B:694:ILE:HD11	1.94	0.50
1:C:595:CYS:HB2	1:C:694:ILE:HD11	1.94	0.50
1:H:595:CYS:HB2	1:H:694:ILE:HD11	1.94	0.50
1:L:595:CYS:HB2	1:L:694:ILE:HD11	1.94	0.50
1:N:373:LEU:HD23	1:N:374:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:595:CYS:HB2	1:O:694:ILE:HD11	1.94	0.50
1:P:616:GLU:OE1	1:P:619:ARG:NH2	2.45	0.50
1:A:595:CYS:HB2	1:A:694:ILE:HD11	1.94	0.50
1:I:373:LEU:HD23	1:I:374:LEU:N	2.26	0.50
1:K:595:CYS:HB2	1:K:694:ILE:HD11	1.94	0.50
1:B:373:LEU:HD23	1:B:374:LEU:N	2.26	0.49
1:F:373:LEU:HD23	1:F:374:LEU:N	2.26	0.49
1:B:616:GLU:OE1	1:B:619:ARG:NH2	2.45	0.49
1:M:373:LEU:HD23	1:M:374:LEU:N	2.26	0.49
1:N:616:GLU:OE1	1:N:619:ARG:NH2	2.45	0.49
1:J:595:CYS:HB2	1:J:694:ILE:HD11	1.94	0.49
1:L:427:ILE:O	1:L:434:VAL:HG12	2.13	0.49
1:N:427:ILE:O	1:N:434:VAL:HG12	2.13	0.49
1:R:373:LEU:HD23	1:R:374:LEU:N	2.26	0.49
1:A:373:LEU:HD23	1:A:374:LEU:N	2.26	0.49
1:B:427:ILE:O	1:B:434:VAL:HG12	2.13	0.49
1:I:427:ILE:O	1:I:434:VAL:HG12	2.13	0.49
1:I:616:GLU:OE1	1:I:619:ARG:NH2	2.45	0.49
1:J:616:GLU:OE1	1:J:619:ARG:NH2	2.45	0.49
1:G:595:CYS:HB2	1:G:694:ILE:HD11	1.94	0.49
1:J:427:ILE:O	1:J:434:VAL:HG12	2.13	0.49
1:L:616:GLU:OE1	1:L:619:ARG:NH2	2.45	0.49
1:A:616:GLU:OE1	1:A:619:ARG:NH2	2.45	0.49
1:C:616:GLU:OE1	1:C:619:ARG:NH2	2.45	0.49
1:G:363:GLU:O	1:H:398:ARG:NH2	2.46	0.49
1:G:427:ILE:O	1:G:434:VAL:HG12	2.13	0.49
1:G:616:GLU:OE1	1:G:619:ARG:NH2	2.45	0.49
1:E:603:ASN:ND2	1:E:693:GLN:O	2.46	0.49
1:M:616:GLU:OE1	1:M:619:ARG:NH2	2.45	0.49
1:O:616:GLU:OE1	1:O:619:ARG:NH2	2.45	0.49
1:Q:603:ASN:ND2	1:Q:693:GLN:O	2.46	0.49
1:F:603:ASN:ND2	1:F:693:GLN:O	2.46	0.49
1:R:603:ASN:ND2	1:R:693:GLN:O	2.46	0.49
1:D:603:ASN:ND2	1:D:693:GLN:O	2.46	0.49
1:P:603:ASN:ND2	1:P:693:GLN:O	2.46	0.49
1:E:427:ILE:O	1:E:434:VAL:HG12	2.13	0.48
1:H:427:ILE:O	1:H:434:VAL:HG12	2.13	0.48
1:D:363:GLU:O	1:E:398:ARG:NH2	2.46	0.48
1:K:478:GLU:H	1:K:478:GLU:CD	2.17	0.48
1:D:427:ILE:O	1:D:434:VAL:HG12	2.13	0.48
1:H:478:GLU:H	1:H:478:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:603:ASN:ND2	1:O:693:GLN:O	2.46	0.48
1:P:427:ILE:O	1:P:434:VAL:HG12	2.13	0.48
1:Q:427:ILE:O	1:Q:434:VAL:HG12	2.13	0.48
1:C:603:ASN:ND2	1:C:693:GLN:O	2.46	0.48
1:K:427:ILE:O	1:K:434:VAL:HG12	2.13	0.48
1:C:427:ILE:O	1:C:434:VAL:HG12	2.13	0.48
1:O:427:ILE:O	1:O:434:VAL:HG12	2.13	0.48
1:B:610:PHE:HE2	1:B:661:LEU:HD11	1.79	0.48
1:F:427:ILE:O	1:F:434:VAL:HG12	2.13	0.48
1:R:427:ILE:O	1:R:434:VAL:HG12	2.13	0.48
1:A:427:ILE:O	1:A:434:VAL:HG12	2.13	0.48
1:M:427:ILE:O	1:M:434:VAL:HG12	2.13	0.48
1:N:603:ASN:ND2	1:N:693:GLN:O	2.46	0.48
1:N:610:PHE:HE2	1:N:661:LEU:HD11	1.79	0.48
1:B:603:ASN:ND2	1:B:693:GLN:O	2.46	0.48
1:D:478:GLU:H	1:D:478:GLU:CD	2.17	0.48
1:E:610:PHE:HE2	1:E:661:LEU:HD11	1.79	0.48
1:I:603:ASN:ND2	1:I:693:GLN:O	2.46	0.48
1:L:598:TYR:CE2	1:L:685:LEU:HD21	2.49	0.48
1:M:603:ASN:ND2	1:M:693:GLN:O	2.46	0.48
1:O:478:GLU:H	1:O:478:GLU:CD	2.17	0.48
1:C:478:GLU:H	1:C:478:GLU:CD	2.17	0.48
1:I:598:TYR:CE2	1:I:685:LEU:HD21	2.49	0.48
1:L:603:ASN:ND2	1:L:693:GLN:O	2.46	0.48
1:P:478:GLU:H	1:P:478:GLU:CD	2.17	0.48
1:Q:610:PHE:HE2	1:Q:661:LEU:HD11	1.79	0.48
1:A:603:ASN:ND2	1:A:693:GLN:O	2.46	0.47
1:D:598:TYR:CE2	1:D:685:LEU:HD21	2.49	0.47
1:P:598:TYR:CE2	1:P:685:LEU:HD21	2.49	0.47
1:A:598:TYR:CE2	1:A:685:LEU:HD21	2.49	0.47
1:A:610:PHE:HE2	1:A:661:LEU:HD11	1.79	0.47
1:H:598:TYR:CE2	1:H:685:LEU:HD21	2.49	0.47
1:J:610:PHE:HE2	1:J:661:LEU:HD11	1.79	0.47
1:K:598:TYR:CE2	1:K:685:LEU:HD21	2.49	0.47
1:M:598:TYR:CE2	1:M:685:LEU:HD21	2.49	0.47
1:M:610:PHE:HE2	1:M:661:LEU:HD11	1.79	0.47
1:F:598:TYR:CE2	1:F:685:LEU:HD21	2.49	0.47
1:G:610:PHE:HE2	1:G:661:LEU:HD11	1.79	0.47
1:R:598:TYR:CE2	1:R:685:LEU:HD21	2.49	0.47
1:E:478:GLU:H	1:E:478:GLU:CD	2.17	0.47
1:F:587:ARG:NH2	1:F:689:GLU:OE1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:603:ASN:ND2	1:H:693:GLN:O	2.46	0.47
1:J:478:GLU:H	1:J:478:GLU:CD	2.17	0.47
1:O:610:PHE:HE2	1:O:661:LEU:HD11	1.79	0.47
1:C:598:TYR:CE2	1:C:685:LEU:HD21	2.49	0.47
1:H:610:PHE:HE2	1:H:661:LEU:HD11	1.79	0.47
1:K:603:ASN:ND2	1:K:693:GLN:O	2.46	0.47
1:Q:478:GLU:H	1:Q:478:GLU:CD	2.17	0.47
1:C:610:PHE:HE2	1:C:661:LEU:HD11	1.79	0.47
1:G:478:GLU:H	1:G:478:GLU:CD	2.17	0.47
1:K:610:PHE:HE2	1:K:661:LEU:HD11	1.79	0.47
1:O:598:TYR:CE2	1:O:685:LEU:HD21	2.49	0.47
1:R:587:ARG:NH2	1:R:689:GLU:OE1	2.47	0.47
1:B:587:ARG:NH2	1:B:689:GLU:OE1	2.47	0.47
1:B:598:TYR:CE2	1:B:685:LEU:HD21	2.49	0.47
1:C:587:ARG:NH2	1:C:689:GLU:OE1	2.47	0.47
1:D:610:PHE:HE2	1:D:661:LEU:HD11	1.79	0.47
1:I:610:PHE:HE2	1:I:661:LEU:HD11	1.79	0.47
1:J:598:TYR:CE2	1:J:685:LEU:HD21	2.49	0.47
1:N:478:GLU:H	1:N:478:GLU:CD	2.17	0.47
1:N:587:ARG:NH2	1:N:689:GLU:OE1	2.47	0.47
1:O:587:ARG:NH2	1:O:689:GLU:OE1	2.47	0.47
1:R:610:PHE:HE2	1:R:661:LEU:HD11	1.79	0.47
1:F:610:PHE:HE2	1:F:661:LEU:HD11	1.79	0.47
1:G:598:TYR:CE2	1:G:685:LEU:HD21	2.49	0.47
1:L:610:PHE:HE2	1:L:661:LEU:HD11	1.79	0.47
1:N:598:TYR:CE2	1:N:685:LEU:HD21	2.49	0.47
1:P:610:PHE:HE2	1:P:661:LEU:HD11	1.79	0.47
1:G:603:ASN:ND2	1:G:693:GLN:O	2.46	0.46
1:H:587:ARG:NH2	1:H:689:GLU:OE1	2.47	0.46
1:H:656:GLN:O	1:H:657:SER:OG	2.31	0.46
1:K:587:ARG:NH2	1:K:689:GLU:OE1	2.47	0.46
1:Q:598:TYR:CE2	1:Q:685:LEU:HD21	2.49	0.46
1:E:598:TYR:CE2	1:E:685:LEU:HD21	2.49	0.46
1:J:603:ASN:ND2	1:J:693:GLN:O	2.46	0.46
1:C:656:GLN:O	1:C:657:SER:OG	2.31	0.46
1:J:587:ARG:NH2	1:J:689:GLU:OE1	2.47	0.46
1:D:522:LEU:HD11	1:D:545:MET:SD	2.56	0.46
1:L:522:LEU:HD11	1:L:545:MET:SD	2.56	0.46
1:P:522:LEU:HD11	1:P:545:MET:SD	2.56	0.46
1:C:452:GLN:NE2	1:C:453:LEU:HG	2.31	0.46
1:G:587:ARG:NH2	1:G:689:GLU:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:522:LEU:HD11	1:I:545:MET:SD	2.56	0.46
1:B:452:GLN:NE2	1:B:453:LEU:HG	2.31	0.46
1:C:447:ARG:HE	1:C:472:THR:CG2	2.29	0.46
1:M:447:ARG:HE	1:M:472:THR:CG2	2.29	0.46
1:M:452:GLN:NE2	1:M:453:LEU:HG	2.31	0.46
1:M:587:ARG:NH2	1:M:689:GLU:OE1	2.47	0.46
1:O:439:LEU:O	1:O:439:LEU:HD12	2.16	0.46
1:O:447:ARG:HE	1:O:472:THR:CG2	2.29	0.46
1:O:452:GLN:NE2	1:O:453:LEU:HG	2.31	0.46
1:A:447:ARG:HE	1:A:472:THR:CG2	2.29	0.46
1:A:587:ARG:NH2	1:A:689:GLU:OE1	2.47	0.46
1:C:439:LEU:O	1:C:439:LEU:HD12	2.16	0.46
1:D:439:LEU:HD12	1:D:439:LEU:O	2.16	0.46
1:D:447:ARG:HE	1:D:472:THR:CG2	2.29	0.46
1:F:452:GLN:NE2	1:F:453:LEU:HG	2.31	0.46
1:I:452:GLN:NE2	1:I:453:LEU:HG	2.31	0.46
1:I:587:ARG:NH2	1:I:689:GLU:OE1	2.47	0.46
1:N:452:GLN:NE2	1:N:453:LEU:HG	2.31	0.46
1:P:439:LEU:HD12	1:P:439:LEU:O	2.16	0.46
1:A:439:LEU:HD12	1:A:439:LEU:O	2.16	0.46
1:A:452:GLN:NE2	1:A:453:LEU:HG	2.31	0.46
1:B:522:LEU:HD11	1:B:545:MET:SD	2.56	0.46
1:D:452:GLN:NE2	1:D:453:LEU:HG	2.31	0.46
1:G:447:ARG:HE	1:G:472:THR:CG2	2.29	0.46
1:H:522:LEU:HD11	1:H:545:MET:SD	2.56	0.46
1:I:447:ARG:HE	1:I:472:THR:CG2	2.29	0.46
1:J:447:ARG:HE	1:J:472:THR:CG2	2.29	0.46
1:L:452:GLN:NE2	1:L:453:LEU:HG	2.31	0.46
1:L:587:ARG:NH2	1:L:689:GLU:OE1	2.47	0.46
1:M:439:LEU:O	1:M:439:LEU:HD12	2.16	0.46
1:N:522:LEU:HD11	1:N:545:MET:SD	2.56	0.46
1:P:447:ARG:HE	1:P:472:THR:CG2	2.29	0.46
1:R:452:GLN:NE2	1:R:453:LEU:HG	2.31	0.46
1:B:439:LEU:HD12	1:B:439:LEU:O	2.16	0.45
1:D:587:ARG:NH2	1:D:689:GLU:OE1	2.47	0.45
1:K:439:LEU:HD12	1:K:439:LEU:O	2.16	0.45
1:L:447:ARG:HE	1:L:472:THR:CG2	2.29	0.45
1:N:439:LEU:HD12	1:N:439:LEU:O	2.16	0.45
1:P:452:GLN:NE2	1:P:453:LEU:HG	2.31	0.45
1:A:522:LEU:HD11	1:A:545:MET:SD	2.56	0.45
1:F:424:GLU:HA	1:F:438:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:439:LEU:HD12	1:I:439:LEU:O	2.16	0.45
1:K:424:GLU:HA	1:K:438:GLU:HA	1.98	0.45
1:K:522:LEU:HD11	1:K:545:MET:SD	2.56	0.45
1:L:439:LEU:HD12	1:L:439:LEU:O	2.16	0.45
1:P:587:ARG:NH2	1:P:689:GLU:OE1	2.47	0.45
1:Q:452:GLN:NE2	1:Q:453:LEU:HG	2.31	0.45
1:Q:522:LEU:HD11	1:Q:545:MET:SD	2.56	0.45
1:R:424:GLU:HA	1:R:438:GLU:HA	1.98	0.45
1:B:522:LEU:HD21	1:B:545:MET:HE1	1.99	0.45
1:C:424:GLU:HA	1:C:438:GLU:HA	1.98	0.45
1:E:447:ARG:HE	1:E:472:THR:CG2	2.29	0.45
1:H:424:GLU:HA	1:H:438:GLU:HA	1.98	0.45
1:H:439:LEU:O	1:H:439:LEU:HD12	2.16	0.45
1:H:452:GLN:NE2	1:H:453:LEU:HG	2.31	0.45
1:H:463:GLY:O	1:H:474:TRP:HD1	2.00	0.45
1:K:463:GLY:O	1:K:474:TRP:HD1	2.00	0.45
1:M:522:LEU:HD11	1:M:545:MET:SD	2.56	0.45
1:B:424:GLU:HA	1:B:438:GLU:HA	1.98	0.45
1:D:447:ARG:HE	1:D:472:THR:HG23	1.82	0.45
1:E:439:LEU:HD12	1:E:439:LEU:O	2.16	0.45
1:E:452:GLN:NE2	1:E:453:LEU:HG	2.31	0.45
1:J:424:GLU:HA	1:J:438:GLU:HA	1.98	0.45
1:J:452:GLN:NE2	1:J:453:LEU:HG	2.31	0.45
1:K:452:GLN:NE2	1:K:453:LEU:HG	2.31	0.45
1:N:424:GLU:HA	1:N:438:GLU:HA	1.98	0.45
1:O:424:GLU:HA	1:O:438:GLU:HA	1.98	0.45
1:P:447:ARG:HE	1:P:472:THR:HG23	1.82	0.45
1:Q:439:LEU:HD12	1:Q:439:LEU:O	2.16	0.45
1:Q:447:ARG:HE	1:Q:472:THR:CG2	2.29	0.45
1:E:463:GLY:O	1:E:474:TRP:HD1	2.00	0.45
1:E:522:LEU:HD11	1:E:545:MET:SD	2.56	0.45
