



## Full wwPDB EM Validation Report ⓘ

May 25, 2025 – 12:38 PM EDT

PDB ID : 8EAO / pdb\_00008eao  
EMDB ID : EMD-27792  
Title : Cryo-EM structure of the in-situ gp1-gp4 complex from bacteriophage P22  
Authors : Wang, C.; Liu, J.; Molineux, I.J.  
Deposited on : 2022-08-29  
Resolution : 3.20 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev118  
MolProbity : 4-5-2 with Phenix2.0rc1  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

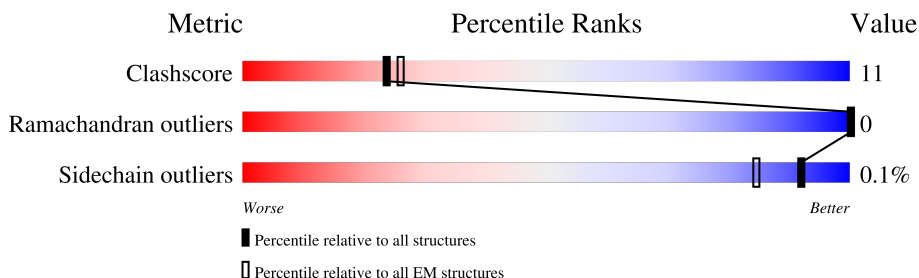
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	149	<div> <div>82%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
1	C	149	<div> <div>83%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
1	E	149	<div> <div>83%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
1	G	149	<div> <div>83%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>
1	I	149	<div> <div>82%</div> <div> <div></div> <div>83%</div> <div>17%</div> </div> </div>
1	K	149	<div> <div>83%</div> <div> <div></div> <div>87%</div> <div>13%</div> </div> </div>
1	M	149	<div> <div>81%</div> <div> <div></div> <div>81%</div> <div>17%</div> </div> </div>
1	O	149	<div> <div>82%</div> <div> <div></div> <div>84%</div> <div>16%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	Q	149	<div> <div>82%</div> <div>85%</div> <div>15%</div> </div>
1	S	149	<div> <div>82%</div> <div>85%</div> <div>15%</div> </div>
1	U	149	<div> <div>82%</div> <div>83%</div> <div>17%</div> </div>
1	W	149	<div> <div>83%</div> <div>83%</div> <div>17%</div> </div>
2	B	621	<div> <div>91%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
2	D	621	<div> <div>91%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	F	621	<div> <div>91%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
2	H	621	<div> <div>91%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
2	J	621	<div> <div>91%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	L	621	<div> <div>91%</div> <div>70%</div> <div>26%</div> <div>.</div> </div>
2	N	621	<div> <div>91%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	P	621	<div> <div>91%</div> <div>68%</div> <div>28%</div> <div>.</div> </div>
2	R	621	<div> <div>91%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
2	T	621	<div> <div>91%</div> <div>67%</div> <div>29%</div> <div>.</div> </div>
2	V	621	<div> <div>91%</div> <div>67%</div> <div>30%</div> <div>.</div> </div>
2	X	621	<div> <div>91%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 71628 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 Peptidoglycan hydrolase gp4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	C	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	E	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	G	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	I	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	K	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	M	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	O	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	Q	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	S	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	U	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		
1	W	149	Total	C	N	O	S	0	0
			1140	716	196	223	5		

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	598	Total	C	N	O	S	0	0
			4829	3043	827	938	21		
2	D	598	Total	C	N	O	S	0	0
			4829	3043	827	938	21		
2	F	598	Total	C	N	O	S	0	0
			4829	3043	827	938	21		

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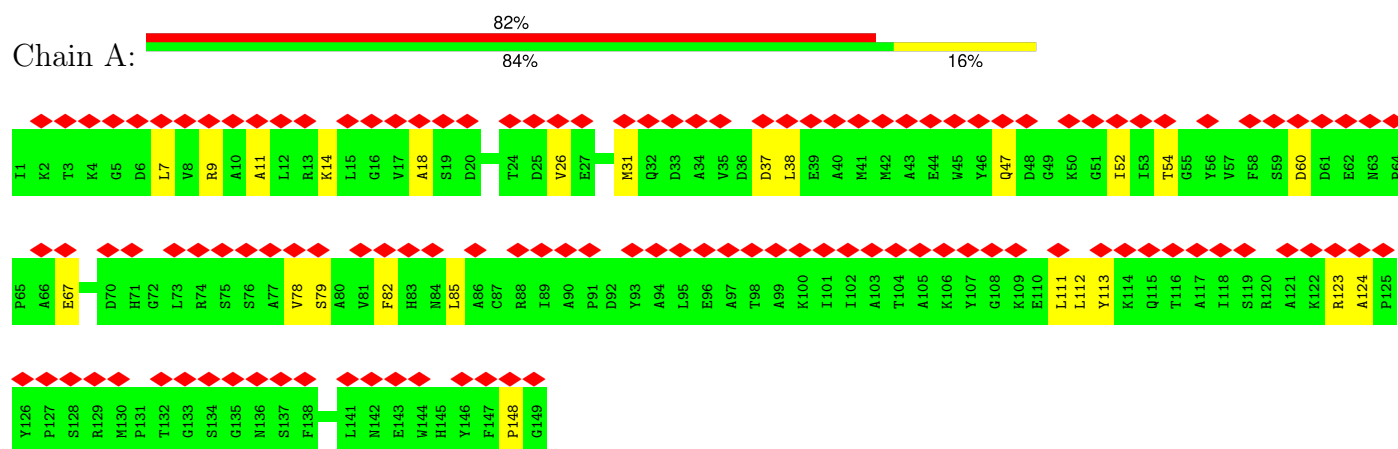
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	J	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	L	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	N	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	P	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	R	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	T	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	V	598	Total 4829	C 3043	N 827	O 938	S 21	0	0
2	X	598	Total 4829	C 3043	N 827	O 938	S 21	0	0

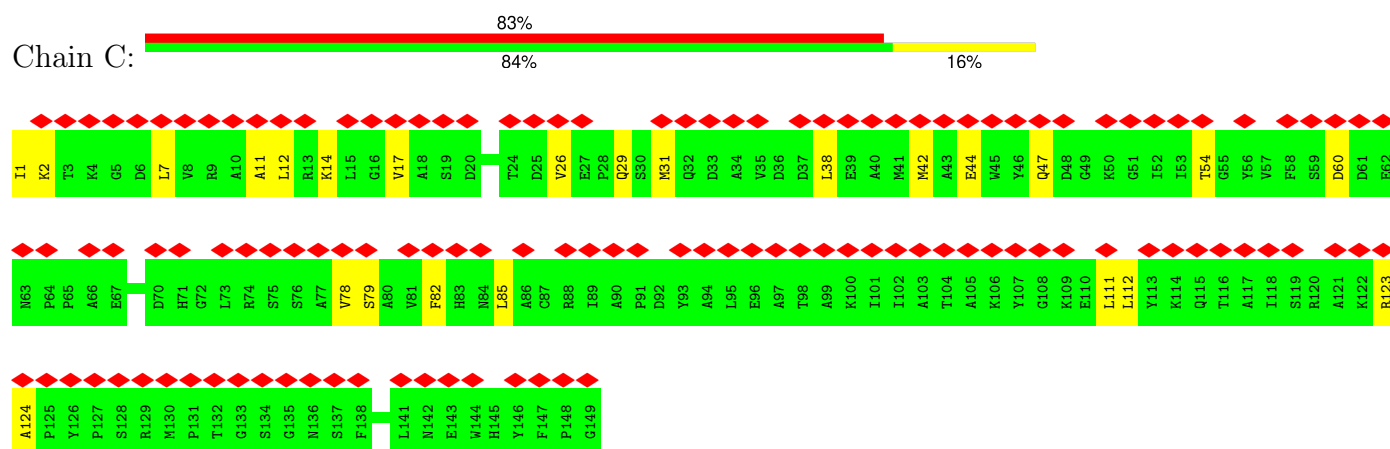
### 3 Residue-property plots

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

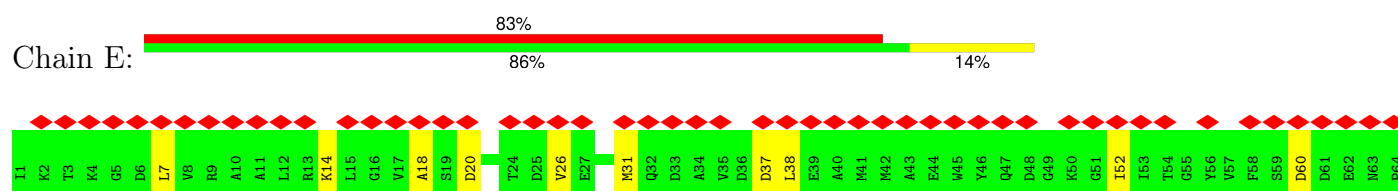
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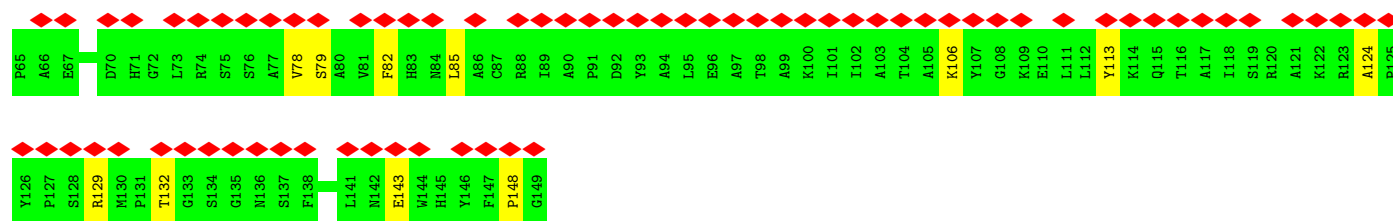


#### • Molecule 1: Peptidoglycan hydrolase gp4

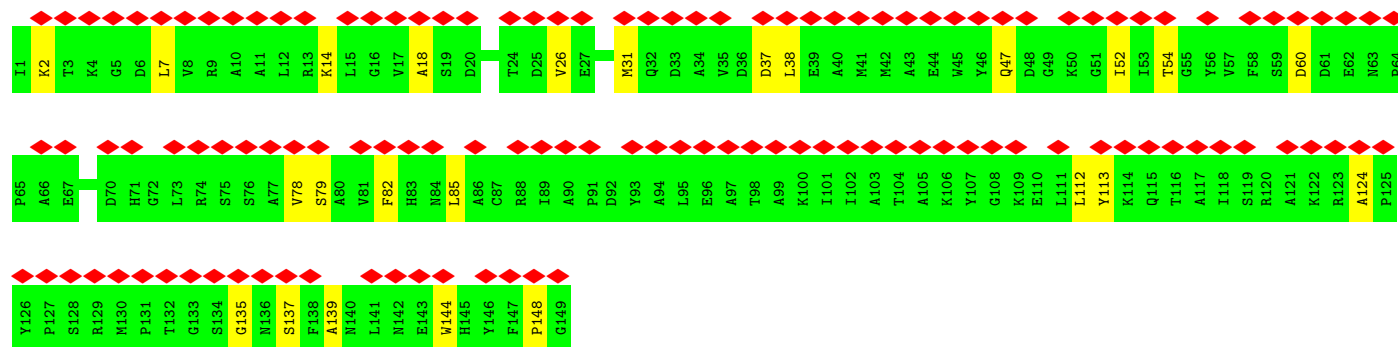
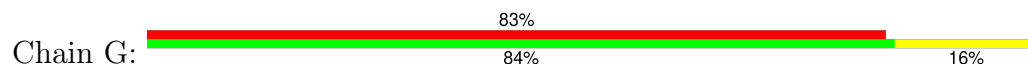


#### • Molecule 1: Peptidoglycan hydrolase gp4

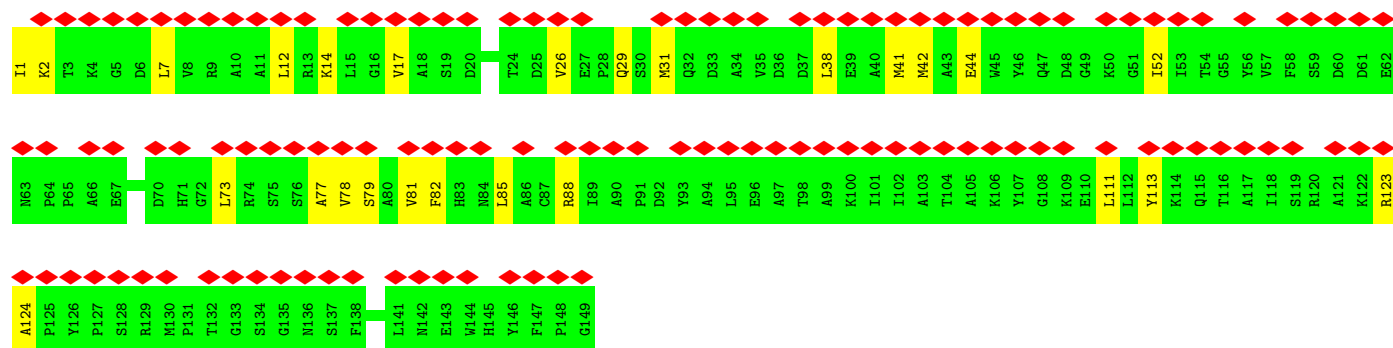
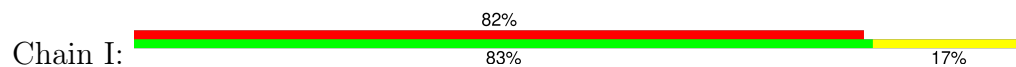




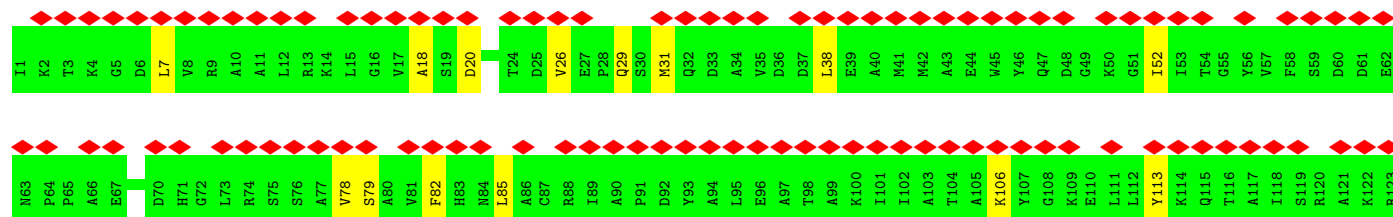
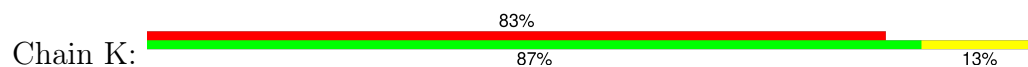
• Molecule 1: Peptidoglycan hydrolase gp4

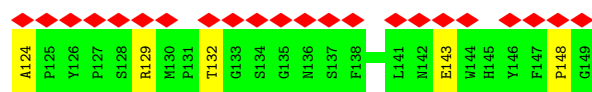


• Molecule 1: Peptidoglycan hydrolase gp4

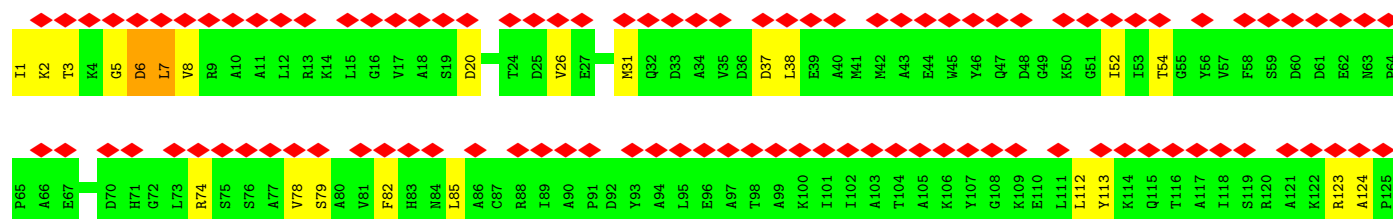
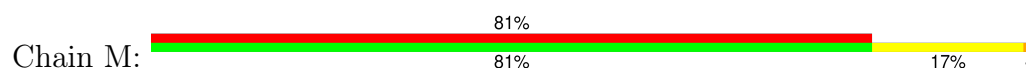


• Molecule 1: Peptidoglycan hydrolase gp4

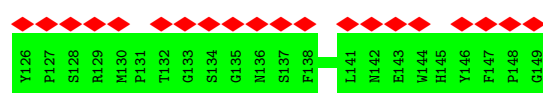
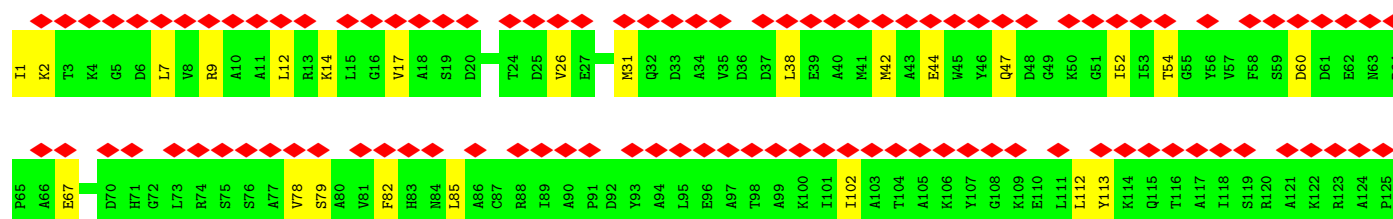
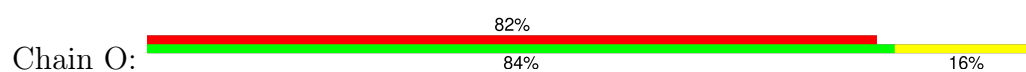




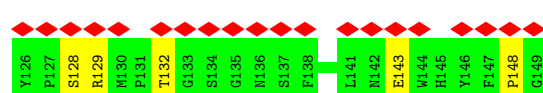
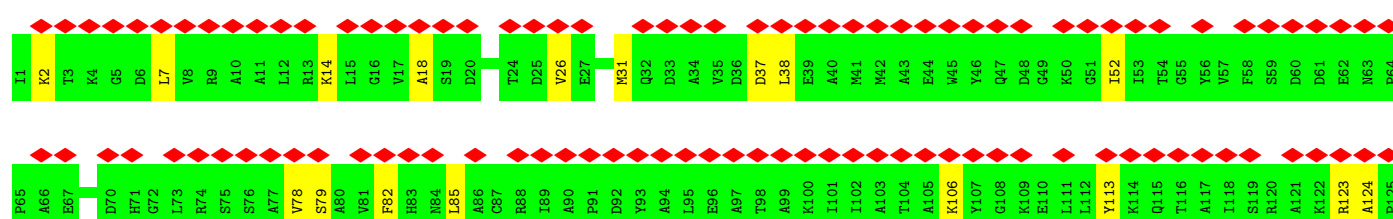
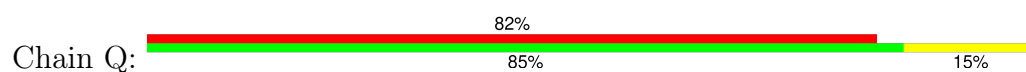
• Molecule 1: Peptidoglycan hydrolase gp4



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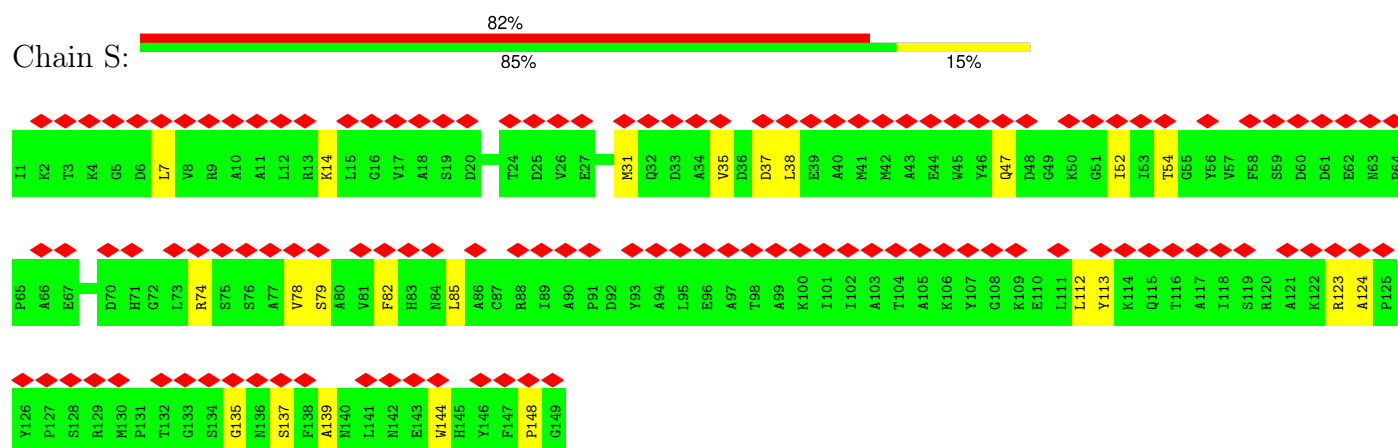


• Molecule 1: Peptidoglycan hydrolase gp4

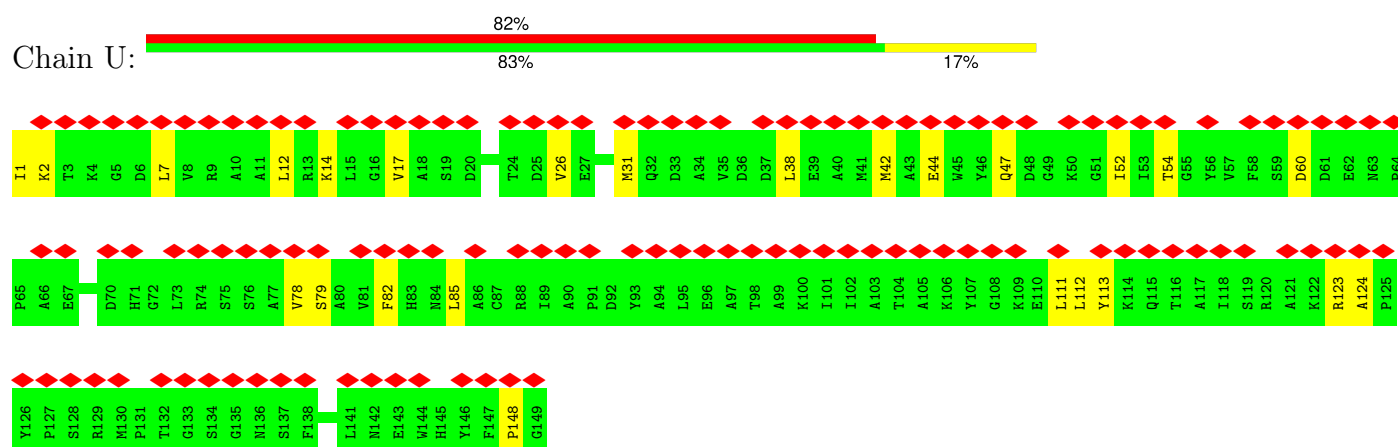


• Molecule 1: Peptidoglycan hydrolase gp4

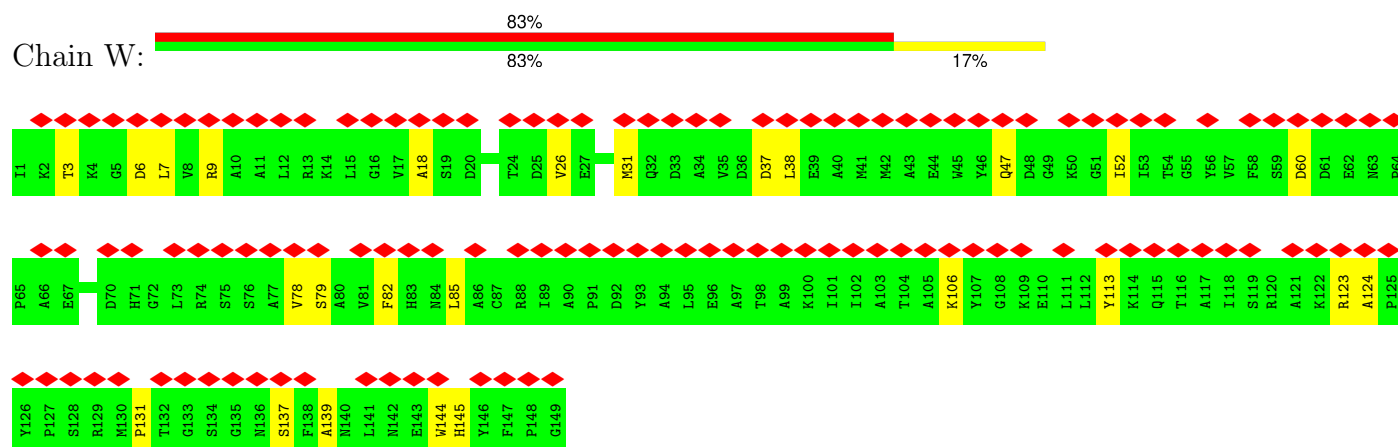




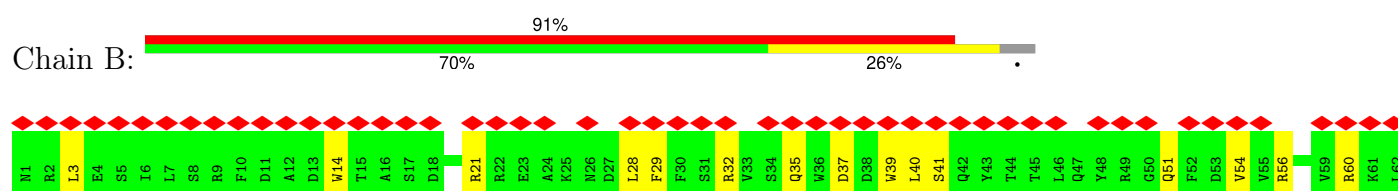
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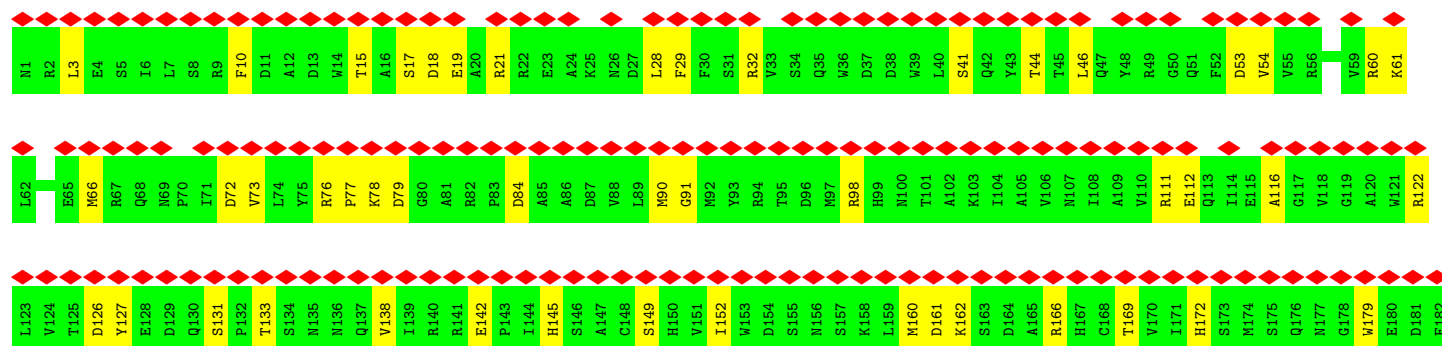
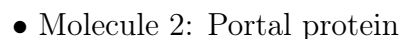


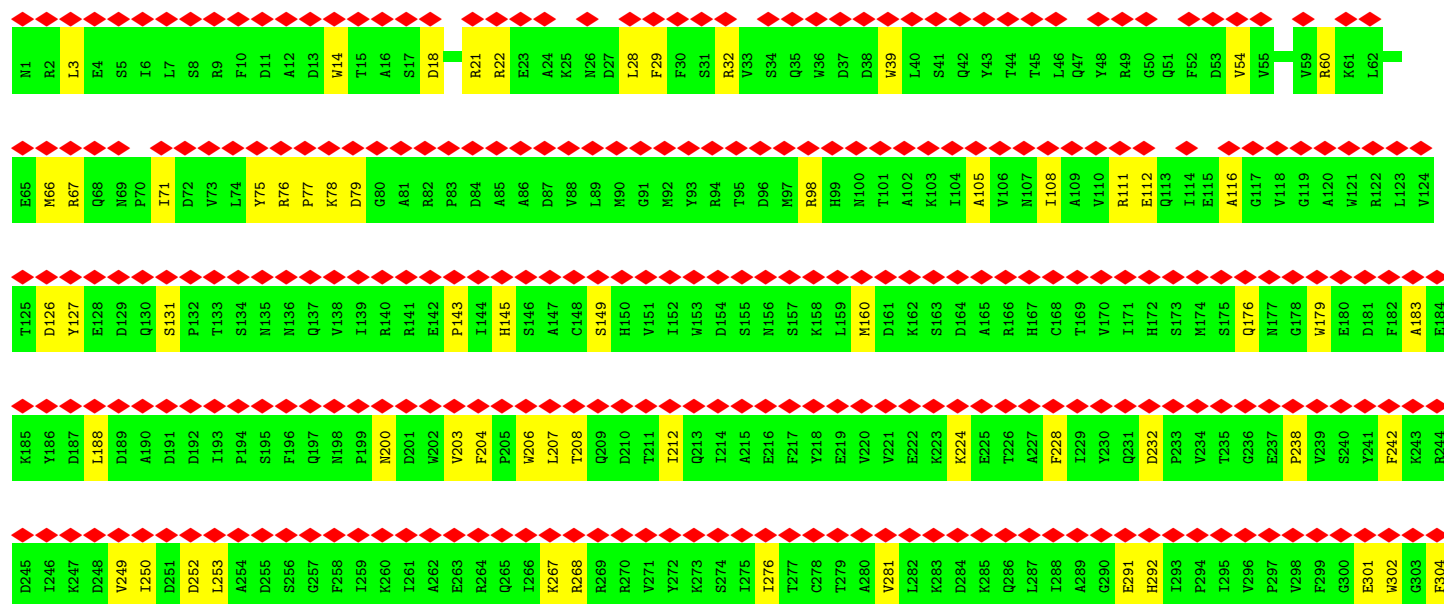
• Molecule 1: Peptidoglycan hydrolase gp4

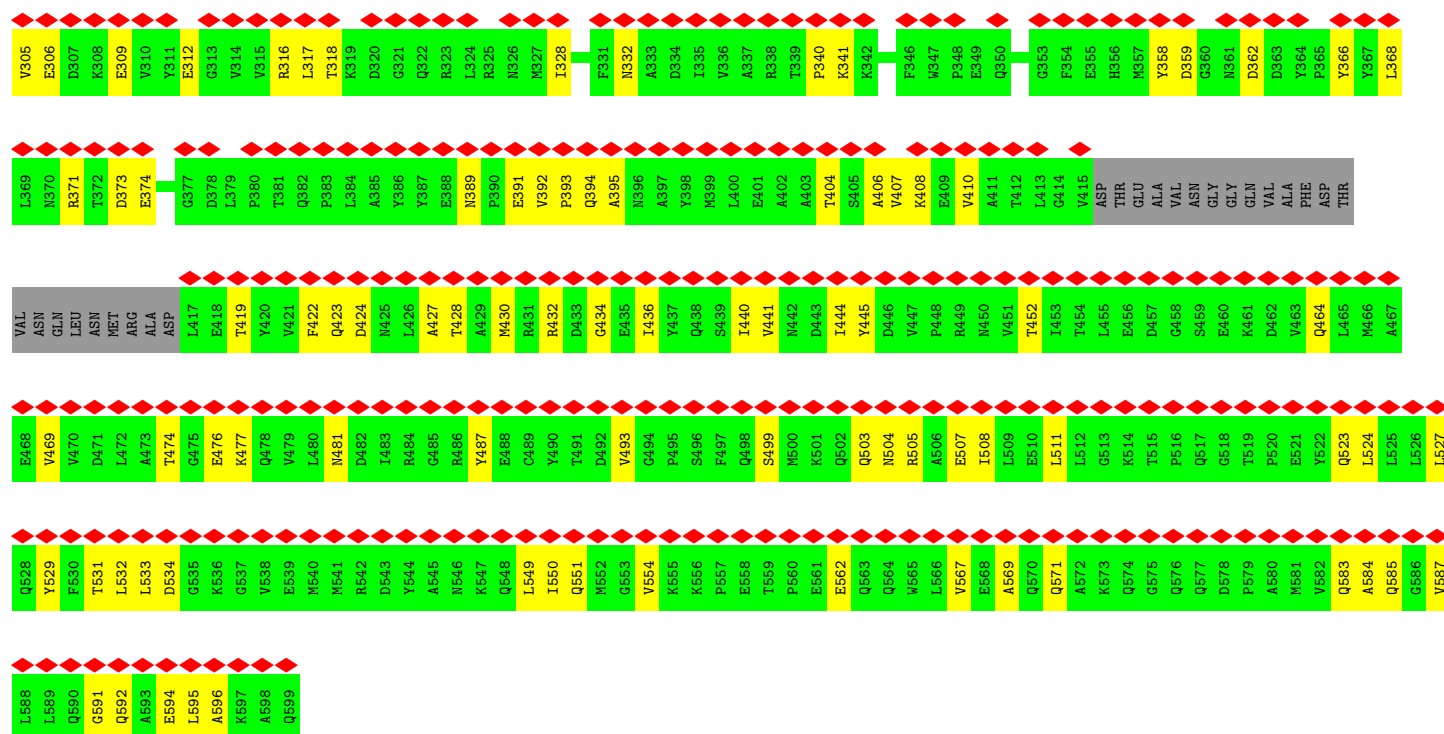


• Molecule 2: Portal protein

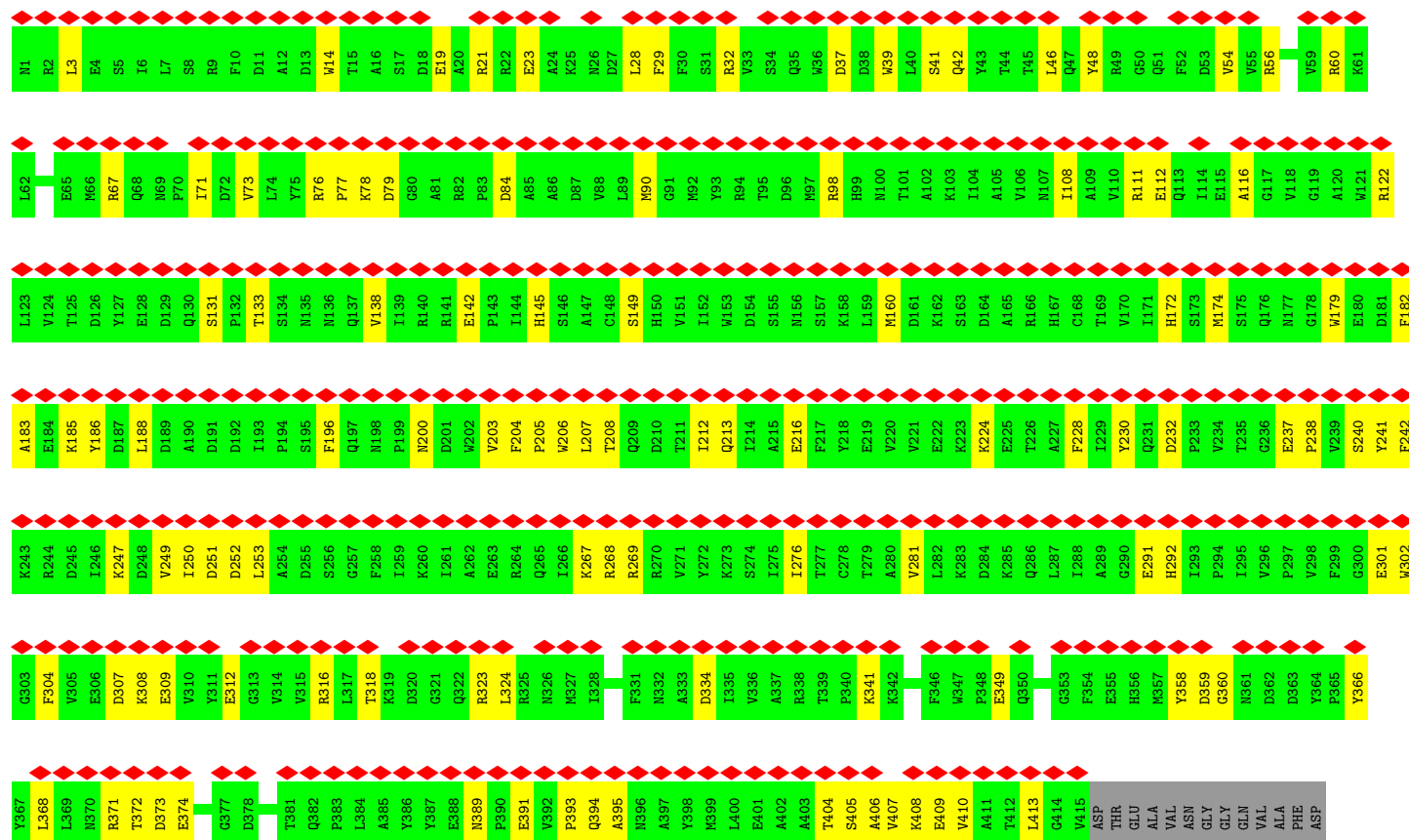


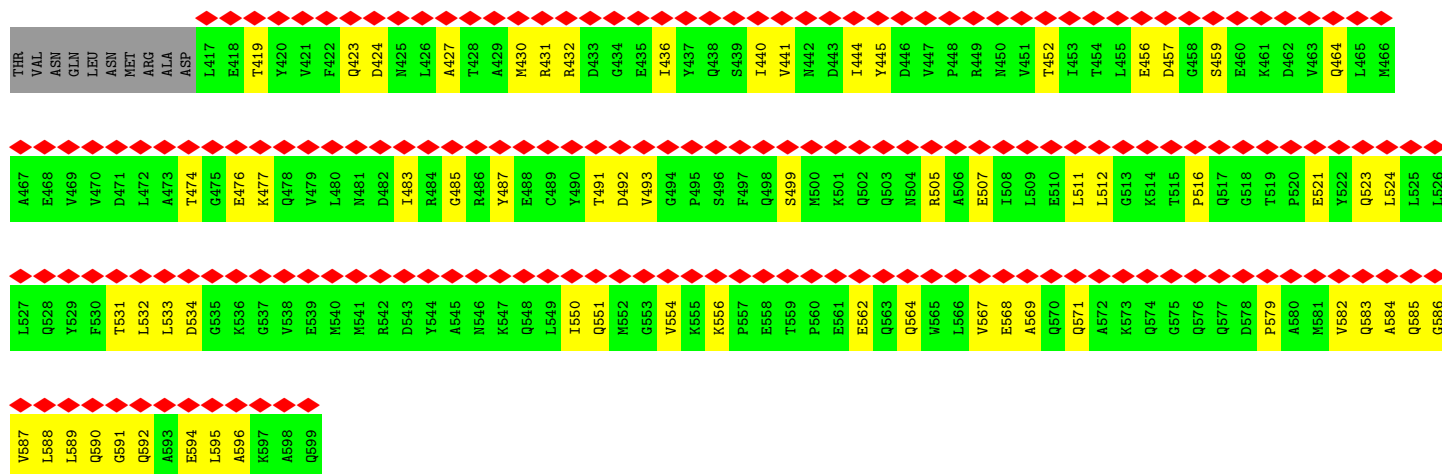




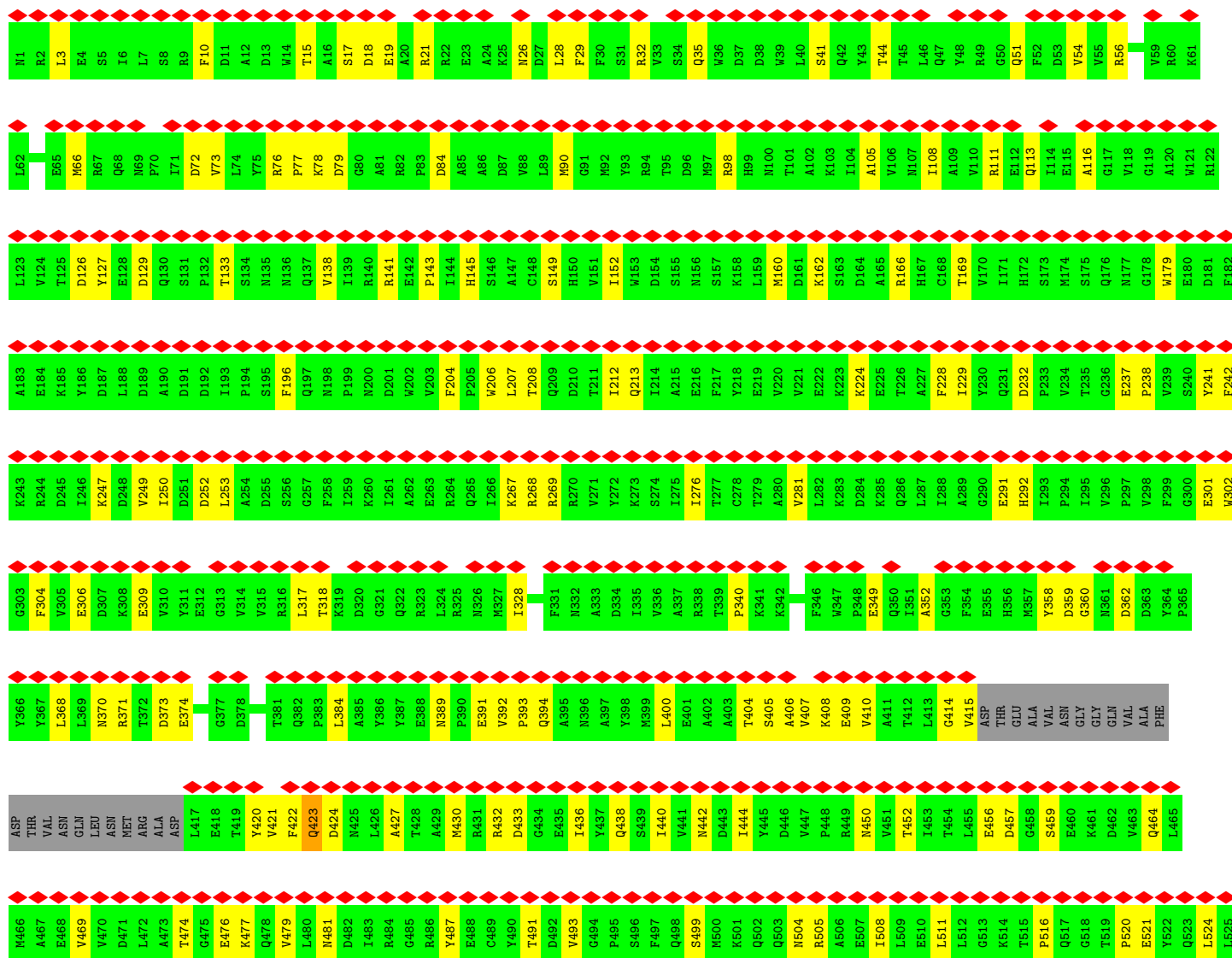
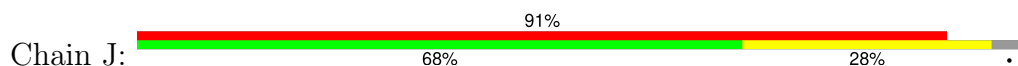


Chain H:



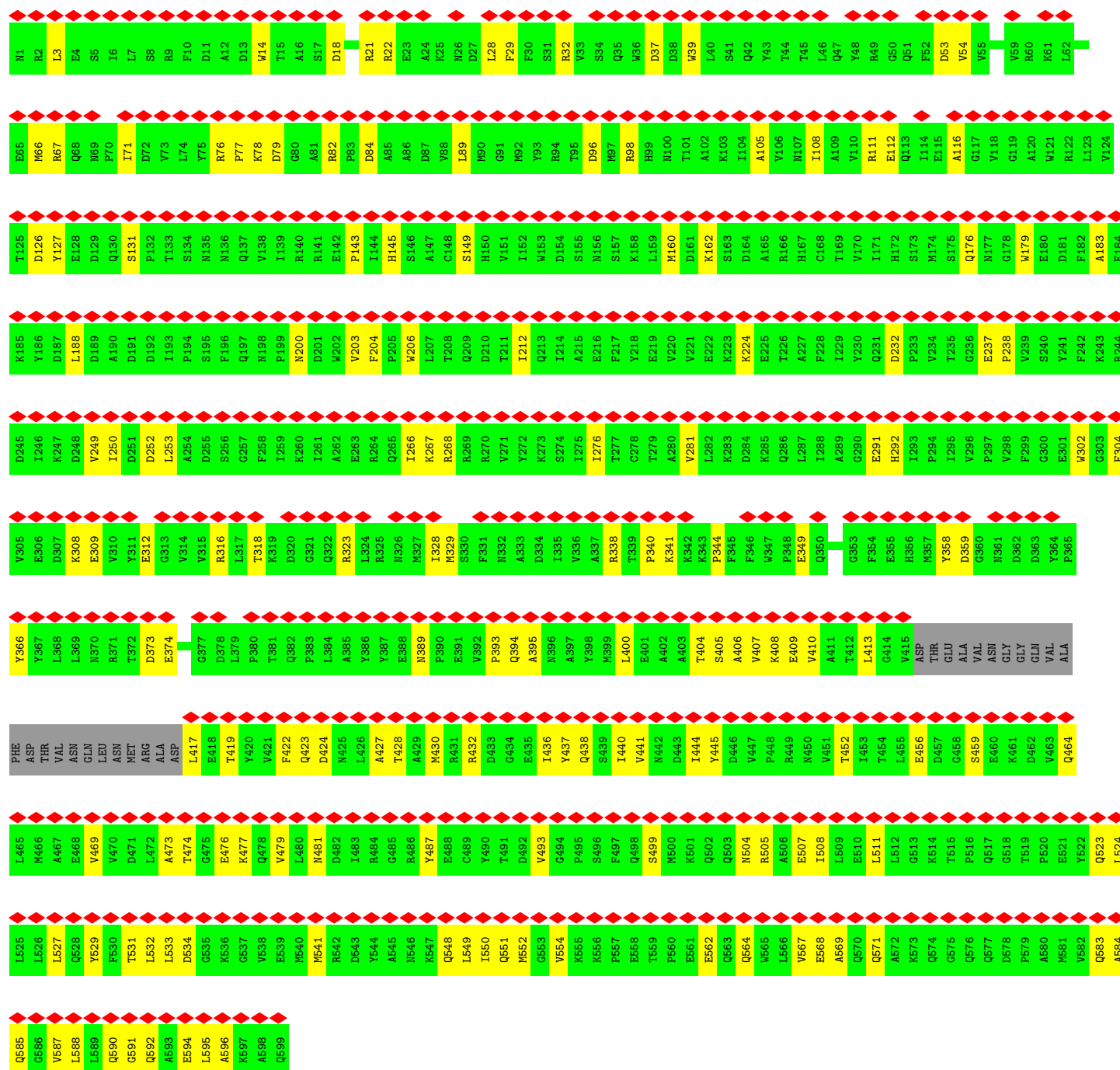


• Molecule 2: Portal protein

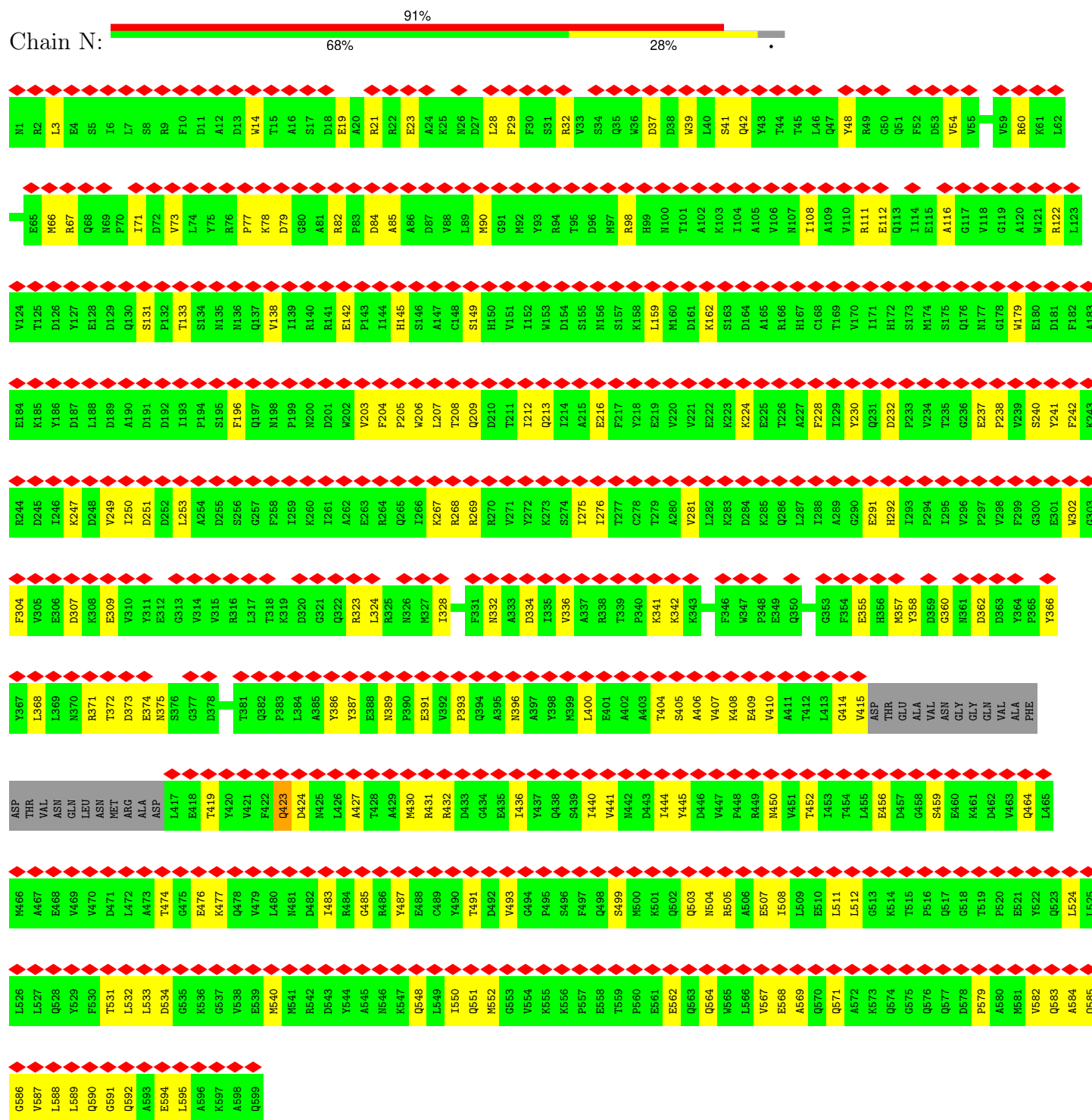




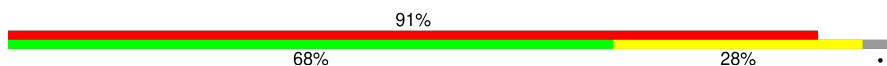
• Molecule 2: Portal protein

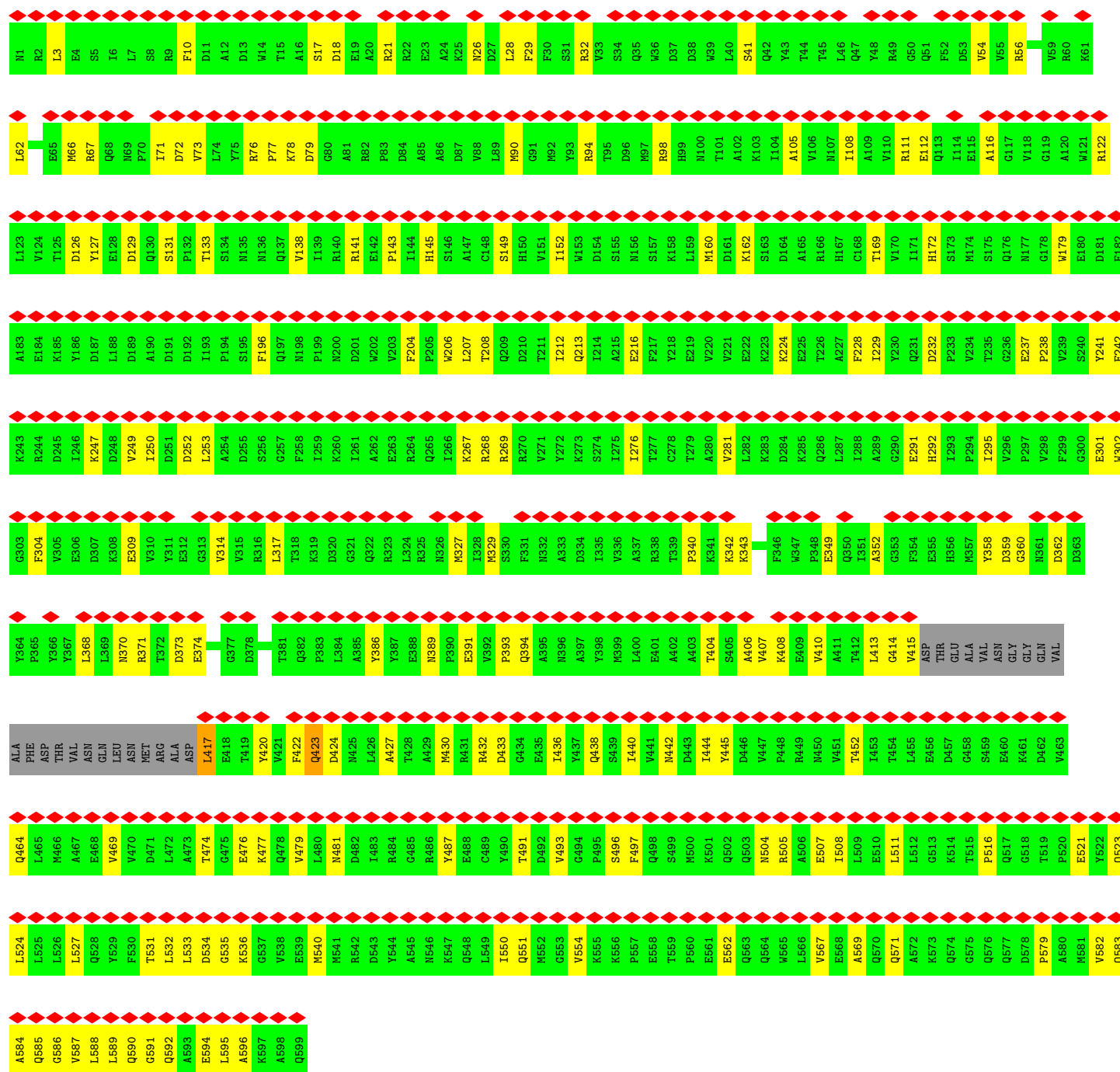


Chain N:

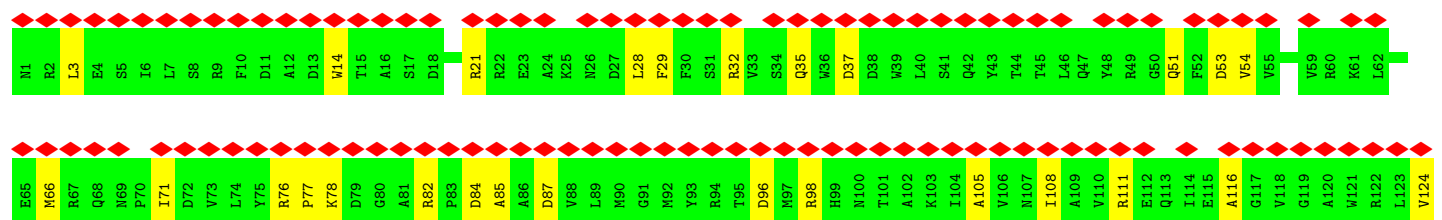
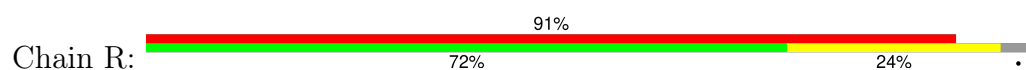


Chain P:

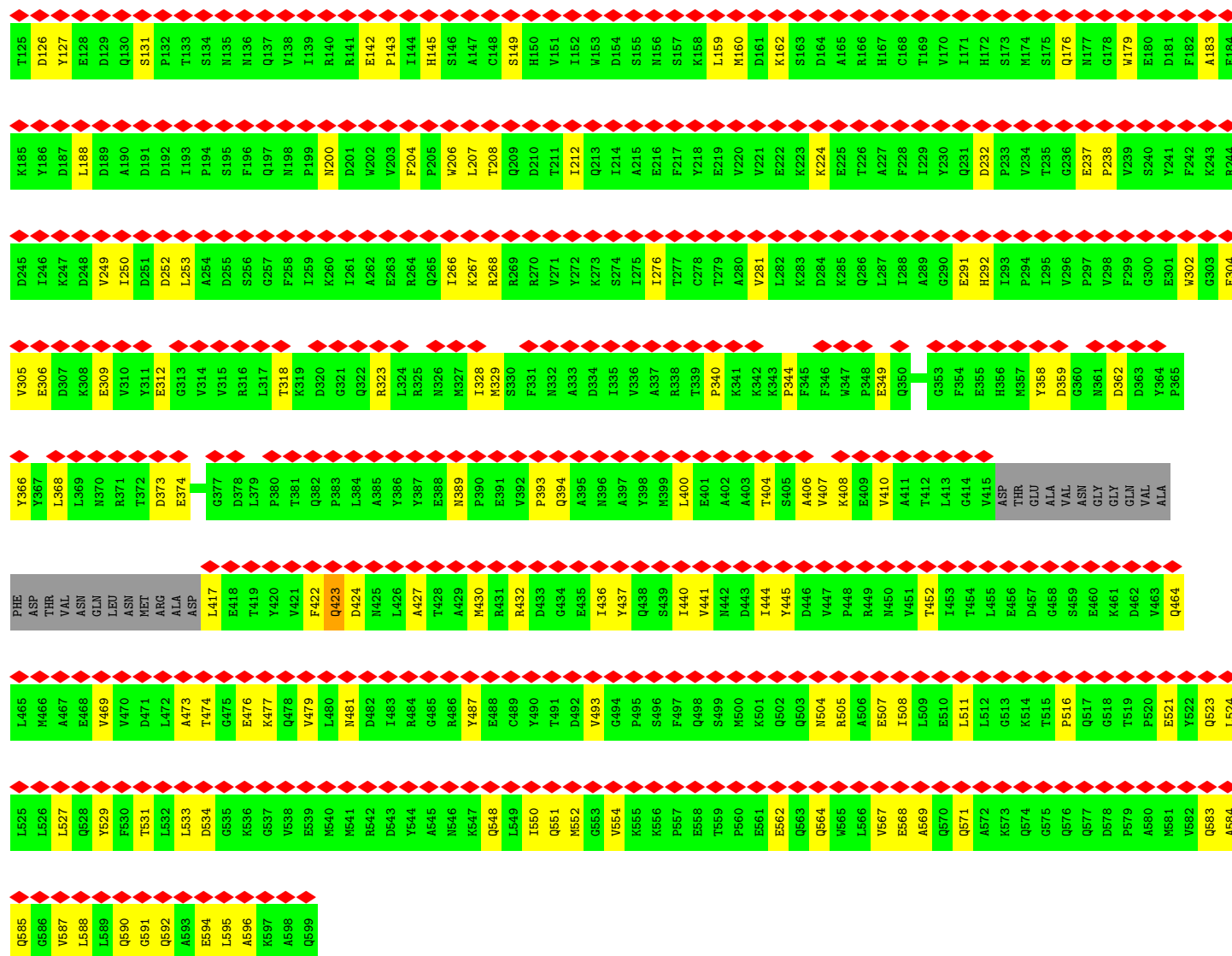




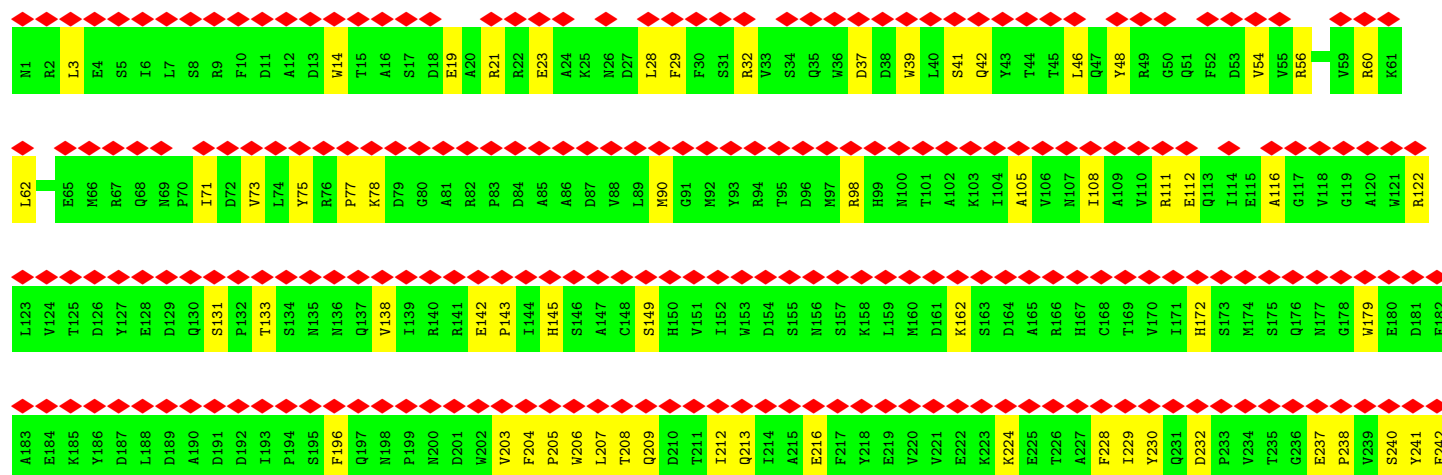
## • Molecule 2: Portal protein

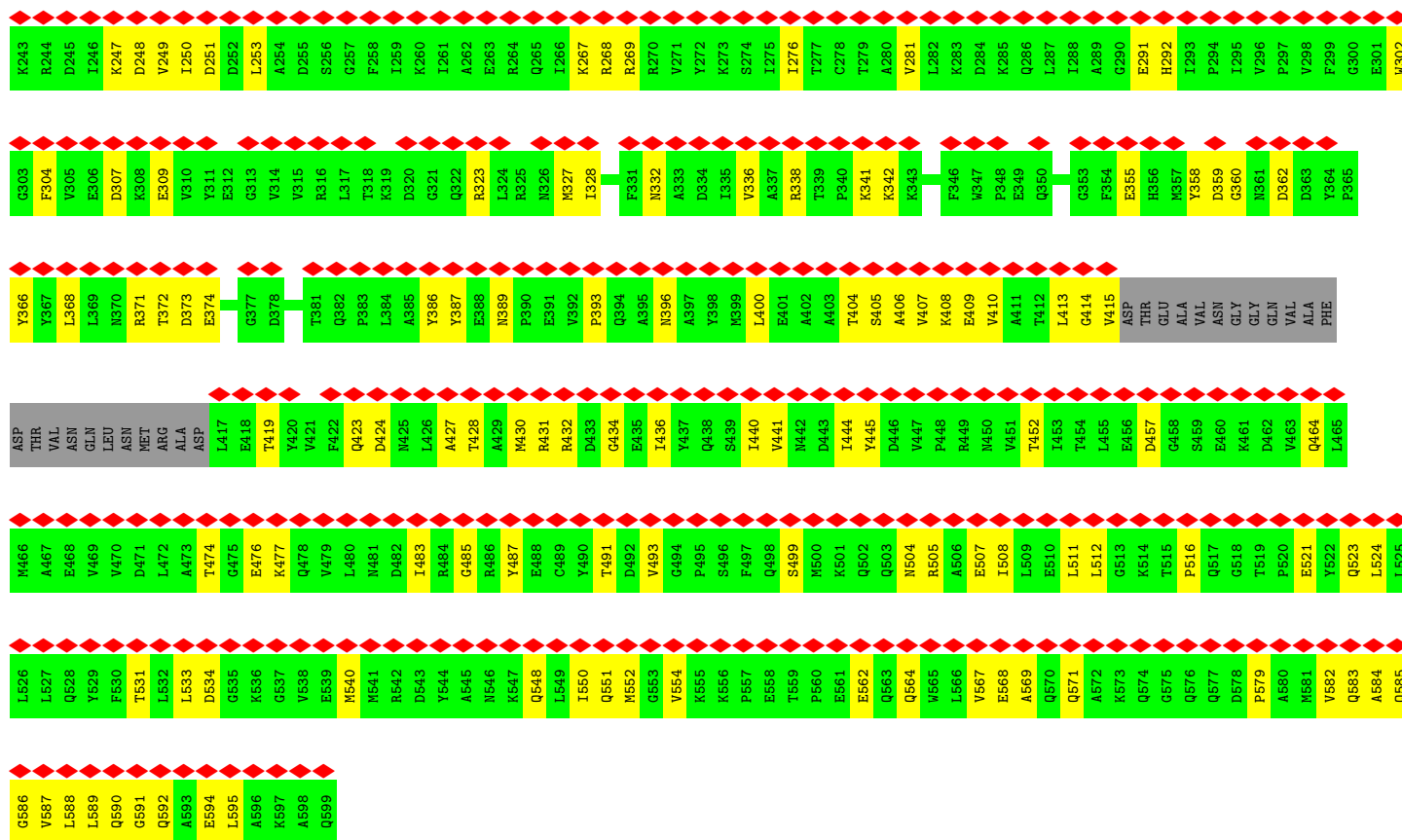




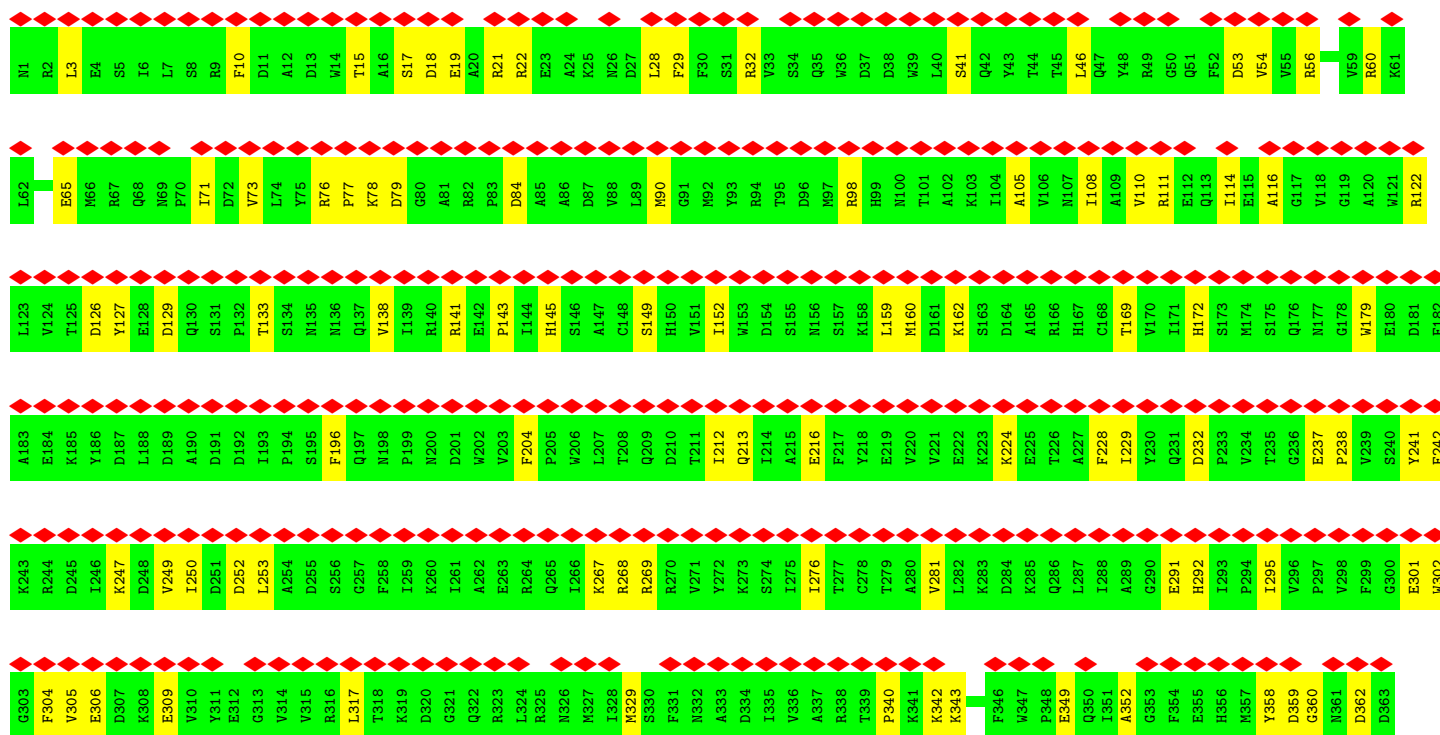


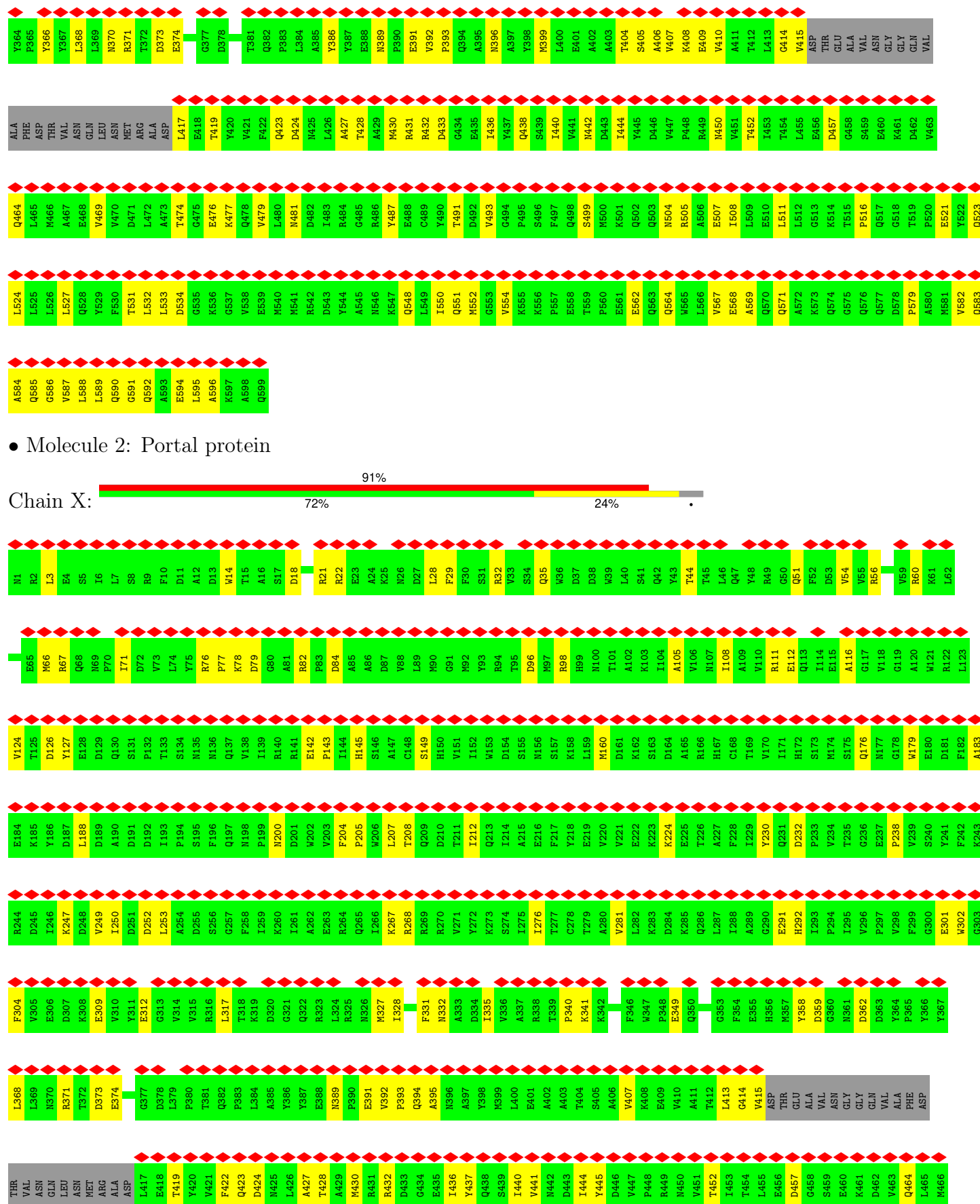
• Molecule 2: Portal protein





• Molecule 2: Portal protein





V587	L588	L589	Q590	G591	Q592	A593	E594	L595	A596	K597	A598	Q599	L527	Q528	Y529	F530	T531	L532	L533	D534	G535	K536	G537	V538	E539	M540	M541	R542	D543	Y544	A545	M546	K547	Q548	L549	T550	G551	M552	G553	V554	K555	M556	P557	E558	T559	P560	E561	E562	Q563	Q564	M565	L566	V567	E568	A569	Q570	Q571	A572	K573	Q574	G575	Q576	Q577	P578	P579	A580	M581	V582	Q583	A584	Q585	G586
A467	E468	V469	W470	D471	L472	A473	T474	G475	E476	K477	Q478	V479	L480	N481	D482	L483	R484	G485	R486	Y487	E488	C489	Y490	T491	D492	V493	C494	P495	S496	P497	Q498	S499	M500	K501	Q502	Q503	N504	R505	A506	E507	L508	L509	E510	L511	L512	G513	K514	T515	P516	Q517	G518	T519	P520	E521	Y522	Q523	L524	L525	L526													

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	73420	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	512.63995, 512.63995, 512.63995	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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	0.27	0/1165	0.43	0/1580
1	C	0.29	0/1165	0.46	0/1580
1	E	0.19	0/1165	0.38	0/1580
1	G	0.26	0/1165	0.41	0/1580
1	I	0.25	0/1165	0.39	0/1580
1	K	0.29	0/1165	0.49	0/1580
1	M	0.26	0/1165	0.52	2/1580 (0.1%)
1	O	0.36	0/1165	0.56	0/1580
1	Q	0.22	0/1165	0.41	0/1580
1	S	0.27	0/1165	0.42	0/1580
1	U	0.28	0/1165	0.45	0/1580
1	W	0.24	0/1165	0.42	0/1580
2	B	0.22	0/4930	0.39	0/6686
2	D	0.18	0/4930	0.33	0/6686
2	F	0.18	0/4930	0.34	0/6686
2	H	0.20	0/4930	0.36	0/6686
2	J	0.18	0/4930	0.35	0/6686
2	L	0.19	0/4930	0.35	0/6686
2	N	0.17	0/4930	0.33	0/6686
2	P	0.20	0/4930	0.35	0/6686
2	R	0.21	0/4930	0.37	0/6686
2	T	0.17	0/4930	0.32	0/6686
2	V	0.16	0/4930	0.31	0/6686
2	X	0.17	0/4930	0.32	0/6686
All	All	0.21	0/73140	0.37	2/99192 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	7	LEU	N-CA-C	-7.52	101.17	110.41
1	M	6	ASP	N-CA-C	-5.86	104.80	111.07