1:F:440:LYS:C	1:F:442:GLY:H	2.20	0.45
1:G:424:GLU:HA	1:G:438:GLU:HA	1.98	0.45
1:G:452:GLN:NE2	1:G:453:LEU:HG	2.31	0.45
1:G:463:GLY:O	1:G:474:TRP:HD1	2.00	0.45
1:J:463:GLY:O	1:J:474:TRP:HD1	2.00	0.45
1:K:447:ARG:HE	1:K:472:THR:CG2	2.29	0.45
1:Q:379:SER:O	1:Q:380:SER:OG	2.26	0.45
1:Q:463:GLY:O	1:Q:474:TRP:HD1	2.00	0.45
1:C:522:LEU:HD11	1:C:545:MET:SD	2.56	0.45
1:F:447:ARG:HE	1:F:472:THR:CG2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:447:ARG:HE	1:G:472:THR:HG23	1.82	0.45
1:G:466:LEU:HD23	1:G:466:LEU:O	2.17	0.45
1:H:447:ARG:HE	1:H:472:THR:CG2	2.29	0.45
1:I:440:LYS:C	1:I:442:GLY:H	2.20	0.45
1:J:440:LYS:C	1:J:442:GLY:H	2.20	0.45
1:J:466:LEU:HD23	1:J:466:LEU:O	2.17	0.45
1:L:440:LYS:C	1:L:442:GLY:H	2.20	0.45
1:L:448:GLU:OE1	1:L:488:LEU:HB3	2.17	0.45
1:O:522:LEU:HD11	1:O:545:MET:SD	2.56	0.45
1:R:439:LEU:HD12	1:R:439:LEU:O	2.16	0.45
1:R:447:ARG:HE	1:R:472:THR:CG2	2.29	0.45
1:F:439:LEU:HD12	1:F:439:LEU:O	2.16	0.45
1:G:439:LEU:HD12	1:G:439:LEU:O	2.16	0.45
1:I:448:GLU:OE1	1:I:488:LEU:HB3	2.17	0.45
1:I:463:GLY:O	1:I:474:TRP:HD1	2.00	0.45
1:J:447:ARG:HE	1:J:472:THR:HG23	1.82	0.45
1:L:447:ARG:HE	1:L:472:THR:HG23	1.82	0.45
1:L:463:GLY:O	1:L:474:TRP:HD1	2.00	0.45
1:A:424:GLU:HA	1:A:438:GLU:HA	1.98	0.45
1:A:447:ARG:HE	1:A:472:THR:HG23	1.82	0.45
1:A:466:LEU:O	1:A:466:LEU:HD23	2.17	0.45
1:B:447:ARG:HE	1:B:472:THR:CG2	2.29	0.45
1:E:379:SER:O	1:E:380:SER:OG	2.26	0.45
1:J:439:LEU:HD12	1:J:439:LEU:O	2.16	0.45
1:M:466:LEU:O	1:M:466:LEU:HD23	2.17	0.45
1:R:440:LYS:C	1:R:442:GLY:H	2.20	0.45
1:B:373:LEU:HD22	1:B:412:ILE:HG23	1.99	0.45
1:C:463:GLY:O	1:C:474:TRP:HD1	2.00	0.45
1:D:424:GLU:HA	1:D:438:GLU:HA	1.98	0.45
1:E:424:GLU:HA	1:E:438:GLU:HA	1.98	0.45
1:G:440:LYS:C	1:G:442:GLY:H	2.20	0.45
1:H:448:GLU:OE1	1:H:488:LEU:HB3	2.17	0.45
1:H:466:LEU:O	1:H:466:LEU:HD23	2.17	0.45
1:I:447:ARG:HE	1:I:472:THR:HG23	1.82	0.45
1:M:447:ARG:HE	1:M:472:THR:HG23	1.82	0.45
1:N:373:LEU:HD22	1:N:412:ILE:HG23	1.99	0.45
1:N:447:ARG:HE	1:N:472:THR:CG2	2.29	0.45
1:O:373:LEU:HD22	1:O:412:ILE:HG23	1.99	0.45
1:O:466:LEU:HD23	1:O:466:LEU:O	2.17	0.45
1:Q:447:ARG:HE	1:Q:472:THR:HG23	1.82	0.45
1:R:447:ARG:HE	1:R:472:THR:HG23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:466:LEU:O	1:R:466:LEU:HD23	2.17	0.45
1:A:463:GLY:O	1:A:474:TRP:HD1	2.00	0.45
1:B:463:GLY:O	1:B:474:TRP:HD1	2.00	0.45
1:C:373:LEU:HD22	1:C:412:ILE:HG23	1.99	0.45
1:E:447:ARG:HE	1:E:472:THR:HG23	1.82	0.45
1:H:440:LYS:C	1:H:442:GLY:H	2.20	0.45
1:K:448:GLU:OE1	1:K:488:LEU:HB3	2.17	0.45
1:K:466:LEU:O	1:K:466:LEU:HD23	2.17	0.45
1:P:424:GLU:HA	1:P:438:GLU:HA	1.98	0.45
1:B:408:PRO:HG3	1:B:521:LEU:HD21	1.99	0.44
1:B:440:LYS:C	1:B:442:GLY:H	2.20	0.44
1:C:466:LEU:HD23	1:C:466:LEU:O	2.17	0.44
1:D:466:LEU:O	1:D:466:LEU:HD23	2.17	0.44
1:F:447:ARG:HE	1:F:472:THR:HG23	1.82	0.44
1:F:463:GLY:O	1:F:474:TRP:HD1	2.00	0.44
1:F:466:LEU:O	1:F:466:LEU:HD23	2.17	0.44
1:G:522:LEU:HD11	1:G:545:MET:SD	2.56	0.44
1:I:408:PRO:HG3	1:I:521:LEU:HD21	2.00	0.44
1:I:424:GLU:HA	1:I:438:GLU:HA	1.98	0.44
1:J:522:LEU:HD11	1:J:545:MET:SD	2.56	0.44
1:L:424:GLU:HA	1:L:438:GLU:HA	1.98	0.44
1:M:424:GLU:HA	1:M:438:GLU:HA	1.98	0.44
1:M:463:GLY:O	1:M:474:TRP:HD1	2.00	0.44
1:N:463:GLY:O	1:N:474:TRP:HD1	2.00	0.44
1:O:447:ARG:HE	1:O:472:THR:HG23	1.82	0.44
1:O:463:GLY:O	1:O:474:TRP:HD1	2.00	0.44
1:Q:424:GLU:HA	1:Q:438:GLU:HA	1.98	0.44
1:R:463:GLY:O	1:R:474:TRP:HD1	2.00	0.44
1:A:448:GLU:OE1	1:A:488:LEU:HB3	2.17	0.44
1:C:443:TYR:CG	1:C:444:LEU:N	2.85	0.44
1:C:447:ARG:HE	1:C:472:THR:HG23	1.82	0.44
1:D:463:GLY:O	1:D:474:TRP:HD1	2.00	0.44
1:F:443:TYR:CG	1:F:444:LEU:N	2.85	0.44
1:M:448:GLU:OE1	1:M:488:LEU:HB3	2.17	0.44
1:O:443:TYR:CG	1:O:444:LEU:N	2.85	0.44
1:P:463:GLY:O	1:P:474:TRP:HD1	2.00	0.44
1:R:443:TYR:CG	1:R:444:LEU:N	2.85	0.44
1:R:522:LEU:HD11	1:R:545:MET:SD	2.56	0.44
1:C:448:GLU:OE1	1:C:488:LEU:HB3	2.17	0.44
1:D:443:TYR:CG	1:D:444:LEU:N	2.85	0.44
1:F:522:LEU:HD11	1:F:545:MET:SD	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:448:GLU:OE1	1:G:488:LEU:HB3	2.17	0.44
1:G:519:ARG:HG2	1:H:531:GLU:CG	2.43	0.44
1:L:408:PRO:HG3	1:L:521:LEU:HD21	2.00	0.44
1:N:408:PRO:HG3	1:N:521:LEU:HD21	2.00	0.44
1:N:440:LYS:C	1:N:442:GLY:H	2.20	0.44
1:O:448:GLU:OE1	1:O:488:LEU:HB3	2.17	0.44
1:P:379:SER:O	1:P:380:SER:OG	2.26	0.44
1:A:373:LEU:HD22	1:A:412:ILE:HG23	1.99	0.44
1:A:408:PRO:HG3	1:A:521:LEU:HD21	2.00	0.44
1:J:443:TYR:CG	1:J:444:LEU:N	2.85	0.44
1:J:448:GLU:OE1	1:J:488:LEU:HB3	2.17	0.44
1:K:440:LYS:C	1:K:442:GLY:H	2.20	0.44
1:M:373:LEU:HD22	1:M:412:ILE:HG23	1.99	0.44
1:M:408:PRO:HG3	1:M:521:LEU:HD21	2.00	0.44
1:P:443:TYR:CG	1:P:444:LEU:N	2.85	0.44
1:P:466:LEU:O	1:P:466:LEU:HD23	2.17	0.44
1:R:448:GLU:OE1	1:R:488:LEU:HB3	2.17	0.44
1:F:448:GLU:OE1	1:F:488:LEU:HB3	2.17	0.44
1:G:443:TYR:CG	1:G:444:LEU:N	2.85	0.44
1:Q:443:TYR:CG	1:Q:444:LEU:N	2.85	0.44
1:Q:466:LEU:HD23	1:Q:466:LEU:O	2.17	0.44
1:K:450:VAL:HB	1:K:488:LEU:HD22	2.00	0.44
1:N:522:LEU:HD21	1:N:545:MET:HE1	2.00	0.44
1:Q:448:GLU:OE1	1:Q:488:LEU:HB3	2.17	0.44
1:B:447:ARG:HE	1:B:472:THR:HG23	1.82	0.44
1:E:443:TYR:CG	1:E:444:LEU:N	2.85	0.44
1:E:448:GLU:OE1	1:E:488:LEU:HB3	2.17	0.44
1:F:450:VAL:HB	1:F:488:LEU:HD22	2.00	0.44
1:H:450:VAL:HB	1:H:488:LEU:HD22	2.00	0.44
1:J:450:VAL:HB	1:J:488:LEU:HD22	2.00	0.44
1:L:450:VAL:HB	1:L:488:LEU:HD22	2.00	0.44
1:L:466:LEU:HD23	1:L:466:LEU:O	2.17	0.44
1:Q:440:LYS:C	1:Q:442:GLY:H	2.20	0.44
1:D:373:LEU:HD22	1:D:412:ILE:HG23	1.99	0.44
1:E:466:LEU:HD23	1:E:466:LEU:O	2.17	0.44
1:G:450:VAL:HB	1:G:488:LEU:HD22	2.00	0.44
1:I:450:VAL:HB	1:I:488:LEU:HD22	2.00	0.44
1:R:450:VAL:HB	1:R:488:LEU:HD22	2.00	0.44
1:C:408:PRO:HG3	1:C:521:LEU:HD21	1.99	0.44
1:C:483:LEU:HD12	1:C:486:SER:HB2	2.00	0.44
1:E:440:LYS:C	1:E:442:GLY:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:373:LEU:HD22	1:F:412:ILE:HG23	1.99	0.44
1:G:408:PRO:HG3	1:G:521:LEU:HD21	2.00	0.44
1:H:408:PRO:HG3	1:H:521:LEU:HD21	2.00	0.44
1:I:466:LEU:HD23	1:I:466:LEU:O	2.17	0.44
1:J:408:PRO:HG3	1:J:521:LEU:HD21	2.00	0.44
1:K:408:PRO:HG3	1:K:521:LEU:HD21	2.00	0.44
1:M:656:GLN:O	1:M:657:SER:OG	2.31	0.44
1:N:447:ARG:HE	1:N:472:THR:HG23	1.82	0.44
1:O:408:PRO:HG3	1:O:521:LEU:HD21	2.00	0.44
1:O:483:LEU:HD12	1:O:486:SER:HB2	2.00	0.44
1:P:373:LEU:HD22	1:P:412:ILE:HG23	1.99	0.44
1:R:373:LEU:HD22	1:R:412:ILE:HG23	1.99	0.44
1:A:450:VAL:HB	1:A:488:LEU:HD22	2.00	0.43
1:D:440:LYS:C	1:D:442:GLY:H	2.20	0.43
1:D:448:GLU:OE1	1:D:488:LEU:HB3	2.17	0.43
1:E:450:VAL:HB	1:E:488:LEU:HD22	2.00	0.43
1:G:373:LEU:HD22	1:G:412:ILE:HG23	1.99	0.43
1:J:373:LEU:HD22	1:J:412:ILE:HG23	1.99	0.43
1:J:398:ARG:NH2	1:R:363:GLU:O	2.51	0.43
1:M:450:VAL:HB	1:M:488:LEU:HD22	2.00	0.43
1:Q:450:VAL:HB	1:Q:488:LEU:HD22	2.00	0.43
1:C:440:LYS:C	1:C:442:GLY:H	2.20	0.43
1:D:690:LEU:HD13	1:D:696:ILE:HD11	2.00	0.43
1:H:447:ARG:HE	1:H:472:THR:HG23	1.82	0.43
1:O:690:LEU:HD13	1:O:696:ILE:HD11	2.00	0.43
1:P:690:LEU:HD13	1:P:696:ILE:HD11	2.00	0.43
1:A:440:LYS:C	1:A:442:GLY:H	2.20	0.43
1:B:483:LEU:HD12	1:B:486:SER:HB2	2.00	0.43
1:C:690:LEU:HD13	1:C:696:ILE:HD11	2.00	0.43
1:D:450:VAL:HB	1:D:488:LEU:HD22	2.00	0.43
1:H:373:LEU:HD22	1:H:412:ILE:HG23	1.99	0.43
1:I:522:LEU:HD21	1:I:545:MET:HE1	2.00	0.43
1:K:373:LEU:HD22	1:K:412:ILE:HG23	1.99	0.43
1:K:447:ARG:HE	1:K:472:THR:HG23	1.82	0.43
1:N:448:GLU:OE1	1:N:488:LEU:HB3	2.17	0.43
1:N:483:LEU:HD12	1:N:486:SER:HB2	2.00	0.43
1:O:440:LYS:C	1:O:442:GLY:H	2.20	0.43
1:P:440:LYS:C	1:P:442:GLY:H	2.20	0.43
1:P:448:GLU:OE1	1:P:488:LEU:HB3	2.17	0.43
1:P:450:VAL:HB	1:P:488:LEU:HD22	2.00	0.43
1:B:448:GLU:OE1	1:B:488:LEU:HB3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HD23	1:B:466:LEU:O	2.17	0.43
1:D:408:PRO:HG3	1:D:521:LEU:HD21	1.99	0.43
1:D:483:LEU:HD12	1:D:486:SER:HB2	2.00	0.43
1:E:587:ARG:NH2	1:E:689:GLU:OE1	2.47	0.43
1:B:450:VAL:HB	1:B:488:LEU:HD22	2.00	0.43
1:E:483:LEU:HD12	1:E:486:SER:HB2	2.00	0.43
1:H:488:LEU:HA	1:H:488:LEU:HD23	1.80	0.43
1:H:598:TYR:CD2	1:H:685:LEU:HD21	2.54	0.43
1:K:488:LEU:HA	1:K:488:LEU:HD23	1.80	0.43
1:K:598:TYR:CD2	1:K:685:LEU:HD21	2.54	0.43
1:L:373:LEU:HD22	1:L:412:ILE:HG23	1.99	0.43
1:L:522:LEU:HD21	1:L:545:MET:HE1	2.00	0.43
1:M:549:LEU:HD23	1:M:549:LEU:HA	1.83	0.43
1:P:483:LEU:HD12	1:P:486:SER:HB2	2.00	0.43
1:B:447:ARG:HG2	1:B:491:PHE:HB2	2.01	0.43
1:E:690:LEU:HD13	1:E:696:ILE:HD11	2.00	0.43
1:G:483:LEU:HD12	1:G:486:SER:HB2	2.00	0.43
1:L:443:TYR:CG	1:L:444:LEU:N	2.85	0.43
1:M:440:LYS:C	1:M:442:GLY:H	2.20	0.43
1:N:450:VAL:HB	1:N:488:LEU:HD22	2.00	0.43
1:Q:483:LEU:HD12	1:Q:486:SER:HB2	2.00	0.43
1:B:598:TYR:CD2	1:B:685:LEU:HD21	2.54	0.43
1:B:690:LEU:HD13	1:B:696:ILE:HD11	2.00	0.43
1:E:373:LEU:HD22	1:E:412:ILE:HG23	1.99	0.43
1:H:483:LEU:HD12	1:H:486:SER:HB2	2.00	0.43
1:I:373:LEU:HD22	1:I:412:ILE:HG23	1.99	0.43