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1140	0	1110	21	0
1	C	1140	0	1110	19	0
1	E	1140	0	1110	18	0
1	G	1140	0	1110	23	0
1	I	1140	0	1110	20	0
1	K	1140	0	1110	17	0
1	M	1140	0	1110	22	0
1	O	1140	0	1110	16	0
1	Q	1140	0	1110	20	0
1	S	1140	0	1110	20	0
1	U	1140	0	1110	20	0
1	W	1140	0	1110	21	0
2	B	4829	0	4698	133	0
2	D	4829	0	4698	135	0
2	F	4829	0	4698	117	0
2	H	4829	0	4698	146	0
2	J	4829	0	4698	142	0
2	L	4829	0	4698	129	0
2	N	4829	0	4698	148	0
2	P	4829	0	4698	142	0
2	R	4829	0	4698	120	0
2	T	4829	0	4698	148	0
2	V	4829	0	4698	139	0
2	X	4829	0	4698	117	0
All	All	71628	0	69696	1508	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (1508) 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)
2:D:540:MET:HE2	2:F:527:LEU:HD13	1.59	0.84
1:W:26:VAL:HG11	1:W:31:MET:HE3	1.63	0.80
1:I:41:MET:HE3	1:I:42:MET:HE2	1.63	0.78
2:J:540:MET:HE2	2:L:527:LEU:HD13	1.64	0.78
2:H:587:VAL:HG11	2:J:588:LEU:HB3	1.68	0.76
2:L:587:VAL:HG11	2:N:588:LEU:HB3	1.67	0.76
1:M:7:LEU:HD21	1:M:78:VAL:HG13	1.66	0.76
1:I:38:LEU:HD13	1:I:85:LEU:HD12	1.67	0.76
2:N:587:VAL:HG11	2:P:588:LEU:HB3	1.68	0.76
2:B:588:LEU:HB3	2:X:587:VAL:HG11	1.67	0.75
2:H:98:ARG:HH12	2:J:78:LYS:HE3	1.52	0.74
2:R:587:VAL:HG11	2:T:588:LEU:HB3	1.68	0.74
2:F:587:VAL:HG11	2:H:588:LEU:HB3	1.68	0.74
2:P:228:PHE:HD2	2:P:247:LYS:HZ1	1.35	0.74
2:F:362:ASP:OD1	1:I:123:ARG:NH2	2.20	0.74
2:T:587:VAL:HG11	2:V:588:LEU:HB3	1.68	0.74
1:W:18:ALA:HB1	1:W:26:VAL:HG22	1.69	0.73
1:C:123:ARG:NH2	2:X:362:ASP:OD1	2.21	0.73
2:N:98:ARG:HH12	2:P:78:LYS:HE3	1.52	0.73
2:D:228:PHE:HD2	2:D:247:LYS:HZ1	1.34	0.73
2:V:228:PHE:HD2	2:V:247:LYS:HZ1	1.36	0.73
2:B:587:VAL:HG11	2:D:588:LEU:HB3	1.68	0.73
2:T:98:ARG:HH12	2:V:78:LYS:HE3	1.54	0.73
2:X:328:ILE:O	2:X:332:ASN:ND2	2.21	0.72
2:R:362:ASP:OD1	1:U:123:ARG:NH1	2.23	0.72
2:B:98:ARG:HH12	2:D:78:LYS:HE3	1.53	0.71
2:J:228:PHE:HD2	2:J:247:LYS:HZ1	1.37	0.71
2:B:586:GLY:HA2	2:B:589:LEU:HD12	1.73	0.71
2:R:359:ASP:HB3	1:S:124:ALA:HB2	1.73	0.70
2:B:78:LYS:HE3	2:X:98:ARG:HH12	1.55	0.70
2:N:586:GLY:HA2	2:N:589:LEU:HD12	1.73	0.70
2:R:249:VAL:HG23	2:R:250:ILE:HG23	1.73	0.70
2:T:586:GLY:HA2	2:T:589:LEU:HD12	1.74	0.70
2:L:249:VAL:HG23	2:L:250:ILE:HG23	1.74	0.69
1:M:1:ILE:HB	1:M:6:ASP:HB3	1.75	0.69
2:F:66:MET:HE1	2:F:422:PHE:HB3	1.74	0.69
2:R:98:ARG:HH12	2:T:78:LYS:HE3	1.57	0.69
2:F:98:ARG:HH12	2:H:78:LYS:HE3	1.58	0.68
2:H:586:GLY:HA2	2:H:589:LEU:HD12	1.74	0.68
2:D:17:SER:OG	2:D:21:ARG:NH2	2.26	0.68
1:Q:37:ASP:OD2	1:S:14:LYS:NZ	2.21	0.68
2:V:17:SER:OG	2:V:21:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:362:ASP:OD1	1:Q:123:ARG:NH2	2.26	0.68
1:M:38:LEU:HD13	1:M:85:LEU:HD12	1.75	0.68
2:L:66:MET:HE1	2:L:422:PHE:HB3	1.75	0.68
2:L:98:ARG:HH12	2:N:78:LYS:HE3	1.59	0.68
2:X:66:MET:HE1	2:X:422:PHE:HB3	1.74	0.67
2:X:249:VAL:HG23	2:X:250:ILE:HG23	1.75	0.67
1:S:47:GLN:HE22	1:U:111:LEU:HB3	1.59	0.67
1:A:47:GLN:HE22	1:C:111:LEU:HB3	1.60	0.67
2:J:17:SER:OG	2:J:21:ARG:NH2	2.27	0.67
1:W:139:ALA:HB1	1:W:144:TRP:CZ3	2.30	0.67
2:P:17:SER:OG	2:P:21:ARG:NH2	2.27	0.67
1:A:124:ALA:HB2	2:X:359:ASP:HB3	1.76	0.67
2:T:414:GLY:O	2:T:415:VAL:C	2.38	0.66
2:F:249:VAL:HG23	2:F:250:ILE:HG23	1.76	0.66
2:D:72:ASP:HA	2:D:430:MET:HE2	1.77	0.66
2:J:72:ASP:HA	2:J:430:MET:HE2	1.77	0.66
2:B:37:ASP:OD2	2:B:323:ARG:NH2	2.28	0.66
1:M:54:THR:HG22	1:M:112:LEU:HD22	1.79	0.65
2:B:394:GLN:NE2	2:X:391:GLU:O	2.30	0.65
1:I:42:MET:HE3	1:I:81:VAL:HG13	1.77	0.65
2:B:389:ASN:HB3	2:D:393:PRO:HB3	1.79	0.64
2:B:312:GLU:HG3	2:B:316:ARG:HD2	1.79	0.64
2:J:98:ARG:HH12	2:L:78:LYS:HE3	1.63	0.64
1:S:38:LEU:HD13	1:S:85:LEU:HD12	1.79	0.64
2:F:389:ASN:HB3	2:H:393:PRO:HB3	1.80	0.64
2:T:362:ASP:OD1	1:W:123:ARG:NH2	2.30	0.64
2:B:302:TRP:NE1	2:B:309:GLU:OE2	2.27	0.64
1:Q:129:ARG:NH1	2:T:48:TYR:O	2.31	0.64
1:C:54:THR:HG22	1:C:112:LEU:HD22	1.80	0.63
1:U:54:THR:HG22	1:U:112:LEU:HD22	1.80	0.63
2:H:391:GLU:O	2:J:394:GLN:NE2	2.32	0.63
2:F:391:GLU:O	2:H:394:GLN:NE2	2.30	0.63
2:V:98:ARG:HH12	2:X:78:LYS:HE3	1.63	0.63
2:V:359:ASP:HB3	1:W:124:ALA:HB2	1.80	0.63
2:P:72:ASP:HA	2:P:430:MET:HE2	1.80	0.63
1:S:54:THR:HG22	1:S:112:LEU:HD22	1.79	0.63
2:B:393:PRO:HB3	2:X:389:ASN:HB3	1.80	0.63
1:I:73:LEU:HD13	1:I:81:VAL:HG21	1.80	0.63
2:D:122:ARG:NH2	2:D:142:GLU:OE1	2.32	0.63
2:H:179:TRP:HB2	2:H:212:ILE:HG21	1.80	0.62
2:L:312:GLU:HG3	2:L:316:ARG:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:249:VAL:HG23	2:T:250:ILE:HG23	1.80	0.62
2:D:98:ARG:HH12	2:F:78:LYS:HE3	1.63	0.62
2:F:328:ILE:O	2:F:332:ASN:ND2	2.32	0.62
2:V:249:VAL:HG23	2:V:250:ILE:HG23	1.81	0.62
1:A:37:ASP:OD2	1:C:14:LYS:NZ	2.25	0.62
2:H:389:ASN:HB3	2:J:393:PRO:HB3	1.80	0.62
2:L:276:ILE:HG22	2:L:281:VAL:HG12	1.81	0.62
2:H:249:VAL:HG23	2:H:250:ILE:HG23	1.81	0.62
2:L:21:ARG:HD3	2:L:149:SER:HA	1.82	0.62
2:P:98:ARG:HH12	2:R:78:LYS:HE3	1.65	0.62
2:X:523:GLN:HE22	2:X:554:VAL:HG11	1.65	0.62
1:E:18:ALA:HB1	1:E:26:VAL:HG22	1.82	0.61
2:L:253:LEU:HD21	2:L:474:THR:HG23	1.81	0.61
2:R:253:LEU:HD21	2:R:474:THR:HG23	1.81	0.61
2:B:391:GLU:O	2:D:394:GLN:NE2	2.31	0.61
2:L:505:ARG:NH1	2:L:531:THR:O	2.34	0.61
2:R:529:TYR:HE1	2:T:511:LEU:HD22	1.65	0.61
2:X:302:TRP:NE1	2:X:309:GLU:OE2	2.29	0.61
2:F:302:TRP:NE1	2:F:309:GLU:OE2	2.29	0.61
2:B:249:VAL:HG23	2:B:250:ILE:HG23	1.81	0.61
2:D:586:GLY:HA2	2:D:589:LEU:HD12	1.83	0.61
2:F:359:ASP:HB3	1:G:124:ALA:HB2	1.82	0.61
2:H:483:ILE:HG13	2:H:485:GLY:H	1.66	0.61
2:X:253:LEU:HD21	2:X:474:THR:HG23	1.82	0.61
1:I:26:VAL:HG13	1:I:31:MET:HE3	1.83	0.61
1:M:7:LEU:O	1:M:8:VAL:HB	2.01	0.61
2:V:532:LEU:HD21	2:X:511:LEU:HD11	1.83	0.60
2:L:499:SER:OG	2:N:79:ASP:OD1	2.20	0.60
2:F:523:GLN:HE22	2:F:554:VAL:HG11	1.67	0.60
2:B:179:TRP:HB2	2:B:212:ILE:HG21	1.83	0.60
2:H:302:TRP:NE1	2:H:309:GLU:OE2	2.26	0.60
2:P:314:VAL:HB	2:P:413:LEU:HD13	1.84	0.60
2:B:32:ARG:NH1	2:D:304:PHE:O	2.34	0.60
1:C:26:VAL:HG13	1:C:31:MET:HE3	1.84	0.60
1:Q:18:ALA:HB1	1:Q:26:VAL:HG22	1.84	0.60
1:S:79:SER:HA	1:S:82:PHE:CE2	2.37	0.60
2:F:505:ARG:NH1	2:F:531:THR:O	2.34	0.60
2:H:21:ARG:HD3	2:H:149:SER:HA	1.82	0.60
1:M:79:SER:HA	1:M:82:PHE:CE2	2.37	0.60
1:U:26:VAL:HG13	1:U:31:MET:HE3	1.83	0.60
2:X:414:GLY:O	2:X:415:VAL:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:54:VAL:HG13	2:R:407:VAL:HG11	1.83	0.60
2:H:73:VAL:HG13	2:H:491:THR:HG23	1.83	0.60
2:N:249:VAL:HG23	2:N:250:ILE:HG23	1.81	0.60
1:Q:128:SER:O	1:Q:129:ARG:HB2	2.01	0.60
2:R:21:ARG:HD3	2:R:149:SER:HA	1.83	0.60
2:T:21:ARG:HD3	2:T:149:SER:HA	1.83	0.60
2:D:540:MET:HE1	2:F:549:LEU:HD13	1.84	0.59
2:F:529:TYR:HE1	2:H:511:LEU:HD22	1.66	0.59
1:G:79:SER:HA	1:G:82:PHE:CE2	2.37	0.59
1:K:38:LEU:HD13	1:K:85:LEU:HD12	1.84	0.59
2:N:37:ASP:OD2	2:N:323:ARG:NH2	2.33	0.59
1:O:79:SER:HA	1:O:82:PHE:CE2	2.38	0.59
2:B:318:THR:HB	2:B:407:VAL:HG13	1.83	0.59
2:F:54:VAL:HG13	2:F:407:VAL:HG11	1.84	0.59
1:C:38:LEU:HD13	1:C:85:LEU:HD12	1.84	0.59
2:L:523:GLN:HE22	2:L:554:VAL:HG11	1.68	0.59
1:M:37:ASP:OD2	1:O:14:LYS:NZ	2.24	0.59
2:R:37:ASP:OD2	2:R:323:ARG:NH2	2.35	0.59
2:T:32:ARG:NH1	2:V:304:PHE:O	2.35	0.59
2:T:483:ILE:HG13	2:T:485:GLY:H	1.67	0.59
1:U:38:LEU:HD13	1:U:85:LEU:HD12	1.84	0.59
2:B:483:ILE:HG13	2:B:485:GLY:H	1.67	0.59
2:D:249:VAL:HG23	2:D:250:ILE:HG23	1.83	0.59
2:F:60:ARG:NE	2:H:301:GLU:OE2	2.34	0.59
1:U:79:SER:HA	1:U:82:PHE:CE2	2.37	0.59
1:A:79:SER:HA	1:A:82:PHE:CE2	2.38	0.59
2:P:586:GLY:HA2	2:P:589:LEU:HD12	1.85	0.59
2:D:32:ARG:NH1	2:F:304:PHE:O	2.36	0.59
1:G:47:GLN:HE21	1:I:111:LEU:HD13	1.66	0.59
1:Q:7:LEU:HD21	1:Q:78:VAL:HG13	1.85	0.59
1:Q:79:SER:HA	1:Q:82:PHE:CE2	2.38	0.59
2:B:73:VAL:HG13	2:B:491:THR:HG23	1.84	0.59
2:B:511:LEU:HD22	2:X:529:TYR:HE1	1.68	0.59
2:B:40:LEU:HG	2:B:41:SER:H	1.68	0.59
1:C:79:SER:HA	1:C:82:PHE:CE2	2.37	0.59
2:D:172:HIS:NE2	2:D:216:GLU:OE1	2.36	0.59
2:L:529:TYR:HE1	2:N:511:LEU:HD22	1.67	0.59
2:N:73:VAL:HG13	2:N:491:THR:HG23	1.84	0.59
2:P:249:VAL:HG23	2:P:250:ILE:HG23	1.83	0.59
1:E:79:SER:HA	1:E:82:PHE:CE2	2.38	0.58
2:F:21:ARG:HD3	2:F:149:SER:HA	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:253:LEU:HD21	2:F:474:THR:HG23	1.83	0.58
2:B:21:ARG:HD3	2:B:149:SER:HA	1.86	0.58
1:I:7:LEU:HD21	1:I:78:VAL:HG13	1.84	0.58
1:W:79:SER:HA	1:W:82:PHE:CE2	2.38	0.58
2:N:483:ILE:HG13	2:N:485:GLY:H	1.68	0.58
2:L:37:ASP:OD2	2:L:323:ARG:NH2	2.35	0.58
2:N:247:LYS:NZ	2:N:251:ASP:OD1	2.34	0.58
2:R:292:HIS:HB3	2:R:432:ARG:HH21	1.69	0.58
2:B:499:SER:OG	2:D:79:ASP:OD1	2.21	0.58
2:H:60:ARG:NE	2:J:301:GLU:OE2	2.36	0.58
2:H:592:GLN:HG2	2:H:595:LEU:HD12	1.86	0.58
2:J:536:LYS:HD3	2:L:464:GLN:HE22	1.68	0.58
2:N:499:SER:OG	2:P:79:ASP:OD1	2.22	0.58
2:V:172:HIS:NE2	2:V:216:GLU:OE1	2.36	0.58
2:D:373:ASP:OD1	2:D:374:GLU:N	2.37	0.58
2:B:60:ARG:NE	2:D:301:GLU:OE2	2.36	0.58
2:H:122:ARG:NH2	2:H:142:GLU:OE1	2.37	0.58
2:J:32:ARG:NH1	2:L:304:PHE:O	2.37	0.58
2:T:73:VAL:HG13	2:T:491:THR:HG23	1.85	0.58
2:T:162:LYS:NZ	2:T:309:GLU:OE1	2.35	0.58
2:B:304:PHE:O	2:X:32:ARG:NH1	2.36	0.58
1:K:79:SER:HA	1:K:82:PHE:CE2	2.39	0.58
2:L:564:GLN:O	2:L:568:GLU:HG3	2.04	0.58
2:N:21:ARG:HD3	2:N:149:SER:HA	1.84	0.58
1:O:26:VAL:HG13	1:O:31:MET:HE3	1.85	0.58
2:P:373:ASP:OD1	2:P:374:GLU:N	2.37	0.58
2:J:105:ALA:HA	2:J:143:PRO:HB3	1.86	0.58
2:L:292:HIS:HB3	2:L:432:ARG:HH21	1.69	0.58
2:P:32:ARG:NH1	2:R:304:PHE:O	2.37	0.58
2:T:60:ARG:NE	2:V:301:GLU:OE2	2.37	0.58
2:V:276:ILE:HG22	2:V:281:VAL:HG12	1.86	0.58
2:V:499:SER:OG	2:X:79:ASP:OD1	2.21	0.58
2:D:318:THR:HB	2:D:407:VAL:HG13	1.84	0.57
2:J:249:VAL:HG23	2:J:250:ILE:HG23	1.83	0.57
2:J:540:MET:HE1	2:L:549:LEU:HD13	1.86	0.57
2:X:292:HIS:HB3	2:X:432:ARG:HH21	1.69	0.57
2:B:301:GLU:OE2	2:X:60:ARG:NE	2.35	0.57
2:F:452:THR:HG22	2:F:464:GLN:HA	1.86	0.57
2:N:60:ARG:NE	2:P:301:GLU:OE2	2.37	0.57
1:O:38:LEU:HD13	1:O:85:LEU:HD12	1.85	0.57
2:V:586:GLY:HA2	2:V:589:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:7:LEU:HD21	1:W:78:VAL:HG13	1.87	0.57
1:G:47:GLN:HE22	1:I:111:LEU:HB3	1.67	0.57
2:L:452:THR:HG22	2:L:464:GLN:HA	1.86	0.57
2:T:499:SER:OG	2:V:79:ASP:OD1	2.22	0.57
2:D:438:GLN:O	2:D:442:ASN:ND2	2.38	0.57
1:E:26:VAL:HG11	1:E:31:MET:HE3	1.86	0.57
2:F:292:HIS:HB3	2:F:432:ARG:HH21	1.70	0.57
2:H:499:SER:OG	2:J:79:ASP:OD1	2.22	0.57
2:J:373:ASP:OD1	2:J:374:GLU:N	2.37	0.57
2:R:452:THR:HG22	2:R:464:GLN:HA	1.87	0.57
2:T:371:ARG:NH2	2:V:349:GLU:OE2	2.38	0.57
2:V:366:TYR:HE1	2:X:358:TYR:HB2	1.69	0.57
2:X:21:ARG:HD3	2:X:149:SER:HA	1.85	0.57
2:X:276:ILE:HG22	2:X:281:VAL:HG12	1.85	0.57
2:D:276:ILE:HG22	2:D:281:VAL:HG12	1.85	0.57
2:D:583:GLN:O	2:D:587:VAL:HG23	2.05	0.57
2:H:32:ARG:NH1	2:J:304:PHE:O	2.37	0.57
2:B:551:GLN:HG2	2:B:569:ALA:HB2	1.86	0.57
2:J:359:ASP:HB3	1:K:124:ALA:HB2	1.87	0.57
2:N:32:ARG:NH1	2:P:304:PHE:O	2.37	0.57
2:P:276:ILE:HG22	2:P:281:VAL:HG12	1.86	0.57
2:P:404:THR:O	2:P:408:LYS:HG2	2.04	0.57
2:J:548:GLN:O	2:J:552:MET:HG3	2.04	0.57
2:N:32:ARG:HH21	2:N:111:ARG:HG2	1.70	0.57
2:L:32:ARG:NH1	2:N:304:PHE:O	2.37	0.57
2:N:533:LEU:HD22	2:P:76:ARG:HH12	1.70	0.57
2:P:452:THR:HG22	2:P:464:GLN:HA	1.87	0.57
1:S:37:ASP:OD2	1:U:14:LYS:NZ	2.24	0.57
2:X:32:ARG:HH21	2:X:111:ARG:HG2	1.70	0.57
2:B:28:LEU:HG	2:B:116:ALA:HB2	1.87	0.56
2:D:532:LEU:HD21	2:F:511:LEU:HD11	1.86	0.56
2:D:60:ARG:NE	2:F:301:GLU:OE2	2.37	0.56
2:F:584:ALA:HB2	2:H:585:GLN:HG2	1.87	0.56
2:H:371:ARG:NH2	2:J:349:GLU:OE2	2.38	0.56
2:P:172:HIS:NE2	2:P:216:GLU:OE1	2.37	0.56
2:R:32:ARG:NH1	2:T:304:PHE:O	2.38	0.56
2:V:65:GLU:HG2	2:V:417:LEU:HD11	1.87	0.56
1:W:3:THR:HG22	1:W:6:ASP:CG	2.30	0.56
2:B:122:ARG:NH2	2:B:142:GLU:OE1	2.37	0.56
1:I:79:SER:HA	1:I:82:PHE:CE2	2.40	0.56
2:J:152:ILE:HB	2:J:169:THR:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:532:LEU:HD21	2:L:511:LEU:HD11	1.86	0.56
2:V:343:LYS:NZ	1:W:123:ARG:HH22	2.03	0.56
2:B:371:ARG:NH2	2:D:349:GLU:OE2	2.39	0.56
1:I:44:GLU:OE2	1:I:88:ARG:NH2	2.36	0.56
2:R:564:GLN:O	2:R:568:GLU:HG3	2.05	0.56
2:X:505:ARG:NH1	2:X:531:THR:O	2.37	0.56
2:B:505:ARG:NH1	2:B:531:THR:O	2.37	0.56
2:F:105:ALA:HA	2:F:143:PRO:HB3	1.88	0.56
2:J:421:VAL:C	2:J:423:GLN:H	2.13	0.56
2:L:419:THR:O	2:L:423:GLN:HB2	2.06	0.56
2:N:122:ARG:NH2	2:N:142:GLU:OE1	2.39	0.56
2:N:371:ARG:NH2	2:P:349:GLU:OE2	2.38	0.56
2:T:32:ARG:HH21	2:T:111:ARG:HG2	1.71	0.56
2:V:73:VAL:HG13	2:V:491:THR:HG23	1.88	0.56
2:V:564:GLN:O	2:V:568:GLU:HG3	2.05	0.56
2:B:564:GLN:O	2:B:568:GLU:HG3	2.06	0.56
2:L:32:ARG:HH21	2:L:111:ARG:HG2	1.71	0.56
2:R:32:ARG:HH21	2:R:111:ARG:HG2	1.71	0.56
2:R:505:ARG:NH1	2:R:531:THR:O	2.38	0.56
2:V:373:ASP:OD1	2:V:374:GLU:N	2.38	0.56
2:V:548:GLN:O	2:V:552:MET:HG3	2.05	0.56
2:X:419:THR:O	2:X:423:GLN:HB2	2.06	0.56
2:F:32:ARG:NH1	2:H:304:PHE:O	2.38	0.56
2:H:228:PHE:N	2:H:242:PHE:O	2.39	0.56
2:J:421:VAL:HG12	2:J:422:PHE:H	1.70	0.56
2:N:505:ARG:NH1	2:N:531:THR:O	2.37	0.56
2:R:276:ILE:HG22	2:R:281:VAL:HG12	1.87	0.56
2:T:358:TYR:OH	2:T:368:LEU:O	2.24	0.56
2:T:564:GLN:O	2:T:568:GLU:HG3	2.06	0.56
2:V:371:ARG:NH1	2:X:349:GLU:OE1	2.39	0.56
2:V:583:GLN:O	2:V:587:VAL:HG23	2.06	0.56
2:P:532:LEU:HD21	2:R:511:LEU:HD11	1.86	0.56
2:V:32:ARG:NH1	2:X:304:PHE:O	2.39	0.56
2:J:196:PHE:O	2:J:213:GLN:NE2	2.39	0.56
1:K:18:ALA:HB1	1:K:26:VAL:HG22	1.87	0.56
2:N:358:TYR:OH	2:N:368:LEU:O	2.24	0.56
1:U:42:MET:HE3	1:U:42:MET:HA	1.88	0.56
2:X:452:THR:HG22	2:X:464:GLN:HA	1.88	0.56
2:F:276:ILE:HG22	2:F:281:VAL:HG12	1.87	0.55
2:H:37:ASP:OD2	2:H:323:ARG:NH2	2.35	0.55
2:P:196:PHE:O	2:P:213:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:583:GLN:O	2:P:587:VAL:HG23	2.06	0.55
2:R:592:GLN:HG2	2:R:595:LEU:HD12	1.89	0.55
2:H:551:GLN:HG2	2:H:569:ALA:HB2	1.88	0.55
2:L:54:VAL:HG13	2:L:407:VAL:HG11	1.87	0.55
2:H:276:ILE:HG22	2:H:281:VAL:HG12	1.88	0.55
2:N:389:ASN:HB3	2:P:393:PRO:HB3	1.89	0.55
2:P:371:ARG:NH1	2:R:349:GLU:OE1	2.39	0.55
2:T:505:ARG:NH1	2:T:531:THR:O	2.37	0.55
1:C:42:MET:HE3	1:C:42:MET:HA	1.88	0.55
2:D:152:ILE:HB	2:D:169:THR:HB	1.88	0.55
2:J:421:VAL:O	2:J:423:GLN:N	2.37	0.55
1:K:7:LEU:HD21	1:K:78:VAL:HG13	1.88	0.55
2:N:414:GLY:O	2:N:415:VAL:C	2.49	0.55
2:N:548:GLN:O	2:N:552:MET:HG3	2.05	0.55
2:P:551:GLN:HG2	2:P:569:ALA:HB2	1.89	0.55
2:X:54:VAL:HG13	2:X:407:VAL:HG11	1.88	0.55
2:D:389:ASN:HB3	2:F:393:PRO:HB3	1.89	0.55
1:E:7:LEU:HD21	1:E:78:VAL:HG13	1.88	0.55
2:L:105:ALA:HA	2:L:143:PRO:HB3	1.89	0.55
2:P:505:ARG:NH1	2:P:531:THR:O	2.38	0.55
1:Q:26:VAL:HG11	1:Q:31:MET:HE3	1.87	0.55
2:R:66:MET:HE1	2:R:422:PHE:HB3	1.88	0.55
2:R:344:PRO:HG3	2:T:387:TYR:HE1	1.71	0.55
2:T:179:TRP:HB2	2:T:212:ILE:HG21	1.88	0.55
2:V:505:ARG:NH1	2:V:531:THR:O	2.39	0.55
2:J:371:ARG:NH1	2:L:349:GLU:OE1	2.39	0.55
2:J:389:ASN:HB3	2:L:393:PRO:HB3	1.89	0.55
1:O:42:MET:HA	1:O:42:MET:HE3	1.87	0.55
2:V:152:ILE:HB	2:V:169:THR:HB	1.88	0.55
2:X:373:ASP:OD1	2:X:374:GLU:N	2.40	0.55
2:J:583:GLN:O	2:J:587:VAL:HG23	2.06	0.55
2:J:586:GLY:HA2	2:J:589:LEU:HD12	1.88	0.55
2:P:389:ASN:HB3	2:R:393:PRO:HB3	1.89	0.55
2:T:592:GLN:HG2	2:T:595:LEU:HD12	1.88	0.55
2:B:247:LYS:NZ	2:B:251:ASP:OD1	2.35	0.55