1:I:443:TYR:CG	1:I:444:LEU:N	2.85	0.43
1:J:483:LEU:HD12	1:J:486:SER:HB2	2.00	0.43
1:N:447:ARG:HG2	1:N:491:PHE:HB2	2.01	0.43
1:N:466:LEU:HD23	1:N:466:LEU:O	2.17	0.43
1:N:690:LEU:HD13	1:N:696:ILE:HD11	2.00	0.43
1:Q:690:LEU:HD13	1:Q:696:ILE:HD11	2.00	0.43
1:A:447:ARG:HG2	1:A:491:PHE:HB2	2.01	0.43
1:A:690:LEU:HD13	1:A:696:ILE:HD11	2.00	0.43
1:C:450:VAL:HB	1:C:488:LEU:HD22	2.00	0.43
1:E:440:LYS:HG2	1:E:474:TRP:CE2	2.54	0.43
1:K:483:LEU:HD12	1:K:486:SER:HB2	2.00	0.43
1:M:447:ARG:HG2	1:M:491:PHE:HB2	2.01	0.43
1:M:598:TYR:CD2	1:M:685:LEU:HD21	2.54	0.43
1:N:598:TYR:CD2	1:N:685:LEU:HD21	2.54	0.43
1:O:440:LYS:HG2	1:O:474:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:408:PRO:HG3	1:P:521:LEU:HD21	2.00	0.43
1:P:440:LYS:HG2	1:P:474:TRP:CE2	2.54	0.43
1:Q:373:LEU:HD22	1:Q:412:ILE:HG23	1.99	0.43
1:Q:408:PRO:HG3	1:Q:521:LEU:HD21	2.00	0.43
1:Q:440:LYS:HG2	1:Q:474:TRP:CE2	2.54	0.43
1:Q:587:ARG:NH2	1:Q:689:GLU:OE1	2.47	0.43
1:R:690:LEU:HD13	1:R:696:ILE:HD11	2.00	0.43
1:A:483:LEU:HD12	1:A:486:SER:HB2	2.00	0.43
1:A:598:TYR:CD2	1:A:685:LEU:HD21	2.54	0.43
1:C:440:LYS:HG2	1:C:474:TRP:CE2	2.54	0.43
1:C:447:ARG:HG2	1:C:491:PHE:HB2	2.01	0.43
1:C:598:TYR:CD2	1:C:685:LEU:HD21	2.54	0.43
1:D:440:LYS:HG2	1:D:474:TRP:CE2	2.54	0.43
1:F:408:PRO:HG3	1:F:521:LEU:HD21	2.00	0.43
1:I:598:TYR:CD2	1:I:685:LEU:HD21	2.54	0.43
1:J:598:TYR:CD2	1:J:685:LEU:HD21	2.54	0.43
1:M:483:LEU:HD12	1:M:486:SER:HB2	2.00	0.43
1:M:690:LEU:HD13	1:M:696:ILE:HD11	2.00	0.43
1:O:447:ARG:HG2	1:O:491:PHE:HB2	2.01	0.43
1:O:450:VAL:HB	1:O:488:LEU:HD22	2.00	0.43
1:B:488:LEU:HA	1:B:488:LEU:HD23	1.80	0.43
1:B:610:PHE:CE2	1:B:661:LEU:HD21	2.54	0.43
1:D:375:ILE:HD11	1:D:501:LEU:HD12	2.01	0.43
1:E:408:PRO:HG3	1:E:521:LEU:HD21	2.00	0.43
1:F:440:LYS:HG2	1:F:474:TRP:CE2	2.54	0.43
1:F:690:LEU:HD13	1:F:696:ILE:HD11	2.00	0.43
1:G:598:TYR:CD2	1:G:685:LEU:HD21	2.54	0.43
1:I:483:LEU:HD12	1:I:486:SER:HB2	2.00	0.43
1:L:483:LEU:HD12	1:L:486:SER:HB2	2.00	0.43
1:R:408:PRO:HG3	1:R:521:LEU:HD21	2.00	0.43
1:A:610:PHE:CE2	1:A:661:LEU:HD21	2.54	0.42
1:F:375:ILE:HD11	1:F:501:LEU:HD12	2.01	0.42
1:G:460:TYR:HB3	1:G:479:TYR:CD1	2.54	0.42
1:I:447:ARG:HG2	1:I:491:PHE:HB2	2.01	0.42
1:J:531:GLU:CG	1:R:519:ARG:HG2	2.47	0.42
1:L:598:TYR:CD2	1:L:685:LEU:HD21	2.54	0.42
1:N:610:PHE:CE2	1:N:661:LEU:HD21	2.54	0.42
1:O:598:TYR:CD2	1:O:685:LEU:HD21	2.54	0.42
1:R:375:ILE:HD11	1:R:501:LEU:HD12	2.01	0.42
1:R:440:LYS:HG2	1:R:474:TRP:CE2	2.54	0.42
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:610:PHE:CE2	1:F:661:LEU:HD21	2.54	0.42
1:G:379:SER:O	1:G:380:SER:OG	2.26	0.42
1:J:460:TYR:HB3	1:J:479:TYR:CD1	2.54	0.42
1:P:375:ILE:HD11	1:P:501:LEU:HD12	2.01	0.42
1:P:598:TYR:CD2	1:P:685:LEU:HD21	2.54	0.42
1:Q:375:ILE:HD11	1:Q:501:LEU:HD12	2.01	0.42
1:R:610:PHE:CE2	1:R:661:LEU:HD21	2.54	0.42
1:A:522:LEU:HD21	1:A:545:MET:HE1	2.01	0.42
1:B:440:LYS:HG2	1:B:474:TRP:CE2	2.54	0.42
1:C:375:ILE:HD11	1:C:501:LEU:HD12	2.01	0.42
1:D:598:TYR:CD2	1:D:685:LEU:HD21	2.54	0.42
1:E:375:ILE:HD11	1:E:501:LEU:HD12	2.01	0.42
1:H:393:GLU:HG3	1:H:498:THR:HG21	2.02	0.42
1:K:393:GLU:HG3	1:K:498:THR:HG21	2.02	0.42
1:L:447:ARG:HG2	1:L:491:PHE:HB2	2.01	0.42
1:M:610:PHE:CE2	1:M:661:LEU:HD21	2.54	0.42
1:N:440:LYS:HG2	1:N:474:TRP:CE2	2.54	0.42
1:N:443:TYR:CG	1:N:444:LEU:N	2.85	0.42
1:O:375:ILE:HD11	1:O:501:LEU:HD12	2.01	0.42
1:P:447:ARG:HG2	1:P:491:PHE:HB2	2.01	0.42
1:Q:598:TYR:CD2	1:Q:685:LEU:HD21	2.54	0.42
1:C:610:PHE:CE2	1:C:661:LEU:HD21	2.54	0.42
1:E:460:TYR:HB3	1:E:479:TYR:CD1	2.55	0.42
1:E:598:TYR:CD2	1:E:685:LEU:HD21	2.54	0.42
1:G:610:PHE:CE2	1:G:661:LEU:HD21	2.54	0.42
1:J:379:SER:O	1:J:380:SER:OG	2.26	0.42
1:J:610:PHE:CE2	1:J:661:LEU:HD21	2.54	0.42
1:N:389:ALA:HB1	1:N:392:ASP:H	1.85	0.42
1:O:610:PHE:CE2	1:O:661:LEU:HD21	2.54	0.42
1:Q:460:TYR:HB3	1:Q:479:TYR:CD1	2.55	0.42
1:R:598:TYR:CD2	1:R:685:LEU:HD21	2.54	0.42
1:A:443:TYR:CG	1:A:444:LEU:N	2.85	0.42
1:B:389:ALA:HB1	1:B:392:ASP:H	1.85	0.42
1:B:443:TYR:CG	1:B:444:LEU:N	2.85	0.42
1:D:447:ARG:HG2	1:D:491:PHE:HB2	2.01	0.42
1:J:375:ILE:HD11	1:J:501:LEU:HD12	2.01	0.42
1:N:488:LEU:HA	1:N:488:LEU:HD23	1.80	0.42
1:P:522:LEU:HD21	1:P:545:MET:HE1	2.01	0.42
1:P:566:LEU:HA	1:P:566:LEU:HD23	1.78	0.42
1:Q:610:PHE:CE2	1:Q:661:LEU:HD21	2.54	0.42
1:A:460:TYR:HB3	1:A:479:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:TYR:HB3	1:B:479:TYR:CD1	2.54	0.42
1:F:393:GLU:HG3	1:F:498:THR:HG21	2.02	0.42
1:F:483:LEU:HD12	1:F:486:SER:HB2	2.00	0.42
1:F:598:TYR:CD2	1:F:685:LEU:HD21	2.54	0.42
1:I:440:LYS:HG2	1:I:474:TRP:CE2	2.54	0.42
1:M:443:TYR:CG	1:M:444:LEU:N	2.85	0.42
1:O:460:TYR:HB3	1:O:479:TYR:CD1	2.54	0.42
1:R:483:LEU:HD12	1:R:486:SER:HB2	2.00	0.42
1:A:393:GLU:HG3	1:A:498:THR:HG21	2.02	0.42
1:B:375:ILE:HD11	1:B:501:LEU:HD12	2.01	0.42
1:D:566:LEU:HA	1:D:566:LEU:HD23	1.78	0.42
1:E:610:PHE:CE2	1:E:661:LEU:HD21	2.54	0.42
1:G:375:ILE:HD11	1:G:501:LEU:HD12	2.01	0.42
1:H:690:LEU:HD13	1:H:696:ILE:HD11	2.00	0.42
1:I:690:LEU:HD13	1:I:696:ILE:HD11	2.00	0.42
1:J:447:ARG:HG2	1:J:491:PHE:HB2	2.01	0.42
1:K:690:LEU:HD13	1:K:696:ILE:HD11	2.00	0.42
1:L:440:LYS:HG2	1:L:474:TRP:CE2	2.54	0.42
1:M:460:TYR:HB3	1:M:479:TYR:CD1	2.55	0.42
1:N:375:ILE:HD11	1:N:501:LEU:HD12	2.01	0.42
1:N:460:TYR:HB3	1:N:479:TYR:CD1	2.55	0.42
1:Q:447:ARG:HG2	1:Q:491:PHE:HB2	2.01	0.42
1:R:393:GLU:HG3	1:R:498:THR:HG21	2.02	0.42
1:A:440:LYS:HG2	1:A:474:TRP:CE2	2.54	0.42
1:C:389:ALA:HB1	1:C:392:ASP:H	1.85	0.42
1:C:460:TYR:HB3	1:C:479:TYR:CD1	2.55	0.42
1:D:542:LEU:HD23	1:D:542:LEU:HA	1.91	0.42
1:F:460:TYR:HB3	1:F:479:TYR:CD1	2.55	0.42
1:G:690:LEU:HD13	1:G:696:ILE:HD11	2.00	0.42
1:I:610:PHE:CE2	1:I:661:LEU:HD21	2.54	0.42
1:J:690:LEU:HD13	1:J:696:ILE:HD11	2.00	0.42
1:M:440:LYS:HG2	1:M:474:TRP:CE2	2.54	0.42
1:M:478:GLU:H	1:M:478:GLU:CD	2.17	0.42
1:P:542:LEU:HD23	1:P:542:LEU:HA	1.91	0.42
1:R:447:ARG:HG2	1:R:491:PHE:HB2	2.01	0.42
1:A:478:GLU:H	1:A:478:GLU:CD	2.17	0.42
1:F:447:ARG:HG2	1:F:491:PHE:HB2	2.01	0.42
1:G:447:ARG:HG2	1:G:491:PHE:HB2	2.01	0.42
1:H:379:SER:O	1:H:380:SER:OG	2.26	0.42
1:H:447:ARG:HG2	1:H:491:PHE:HB2	2.01	0.42
1:I:389:ALA:HB1	1:I:392:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:389:ALA:HB1	1:L:392:ASP:H	1.85	0.42
1:L:690:LEU:HD13	1:L:696:ILE:HD11	2.00	0.42
1:M:393:GLU:HG3	1:M:498:THR:HG21	2.02	0.42
1:N:393:GLU:HG3	1:N:498:THR:HG21	2.02	0.42
1:O:389:ALA:HB1	1:O:392:ASP:H	1.85	0.42
1:Q:389:ALA:HB1	1:Q:392:ASP:H	1.85	0.42
1:R:460:TYR:HB3	1:R:479:TYR:CD1	2.54	0.42
1:B:393:GLU:HG3	1:B:498:THR:HG21	2.02	0.42
1:B:542:LEU:HD23	1:B:542:LEU:HA	1.91	0.42
1:E:389:ALA:HB1	1:E:392:ASP:H	1.85	0.42
1:E:447:ARG:HG2	1:E:491:PHE:HB2	2.01	0.42
1:H:440:LYS:HG2	1:H:474:TRP:CE2	2.54	0.42
1:K:440:LYS:HG2	1:K:474:TRP:CE2	2.54	0.42
1:L:610:PHE:CE2	1:L:661:LEU:HD21	2.54	0.42
1:P:610:PHE:CE2	1:P:661:LEU:HD21	2.54	0.42
1:E:393:GLU:HG3	1:E:498:THR:HG21	2.02	0.41
1:H:389:ALA:HB1	1:H:392:ASP:H	1.85	0.41
1:I:375:ILE:HD11	1:I:501:LEU:HD12	2.01	0.41
1:K:389:ALA:HB1	1:K:392:ASP:H	1.85	0.41
1:K:447:ARG:HG2	1:K:491:PHE:HB2	2.01	0.41
1:L:375:ILE:HD11	1:L:501:LEU:HD12	2.01	0.41
1:D:610:PHE:CE2	1:D:661:LEU:HD21	2.54	0.41
1:H:389:ALA:C	1:H:391:ASN:H	2.24	0.41
1:I:460:TYR:HB3	1:I:479:TYR:CD1	2.55	0.41
1:K:389:ALA:C	1:K:391:ASN:H	2.24	0.41
1:R:566:LEU:HD23	1:R:566:LEU:HA	1.78	0.41
1:A:690:LEU:HD23	1:A:690:LEU:HA	1.80	0.41
1:D:460:TYR:HB3	1:D:479:TYR:CD1	2.55	0.41
1:D:488:LEU:HD23	1:D:488:LEU:HA	1.80	0.41
1:G:440:LYS:HG2	1:G:474:TRP:CE2	2.54	0.41
1:H:443:TYR:CG	1:H:444:LEU:N	2.85	0.41
1:H:497:LEU:HA	1:H:497:LEU:HD12	1.79	0.41
1:J:389:ALA:C	1:J:391:ASN:H	2.24	0.41
1:J:389:ALA:HB1	1:J:392:ASP:H	1.85	0.41
1:J:440:LYS:HG2	1:J:474:TRP:CE2	2.54	0.41
1:K:367:PHE:CD2	1:L:524:GLN:HG2	2.55	0.41
1:K:379:SER:O	1:K:380:SER:OG	2.26	0.41
1:K:443:TYR:CG	1:K:444:LEU:N	2.85	0.41
1:K:610:PHE:CE2	1:K:661:LEU:HD21	2.54	0.41
1:L:367:PHE:CD2	1:M:524:GLN:HG2	2.56	0.41
1:L:393:GLU:HG3	1:L:498:THR:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:460:TYR:HB3	1:L:479:TYR:CD1	2.55	0.41
1:O:488:LEU:HD23	1:O:488:LEU:HA	1.80	0.41
1:P:460:TYR:HB3	1:P:479:TYR:CD1	2.55	0.41
1:P:488:LEU:HD23	1:P:488:LEU:HA	1.80	0.41
1:P:663:VAL:O	1:P:686:SER:HA	2.21	0.41
1:Q:393:GLU:HG3	1:Q:498:THR:HG21	2.02	0.41
1:A:460:TYR:OH	1:A:482:ARG:HD2	2.21	0.41
1:A:524:GLN:HG2	1:I:367:PHE:CD2	2.56	0.41
1:B:460:TYR:OH	1:B:482:ARG:HD2	2.21	0.41
1:B:634:ASP:O	1:B:638:THR:OG1	2.39	0.41
1:C:663:VAL:O	1:C:686:SER:HA	2.21	0.41
1:D:663:VAL:O	1:D:686:SER:HA	2.21	0.41
1:G:389:ALA:C	1:G:391:ASN:H	2.24	0.41
1:G:389:ALA:HB1	1:G:392:ASP:H	1.85	0.41
1:I:523:GLU:HA	1:I:526:GLU:HG2	2.02	0.41
1:I:542:LEU:HD23	1:I:542:LEU:HA	1.91	0.41
1:K:460:TYR:HB3	1:K:479:TYR:CD1	2.55	0.41
1:L:566:LEU:HD23	1:L:566:LEU:HA	1.78	0.41