2:B:592:GLN:HG2	2:B:595:LEU:HD12	1.89	0.55
2:L:567:VAL:O	2:L:571:GLN:HG3	2.07	0.55
2:B:276:ILE:HG22	2:B:281:VAL:HG12	1.88	0.55
1:C:7:LEU:HD21	1:C:78:VAL:HG13	1.89	0.55
2:N:292:HIS:HB3	2:N:432:ARG:HH21	1.72	0.55
2:N:564:GLN:O	2:N:568:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:84:ASP:OD2	2:R:464:GLN:NE2	2.40	0.55
2:V:179:TRP:HB2	2:V:212:ILE:HG21	1.89	0.55
1:A:54:THR:HG22	1:A:112:LEU:HD22	1.89	0.54
2:F:551:GLN:HG2	2:F:569:ALA:HB2	1.90	0.54
2:T:37:ASP:OD2	2:T:323:ARG:NH2	2.33	0.54
2:V:54:VAL:HG13	2:V:407:VAL:HG11	1.89	0.54
2:N:179:TRP:HB2	2:N:212:ILE:HG21	1.89	0.54
2:N:511:LEU:HB3	2:N:524:LEU:HD21	1.89	0.54
2:P:54:VAL:HG13	2:P:407:VAL:HG11	1.89	0.54
1:A:38:LEU:HD13	1:A:85:LEU:HD12	1.89	0.54
2:D:551:GLN:HG2	2:D:569:ALA:HB2	1.89	0.54
2:H:28:LEU:HG	2:H:116:ALA:HB2	1.89	0.54
2:H:532:LEU:HD21	2:J:511:LEU:HD11	1.90	0.54
2:T:276:ILE:HG22	2:T:281:VAL:HG12	1.88	0.54
2:F:32:ARG:HH21	2:F:111:ARG:HG2	1.73	0.54
2:F:67:ARG:HD3	2:H:424:ASP:OD2	2.07	0.54
2:J:276:ILE:HG22	2:J:281:VAL:HG12	1.88	0.54
2:J:362:ASP:OD1	1:M:123:ARG:NH2	2.37	0.54
2:L:67:ARG:HD3	2:N:424:ASP:OD2	2.08	0.54
2:L:291:GLU:OE1	2:L:487:TYR:OH	2.24	0.54
2:H:583:GLN:HE22	2:J:585:GLN:C	2.15	0.54
2:J:32:ARG:HH21	2:J:111:ARG:HG2	1.72	0.54
2:L:344:PRO:HG3	2:N:387:TYR:HE1	1.72	0.54
2:L:592:GLN:HG2	2:L:595:LEU:HD12	1.89	0.54
2:P:32:ARG:HH21	2:P:111:ARG:HG2	1.73	0.54
2:B:206:TRP:CD1	2:B:209:GLN:HE21	2.26	0.54
2:F:291:GLU:OE1	2:F:487:TYR:OH	2.25	0.54
2:F:373:ASP:OD1	2:F:374:GLU:N	2.40	0.54
2:L:28:LEU:HG	2:L:116:ALA:HB2	1.89	0.54
2:N:276:ILE:HG22	2:N:281:VAL:HG12	1.88	0.54
2:P:592:GLN:HG2	2:P:595:LEU:HD12	1.89	0.54
2:T:291:GLU:OE1	2:T:487:TYR:OH	2.25	0.54
2:T:567:VAL:O	2:T:571:GLN:HG3	2.08	0.54
2:V:414:GLY:O	2:V:415:VAL:C	2.51	0.54
2:V:567:VAL:O	2:V:571:GLN:HG3	2.08	0.54
2:H:505:ARG:NH1	2:H:531:THR:O	2.37	0.54
2:N:452:THR:HG22	2:N:464:GLN:HA	1.90	0.54
2:P:3:LEU:HD13	2:P:281:VAL:HG13	1.90	0.54
2:P:152:ILE:HB	2:P:169:THR:HB	1.89	0.54
2:T:551:GLN:HG2	2:T:569:ALA:HB2	1.90	0.54
1:G:38:LEU:HD13	1:G:85:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:206:TRP:CD1	2:N:209:GLN:HE21	2.25	0.54
2:X:567:VAL:O	2:X:571:GLN:HG3	2.08	0.54
2:D:366:TYR:HE1	2:F:358:TYR:HB2	1.71	0.54
2:H:3:LEU:HD13	2:H:281:VAL:HG13	1.90	0.54
2:L:404:THR:O	2:L:408:LYS:HG2	2.07	0.54
2:B:567:VAL:O	2:B:571:GLN:HG3	2.07	0.54
2:N:3:LEU:HD13	2:N:281:VAL:HG13	1.90	0.54
2:V:60:ARG:NE	2:X:301:GLU:OE2	2.38	0.54
2:V:534:ASP:HB2	2:X:77:PRO:HD3	1.90	0.54
2:B:14:TRP:O	2:B:21:ARG:NH2	2.40	0.53
2:D:3:LEU:HD13	2:D:281:VAL:HG13	1.90	0.53
2:D:452:THR:HG22	2:D:464:GLN:HA	1.90	0.53
2:F:3:LEU:HD13	2:F:281:VAL:HG13	1.91	0.53
2:F:71:ILE:HG22	2:F:430:MET:HG3	1.90	0.53
2:V:28:LEU:O	2:V:32:ARG:HB2	2.08	0.53
2:V:452:THR:HG22	2:V:464:GLN:HA	1.91	0.53
2:X:82:ARG:NH1	2:X:84:ASP:OD1	2.37	0.53
2:J:452:THR:HG22	2:J:464:GLN:HA	1.90	0.53
1:K:129:ARG:NH2	2:N:334:ASP:OD2	2.38	0.53
2:L:302:TRP:NE1	2:L:309:GLU:OE2	2.32	0.53
1:M:26:VAL:HG13	1:M:31:MET:HE3	1.91	0.53
2:N:196:PHE:O	2:N:213:GLN:NE2	2.41	0.53
2:N:583:GLN:HE22	2:P:585:GLN:C	2.15	0.53
2:H:534:ASP:HB2	2:J:77:PRO:HD3	1.91	0.53
2:J:162:LYS:NZ	2:J:309:GLU:OE1	2.41	0.53
2:N:567:VAL:O	2:N:571:GLN:HG3	2.07	0.53
2:V:105:ALA:HA	2:V:143:PRO:HB3	1.90	0.53
1:G:18:ALA:HB1	1:G:26:VAL:HG22	1.90	0.53
2:H:564:GLN:O	2:H:568:GLU:HG3	2.07	0.53
2:L:71:ILE:HG22	2:L:430:MET:HG3	1.91	0.53
2:N:532:LEU:HD21	2:P:511:LEU:HD11	1.90	0.53
2:P:540:MET:HE2	2:R:527:LEU:HD22	1.90	0.53
2:V:389:ASN:HB3	2:X:393:PRO:HB3	1.91	0.53
2:D:505:ARG:NH1	2:D:531:THR:O	2.39	0.53
2:D:534:ASP:HB2	2:F:77:PRO:HD3	1.89	0.53
2:J:179:TRP:HB2	2:J:212:ILE:HG21	1.90	0.53
2:L:389:ASN:HB3	2:N:393:PRO:HB3	1.90	0.53
2:T:583:GLN:HE22	2:V:585:GLN:C	2.15	0.53
2:V:3:LEU:HD13	2:V:281:VAL:HG13	1.90	0.53
2:X:14:TRP:O	2:X:21:ARG:NH2	2.42	0.53
2:B:253:LEU:HD21	2:B:474:THR:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:LEU:HD21	2:D:474:THR:HG23	1.91	0.53
2:H:204:PHE:HB3	2:H:206:TRP:NE1	2.23	0.53
2:J:28:LEU:O	2:J:32:ARG:HB2	2.08	0.53
2:V:358:TYR:OH	2:V:368:LEU:O	2.25	0.53
2:X:126:ASP:OD1	2:X:127:TYR:N	2.42	0.53
2:B:550:ILE:HD13	2:B:562:GLU:HB3	1.90	0.53
2:F:28:LEU:HG	2:F:116:ALA:HB2	1.90	0.53
2:F:305:VAL:HG22	2:F:306:GLU:HG2	1.90	0.53
2:F:404:THR:O	2:F:408:LYS:HG2	2.09	0.53
2:F:499:SER:OG	2:H:79:ASP:OD1	2.27	0.53
2:H:207:LEU:HD23	2:H:208:THR:HG23	1.89	0.53
1:O:54:THR:HG22	1:O:112:LEU:HD22	1.89	0.53
2:T:3:LEU:HD13	2:T:281:VAL:HG13	1.90	0.53
2:X:252:ASP:N	2:X:252:ASP:OD1	2.41	0.53
1:A:111:LEU:HD23	1:W:47:GLN:HE21	1.73	0.53
2:D:32:ARG:HH21	2:D:111:ARG:HG2	1.74	0.53
2:D:291:GLU:OE1	2:D:487:TYR:OH	2.26	0.53
2:F:427:ALA:HB1	2:F:493:VAL:HG21	1.90	0.53
2:L:551:GLN:HG2	2:L:569:ALA:HB2	1.89	0.53
2:P:67:ARG:HD3	2:R:424:ASP:OD2	2.08	0.53
2:P:105:ALA:HA	2:P:143:PRO:HB3	1.90	0.53
2:R:291:GLU:OE1	2:R:487:TYR:OH	2.25	0.53
2:R:366:TYR:HE1	2:T:358:TYR:HB2	1.74	0.53
2:B:583:GLN:HE22	2:D:585:GLN:C	2.16	0.53
2:D:28:LEU:O	2:D:32:ARG:HB2	2.08	0.53
2:N:405:SER:O	2:N:409:GLU:HG3	2.09	0.53
2:P:567:VAL:O	2:P:571:GLN:HG3	2.09	0.53
1:U:7:LEU:HD21	1:U:78:VAL:HG13	1.91	0.53
2:V:84:ASP:OD1	2:V:450:ASN:ND2	2.42	0.53
2:V:228:PHE:N	2:V:242:PHE:O	2.41	0.53
2:V:592:GLN:HG2	2:V:595:LEU:HD12	1.90	0.53
2:B:406:ALA:O	2:B:410:VAL:HG23	2.08	0.53
1:C:29:GLN:NE2	1:E:20:ASP:OD2	2.41	0.53
2:J:28:LEU:HG	2:J:116:ALA:HB2	1.90	0.53
2:J:404:THR:O	2:J:408:LYS:HG2	2.08	0.53
2:L:373:ASP:OD1	2:L:374:GLU:N	2.42	0.53
2:R:28:LEU:HG	2:R:116:ALA:HB2	1.89	0.53
2:X:427:ALA:HB1	2:X:493:VAL:HG21	1.91	0.53
2:D:162:LYS:NZ	2:D:309:GLU:OE1	2.41	0.52
2:J:534:ASP:HB2	2:L:77:PRO:HD3	1.90	0.52
2:F:126:ASP:OD1	2:F:127:TYR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:476:GLU:HG2	2:N:477:LYS:HG3	1.92	0.52
2:R:305:VAL:HG22	2:R:306:GLU:HG2	1.91	0.52
2:V:343:LYS:HZ1	1:W:123:ARG:HH22	1.56	0.52
2:D:317:LEU:HB3	2:D:410:VAL:HG11	1.91	0.52
2:F:419:THR:O	2:F:423:GLN:HB2	2.09	0.52
2:J:551:GLN:HG2	2:J:569:ALA:HB2	1.90	0.52
1:S:148:PRO:HD3	2:V:41:SER:HB2	1.91	0.52
2:T:253:LEU:HD21	2:T:474:THR:HG23	1.90	0.52
2:T:452:THR:HG22	2:T:464:GLN:HA	1.91	0.52
2:D:592:GLN:HG2	2:D:595:LEU:HD12	1.91	0.52
2:J:317:LEU:HB3	2:J:410:VAL:HG11	1.92	0.52
2:N:232:ASP:HB3	2:N:238:PRO:HG3	1.91	0.52
2:N:592:GLN:HG2	2:N:595:LEU:HD12	1.89	0.52
2:R:3:LEU:HD13	2:R:281:VAL:HG13	1.91	0.52
2:T:476:GLU:HG2	2:T:477:LYS:HG3	1.92	0.52
2:X:551:GLN:HG2	2:X:569:ALA:HB2	1.92	0.52
2:B:54:VAL:HG13	2:B:407:VAL:HG11	1.92	0.52
2:H:71:ILE:HG22	2:H:430:MET:HG3	1.92	0.52
2:H:292:HIS:HB3	2:H:432:ARG:HH21	1.74	0.52
2:H:358:TYR:OH	2:H:368:LEU:O	2.24	0.52
2:P:28:LEU:HG	2:P:116:ALA:HB2	1.90	0.52
1:W:38:LEU:HD13	1:W:85:LEU:HD12	1.92	0.52
2:X:71:ILE:HG22	2:X:430:MET:HG3	1.92	0.52
2:B:32:ARG:HH21	2:B:111:ARG:HG2	1.73	0.52
2:F:252:ASP:OD1	2:F:252:ASP:N	2.41	0.52
1:G:148:PRO:HD3	2:J:41:SER:HB2	1.92	0.52
2:H:404:THR:O	2:H:408:LYS:HG2	2.09	0.52
2:N:228:PHE:N	2:N:242:PHE:O	2.39	0.52
2:R:162:LYS:NZ	2:R:309:GLU:OE2	2.42	0.52
2:R:358:TYR:OH	2:R:368:LEU:O	2.26	0.52
2:R:373:ASP:OD1	2:R:374:GLU:N	2.42	0.52
2:V:196:PHE:O	2:V:213:GLN:NE2	2.43	0.52
2:B:228:PHE:N	2:B:242:PHE:O	2.41	0.52
2:D:54:VAL:HG13	2:D:407:VAL:HG11	1.92	0.52
2:H:567:VAL:O	2:H:571:GLN:HG3	2.10	0.52
2:J:291:GLU:OE1	2:J:487:TYR:OH	2.27	0.52
2:J:505:ARG:NH1	2:J:531:THR:O	2.40	0.52
2:J:592:GLN:HG2	2:J:595:LEU:HD12	1.90	0.52
2:L:359:ASP:HB3	1:M:124:ALA:HB2	1.91	0.52
2:L:406:ALA:O	2:L:410:VAL:HG23	2.10	0.52
2:N:253:LEU:HD21	2:N:474:THR:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:179:TRP:HB2	2:P:212:ILE:HG21	1.92	0.52
2:R:71:ILE:HG22	2:R:430:MET:HG3	1.90	0.52
2:R:126:ASP:OD1	2:R:127:TYR:N	2.42	0.52
2:R:404:THR:O	2:R:408:LYS:HG2	2.09	0.52
2:V:126:ASP:OD1	2:V:127:TYR:N	2.42	0.52
2:X:28:LEU:HG	2:X:116:ALA:HB2	1.92	0.52
2:B:360:GLY:HA2	2:D:340:PRO:HG3	1.91	0.52
2:B:452:THR:HG22	2:B:464:GLN:HA	1.92	0.52
2:D:126:ASP:OD1	2:D:127:TYR:N	2.42	0.52
2:D:196:PHE:O	2:D:213:GLN:NE2	2.43	0.52
2:J:113:GLN:NE2	2:J:422:PHE:HA	2.24	0.52
2:J:567:VAL:O	2:J:571:GLN:HG3	2.09	0.52
2:N:28:LEU:HG	2:N:116:ALA:HB2	1.92	0.52
2:T:196:PHE:O	2:T:213:GLN:NE2	2.42	0.52
1:G:54:THR:HG22	1:G:112:LEU:HD22	1.90	0.52
2:L:131:SER:O	2:L:131:SER:OG	2.28	0.52
2:P:56:ARG:NH2	2:R:312:GLU:OE1	2.43	0.52
1:S:47:GLN:NE2	1:U:111:LEU:HB3	2.23	0.52
2:T:206:TRP:CD1	2:T:209:GLN:HE21	2.28	0.52
2:T:224:LYS:HA	2:T:267:LYS:HA	1.92	0.52
2:V:224:LYS:HA	2:V:267:LYS:HA	1.92	0.52
2:B:584:ALA:HB2	2:D:585:GLN:HG2	1.92	0.52
2:D:567:VAL:O	2:D:571:GLN:HG3	2.09	0.52
1:G:47:GLN:NE2	1:I:111:LEU:HB3	2.25	0.52
2:L:252:ASP:N	2:L:252:ASP:OD1	2.42	0.52
2:L:427:ALA:HB1	2:L:493:VAL:HG21	1.92	0.52
1:M:3:THR:HG23	1:M:6:ASP:H	1.75	0.52
2:N:14:TRP:O	2:N:21:ARG:NH2	2.42	0.52
2:N:269:ARG:HB2	2:N:291:GLU:HG2	1.92	0.52
2:P:413:LEU:HD11	2:P:422:PHE:CZ	2.45	0.52
2:V:253:LEU:HD21	2:V:474:THR:HG23	1.91	0.52
2:V:438:GLN:O	2:V:442:ASN:ND2	2.43	0.52
2:D:28:LEU:HG	2:D:116:ALA:HB2	1.91	0.51
2:V:291:GLU:OE1	2:V:487:TYR:OH	2.27	0.51
2:B:3:LEU:HD13	2:B:281:VAL:HG13	1.90	0.51
2:F:200:ASN:ND2	2:H:307:ASP:OD2	2.43	0.51
2:H:32:ARG:HH21	2:H:111:ARG:HG2	1.75	0.51
2:H:476:GLU:HG2	2:H:477:LYS:HG3	1.91	0.51
2:T:373:ASP:OD1	2:T:374:GLU:N	2.44	0.51
2:B:404:THR:O	2:B:408:LYS:HG2	2.11	0.51
2:D:160:MET:HE2	2:D:302:TRP:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:76:ARG:NE	2:H:492:ASP:OD2	2.41	0.51
2:L:366:TYR:HE1	2:N:358:TYR:HB2	1.75	0.51
2:P:28:LEU:O	2:P:32:ARG:HB2	2.09	0.51
2:T:14:TRP:O	2:T:21:ARG:NH2	2.42	0.51
2:T:406:ALA:O	2:T:410:VAL:HG23	2.10	0.51
1:A:18:ALA:HB1	1:A:26:VAL:HG22	1.93	0.51
2:B:373:ASP:OD1	2:B:374:GLU:N	2.44	0.51
2:N:162:LYS:NZ	2:N:309:GLU:OE1	2.36	0.51
2:P:126:ASP:OD1	2:P:127:TYR:N	2.43	0.51
2:P:129:ASP:HB3	2:R:266:ILE:HG23	1.93	0.51
2:B:476:GLU:HG2	2:B:477:LYS:HG3	1.92	0.51
2:H:312:GLU:HG3	2:H:316:ARG:HD2	1.92	0.51
2:L:430:MET:HE3	2:L:430:MET:HA	1.93	0.51
2:N:406:ALA:O	2:N:410:VAL:HG23	2.10	0.51
2:T:232:ASP:HB3	2:T:238:PRO:HG3	1.91	0.51
2:V:28:LEU:HG	2:V:116:ALA:HB2	1.92	0.51
2:D:54:VAL:CG2	2:D:408:LYS:HE3	2.41	0.51
2:D:73:VAL:HG13	2:D:491:THR:HG23	1.92	0.51
2:F:532:LEU:HD21	2:H:511:LEU:HD11	1.92	0.51
2:T:511:LEU:HB3	2:T:524:LEU:HD21	1.93	0.51
2:X:232:ASP:HB3	2:X:238:PRO:HG3	1.92	0.51
1:A:148:PRO:HD3	2:D:41:SER:HB2	1.91	0.51
2:H:232:ASP:HB3	2:H:238:PRO:HG3	1.91	0.51
1:I:29:GLN:NE2	1:K:20:ASP:OD2	2.44	0.51
2:N:584:ALA:O	2:N:587:VAL:HB	2.11	0.51
2:T:405:SER:O	2:T:409:GLU:HG3	2.11	0.51
2:T:533:LEU:HD22	2:V:76:ARG:HH12	1.75	0.51
2:B:232:ASP:HB3	2:B:238:PRO:HG3	1.92	0.51
2:B:427:ALA:HB1	2:B:493:VAL:HG21	1.92	0.51
2:H:200:ASN:HB2	2:J:306:GLU:OE1	2.10	0.51
2:H:373:ASP:OD1	2:H:374:GLU:N	2.44	0.51
2:N:404:THR:O	2:N:408:LYS:HG2	2.11	0.51
1:O:7:LEU:HD21	1:O:78:VAL:HG13	1.93	0.51
2:P:291:GLU:OE1	2:P:487:TYR:OH	2.28	0.51
2:T:247:LYS:NZ	2:T:251:ASP:OD1	2.34	0.51
2:B:511:LEU:HB3	2:B:524:LEU:HD21	1.93	0.51
2:D:232:ASP:HB3	2:D:238:PRO:HG3	1.93	0.51
2:F:592:GLN:HG2	2:F:595:LEU:HD12	1.93	0.51
2:J:126:ASP:OD1	2:J:127:TYR:N	2.43	0.51
2:N:373:ASP:OD1	2:N:374:GLU:N	2.43	0.51
2:P:224:LYS:HA	2:P:267:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:14:TRP:O	2:R:21:ARG:NH2	2.44	0.51
2:R:427:ALA:HB1	2:R:493:VAL:HG21	1.91	0.51
2:X:230:TYR:HE2	2:X:247:LYS:HZ1	1.59	0.51
2:F:358:TYR:OH	2:F:368:LEU:O	2.28	0.51
2:H:452:THR:HG22	2:H:464:GLN:HA	1.92	0.51
2:J:129:ASP:HB3	2:L:266:ILE:HG23	1.93	0.51
2:J:253:LEU:HD21	2:J:474:THR:HG23	1.92	0.51
2:L:224:LYS:HA	2:L:267:LYS:HA	1.93	0.51
2:L:292:HIS:HB2	2:L:436:ILE:HG12	1.93	0.51
2:N:82:ARG:HG2	2:N:85:ALA:HB2	1.93	0.51
2:R:430:MET:HE3	2:R:430:MET:HA	1.93	0.51
2:T:584:ALA:O	2:T:587:VAL:HB	2.11	0.51
2:N:71:ILE:HG22	2:N:430:MET:HG3	1.93	0.50
2:N:224:LYS:HA	2:N:267:LYS:HA	1.92	0.50
2:N:430:MET:HA	2:N:430:MET:HE3	1.93	0.50
2:P:73:VAL:HG13	2:P:491:THR:HG23	1.92	0.50
2:R:252:ASP:OD1	2:R:252:ASP:N	2.43	0.50
2:T:430:MET:HE3	2:T:430:MET:HA	1.93	0.50
1:A:47:GLN:NE2	1:C:111:LEU:HB3	2.25	0.50
2:B:28:LEU:O	2:B:32:ARG:HB2	2.11	0.50
2:D:133:THR:H	2:D:138:VAL:HG12	1.75	0.50
2:D:228:PHE:N	2:D:242:PHE:O	2.41	0.50
2:H:14:TRP:O	2:H:21:ARG:NH2	2.44	0.50
2:N:291:GLU:OE1	2:N:487:TYR:OH	2.29	0.50
2:T:28:LEU:HG	2:T:116:ALA:HB2	1.92	0.50
2:V:232:ASP:HB3	2:V:238:PRO:HG3	1.93	0.50
2:X:291:GLU:OE1	2:X:487:TYR:OH	2.29	0.50
2:D:404:THR:O	2:D:408:LYS:HG2	2.12	0.50
2:F:206:TRP:CE3	2:H:308:LYS:HD3	2.46	0.50
2:F:232:ASP:HB3	2:F:238:PRO:HG3	1.93	0.50
2:H:430:MET:HE3	2:H:430:MET:HA	1.93	0.50
2:P:133:THR:H	2:P:138:VAL:HG12	1.77	0.50
1:G:37:ASP:OD2	1:I:14:LYS:NZ	2.25	0.50
2:H:54:VAL:HG13	2:H:407:VAL:HG11	1.93	0.50
2:H:406:ALA:O	2:H:410:VAL:HG23	2.11	0.50
2:H:427:ALA:HB1	2:H:493:VAL:HG21	1.93	0.50
2:J:160:MET:HE2	2:J:302:TRP:HB3	1.94	0.50
2:L:232:ASP:HB3	2:L:238:PRO:HG3	1.92	0.50
2:R:232:ASP:HB3	2:R:238:PRO:HG3	1.92	0.50
2:R:551:GLN:HG2	2:R:569:ALA:HB2	1.94	0.50
2:V:523:GLN:HE21	2:V:554:VAL:HG21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:LYS:HA	2:B:267:LYS:HA	1.93	0.50
2:B:584:ALA:O	2:B:587:VAL:HB	2.11	0.50
2:F:14:TRP:O	2:F:21:ARG:NH2	2.45	0.50
2:F:179:TRP:HB2	2:F:212:ILE:HG21	1.92	0.50
2:H:584:ALA:O	2:H:587:VAL:HB	2.12	0.50
1:M:148:PRO:HD3	2:P:41:SER:HB2	1.93	0.50
2:P:362:ASP:OD1	1:S:123:ARG:NH2	2.39	0.50
2:F:430:MET:HE3	2:F:430:MET:HA	1.93	0.50
2:H:84:ASP:OD2	2:H:464:GLN:NE2	2.45	0.50
2:H:431:ARG:HA	2:H:491:THR:HG21	1.93	0.50
2:J:73:VAL:HG13	2:J:491:THR:HG23	1.93	0.50
2:P:253:LEU:HD21	2:P:474:THR:HG23	1.92	0.50
2:R:224:LYS:HA	2:R:267:LYS:HA	1.93	0.50
2:R:292:HIS:HB2	2:R:436:ILE:HG12	1.93	0.50
2:R:548:GLN:O	2:R:552:MET:HG3	2.12	0.50
2:T:584:ALA:HB2	2:V:585:GLN:HG2	1.94	0.50
2:X:358:TYR:OH	2:X:368:LEU:O	2.27	0.50
2:D:268:ARG:HH21	2:D:291:GLU:HG3	1.77	0.50
2:D:523:GLN:HE21	2:D:554:VAL:HG21	1.77	0.50
2:F:292:HIS:HB2	2:F:436:ILE:HG12	1.94	0.50
2:J:268:ARG:HH21	2:J:291:GLU:HG3	1.77	0.50
2:J:421:VAL:C	2:J:423:GLN:N	2.70	0.50
2:V:584:ALA:HB2	2:X:585:GLN:HG2	1.94	0.50
2:J:224:LYS:HA	2:J:267:LYS:HA	1.92	0.50
2:J:499:SER:OG	2:L:79:ASP:OD1	2.30	0.50
2:P:292:HIS:HB3	2:P:432:ARG:HH21	1.77	0.50
2:P:579:PRO:HB2	2:P:582:VAL:HB	1.94	0.50
2:R:183:ALA:HA	2:R:188:LEU:HB2	1.94	0.50
1:E:38:LEU:HD13	1:E:85:LEU:HD12	1.94	0.49
2:J:414:GLY:O	2:J:415:VAL:C	2.54	0.49
2:N:436:ILE:O	2:N:440:ILE:HG13	2.12	0.49
2:P:162:LYS:NZ	2:P:309:GLU:OE1	2.45	0.49
2:X:592:GLN:HG2	2:X:595:LEU:HD12	1.93	0.49
2:B:430:MET:HE3	2:B:430:MET:HA	1.93	0.49
2:H:224:LYS:HA	2:H:267:LYS:HA	1.93	0.49
2:J:232:ASP:HB3	2:J:238:PRO:HG3	1.93	0.49
2:L:126:ASP:OD1	2:L:127:TYR:N	2.44	0.49
2:N:29:PHE:HE2	2:N:204:PHE:HB2	1.77	0.49
2:P:358:TYR:OH	2:P:368:LEU:O	2.27	0.49
2:B:436:ILE:O	2:B:440:ILE:HG13	2.12	0.49
2:D:224:LYS:HA	2:D:267:LYS:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:499:SER:OG	2:F:79:ASP:OD1	2.30	0.49
2:F:176:GLN:O	2:F:179:TRP:N	2.45	0.49
2:L:28:LEU:O	2:L:32:ARG:HB2	2.12	0.49
1:Q:7:LEU:CD2	1:Q:78:VAL:HG13	2.41	0.49
2:T:207:LEU:HD23	2:T:208:THR:HG23	1.94	0.49