1:M:460:TYR:OH	1:M:482:ARG:HD2	2.21	0.41
1:N:460:TYR:OH	1:N:482:ARG:HD2	2.21	0.41
1:N:542:LEU:HD23	1:N:542:LEU:HA	1.91	0.41
1:A:389:ALA:HB1	1:A:392:ASP:H	1.85	0.41
1:D:389:ALA:C	1:D:391:ASN:H	2.24	0.41
1:D:389:ALA:HB1	1:D:392:ASP:H	1.85	0.41
1:D:497:LEU:HD12	1:D:497:LEU:HA	1.79	0.41
1:E:488:LEU:HD23	1:E:488:LEU:HA	1.80	0.41
1:H:375:ILE:HD11	1:H:501:LEU:HD12	2.01	0.41
1:H:610:PHE:CE2	1:H:661:LEU:HD21	2.54	0.41
1:I:393:GLU:HG3	1:I:498:THR:HG21	2.02	0.41
1:I:478:GLU:H	1:I:478:GLU:CD	2.17	0.41
1:K:497:LEU:HD12	1:K:497:LEU:HA	1.79	0.41
1:L:478:GLU:H	1:L:478:GLU:CD	2.17	0.41
1:L:523:GLU:HA	1:L:526:GLU:HG2	2.03	0.41
1:M:690:LEU:HD23	1:M:690:LEU:HA	1.80	0.41
1:N:367:PHE:CD2	1:O:524:GLN:HG2	2.56	0.41
1:N:634:ASP:O	1:N:638:THR:OG1	2.39	0.41
1:O:663:VAL:O	1:O:686:SER:HA	2.21	0.41
1:P:389:ALA:HB1	1:P:392:ASP:H	1.85	0.41
1:Q:488:LEU:HD23	1:Q:488:LEU:HA	1.80	0.41
1:B:389:ALA:C	1:B:391:ASN:H	2.24	0.41
1:C:389:ALA:C	1:C:391:ASN:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:488:LEU:HD23	1:C:488:LEU:HA	1.80	0.41
1:F:500:HIS:O	1:F:504:VAL:N	2.53	0.41
1:F:566:LEU:HD23	1:F:566:LEU:HA	1.78	0.41
1:H:367:PHE:CD2	1:I:524:GLN:HG2	2.56	0.41
1:H:390:LEU:HD13	1:H:390:LEU:HA	1.95	0.41
1:H:443:TYR:CD2	1:H:444:LEU:N	2.88	0.41
1:H:460:TYR:HB3	1:H:479:TYR:CD1	2.55	0.41
1:I:566:LEU:HD23	1:I:566:LEU:HA	1.78	0.41
1:I:690:LEU:HD23	1:I:690:LEU:HA	1.80	0.41
1:K:375:ILE:HD11	1:K:501:LEU:HD12	2.01	0.41
1:M:389:ALA:HB1	1:M:392:ASP:H	1.85	0.41
1:M:523:GLU:HA	1:M:526:GLU:HG2	2.02	0.41
1:O:389:ALA:C	1:O:391:ASN:H	2.24	0.41
1:P:367:PHE:CD2	1:Q:524:GLN:HG2	2.56	0.41
1:P:389:ALA:C	1:P:391:ASN:H	2.24	0.41
1:E:367:PHE:CD2	1:F:524:GLN:HG2	2.56	0.41
1:F:389:ALA:C	1:F:391:ASN:H	2.24	0.41
1:G:663:VAL:O	1:G:686:SER:HA	2.21	0.41
1:I:634:ASP:O	1:I:638:THR:OG1	2.38	0.41
1:J:663:VAL:O	1:J:686:SER:HA	2.21	0.41
1:K:443:TYR:CD2	1:K:444:LEU:N	2.88	0.41
1:M:367:PHE:CD2	1:N:524:GLN:HG2	2.56	0.41
1:M:390:LEU:HD13	1:M:390:LEU:HA	1.95	0.41
1:O:542:LEU:HD23	1:O:542:LEU:HA	1.91	0.41
1:R:389:ALA:C	1:R:391:ASN:H	2.24	0.41
1:R:500:HIS:O	1:R:504:VAL:N	2.53	0.41
1:A:523:GLU:HA	1:A:526:GLU:HG2	2.03	0.41
1:G:393:GLU:HG3	1:G:498:THR:HG21	2.02	0.41
1:I:389:ALA:C	1:I:391:ASN:H	2.24	0.41
1:J:367:PHE:CD2	1:K:524:GLN:HG2	2.56	0.41
1:K:390:LEU:HD13	1:K:390:LEU:HA	1.95	0.41
1:L:634:ASP:O	1:L:638:THR:OG1	2.38	0.41
1:L:690:LEU:HD23	1:L:690:LEU:HA	1.80	0.41
1:Q:500:HIS:O	1:Q:504:VAL:N	2.53	0.41
1:A:367:PHE:CD2	1:B:524:GLN:HG2	2.56	0.41
1:A:375:ILE:HD11	1:A:501:LEU:HD12	2.01	0.41
1:A:390:LEU:HD13	1:A:390:LEU:HA	1.95	0.41
1:B:523:GLU:HA	1:B:526:GLU:HG2	2.03	0.41
1:C:456:LEU:HD23	1:C:462:LYS:HE3	2.03	0.41
1:C:542:LEU:HD23	1:C:542:LEU:HA	1.91	0.41
1:E:460:TYR:OH	1:E:482:ARG:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:500:HIS:O	1:E:504:VAL:N	2.53	0.41
1:F:389:ALA:HB1	1:F:392:ASP:H	1.85	0.41
1:G:500:HIS:O	1:G:504:VAL:N	2.53	0.41
1:I:460:TYR:OH	1:I:482:ARG:HD2	2.21	0.41
1:J:393:GLU:HG3	1:J:498:THR:HG21	2.02	0.41
1:J:497:LEU:HA	1:J:497:LEU:HD12	1.79	0.41
1:L:389:ALA:C	1:L:391:ASN:H	2.24	0.41
1:L:460:TYR:OH	1:L:482:ARG:HD2	2.21	0.41
1:M:375:ILE:HD11	1:M:501:LEU:HD12	2.01	0.41
1:M:663:VAL:O	1:M:686:SER:HA	2.21	0.41
1:N:389:ALA:C	1:N:391:ASN:H	2.24	0.41
1:N:523:GLU:HA	1:N:526:GLU:HG2	2.03	0.41
1:O:456:LEU:HD23	1:O:462:LYS:HE3	2.03	0.41
1:P:497:LEU:HD12	1:P:497:LEU:HA	1.79	0.41
1:Q:460:TYR:OH	1:Q:482:ARG:HD2	2.21	0.41
1:Q:663:VAL:O	1:Q:686:SER:HA	2.21	0.41
1:R:389:ALA:HB1	1:R:392:ASP:H	1.85	0.41
1:A:663:VAL:O	1:A:686:SER:HA	2.21	0.41
1:B:367:PHE:CD2	1:C:524:GLN:HG2	2.56	0.41
1:B:456:LEU:HD23	1:B:462:LYS:HE3	2.03	0.41
1:C:379:SER:O	1:C:380:SER:OG	2.26	0.41
1:E:389:ALA:C	1:E:391:ASN:H	2.24	0.41
1:E:523:GLU:HA	1:E:526:GLU:HG2	2.03	0.41
1:E:663:VAL:O	1:E:686:SER:HA	2.21	0.41
1:F:460:TYR:OH	1:F:482:ARG:HD2	2.21	0.41
1:G:423:GLY:O	1:G:439:LEU:HG	2.21	0.41
1:G:497:LEU:HA	1:G:497:LEU:HD12	1.79	0.41
1:I:423:GLY:O	1:I:439:LEU:HG	2.21	0.41
1:J:423:GLY:O	1:J:439:LEU:HG	2.21	0.41
1:J:500:HIS:O	1:J:504:VAL:N	2.53	0.41
1:L:423:GLY:O	1:L:439:LEU:HG	2.21	0.41
1:L:542:LEU:HD23	1:L:542:LEU:HA	1.91	0.41
1:O:367:PHE:CD2	1:P:524:GLN:HG2	2.56	0.41
1:O:460:TYR:OH	1:O:482:ARG:HD2	2.21	0.41
1:P:634:ASP:O	1:P:638:THR:OG1	2.39	0.41
1:Q:523:GLU:HA	1:Q:526:GLU:HG2	2.03	0.41
1:C:460:TYR:OH	1:C:482:ARG:HD2	2.21	0.40
1:G:443:TYR:CD2	1:G:444:LEU:N	2.88	0.40
1:J:443:TYR:CD2	1:J:444:LEU:N	2.88	0.40
1:K:523:GLU:HA	1:K:526:GLU:HG2	2.03	0.40
1:N:456:LEU:HD23	1:N:462:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:393:GLU:HG3	1:O:498:THR:HG21	2.02	0.40
1:P:432:VAL:HA	1:P:433:PRO:HD2	1.98	0.40
1:Q:389:ALA:C	1:Q:391:ASN:H	2.24	0.40
1:A:456:LEU:HD23	1:A:462:LYS:HE3	2.03	0.40
1:B:623:ARG:O	1:B:625:THR:HG23	2.21	0.40
1:C:393:GLU:HG3	1:C:498:THR:HG21	2.02	0.40
1:H:523:GLU:HA	1:H:526:GLU:HG2	2.03	0.40
1:I:544:ARG:HH22	1:I:577:LYS:HA	1.86	0.40
1:L:656:GLN:O	1:L:657:SER:OG	2.31	0.40
1:M:456:LEU:HD23	1:M:462:LYS:HE3	2.03	0.40
1:M:544:ARG:HH22	1:M:577:LYS:HA	1.87	0.40
1:N:423:GLY:O	1:N:439:LEU:HG	2.21	0.40
1:N:623:ARG:O	1:N:625:THR:HG23	2.21	0.40
1:O:623:ARG:O	1:O:625:THR:HG23	2.21	0.40
1:P:523:GLU:HA	1:P:526:GLU:HG2	2.03	0.40
1:R:460:TYR:OH	1:R:482:ARG:HD2	2.21	0.40
1:B:423:GLY:O	1:B:439:LEU:HG	2.21	0.40
1:B:478:GLU:H	1:B:478:GLU:CD	2.17	0.40
1:C:623:ARG:O	1:C:625:THR:HG23	2.21	0.40
1:D:432:VAL:HA	1:D:433:PRO:HD2	1.98	0.40
1:E:445:LEU:HD12	1:E:445:LEU:HA	1.93	0.40
1:E:542:LEU:HD23	1:E:542:LEU:HA	1.91	0.40
1:G:390:LEU:HD13	1:G:390:LEU:HA	1.95	0.40
1:G:460:TYR:OH	1:G:482:ARG:HD2	2.21	0.40
1:G:488:LEU:HA	1:G:488:LEU:HD23	1.80	0.40
1:G:523:GLU:HA	1:G:526:GLU:HG2	2.02	0.40
1:H:663:VAL:O	1:H:686:SER:HA	2.21	0.40
1:J:460:TYR:OH	1:J:482:ARG:HD2	2.21	0.40
1:J:488:LEU:HA	1:J:488:LEU:HD23	1.80	0.40
1:J:523:GLU:HA	1:J:526:GLU:HG2	2.02	0.40
1:K:623:ARG:O	1:K:625:THR:HG23	2.21	0.40
1:K:634:ASP:O	1:K:638:THR:OG1	2.38	0.40
1:K:663:VAL:O	1:K:686:SER:HA	2.21	0.40
1:L:544:ARG:HH22	1:L:577:LYS:HA	1.87	0.40
1:M:646:ARG:NH1	1:M:678:GLU:OE1	2.54	0.40
1:O:646:ARG:NH1	1:O:678:GLU:OE1	2.53	0.40
1:Q:367:PHE:CD2	1:R:524:GLN:HG2	2.56	0.40
1:A:544:ARG:HH22	1:A:577:LYS:HA	1.87	0.40
1:A:646:ARG:NH1	1:A:678:GLU:OE1	2.54	0.40
1:C:646:ARG:NH1	1:C:678:GLU:OE1	2.53	0.40
1:D:523:GLU:HA	1:D:526:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:ARG:O	1:D:625:THR:HG23	2.21	0.40
1:F:663:VAL:O	1:F:686:SER:HA	2.21	0.40
1:H:623:ARG:O	1:H:625:THR:HG23	2.21	0.40
1:J:390:LEU:HD13	1:J:390:LEU:HA	1.95	0.40
1:J:456:LEU:CD2	1:J:462:LYS:HE3	2.52	0.40
1:L:456:LEU:HD23	1:L:462:LYS:HE3	2.03	0.40
1:M:389:ALA:C	1:M:391:ASN:H	2.24	0.40
1:Q:423:GLY:O	1:Q:439:LEU:HG	2.21	0.40
1:Q:462:LYS:HB3	1:Q:473:PHE:HD1	1.87	0.40
1:Q:544:ARG:HH22	1:Q:577:LYS:HA	1.87	0.40
1:A:623:ARG:O	1:A:625:THR:HG23	2.21	0.40
1:B:544:ARG:HH22	1:B:577:LYS:HA	1.87	0.40
1:B:663:VAL:O	1:B:686:SER:HA	2.21	0.40
1:C:467:LEU:HB3	1:C:472:THR:OG1	2.22	0.40
1:D:393:GLU:HG3	1:D:498:THR:HG21	2.02	0.40
1:D:456:LEU:HD23	1:D:462:LYS:HE3	2.03	0.40
1:E:462:LYS:HB3	1:E:473:PHE:HD1	1.87	0.40
1:E:544:ARG:HH22	1:E:577:LYS:HA	1.87	0.40
1:G:456:LEU:CD2	1:G:462:LYS:HE3	2.52	0.40
1:I:456:LEU:HD23	1:I:462:LYS:HE3	2.03	0.40
1:M:462:LYS:HB3	1:M:473:PHE:HD1	1.87	0.40
1:M:623:ARG:O	1:M:625:THR:HG23	2.21	0.40
1:N:544:ARG:HH22	1:N:577:LYS:HA	1.86	0.40
1:O:379:SER:O	1:O:380:SER:OG	2.26	0.40
1:O:467:LEU:HB3	1:O:472:THR:OG1	2.22	0.40
1:O:523:GLU:HA	1:O:526:GLU:HG2	2.02	0.40
1:P:623:ARG:O	1:P:625:THR:HG23	2.21	0.40
1:Q:542:LEU:HD23	1:Q:542:LEU:HA	1.91	0.40
1:R:544:ARG:HH22	1:R:577:LYS:HA	1.86	0.40
1:R:634:ASP:O	1:R:638:THR:OG1	2.38	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	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	B	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	C	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	D	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	E	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	F	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	G	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	41	74
1	H	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	41	74
1	I	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	41	74
1	J	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	K	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	41	74
1	L	342/710 (48%)	281 (82%)	60 (18%)	1 (0%)	41	74
1	M	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	N	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	O	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	P	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	Q	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
1	R	342/710 (48%)	282 (82%)	59 (17%)	1 (0%)	41	74
All	All	6156/12780 (48%)	5071 (82%)	1067 (17%)	18 (0%)	44	74

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	GLU
1	B	386	GLU
1	C	386	GLU
1	D	386	GLU
1	E	386	GLU
1	F	386	GLU
1	G	386	GLU
1	H	386	GLU
1	I	386	GLU
1	J	386	GLU
1	K	386	GLU

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Mol	Chain	Res	Type
1	L	386	GLU
1	M	386	GLU
1	N	386	GLU
1	O	386	GLU
1	P	386	GLU
1	Q	386	GLU
1	R	386	GLU

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	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	B	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	C	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	D	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	E	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	F	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	G	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	H	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	I	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	J	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	K	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	L	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	M	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	N	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	O	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	P	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	Q	306/605 (51%)	302 (99%)	4 (1%)	69	83
1	R	306/605 (51%)	302 (99%)	4 (1%)	69	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5508/10890 (51%)	5436 (99%)	72 (1%)	70 83

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	GLU
1	A	503	HIS
1	A	592	ARG
1	A	638	THR
1	B	480	GLU
1	B	503	HIS
1	B	592	ARG
1	B	638	THR
1	C	480	GLU
1	C	503	HIS
1	C	592	ARG
1	C	638	THR
1	D	480	GLU
1	D	503	HIS
1	D	592	ARG
1	D	638	THR
1	E	480	GLU
1	E	503	HIS
1	E	592	ARG
1	E	638	THR
1	F	480	GLU
1	F	503	HIS
1	F	592	ARG
1	F	638	THR
1	G	480	GLU
1	G	503	HIS
1	G	592	ARG
1	G	638	THR
1	H	480	GLU
1	H	503	HIS
1	H	592	ARG
1	H	638	THR
1	I	480	GLU
1	I	503	HIS
1	I	592	ARG
1	I	638	THR
1	J	480	GLU

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Mol	Chain	Res	Type
1	J	503	HIS
1	J	592	ARG
1	J	638	THR
1	K	480	GLU
1	K	503	HIS
1	K	592	ARG
1	K	638	THR
1	L	480	GLU
1	L	503	HIS
1	L	592	ARG
1	L	638	THR
1	M	480	GLU
1	M	503	HIS
1	M	592	ARG
1	M	638	THR
1	N	480	GLU
1	N	503	HIS
1	N	592	ARG
1	N	638	THR
1	O	480	GLU
1	O	503	HIS
1	O	592	ARG
1	O	638	THR
1	P	480	GLU
1	P	503	HIS
1	P	592	ARG
1	P	638	THR
1	Q	480	GLU
1	Q	503	HIS
1	Q	592	ARG
1	Q	638	THR
1	R	480	GLU
1	R	503	HIS
1	R	592	ARG
1	R	638	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	561	ASN
1	B	561	ASN
1	C	561	ASN

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Mol	Chain	Res	Type
1	D	561	ASN
1	E	561	ASN
1	F	561	ASN
1	G	561	ASN
1	H	561	ASN
1	I	561	ASN
1	J	561	ASN
1	K	561	ASN
1	L	561	ASN
1	M	561	ASN
1	N	561	ASN
1	O	561	ASN
1	P	561	ASN
1	Q	561	ASN
1	R	561	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

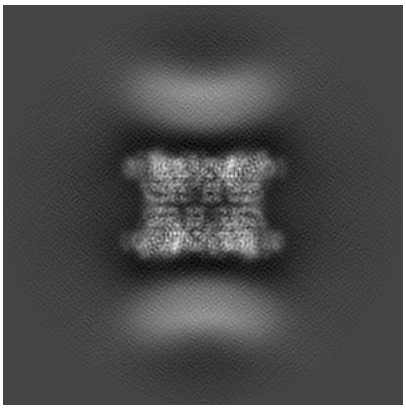
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11820. These allow visual inspection of the internal detail of the map and identification of artifacts.