2:V:133:THR:H	2:V:138:VAL:HG12	1.76	0.49
2:V:551:GLN:HG2	2:V:569:ALA:HB2	1.94	0.49
2:B:371:ARG:HE	2:B:372:THR:HG23	1.78	0.49
2:B:424:ASP:OD2	2:X:67:ARG:HD3	2.13	0.49
2:B:585:GLN:C	2:X:583:GLN:HE22	2.20	0.49
2:H:133:THR:H	2:H:138:VAL:HG12	1.77	0.49
1:K:7:LEU:CD2	1:K:78:VAL:HG13	2.42	0.49
2:L:179:TRP:HB2	2:L:212:ILE:HG21	1.95	0.49
2:T:371:ARG:HE	2:T:372:THR:HG23	1.78	0.49
2:T:436:ILE:O	2:T:440:ILE:HG13	2.12	0.49
2:X:430:MET:HE3	2:X:430:MET:HA	1.93	0.49
2:J:579:PRO:HB2	2:J:582:VAL:HB	1.94	0.49
2:L:84:ASP:OD2	2:L:464:GLN:NE2	2.46	0.49
2:L:583:GLN:HE22	2:N:585:GLN:C	2.20	0.49
2:R:28:LEU:O	2:R:32:ARG:HB2	2.12	0.49
2:T:427:ALA:HB1	2:T:493:VAL:HG21	1.94	0.49
2:X:176:GLN:O	2:X:179:TRP:N	2.45	0.49
2:B:291:GLU:OE1	2:B:487:TYR:OH	2.31	0.49
2:F:75:TYR:OH	2:F:434:GLY:O	2.28	0.49
2:F:108:ILE:HD11	2:H:302:TRP:HZ3	1.76	0.49
2:F:584:ALA:O	2:F:587:VAL:HB	2.12	0.49
2:L:108:ILE:HD11	2:N:302:TRP:HZ3	1.77	0.49
2:N:371:ARG:HE	2:N:372:THR:HG23	1.78	0.49
2:P:550:ILE:HD13	2:P:562:GLU:HB3	1.95	0.49
1:Q:38:LEU:HD13	1:Q:85:LEU:HD12	1.94	0.49
2:R:583:GLN:HE22	2:T:585:GLN:C	2.20	0.49
2:R:584:ALA:O	2:R:587:VAL:HB	2.12	0.49
1:W:131:PRO:HA	1:W:145:HIS:HA	1.95	0.49
2:J:228:PHE:N	2:J:242:PHE:O	2.42	0.49
2:L:14:TRP:O	2:L:21:ARG:NH2	2.44	0.49
2:L:436:ILE:O	2:L:440:ILE:HG13	2.13	0.49
2:N:216:GLU:HG2	2:N:275:ILE:HG13	1.94	0.49
2:R:389:ASN:HB3	2:T:393:PRO:HB3	1.94	0.49
2:V:436:ILE:O	2:V:440:ILE:HG13	2.13	0.49
2:X:183:ALA:HA	2:X:188:LEU:HB2	1.94	0.49
2:D:84:ASP:OD1	2:D:450:ASN:ND2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:224:LYS:HA	2:F:267:LYS:HA	1.95	0.49
2:H:436:ILE:O	2:H:440:ILE:HG13	2.12	0.49
1:I:52:ILE:HD13	1:I:113:TYR:HA	1.95	0.49
2:X:584:ALA:O	2:X:587:VAL:HB	2.12	0.49
2:B:65:GLU:HG2	2:B:417:LEU:HD11	1.95	0.49
2:H:145:HIS:CD2	2:J:304:PHE:HB2	2.48	0.49
2:N:133:THR:H	2:N:138:VAL:HG12	1.78	0.49
2:P:232:ASP:HB3	2:P:238:PRO:HG3	1.93	0.49
2:P:438:GLN:O	2:P:442:ASN:ND2	2.45	0.49
2:R:176:GLN:O	2:R:179:TRP:N	2.44	0.49
2:V:533:LEU:HD22	2:X:76:ARG:HH12	1.78	0.49
1:A:11:ALA:CB	1:A:85:LEU:HD22	2.43	0.49
2:D:29:PHE:HE2	2:D:204:PHE:HB2	1.78	0.49
2:F:54:VAL:CG2	2:F:408:LYS:HE3	2.42	0.49
2:J:84:ASP:OD1	2:J:450:ASN:ND2	2.46	0.49
2:L:584:ALA:O	2:L:587:VAL:HB	2.12	0.49
2:T:268:ARG:HH21	2:T:291:GLU:HG3	1.78	0.49
2:T:269:ARG:HB2	2:T:291:GLU:HG2	1.94	0.49
2:V:268:ARG:HH21	2:V:291:GLU:HG3	1.78	0.49
2:D:584:ALA:O	2:D:587:VAL:HB	2.13	0.48
2:P:469:VAL:HG12	2:P:481:ASN:HD22	1.78	0.48
2:P:534:ASP:HB2	2:R:77:PRO:HD3	1.95	0.48
2:D:179:TRP:HB2	2:D:212:ILE:HG21	1.95	0.48
2:F:28:LEU:O	2:F:32:ARG:HB2	2.13	0.48
2:F:583:GLN:HE22	2:H:585:GLN:C	2.21	0.48
2:N:84:ASP:OD1	2:N:450:ASN:ND2	2.45	0.48
2:N:342:LYS:HG3	2:N:386:TYR:HB3	1.95	0.48
2:P:436:ILE:O	2:P:440:ILE:HG13	2.14	0.48
2:X:29:PHE:HE1	2:X:204:PHE:HB2	1.78	0.48
2:B:292:HIS:HB3	2:B:432:ARG:HH21	1.78	0.48
2:D:131:SER:O	2:D:131:SER:OG	2.27	0.48
2:F:29:PHE:HE2	2:F:204:PHE:HB2	1.78	0.48
2:J:73:VAL:O	2:J:90:MET:HE1	2.13	0.48
2:J:318:THR:HB	2:J:407:VAL:HG13	1.94	0.48
2:J:584:ALA:O	2:J:587:VAL:HB	2.12	0.48
2:N:54:VAL:HG13	2:N:407:VAL:HG11	1.95	0.48
2:R:268:ARG:HH21	2:R:291:GLU:HG3	1.79	0.48
2:R:436:ILE:O	2:R:440:ILE:HG13	2.13	0.48
2:T:131:SER:O	2:T:131:SER:OG	2.27	0.48
2:X:268:ARG:HH21	2:X:291:GLU:HG3	1.78	0.48
2:B:71:ILE:HG22	2:B:430:MET:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:533:LEU:HD22	2:J:76:ARG:HH12	1.79	0.48
2:L:176:GLN:O	2:L:179:TRP:N	2.45	0.48
2:R:179:TRP:HB2	2:R:212:ILE:HG21	1.95	0.48
2:V:292:HIS:HB3	2:V:432:ARG:HH21	1.78	0.48
2:V:579:PRO:HB2	2:V:582:VAL:HB	1.94	0.48
2:D:358:TYR:OH	2:D:368:LEU:O	2.29	0.48
2:J:436:ILE:O	2:J:440:ILE:HG13	2.13	0.48
2:R:54:VAL:CG2	2:R:408:LYS:HE3	2.44	0.48
2:T:332:ASN:OD1	2:T:396:ASN:ND2	2.45	0.48
2:T:424:ASP:O	2:T:428:THR:HG23	2.13	0.48
2:V:406:ALA:O	2:V:410:VAL:HG23	2.13	0.48
2:X:424:ASP:O	2:X:428:THR:HG23	2.13	0.48
2:D:359:ASP:HB3	1:E:124:ALA:HB2	1.96	0.48
2:F:183:ALA:HA	2:F:188:LEU:HB2	1.96	0.48
2:L:550:ILE:HD13	2:L:562:GLU:HB3	1.94	0.48
1:Q:26:VAL:CG1	1:Q:31:MET:HE3	2.43	0.48
2:R:441:VAL:HG22	2:R:445:TYR:CD2	2.49	0.48
2:B:307:ASP:OD2	2:X:200:ASN:ND2	2.47	0.48
2:D:73:VAL:O	2:D:90:MET:HE1	2.13	0.48
2:H:160:MET:HE2	2:H:302:TRP:HB3	1.96	0.48
2:H:268:ARG:HH21	2:H:291:GLU:HG3	1.79	0.48
2:N:67:ARG:HD3	2:P:424:ASP:OD2	2.14	0.48
2:P:584:ALA:O	2:P:587:VAL:HB	2.13	0.48
2:F:424:ASP:O	2:F:428:THR:HG23	2.13	0.48
2:N:28:LEU:O	2:N:32:ARG:HB2	2.14	0.48
2:P:523:GLN:HE21	2:P:554:VAL:HG21	1.77	0.48
2:P:533:LEU:HD22	2:R:76:ARG:HH12	1.78	0.48
2:V:584:ALA:O	2:V:587:VAL:HB	2.13	0.48
2:B:145:HIS:CD2	2:D:304:PHE:HB2	2.48	0.48
2:J:438:GLN:O	2:J:442:ASN:ND2	2.47	0.48
2:N:19:GLU:O	2:N:23:GLU:HG3	2.14	0.48
2:N:268:ARG:HH21	2:N:291:GLU:HG3	1.78	0.48
2:P:73:VAL:O	2:P:90:MET:HE1	2.14	0.48
2:P:359:ASP:HB3	1:Q:124:ALA:HB2	1.96	0.48
2:B:133:THR:H	2:B:138:VAL:HG12	1.78	0.48
2:B:268:ARG:HH21	2:B:291:GLU:HG3	1.79	0.48
2:B:534:ASP:HB2	2:D:77:PRO:HD3	1.95	0.48
2:D:436:ILE:O	2:D:440:ILE:HG13	2.13	0.48
2:P:268:ARG:HH21	2:P:291:GLU:HG3	1.79	0.48
2:V:550:ILE:HD13	2:V:562:GLU:HB3	1.96	0.48
2:X:28:LEU:O	2:X:32:ARG:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:292:HIS:HB2	2:X:436:ILE:HG12	1.95	0.48
2:B:39:TRP:HB3	2:B:203:VAL:HG23	1.94	0.47
2:F:145:HIS:CD2	2:H:304:PHE:HB2	2.49	0.47
2:J:3:LEU:HD13	2:J:281:VAL:HG13	1.96	0.47
2:L:424:ASP:O	2:L:428:THR:HG23	2.13	0.47
2:N:427:ALA:HB1	2:N:493:VAL:HG21	1.95	0.47
2:R:200:ASN:ND2	2:T:307:ASP:OD2	2.47	0.47
2:D:292:HIS:HB3	2:D:432:ARG:HH21	1.79	0.47
2:H:247:LYS:NZ	2:H:251:ASP:OD1	2.34	0.47
2:T:512:LEU:HG	2:T:524:LEU:HB3	1.96	0.47
2:D:328:ILE:HG21	2:D:400:LEU:HB2	1.97	0.47
1:E:26:VAL:CG1	1:E:31:MET:HE3	2.43	0.47
2:F:268:ARG:HH21	2:F:291:GLU:HG3	1.78	0.47
2:F:318:THR:HB	2:F:407:VAL:HG13	1.96	0.47
2:J:292:HIS:HB3	2:J:432:ARG:HH21	1.79	0.47
2:N:534:ASP:HB2	2:P:77:PRO:HD3	1.96	0.47
2:P:29:PHE:HE2	2:P:204:PHE:HB2	1.79	0.47
2:V:424:ASP:O	2:V:428:THR:HG23	2.15	0.47
2:V:427:ALA:HB1	2:V:493:VAL:HG21	1.96	0.47
2:H:291:GLU:OE1	2:H:487:TYR:OH	2.32	0.47
2:J:391:GLU:O	2:L:394:GLN:NE2	2.45	0.47
2:L:548:GLN:O	2:L:552:MET:HG3	2.14	0.47
2:R:366:TYR:CE1	2:T:358:TYR:HB2	2.49	0.47
2:T:328:ILE:HG21	2:T:400:LEU:HB2	1.95	0.47
1:A:111:LEU:HB3	1:W:47:GLN:HE22	1.80	0.47
2:B:523:GLN:NE2	2:B:554:VAL:HG21	2.29	0.47
2:D:406:ALA:O	2:D:410:VAL:HG23	2.15	0.47
1:K:26:VAL:CG1	1:K:31:MET:HE3	2.45	0.47
2:L:183:ALA:HA	2:L:188:LEU:HB2	1.97	0.47
2:P:160:MET:HE2	2:P:302:TRP:HB3	1.95	0.47
2:H:371:ARG:HE	2:H:372:THR:HG23	1.78	0.47
2:H:511:LEU:HB3	2:H:524:LEU:HD21	1.95	0.47
2:L:268:ARG:HH21	2:L:291:GLU:HG3	1.79	0.47
2:N:550:ILE:HD13	2:N:562:GLU:HB3	1.95	0.47
1:S:52:ILE:HD13	1:S:113:TYR:HA	1.96	0.47
2:V:160:MET:HE2	2:V:302:TRP:HB3	1.95	0.47
2:B:131:SER:O	2:B:131:SER:OG	2.27	0.47
1:E:37:ASP:OD2	1:G:14:LYS:NZ	2.28	0.47
2:F:550:ILE:HD13	2:F:562:GLU:HB3	1.96	0.47
2:H:71:ILE:HD11	2:H:423:GLN:HG3	1.96	0.47
2:J:29:PHE:HE2	2:J:204:PHE:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:584:ALA:HB2	2:L:585:GLN:HG2	1.96	0.47
2:P:406:ALA:O	2:P:410:VAL:HG23	2.15	0.47
2:T:19:GLU:O	2:T:23:GLU:HG3	2.14	0.47
2:T:292:HIS:HB3	2:T:432:ARG:HH21	1.80	0.47
2:T:328:ILE:O	2:T:332:ASN:ND2	2.48	0.47
2:T:583:GLN:HE21	2:V:589:LEU:HG	1.80	0.47
2:V:56:ARG:NH2	2:X:312:GLU:OE1	2.48	0.47
2:V:405:SER:O	2:V:409:GLU:HG3	2.14	0.47
2:D:342:LYS:HG3	2:D:386:TYR:HB3	1.96	0.47
2:F:436:ILE:O	2:F:440:ILE:HG13	2.14	0.47
2:F:533:LEU:HD12	2:H:507:GLU:OE2	2.15	0.47
2:H:19:GLU:O	2:H:23:GLU:HG3	2.15	0.47
2:J:360:GLY:HA2	2:L:340:PRO:HG3	1.97	0.47
2:P:108:ILE:HD11	2:R:302:TRP:HZ3	1.79	0.47
2:P:292:HIS:HB2	2:P:436:ILE:HG12	1.97	0.47
2:P:584:ALA:HB2	2:R:585:GLN:HG2	1.97	0.47
2:T:71:ILE:HG22	2:T:430:MET:HG3	1.95	0.47
2:T:133:THR:H	2:T:138:VAL:HG12	1.79	0.47
2:V:292:HIS:HB2	2:V:436:ILE:HG12	1.96	0.47
2:D:424:ASP:O	2:D:428:THR:HG23	2.14	0.47
2:F:131:SER:O	2:F:131:SER:OG	2.27	0.47
2:H:54:VAL:CG2	2:H:408:LYS:HE3	2.44	0.47
2:P:228:PHE:N	2:P:242:PHE:O	2.41	0.47
2:B:512:LEU:HG	2:B:524:LEU:HB3	1.96	0.47
2:F:312:GLU:HG3	2:F:316:ARG:HD2	1.95	0.47
2:P:10:PHE:HE1	2:P:152:ILE:HG13	1.81	0.47
2:D:469:VAL:HG12	2:D:481:ASN:HD22	1.80	0.46
2:H:28:LEU:O	2:H:32:ARG:HB2	2.15	0.46
2:H:253:LEU:HD21	2:H:474:THR:HG23	1.97	0.46
2:N:372:THR:HG21	1:Q:106:LYS:HB3	1.97	0.46
2:R:523:GLN:NE2	2:R:554:VAL:HG21	2.30	0.46
2:V:122:ARG:HG3	2:V:295:ILE:HG13	1.97	0.46
2:D:250:ILE:HD13	2:D:479:VAL:HB	1.97	0.46
2:H:583:GLN:HE21	2:J:589:LEU:HG	1.80	0.46
2:J:54:VAL:HG13	2:J:407:VAL:HG11	1.97	0.46
1:K:148:PRO:HD3	2:N:41:SER:HB2	1.95	0.46
2:L:54:VAL:CG2	2:L:408:LYS:HE3	2.45	0.46
2:N:391:GLU:HA	2:P:394:GLN:HE21	1.79	0.46
2:N:551:GLN:HG2	2:N:569:ALA:HB2	1.95	0.46
2:T:372:THR:HG21	1:W:106:LYS:HB3	1.97	0.46
2:V:10:PHE:HE1	2:V:152:ILE:HG13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:224:LYS:HA	2:X:267:LYS:HA	1.96	0.46
2:J:206:TRP:CE3	2:L:308:LYS:HD3	2.50	0.46
2:L:328:ILE:HG21	2:L:400:LEU:HB2	1.97	0.46
1:M:135:GLY:O	2:N:42:GLN:NE2	2.49	0.46
2:T:29:PHE:HE2	2:T:204:PHE:HB2	1.81	0.46
2:X:3:LEU:HD13	2:X:281:VAL:HG13	1.98	0.46
2:X:436:ILE:O	2:X:440:ILE:HG13	2.15	0.46
2:B:359:ASP:HB3	1:C:124:ALA:HB2	1.96	0.46
2:D:579:PRO:HB2	2:D:582:VAL:HB	1.96	0.46
1:E:129:ARG:NH1	2:H:48:TYR:O	2.44	0.46
2:F:207:LEU:HD23	2:F:208:THR:HG23	1.96	0.46
2:J:250:ILE:HD13	2:J:479:VAL:HB	1.98	0.46
2:J:427:ALA:HB1	2:J:493:VAL:HG21	1.98	0.46
2:N:419:THR:O	2:N:423:GLN:HB2	2.15	0.46
2:D:533:LEU:HD12	2:F:507:GLU:OE1	2.16	0.46
2:L:469:VAL:HG12	2:L:481:ASN:HD22	1.81	0.46
2:R:406:ALA:O	2:R:410:VAL:HG23	2.16	0.46
2:V:108:ILE:HD11	2:X:302:TRP:HZ3	1.80	0.46
2:D:427:ALA:HB1	2:D:493:VAL:HG21	1.97	0.46
1:G:7:LEU:CD2	1:G:78:VAL:HG13	2.46	0.46
2:J:469:VAL:HG12	2:J:481:ASN:HD22	1.79	0.46
2:J:533:LEU:HD22	2:L:76:ARG:HH12	1.79	0.46
1:Q:148:PRO:HD3	2:T:41:SER:HB2	1.97	0.46
2:R:96:ASP:OD2	2:R:437:TYR:OH	2.31	0.46
2:R:358:TYR:HD1	2:T:387:TYR:OH	1.98	0.46
2:R:550:ILE:HD13	2:R:562:GLU:HB3	1.98	0.46
2:V:469:VAL:HG12	2:V:481:ASN:HD22	1.79	0.46
2:H:318:THR:HB	2:H:407:VAL:HG13	1.97	0.46
2:L:3:LEU:HD13	2:L:281:VAL:HG13	1.97	0.46
2:L:200:ASN:ND2	2:N:307:ASP:OD2	2.49	0.46
2:L:583:GLN:O	2:L:587:VAL:HG23	2.16	0.46
2:N:230:TYR:HE2	2:N:247:LYS:HZ1	1.62	0.46
2:P:413:LEU:HD21	2:P:422:PHE:CD2	2.51	0.46
2:R:583:GLN:O	2:R:587:VAL:HG23	2.16	0.46
2:V:29:PHE:HE2	2:V:204:PHE:HB2	1.80	0.46
2:V:73:VAL:O	2:V:90:MET:HE1	2.15	0.46
2:B:304:PHE:HB2	2:X:145:HIS:CD2	2.50	0.46
2:F:583:GLN:O	2:F:587:VAL:HG23	2.16	0.46
2:F:591:GLY:HA2	2:F:594:GLU:OE1	2.16	0.46
2:L:160:MET:HE2	2:L:302:TRP:HB3	1.97	0.46
2:N:583:GLN:HE21	2:P:589:LEU:HG	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:160:MET:HE2	2:R:302:TRP:HB3	1.97	0.46
2:T:534:ASP:HB2	2:V:77:PRO:HD3	1.96	0.46
2:X:341:LYS:HD2	2:X:341:LYS:N	2.31	0.46
2:H:341:LYS:N	2:H:341:LYS:HD2	2.30	0.46
2:J:533:LEU:HD12	2:L:507:GLU:OE1	2.16	0.46
2:L:366:TYR:CE1	2:N:358:TYR:HB2	2.50	0.46
2:P:360:GLY:HA2	2:R:340:PRO:HG3	1.98	0.46
2:R:440:ILE:O	2:R:444:ILE:HG12	2.15	0.46
2:V:250:ILE:HD13	2:V:479:VAL:HB	1.97	0.46
2:V:399:MET:HE2	2:V:399:MET:HB2	1.73	0.46
1:O:1:ILE:HG22	1:O:2:LYS:HG3	1.97	0.46
2:T:548:GLN:O	2:T:552:MET:HG3	2.16	0.46
2:B:172:HIS:NE2	2:B:216:GLU:OE1	2.49	0.45
2:B:556:LYS:HB3	2:B:556:LYS:HE3	1.85	0.45
1:E:7:LEU:CD2	1:E:78:VAL:HG13	2.46	0.45
2:P:122:ARG:HG3	2:P:295:ILE:HG13	1.98	0.45
2:P:250:ILE:HD13	2:P:479:VAL:HB	1.98	0.45
2:P:535:GLY:HA2	2:R:87:ASP:OD1	2.16	0.45
1:U:14:LYS:HD3	1:U:14:LYS:HA	1.75	0.45
1:A:14:LYS:NZ	1:W:37:ASP:OD2	2.45	0.45
2:L:89:LEU:HD11	2:L:438:GLN:HG3	1.99	0.45
2:V:419:THR:O	2:V:423:GLN:HB2	2.16	0.45
1:C:1:ILE:HG22	1:C:2:LYS:HG3	1.98	0.45
2:D:21:ARG:HH11	2:D:149:SER:HA	1.81	0.45
2:H:483:ILE:HG13	2:H:485:GLY:N	2.31	0.45
2:T:75:TYR:OH	2:T:434:GLY:O	2.34	0.45
2:T:228:PHE:HD2	2:T:247:LYS:NZ	2.15	0.45
1:A:7:LEU:CD2	1:A:78:VAL:HG13	2.46	0.45
2:B:532:LEU:HG	2:B:533:LEU:H	1.81	0.45
2:B:583:GLN:HE21	2:D:589:LEU:HG	1.82	0.45
2:D:511:LEU:HB3	2:D:524:LEU:HD21	1.98	0.45
1:E:148:PRO:HD3	2:H:41:SER:HB2	1.97	0.45
2:L:440:ILE:O	2:L:444:ILE:HG12	2.16	0.45
1:S:7:LEU:CD2	1:S:78:VAL:HG13	2.46	0.45
1:S:31:MET:O	1:S:35:VAL:HG23	2.17	0.45
2:D:423:GLN:HE21	2:D:423:GLN:HB2	1.50	0.45
2:F:341:LYS:HD2	2:F:341:LYS:N	2.31	0.45
1:M:52:ILE:HD13	1:M:113:TYR:HA	1.99	0.45
2:T:39:TRP:HB3	2:T:203:VAL:HG23	1.98	0.45
2:B:301:GLU:OE1	2:X:56:ARG:NH2	2.50	0.45
2:B:341:LYS:HD2	2:B:341:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:THR:HG21	1:E:106:LYS:HB3	1.99	0.45
2:F:160:MET:HE2	2:F:302:TRP:HB3	1.97	0.45
2:F:328:ILE:HG22	2:F:332:ASN:HD21	1.81	0.45
2:N:84:ASP:OD2	2:N:464:GLN:NE2	2.50	0.45
2:P:533:LEU:HD12	2:R:507:GLU:OE1	2.16	0.45
2:P:536:LYS:HE2	2:R:87:ASP:OD2	2.17	0.45
2:T:28:LEU:O	2:T:32:ARG:HB2	2.15	0.45
2:V:329:MET:HE3	2:V:329:MET:HB3	1.85	0.45
2:V:342:LYS:HG3	2:V:386:TYR:HB3	1.98	0.45
2:X:583:GLN:O	2:X:587:VAL:HG23	2.16	0.45
1:A:123:ARG:NH2	2:V:362:ASP:OD1	2.49	0.45
2:B:440:ILE:O	2:B:444:ILE:HG12	2.17	0.45
2:D:550:ILE:HD13	2:D:562:GLU:HB3	1.97	0.45
2:H:372:THR:HG21	1:K:106:LYS:HB3	1.99	0.45
2:J:166:ARG:HG2	2:J:166:ARG:HH11	1.82	0.45
1:K:26:VAL:HG11	1:K:31:MET:HE3	1.98	0.45
2:P:94:ARG:HH21	2:P:497:PHE:HD2	1.63	0.45
2:X:160:MET:HE2	2:X:302:TRP:HB3	1.98	0.45
2:B:54:VAL:CG2	2:B:408:LYS:HE3	2.47	0.45
2:B:207:LEU:HD23	2:B:208:THR:HG23	1.97	0.45
2:H:73:VAL:O	2:H:90:MET:HE1	2.17	0.45
2:J:108:ILE:HD11	2:L:302:TRP:HZ3	1.81	0.45
2:R:567:VAL:O	2:R:571:GLN:HG3	2.16	0.45
2:T:145:HIS:CD2	2:V:304:PHE:HB2	2.51	0.45
2:T:359:ASP:HB3	1:U:124:ALA:HB2	1.98	0.45
2:X:476:GLU:HG2	2:X:477:LYS:HG3	1.98	0.45
2:B:160:MET:HE2	2:B:302:TRP:HB3	1.97	0.45
2:D:457:ASP:OD1	2:D:457:ASP:N	2.49	0.45
1:I:1:ILE:HG22	1:I:2:LYS:HG3	1.98	0.45
2:J:66:MET:HE1	2:J:422:PHE:HB3	1.99	0.45
2:J:358:TYR:OH	2:J:368:LEU:O	2.27	0.45
2:L:29:PHE:HE1	2:L:204:PHE:HB2	1.82	0.45
2:P:72:ASP:HB2	2:P:496:SER:CB	2.47	0.45
2:R:131:SER:O	2:R:131:SER:OG	2.27	0.45
2:R:469:VAL:HG12	2:R:481:ASN:HD22	1.82	0.45
2:T:342:LYS:HG3	2:T:386:TYR:HB3	1.98	0.45
1:U:1:ILE:HG22	1:U:2:LYS:HG3	1.99	0.45
2:V:523:GLN:NE2	2:V:554:VAL:HG21	2.32	0.45
2:X:179:TRP:HB2	2:X:212:ILE:HG21	1.98	0.45
1:A:52:ILE:HD13	1:A:113:TYR:HA	1.99	0.45
2:B:419:THR:O	2:B:423:GLN:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:ASP:OD1	2:B:457:ASP:N	2.50	0.45
2:H:185:LYS:HD2	2:H:186:TYR:CE2	2.52	0.45
2:H:405:SER:O	2:H:409:GLU:HG3	2.17	0.45
1:I:7:LEU:CD2	1:I:78:VAL:HG13	2.47	0.45
2:J:21:ARG:HH11	2:J:149:SER:HA	1.81	0.45
2:L:541:MET:HE2	2:N:524:LEU:HD11	1.99	0.45
2:N:360:GLY:HA2	2:P:340:PRO:HG3	1.99	0.45
2:P:21:ARG:HH11	2:P:149:SER:HA	1.82	0.45
2:R:82:ARG:HG2	2:R:85:ALA:HB2	1.99	0.45
2:T:204:PHE:HB3	2:T:206:TRP:NE1	2.32	0.45
2:V:71:ILE:O	2:V:430:MET:HE3	2.18	0.45
2:B:292:HIS:HB2	2:B:436:ILE:HG12	2.00	0.44
2:B:579:PRO:HB2	2:B:582:VAL:HB	1.99	0.44
2:D:523:GLN:NE2	2:D:554:VAL:HG21	2.32	0.44
2:H:207:LEU:HD22	2:J:15:THR:HG23	1.99	0.44
2:J:317:LEU:HD23	2:J:317:LEU:HA	1.85	0.44