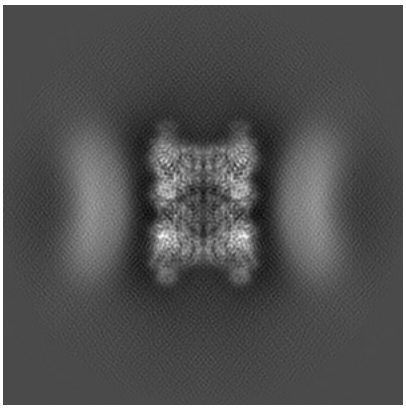
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

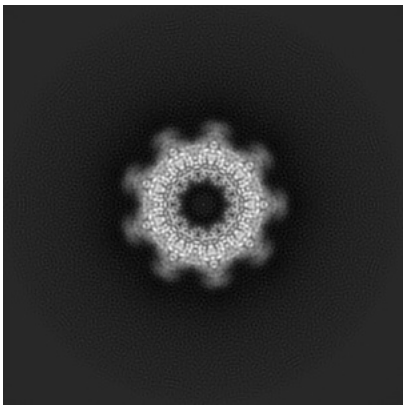
6.1.1 Primary map



X

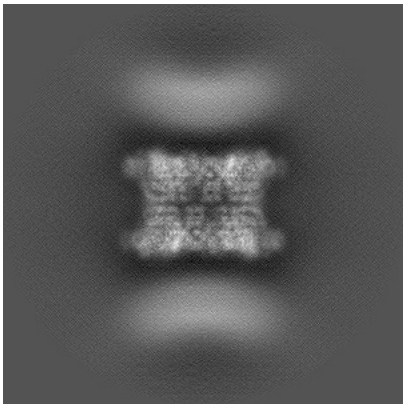


Y

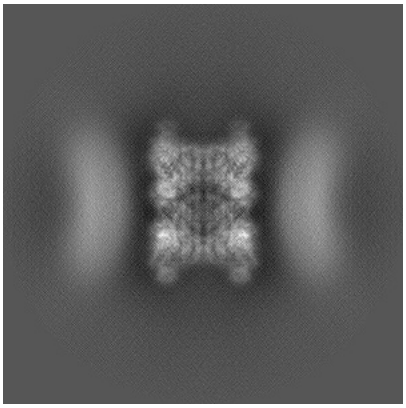


Z

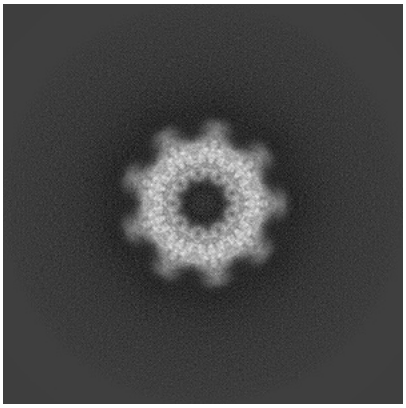
6.1.2 Raw map



X



Y

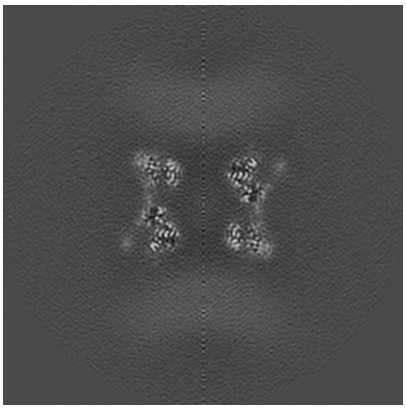


Z

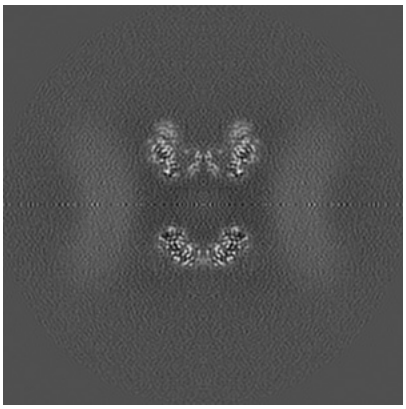
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

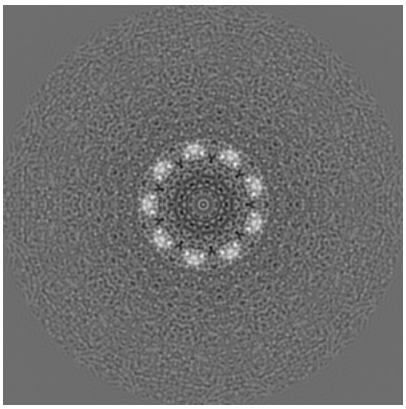
6.2.1 Primary map



X Index: 256

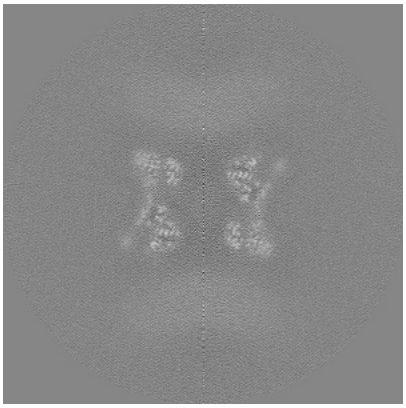


Y Index: 256

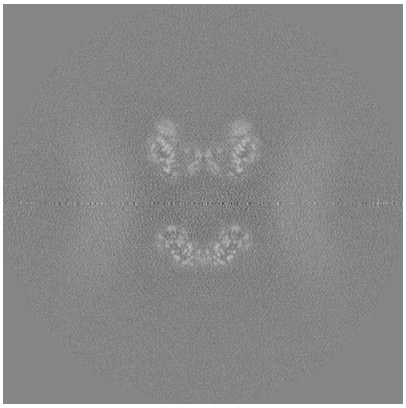


Z Index: 256

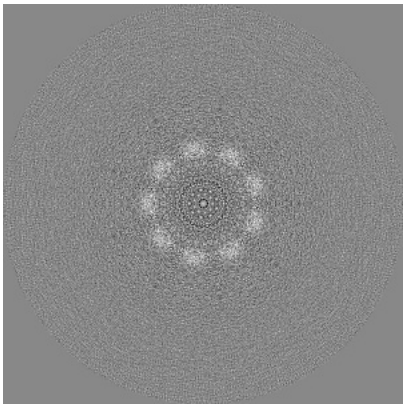
6.2.2 Raw map



X Index: 256



Y Index: 256

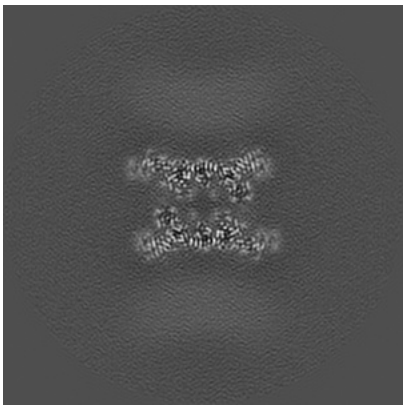


Z Index: 256

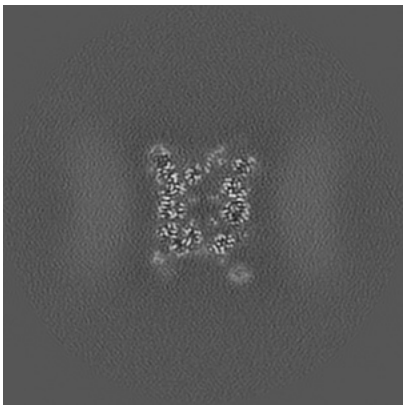
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

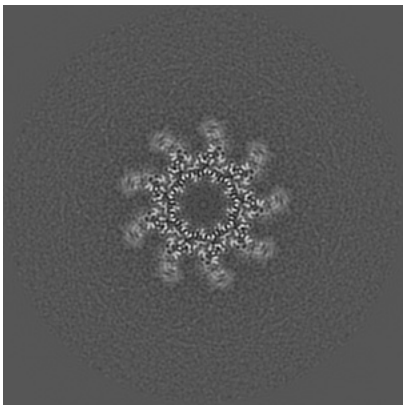
6.3.1 Primary map



X Index: 216

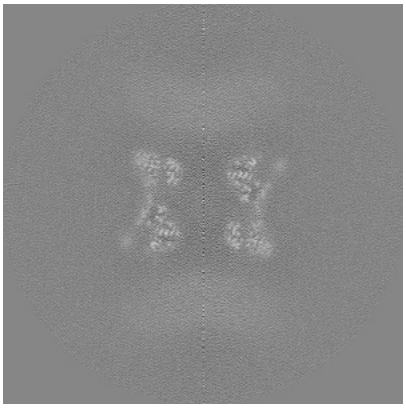


Y Index: 214

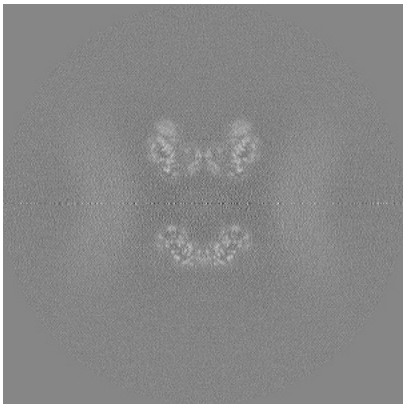


Z Index: 303

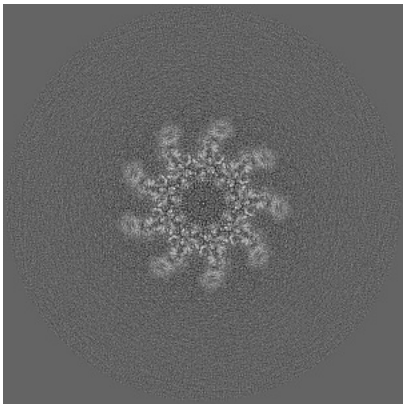
6.3.2 Raw map



X Index: 256



Y Index: 256

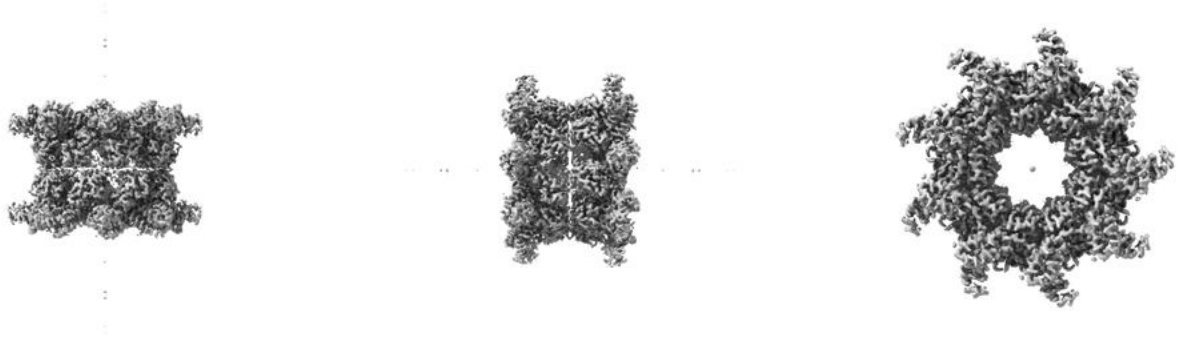


Z Index: 209

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

6.4 Orthogonal surface views (i)

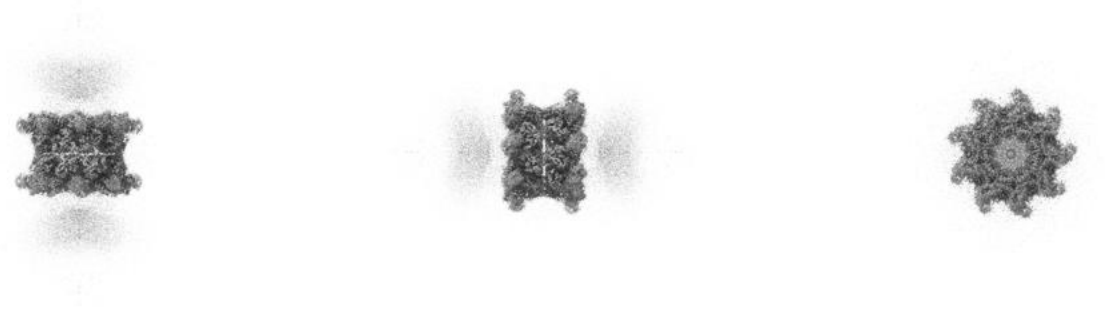
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

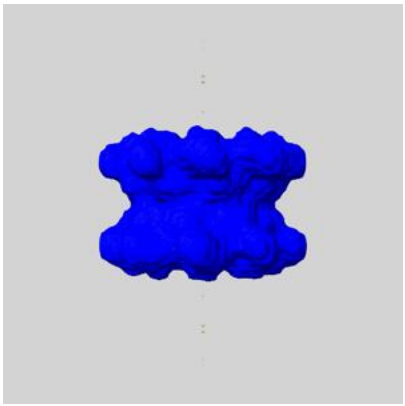
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

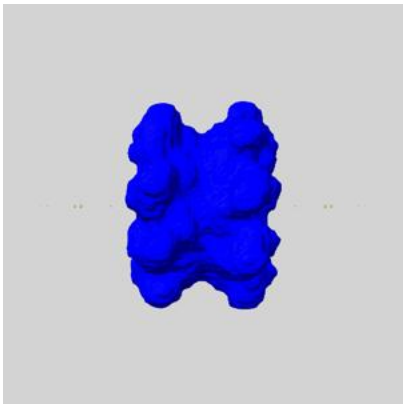
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

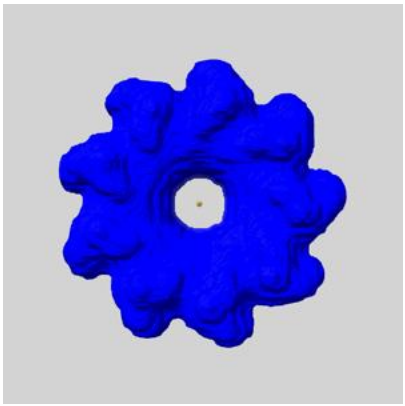
6.5.1 emd_11820_msk_1.map (i)



X



Y

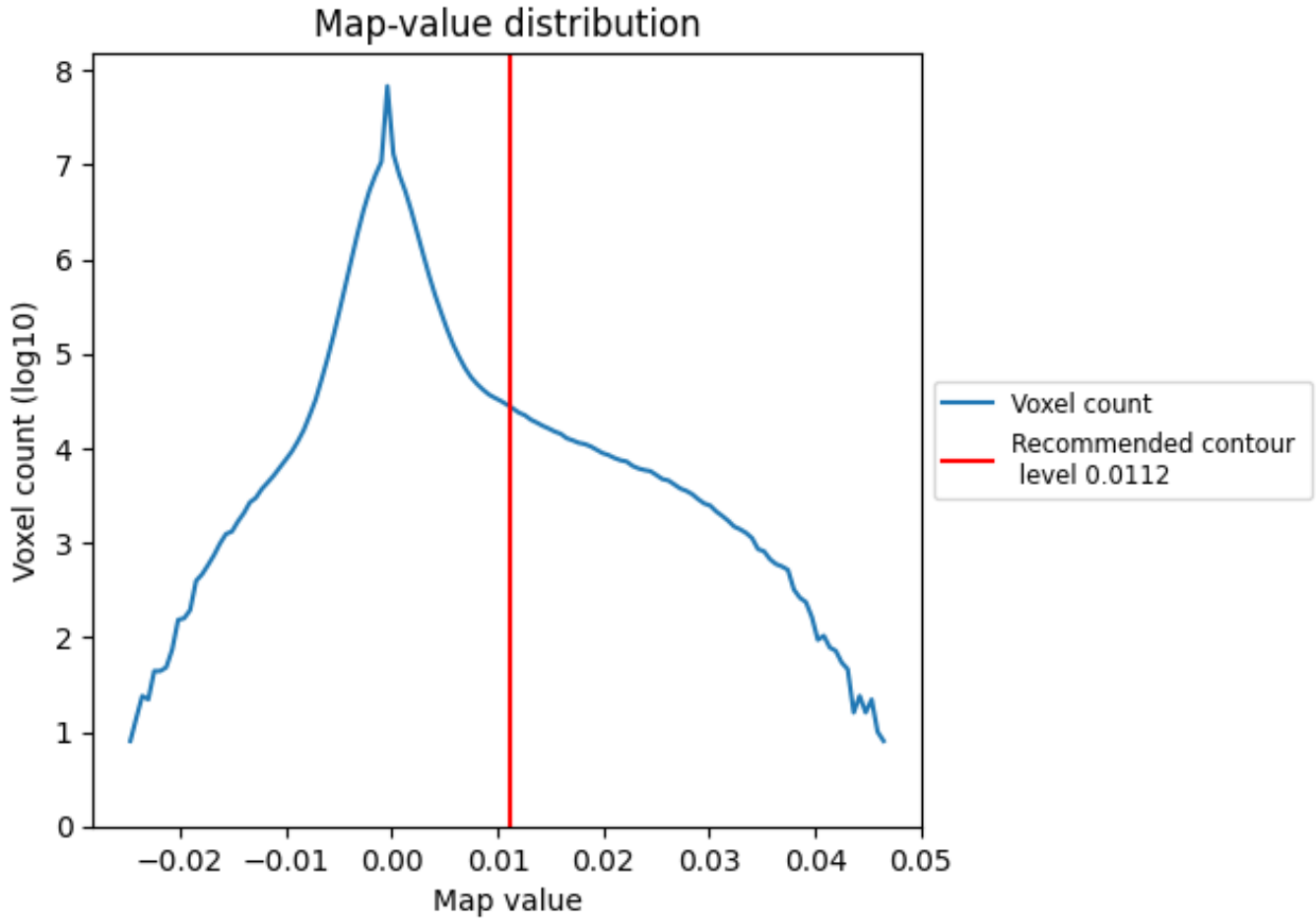


Z

7 Map analysis

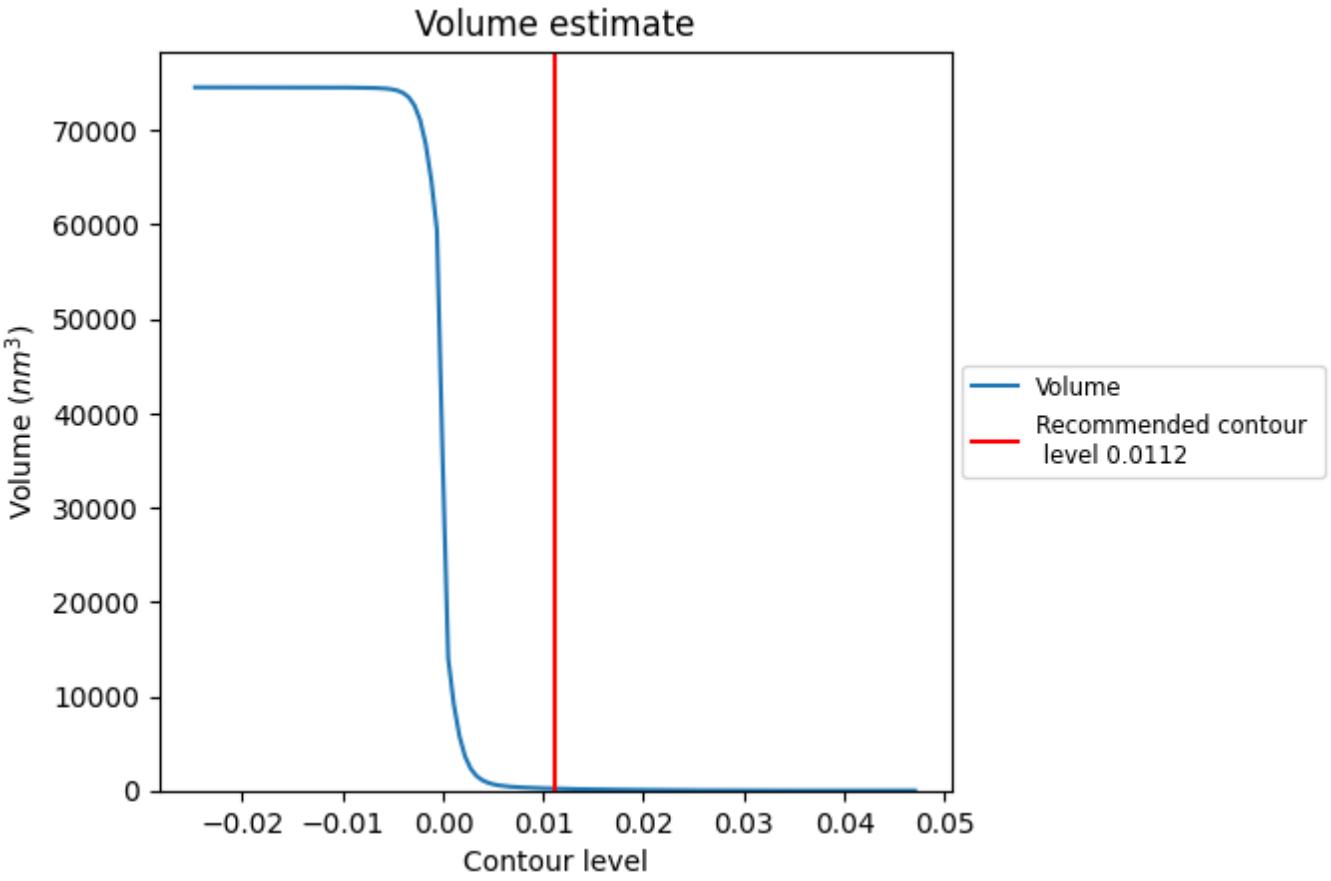
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

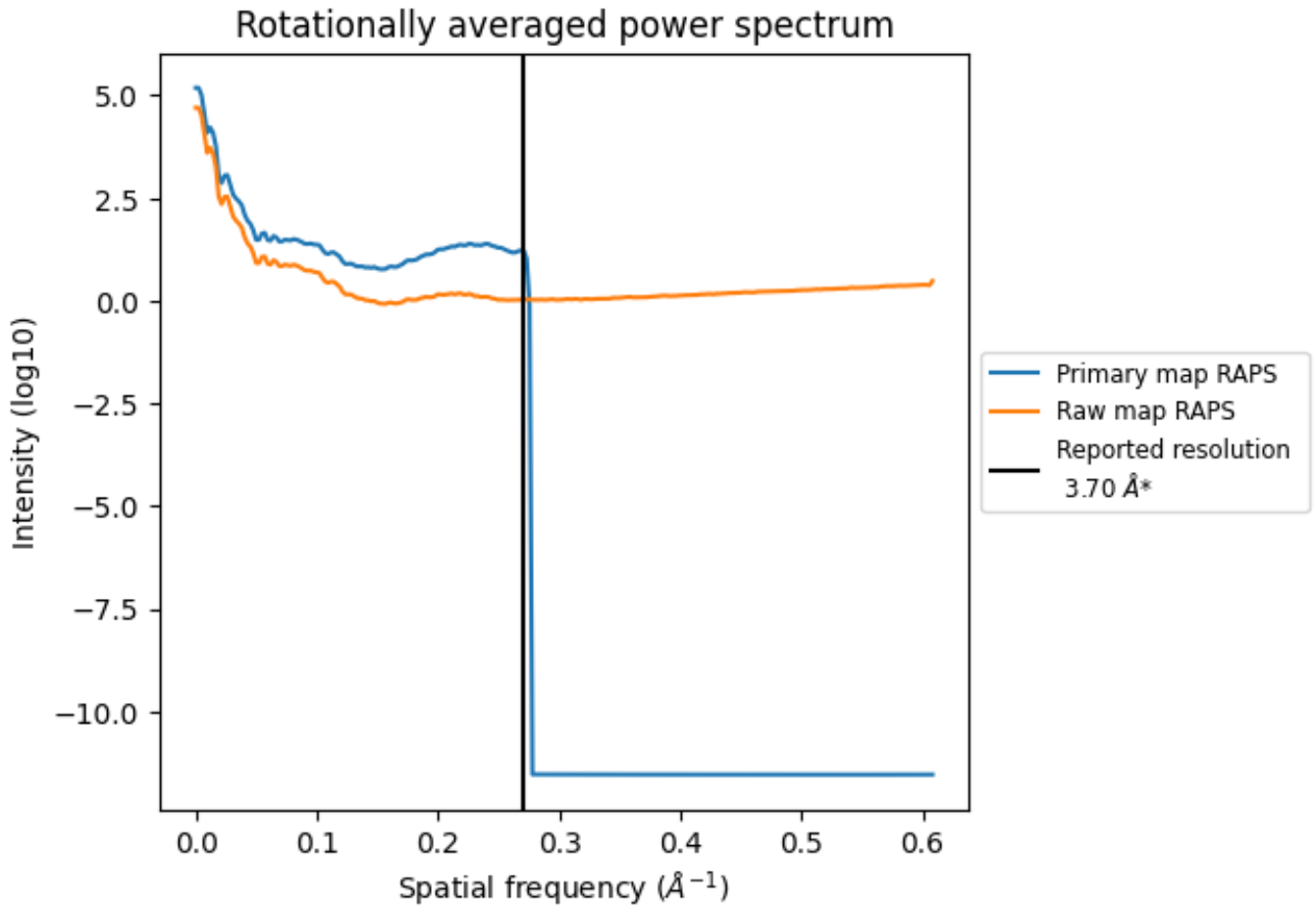
7.2 Volume estimate



The volume at the recommended contour level is 207 nm^3; this corresponds to an approximate mass of 187 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)

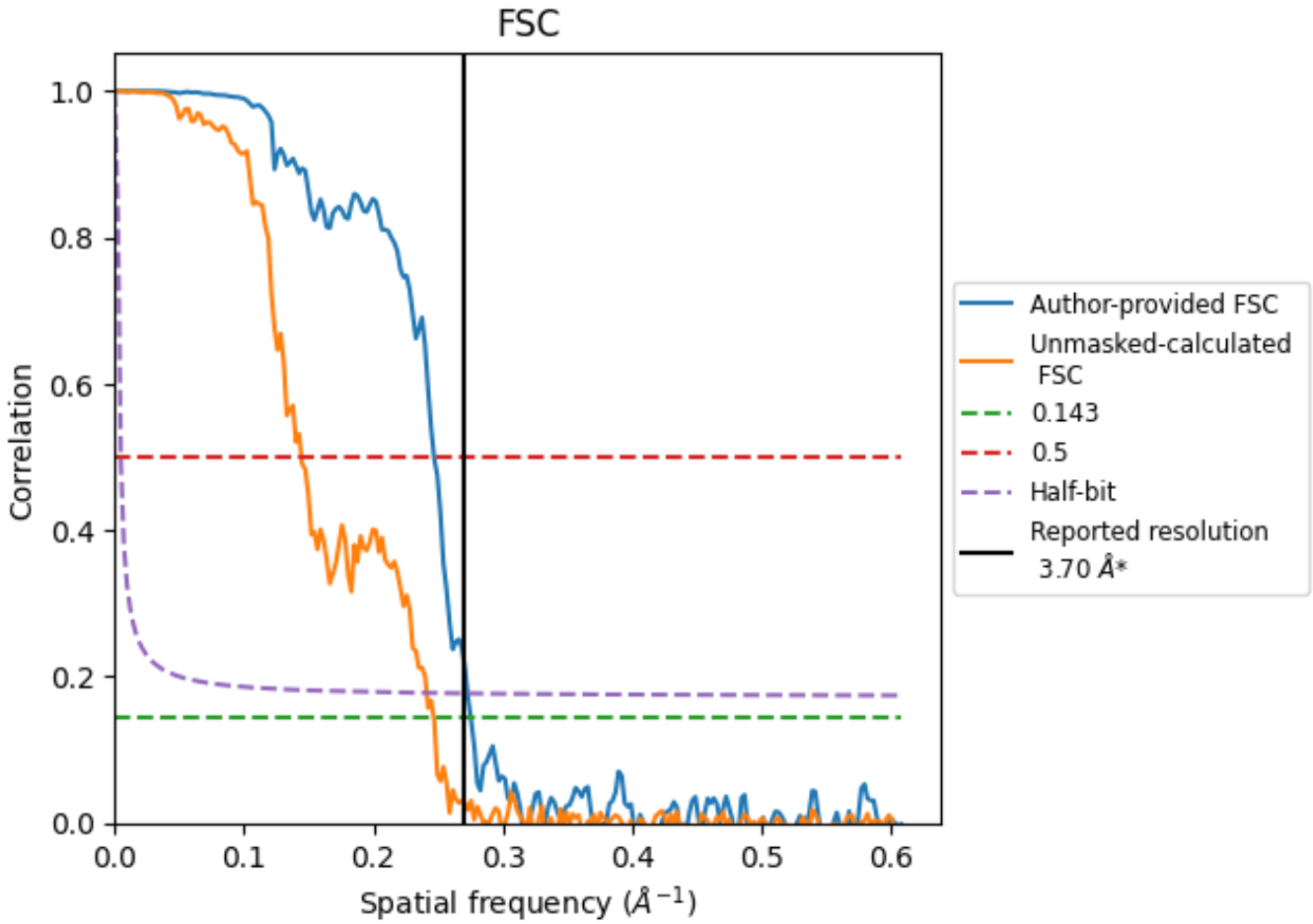


*Reported resolution corresponds to spatial frequency of 0.270 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.270 Å^{-1}

8.2 Resolution estimates (i)

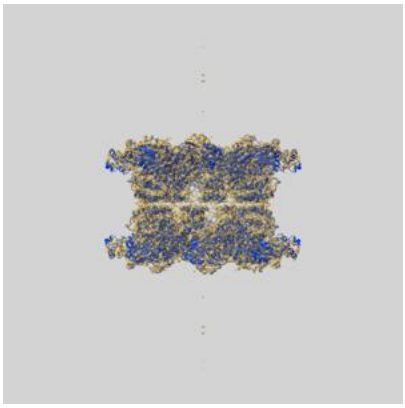
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.63	4.05	3.66
Unmasked-calculated*	4.05	6.93	4.15

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

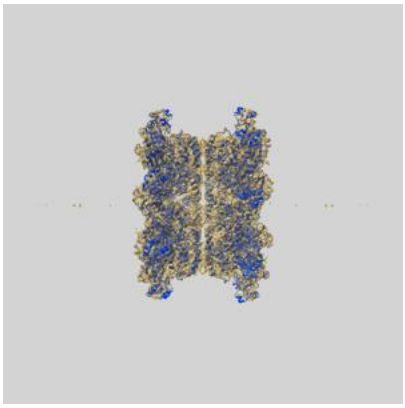
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11820 and PDB model 7ALW. Per-residue inclusion information can be found in section 3 on page 9.

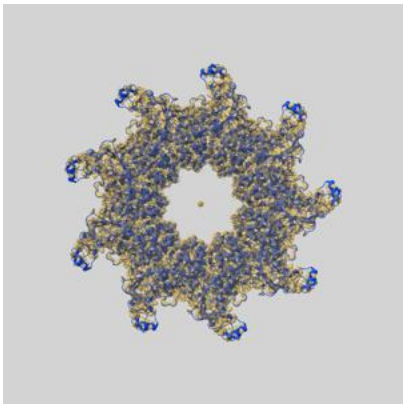
9.1 Map-model overlay



X



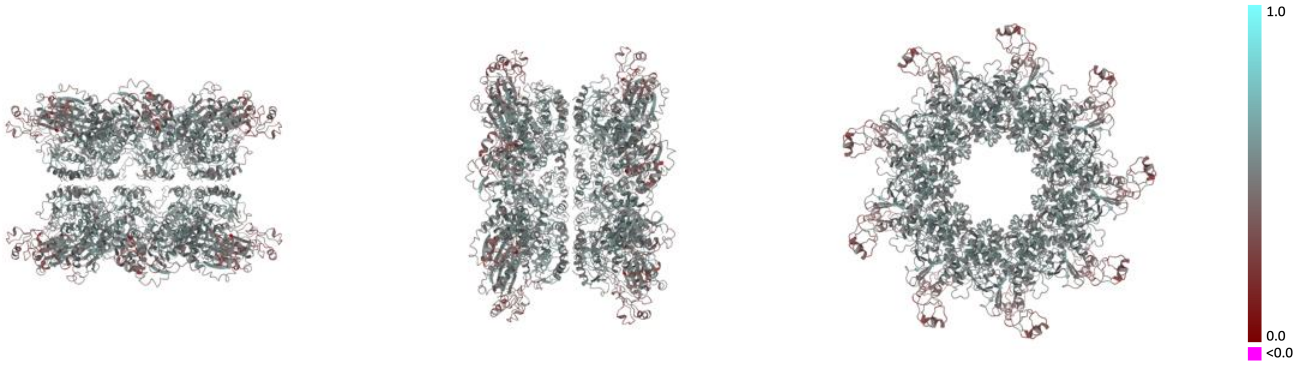
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0112 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.

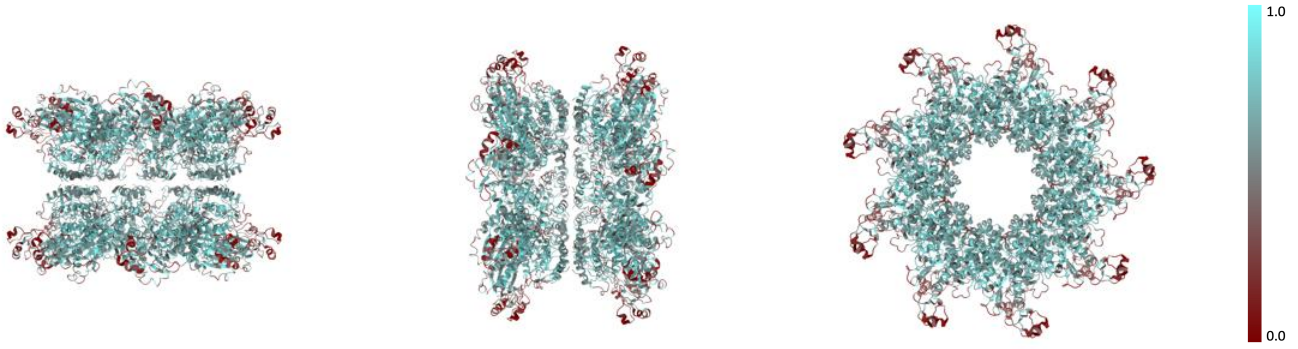
9.2 Q-score mapped to coordinate model (i)



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.

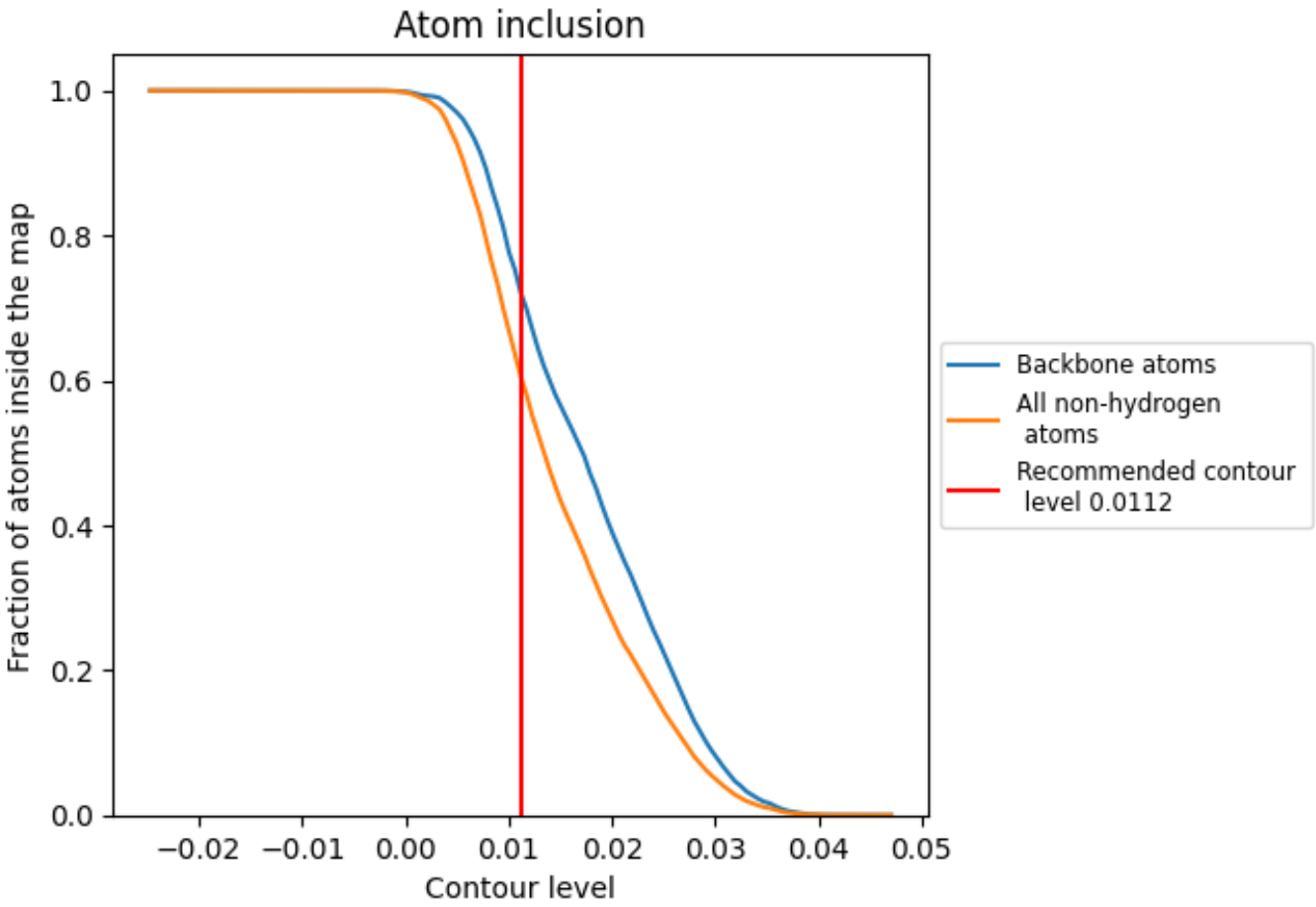
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0112).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.0112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6044	0.4790
A	0.6072	0.4790
B	0.6024	0.4780
C	0.6050	0.4780
D	0.6079	0.4780
E	0.6013	0.4800
F	0.6057	0.4800
G	0.6083	0.4800
H	0.6035	0.4800
I	0.6021	0.4790
J	0.6046	0.4790
K	0.6039	0.4810
L	0.6024	0.4800
M	0.6076	0.4800
N	0.6024	0.4790
O	0.6046	0.4780
P	0.6043	0.4780
Q	0.6013	0.4790
R	0.6046	0.4790