2:J:421:VAL:O	2:J:422:PHE:HB2	2.15	0.44
2:P:523:GLN:NE2	2:P:554:VAL:HG21	2.33	0.44
2:J:406:ALA:O	2:J:410:VAL:HG23	2.17	0.44
2:N:391:GLU:O	2:P:394:GLN:NE2	2.46	0.44
2:P:511:LEU:HB3	2:P:524:LEU:HD21	1.98	0.44
2:V:404:THR:O	2:V:408:LYS:HG2	2.17	0.44
2:V:457:ASP:OD1	2:V:457:ASP:N	2.50	0.44
1:A:9:ARG:NH1	1:A:67:GLU:OE2	2.47	0.44
2:B:89:LEU:HD11	2:B:438:GLN:HG3	1.99	0.44
2:B:591:GLY:HA2	2:B:594:GLU:OE1	2.18	0.44
2:D:166:ARG:HH11	2:D:166:ARG:HG2	1.82	0.44
2:F:476:GLU:HG2	2:F:477:LYS:HG3	1.98	0.44
2:L:583:GLN:HE21	2:N:589:LEU:HG	1.83	0.44
2:N:73:VAL:O	2:N:90:MET:HE1	2.17	0.44
2:N:145:HIS:CD2	2:P:304:PHE:HB2	2.52	0.44
2:P:343:LYS:NZ	1:Q:123:ARG:HH22	2.15	0.44
2:R:523:GLN:HE22	2:R:554:VAL:HG11	1.82	0.44
2:T:54:VAL:HG13	2:T:407:VAL:HG11	1.98	0.44
2:V:533:LEU:HD12	2:X:507:GLU:OE2	2.17	0.44
2:V:587:VAL:HG11	2:X:588:LEU:HB3	1.99	0.44
2:X:457:ASP:OD1	2:X:457:ASP:N	2.50	0.44
1:C:11:ALA:CB	1:C:85:LEU:HD22	2.46	0.44
2:D:10:PHE:HE1	2:D:152:ILE:HG13	1.82	0.44
2:D:516:PRO:O	2:D:521:GLU:HB2	2.18	0.44
2:D:533:LEU:HD22	2:F:76:ARG:HH12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:328:ILE:HG21	2:J:400:LEU:HB2	2.00	0.44
2:L:533:LEU:HD12	2:N:507:GLU:OE1	2.17	0.44
2:P:252:ASP:OD1	2:P:253:LEU:N	2.50	0.44
2:R:328:ILE:HG21	2:R:400:LEU:HB2	1.98	0.44
2:R:476:GLU:HG2	2:R:477:LYS:HG3	2.00	0.44
2:T:241:TYR:O	2:T:483:ILE:HA	2.17	0.44
2:V:392:VAL:HG23	2:X:395:ALA:HB1	2.00	0.44
2:B:71:ILE:HD11	2:B:423:GLN:HG3	1.99	0.44
1:C:7:LEU:CD2	1:C:78:VAL:HG13	2.47	0.44
2:F:567:VAL:O	2:F:571:GLN:HG3	2.18	0.44
2:J:145:HIS:CD2	2:L:304:PHE:HB2	2.53	0.44
2:J:292:HIS:HB2	2:J:436:ILE:HG12	2.00	0.44
2:N:207:LEU:HD23	2:N:208:THR:HG23	1.99	0.44
2:N:332:ASN:OD1	2:N:396:ASN:ND2	2.48	0.44
2:N:512:LEU:HG	2:N:524:LEU:HB3	1.99	0.44
2:P:417:LEU:HD12	2:P:420:TYR:HB2	2.00	0.44
2:R:533:LEU:HD12	2:T:507:GLU:OE2	2.18	0.44
2:R:583:GLN:HE21	2:T:589:LEU:HG	1.83	0.44
2:X:328:ILE:HG22	2:X:332:ASN:HD21	1.81	0.44
1:E:132:THR:OG1	1:E:143:GLU:O	2.32	0.44
2:F:228:PHE:N	2:F:242:PHE:O	2.51	0.44
2:F:534:ASP:HB2	2:H:77:PRO:HD3	1.98	0.44
2:F:583:GLN:HE21	2:H:589:LEU:HG	1.83	0.44
2:H:29:PHE:HE2	2:H:204:PHE:HB2	1.82	0.44
2:L:476:GLU:HG2	2:L:477:LYS:HG3	2.00	0.44
2:L:584:ALA:HB2	2:N:585:GLN:HG2	1.99	0.44
1:O:14:LYS:HA	1:O:14:LYS:HD3	1.72	0.44
2:T:73:VAL:O	2:T:90:MET:HE1	2.18	0.44
2:T:172:HIS:NE2	2:T:216:GLU:OE2	2.50	0.44
2:B:524:LEU:HD11	2:X:541:MET:HE2	1.98	0.44
2:B:583:GLN:O	2:B:587:VAL:HG23	2.18	0.44
2:F:440:ILE:O	2:F:444:ILE:HG12	2.17	0.44
2:H:39:TRP:HB3	2:H:203:VAL:HG23	1.99	0.44
1:I:77:ALA:O	1:I:81:VAL:HG23	2.18	0.44
2:J:54:VAL:CG2	2:J:408:LYS:HE3	2.48	0.44
2:T:108:ILE:HD11	2:V:302:TRP:HZ3	1.82	0.44
2:T:550:ILE:HD13	2:T:562:GLU:HB3	1.99	0.44
2:D:252:ASP:OD1	2:D:253:LEU:N	2.50	0.44
2:F:366:TYR:HE1	2:H:358:TYR:HB2	1.83	0.44
1:G:52:ILE:HD13	1:G:113:TYR:HA	2.00	0.44
2:H:247:LYS:HD2	2:H:247:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:419:THR:O	2:H:423:GLN:HB2	2.17	0.44
2:H:556:LYS:HB3	2:H:556:LYS:HE3	1.84	0.44
1:K:29:GLN:NE2	1:M:20:ASP:OD2	2.51	0.44
1:K:129:ARG:NH1	2:N:48:TYR:O	2.45	0.44
2:L:532:LEU:HD21	2:N:511:LEU:HD11	2.00	0.44
2:N:533:LEU:HD12	2:P:507:GLU:OE1	2.18	0.44
2:T:105:ALA:HA	2:T:143:PRO:HB3	2.00	0.44
2:B:185:LYS:HD2	2:B:186:TYR:CE2	2.53	0.44
2:B:247:LYS:HD2	2:B:247:LYS:O	2.18	0.44
2:B:507:GLU:OE2	2:X:533:LEU:HD12	2.18	0.44
2:D:247:LYS:HD2	2:D:247:LYS:O	2.18	0.44
2:D:292:HIS:HB2	2:D:436:ILE:HG12	2.00	0.44
2:H:440:ILE:O	2:H:444:ILE:HG12	2.18	0.44
2:H:583:GLN:O	2:H:587:VAL:HG23	2.18	0.44
2:L:341:LYS:HA	2:L:341:LYS:HD3	1.77	0.44
2:N:292:HIS:HB2	2:N:436:ILE:HG12	2.00	0.44
2:P:427:ALA:HB1	2:P:493:VAL:HG21	1.98	0.44
2:T:483:ILE:HG13	2:T:485:GLY:N	2.32	0.44
2:X:441:VAL:HG22	2:X:445:TYR:CD2	2.53	0.44
1:A:26:VAL:HG13	1:A:31:MET:HE3	1.98	0.43
2:B:73:VAL:O	2:B:90:MET:HE1	2.18	0.43
2:B:228:PHE:HD2	2:B:247:LYS:NZ	2.16	0.43
2:B:483:ILE:HG13	2:B:485:GLY:N	2.32	0.43
2:F:406:ALA:O	2:F:410:VAL:HG23	2.18	0.43
2:N:503:GLN:O	2:N:507:GLU:HG3	2.18	0.43
2:N:584:ALA:HB2	2:P:585:GLN:HG2	1.99	0.43
1:S:124:ALA:O	2:T:338:ARG:NH2	2.34	0.43
2:T:229:ILE:HG12	2:T:241:TYR:CE1	2.53	0.43
2:T:583:GLN:O	2:T:587:VAL:HG23	2.18	0.43
2:V:162:LYS:NZ	2:V:309:GLU:OE1	2.46	0.43
2:V:269:ARG:HB2	2:V:291:GLU:HG2	1.99	0.43
2:X:504:ASN:O	2:X:508:ILE:HG12	2.18	0.43
1:A:7:LEU:HD21	1:A:78:VAL:HG13	2.00	0.43
2:B:77:PRO:HD3	2:X:534:ASP:HB2	2.01	0.43
2:B:343:LYS:NZ	1:C:123:ARG:HH22	2.17	0.43
2:F:392:VAL:HG23	2:H:395:ALA:HB1	1.99	0.43
1:G:26:VAL:HG13	1:G:31:MET:HE3	2.00	0.43
2:H:457:ASP:N	2:H:457:ASP:OD1	2.50	0.43
2:P:131:SER:O	2:P:131:SER:OG	2.27	0.43
2:T:457:ASP:OD1	2:T:457:ASP:N	2.50	0.43
2:V:360:GLY:HA2	2:X:340:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:LEU:HG	2:X:583:GLN:HE21	1.83	0.43
2:D:392:VAL:HG23	2:F:395:ALA:HB1	1.99	0.43
2:H:292:HIS:HB2	2:H:436:ILE:HG12	2.00	0.43
2:J:10:PHE:HE1	2:J:152:ILE:HG13	1.83	0.43
2:J:207:LEU:HD23	2:J:208:THR:HG23	1.99	0.43
2:J:269:ARG:HB2	2:J:291:GLU:HG2	2.00	0.43
1:M:5:GLY:O	1:M:7:LEU:O	2.36	0.43
2:P:94:ARG:NH2	2:P:497:PHE:HD2	2.16	0.43
2:R:591:GLY:HA2	2:R:594:GLU:OE1	2.18	0.43
2:T:228:PHE:HD2	2:T:247:LYS:HZ1	1.65	0.43
2:V:53:ASP:OD2	2:X:317:LEU:HD22	2.18	0.43
2:X:124:VAL:HG21	2:X:142:GLU:OE2	2.18	0.43
2:D:341:LYS:HD2	2:D:341:LYS:N	2.32	0.43
2:D:590:GLN:O	2:D:594:GLU:HG3	2.19	0.43
1:E:129:ARG:NH2	2:H:334:ASP:OD2	2.42	0.43
2:F:504:ASN:O	2:F:508:ILE:HG12	2.18	0.43
1:S:135:GLY:O	2:T:42:GLN:NE2	2.52	0.43
2:T:292:HIS:HB2	2:T:436:ILE:HG12	2.00	0.43
2:V:247:LYS:HD2	2:V:247:LYS:O	2.19	0.43
1:W:6:ASP:OD1	1:W:9:ARG:NH2	2.52	0.43
2:X:550:ILE:HD13	2:X:562:GLU:HB3	2.00	0.43
2:B:241:TYR:O	2:B:483:ILE:HA	2.18	0.43
2:B:349:GLU:OE2	2:X:371:ARG:NH2	2.43	0.43
2:D:145:HIS:CD2	2:F:304:PHE:HB2	2.54	0.43
2:L:504:ASN:O	2:L:508:ILE:HG12	2.18	0.43
2:L:523:GLN:NE2	2:L:554:VAL:HG21	2.33	0.43
2:N:247:LYS:HD2	2:N:247:LYS:O	2.18	0.43
2:T:440:ILE:O	2:T:444:ILE:HG12	2.18	0.43
2:X:440:ILE:O	2:X:444:ILE:HG12	2.18	0.43
2:L:591:GLY:HA2	2:L:594:GLU:OE1	2.18	0.43
2:N:341:LYS:HD2	2:N:341:LYS:N	2.34	0.43
2:P:476:GLU:HG2	2:P:477:LYS:HG3	2.01	0.43
2:R:318:THR:HB	2:R:407:VAL:HG13	1.99	0.43
2:V:46:LEU:HD12	2:V:46:LEU:HA	1.89	0.43
2:X:591:GLY:HA2	2:X:594:GLU:OE1	2.18	0.43
2:B:302:TRP:HZ3	2:X:108:ILE:HD11	1.84	0.43
2:H:67:ARG:HD3	2:J:424:ASP:OD2	2.19	0.43
2:N:579:PRO:HB2	2:N:582:VAL:HB	2.01	0.43
2:N:583:GLN:O	2:N:587:VAL:HG23	2.18	0.43
2:P:145:HIS:CD2	2:R:304:PHE:HB2	2.53	0.43
2:P:352:ALA:HB3	2:P:370:ASN:HD21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:29:PHE:HE1	2:R:204:PHE:HB2	1.84	0.43
2:R:108:ILE:HD11	2:T:302:TRP:HZ3	1.82	0.43
2:R:504:ASN:O	2:R:508:ILE:HG12	2.18	0.43
2:V:476:GLU:HG2	2:V:477:LYS:HG3	2.00	0.43
2:V:591:GLY:HA2	2:V:594:GLU:OE1	2.19	0.43
2:D:91:GLY:HA2	2:D:500:MET:HG3	2.01	0.43
2:F:441:VAL:HG22	2:F:445:TYR:CD2	2.53	0.43
2:J:476:GLU:HG2	2:J:477:LYS:HG3	2.01	0.43
2:P:391:GLU:HA	2:R:394:GLN:HE21	1.83	0.43
2:T:579:PRO:HB2	2:T:582:VAL:HB	2.01	0.43
2:V:21:ARG:HH11	2:V:149:SER:HA	1.83	0.43
2:D:66:MET:HE1	2:D:422:PHE:HB3	2.01	0.43
2:F:523:GLN:NE2	2:F:554:VAL:HG21	2.33	0.43
1:K:124:ALA:O	2:L:338:ARG:NH2	2.40	0.43
2:L:145:HIS:CD2	2:N:304:PHE:HB2	2.53	0.43
2:L:511:LEU:HB3	2:L:524:LEU:HD21	2.01	0.43
1:Q:2:LYS:HE3	1:Q:2:LYS:HB2	1.88	0.43
2:R:417:LEU:N	2:R:417:LEU:HD22	2.34	0.43
1:U:7:LEU:CD2	1:U:78:VAL:HG13	2.48	0.43
1:U:148:PRO:HG3	2:X:44:THR:HG21	2.00	0.43
2:X:331:PHE:O	2:X:335:ILE:HG13	2.19	0.43
2:H:172:HIS:CD2	2:H:216:GLU:HG3	2.54	0.43
2:H:512:LEU:HG	2:H:524:LEU:HB3	2.01	0.43
2:J:247:LYS:HD2	2:J:247:LYS:O	2.18	0.43
2:J:516:PRO:O	2:J:521:GLU:HB2	2.19	0.43
2:L:541:MET:HE2	2:N:524:LEU:CD1	2.49	0.43
1:S:31:MET:HE3	1:S:31:MET:HB3	1.90	0.43
2:V:18:ASP:O	2:V:21:ARG:HG2	2.19	0.43
1:G:7:LEU:HD21	1:G:78:VAL:HG13	2.01	0.42
2:J:98:ARG:NH1	2:L:78:LYS:HE3	2.33	0.42
2:J:591:GLY:HA2	2:J:594:GLU:OE1	2.18	0.42
2:L:82:ARG:NE	2:L:84:ASP:OD1	2.46	0.42
2:N:328:ILE:HG21	2:N:400:LEU:HB2	2.00	0.42
2:N:431:ARG:HA	2:N:491:THR:HG21	2.01	0.42
2:T:366:TYR:HE1	2:V:358:TYR:HB2	1.83	0.42
2:T:540:MET:HE2	2:V:527:LEU:HD22	2.00	0.42
2:T:591:GLY:HA2	2:T:594:GLU:OE1	2.18	0.42
2:J:18:ASP:O	2:J:21:ARG:HG2	2.19	0.42
2:L:39:TRP:HB3	2:L:203:VAL:HG23	2.01	0.42
2:P:207:LEU:HD23	2:P:208:THR:HG23	2.00	0.42
2:R:511:LEU:HB3	2:R:524:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:112:GLU:O	2:T:116:ALA:N	2.52	0.42
2:N:355:GLU:OE2	1:O:113:TYR:OH	2.32	0.42
2:N:591:GLY:HA2	2:N:594:GLU:OE1	2.18	0.42
1:O:52:ILE:HD13	1:O:113:TYR:HA	2.01	0.42
2:P:391:GLU:O	2:R:394:GLN:NE2	2.46	0.42
2:R:105:ALA:HA	2:R:143:PRO:HB3	2.00	0.42
2:V:229:ILE:HG12	2:V:241:TYR:CD1	2.55	0.42
2:D:360:GLY:HA2	2:F:340:PRO:HG3	2.01	0.42
2:D:391:GLU:HA	2:F:394:GLN:HE21	1.84	0.42
2:H:579:PRO:HB2	2:H:582:VAL:HB	2.01	0.42
2:L:250:ILE:HD13	2:L:479:VAL:HB	2.01	0.42
2:L:444:ILE:HG13	2:L:445:TYR:CD1	2.54	0.42
2:P:591:GLY:HA2	2:P:594:GLU:OE1	2.19	0.42
2:T:341:LYS:N	2:T:341:LYS:HD2	2.34	0.42
2:T:355:GLU:OE1	2:T:355:GLU:N	2.49	0.42
2:V:141:ARG:NH2	2:V:433:ASP:OD2	2.53	0.42
2:V:145:HIS:CD2	2:X:304:PHE:HB2	2.53	0.42
2:V:159:LEU:HD23	2:V:159:LEU:HA	1.90	0.42
2:V:511:LEU:HB3	2:V:524:LEU:HD21	2.01	0.42
1:W:7:LEU:CD2	1:W:78:VAL:HG13	2.48	0.42
2:B:230:TYR:HE2	2:B:247:LYS:HZ1	1.68	0.42
2:D:53:ASP:OD2	2:F:317:LEU:HD22	2.19	0.42
2:D:207:LEU:HD23	2:D:208:THR:HG23	2.00	0.42
2:H:206:TRP:HA	2:J:19:GLU:OE2	2.18	0.42
2:H:590:GLN:O	2:H:594:GLU:HG3	2.20	0.42
2:H:591:GLY:HA2	2:H:594:GLU:OE1	2.20	0.42
2:J:133:THR:H	2:J:138:VAL:HG12	1.85	0.42
2:J:594:GLU:CD	2:L:596:ALA:HB2	2.45	0.42
1:O:9:ARG:NH1	1:O:67:GLU:OE2	2.53	0.42
2:P:72:ASP:HB2	2:P:496:SER:HB3	2.01	0.42
2:P:269:ARG:HB2	2:P:291:GLU:HG2	1.99	0.42
2:R:124:VAL:HG21	2:R:142:GLU:OE2	2.20	0.42
2:T:336:VAL:HG13	2:V:396:ASN:OD1	2.19	0.42
2:T:404:THR:O	2:T:408:LYS:HG2	2.19	0.42
2:X:523:GLN:NE2	2:X:554:VAL:HG21	2.34	0.42
2:F:511:LEU:HB3	2:F:524:LEU:HD21	2.02	0.42
1:G:2:LYS:HE3	1:G:2:LYS:HB2	1.89	0.42
2:H:228:PHE:HD2	2:H:247:LYS:NZ	2.17	0.42
1:K:132:THR:OG1	1:K:143:GLU:O	2.36	0.42
1:M:5:GLY:C	1:M:7:LEU:O	2.62	0.42
1:M:137:SER:OG	2:N:205:PRO:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:71:ILE:HD11	2:N:423:GLN:HG3	2.00	0.42
2:P:414:GLY:O	2:P:415:VAL:C	2.63	0.42
2:R:250:ILE:HD13	2:R:479:VAL:HB	2.02	0.42
1:S:7:LEU:HD21	1:S:78:VAL:HG13	2.02	0.42
2:T:56:ARG:NH1	2:V:317:LEU:HD11	2.35	0.42
2:T:206:TRP:HA	2:V:19:GLU:OE2	2.20	0.42
2:T:413:LEU:HD23	2:T:413:LEU:HA	1.90	0.42
2:V:516:PRO:O	2:V:521:GLU:HB2	2.19	0.42
2:J:392:VAL:HG23	2:L:395:ALA:HB1	2.02	0.42
2:J:550:ILE:HD13	2:J:562:GLU:HB3	2.00	0.42
2:N:228:PHE:HD2	2:N:247:LYS:NZ	2.17	0.42
2:N:441:VAL:HG22	2:N:445:TYR:CD2	2.55	0.42
2:P:229:ILE:HG12	2:P:241:TYR:CD1	2.55	0.42
2:P:247:LYS:HD2	2:P:247:LYS:O	2.18	0.42
2:P:516:PRO:O	2:P:521:GLU:HB2	2.19	0.42
2:R:71:ILE:HD11	2:R:423:GLN:HG3	2.00	0.42
2:R:253:LEU:HD22	2:R:473:ALA:HA	2.02	0.42
2:B:176:GLN:O	2:B:179:TRP:N	2.52	0.42
2:D:269:ARG:HB2	2:D:291:GLU:HG2	2.01	0.42
2:D:504:ASN:O	2:D:508:ILE:HG12	2.20	0.42
2:F:39:TRP:HB3	2:F:203:VAL:HG23	2.00	0.42
2:L:358:TYR:HD1	2:N:387:TYR:OH	2.03	0.42
2:L:590:GLN:O	2:L:594:GLU:HG3	2.20	0.42
2:P:62:LEU:HD13	2:P:413:LEU:HD22	2.02	0.42
1:Q:52:ILE:HD13	1:Q:113:TYR:HA	2.02	0.42
2:V:32:ARG:HH21	2:V:111:ARG:HG2	1.85	0.42
2:D:229:ILE:HG12	2:D:241:TYR:CD1	2.55	0.42
2:J:391:GLU:HA	2:L:394:GLN:HE21	1.84	0.42
2:J:520:PRO:O	2:J:524:LEU:HD13	2.20	0.42
2:J:590:GLN:O	2:J:594:GLU:HG3	2.20	0.42
1:M:74:ARG:HH22	1:M:112:LEU:HD23	1.85	0.42
2:N:39:TRP:HB3	2:N:203:VAL:HG23	2.01	0.42
1:S:137:SER:OG	2:T:205:PRO:HG2	2.19	0.42
2:X:469:VAL:HG12	2:X:481:ASN:HD22	1.85	0.42
2:F:533:LEU:HD22	2:H:76:ARG:HH12	1.85	0.42
2:H:196:PHE:O	2:H:213:GLN:NE2	2.53	0.42
2:J:229:ILE:HG12	2:J:241:TYR:CD1	2.55	0.42
1:K:52:ILE:HD13	1:K:113:TYR:HA	2.02	0.42
2:R:35:GLN:H	2:R:51:GLN:HE22	1.67	0.42
2:R:159:LEU:HD23	2:R:159:LEU:HA	1.90	0.42
2:T:230:TYR:O	2:T:240:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:440:ILE:O	2:V:444:ILE:HG12	2.20	0.42
2:X:590:GLN:O	2:X:594:GLU:HG3	2.20	0.42
1:A:60:ASP:N	1:A:60:ASP:OD1	2.53	0.41
2:B:56:ARG:NH1	2:D:317:LEU:HD11	2.35	0.41
2:B:351:ILE:O	2:B:355:GLU:HG3	2.19	0.41
2:D:204:PHE:HB3	2:D:206:TRP:NE1	2.35	0.41
2:F:371:ARG:NH2	2:H:349:GLU:OE2	2.43	0.41
2:H:241:TYR:O	2:H:483:ILE:HA	2.20	0.41
2:J:204:PHE:HB3	2:J:206:TRP:NE1	2.36	0.41
2:N:108:ILE:HD11	2:P:302:TRP:HZ3	1.85	0.41
2:N:131:SER:O	2:N:131:SER:OG	2.32	0.41
2:N:440:ILE:O	2:N:444:ILE:HG12	2.19	0.41
1:O:60:ASP:OD1	1:O:60:ASP:N	2.53	0.41
2:T:355:GLU:OE2	1:U:113:TYR:OH	2.31	0.41
2:V:352:ALA:HB3	2:V:370:ASN:HD21	1.85	0.41
2:V:504:ASN:O	2:V:508:ILE:HG12	2.20	0.41
2:V:594:GLU:CD	2:X:596:ALA:HB2	2.45	0.41
1:W:52:ILE:HD13	1:W:113:TYR:HA	2.01	0.41
1:A:148:PRO:HG3	2:D:44:THR:HG21	2.02	0.41
2:B:230:TYR:O	2:B:240:SER:N	2.53	0.41
2:D:112:GLU:O	2:D:116:ALA:N	2.53	0.41
2:D:476:GLU:HG2	2:D:477:LYS:HG3	2.01	0.41
1:G:14:LYS:HA	1:G:14:LYS:HD3	1.81	0.41
1:G:60:ASP:OD1	1:G:60:ASP:N	2.53	0.41
2:H:112:GLU:O	2:H:116:ALA:N	2.52	0.41
2:H:269:ARG:HB2	2:H:291:GLU:HG2	2.02	0.41
2:H:360:GLY:HA2	2:J:340:PRO:HG3	2.01	0.41
2:H:516:PRO:O	2:H:521:GLU:HB2	2.20	0.41
2:J:352:ALA:HB3	2:J:370:ASN:HD21	1.85	0.41
2:L:18:ASP:O	2:L:22:ARG:HG3	2.21	0.41
2:N:241:TYR:O	2:N:483:ILE:HA	2.20	0.41
2:N:324:LEU:HD12	2:N:324:LEU:HA	1.94	0.41
2:P:342:LYS:HG3	2:P:386:TYR:HB3	2.01	0.41
2:P:504:ASN:O	2:P:508:ILE:HG12	2.20	0.41
2:R:590:GLN:O	2:R:594:GLU:HG3	2.19	0.41
2:T:237:GLU:N	2:T:238:PRO:HD3	2.36	0.41
1:U:12:LEU:HB3	1:U:17:VAL:O	2.20	0.41
2:V:366:TYR:CE1	2:X:358:TYR:HB2	2.51	0.41
2:X:207:LEU:HD23	2:X:208:THR:HG23	2.03	0.41
1:C:44:GLU:O	1:C:47:GLN:HG2	2.21	0.41
2:F:112:GLU:O	2:F:116:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:366:TYR:HE1	2:P:358:TYR:HB2	1.85	0.41
1:Q:132:THR:OG1	1:Q:143:GLU:O	2.36	0.41
2:R:71:ILE:CD1	2:R:423:GLN:HG3	2.50	0.41
2:T:46:LEU:HD12	2:T:46:LEU:HA	1.88	0.41
2:V:237:GLU:N	2:V:238:PRO:HD3	2.35	0.41
2:X:105:ALA:HA	2:X:143:PRO:HB3	2.01	0.41
2:X:332:ASN:OD1	2:X:392:VAL:HG13	2.21	0.41
2:D:237:GLU:N	2:D:238:PRO:HD3	2.35	0.41
2:F:469:VAL:HG12	2:F:481:ASN:HD22	1.84	0.41
1:G:137:SER:OG	2:H:205:PRO:HG2	2.20	0.41
1:G:148:PRO:HG3	2:J:44:THR:HG21	2.02	0.41
2:H:56:ARG:NH1	2:J:317:LEU:HD11	2.35	0.41
2:H:230:TYR:O	2:H:240:SER:N	2.54	0.41
2:J:237:GLU:N	2:J:238:PRO:HD3	2.35	0.41
2:J:384:LEU:HD23	2:J:384:LEU:HA	1.92	0.41
2:J:405:SER:O	2:J:409:GLU:HG3	2.20	0.41
2:L:413:LEU:HD23	2:L:413:LEU:HA	1.85	0.41
2:N:590:GLN:O	2:N:594:GLU:HG3	2.20	0.41
2:P:237:GLU:N	2:P:238:PRO:HD3	2.36	0.41
2:P:444:ILE:HG13	2:P:445:TYR:CD1	2.55	0.41
2:P:594:GLU:CD	2:R:596:ALA:HB2	2.45	0.41
2:R:534:ASP:HB2	2:T:77:PRO:HD3	2.02	0.41
2:R:584:ALA:HB2	2:T:585:GLN:HG2	2.02	0.41
2:T:360:GLY:HA2	2:V:340:PRO:HG3	2.02	0.41
2:T:419:THR:O	2:T:423:GLN:HB2	2.20	0.41
2:T:516:PRO:O	2:T:521:GLU:HB2	2.20	0.41
2:V:391:GLU:HA	2:X:394:GLN:HE21	1.85	0.41
2:B:29:PHE:HE2	2:B:204:PHE:HB2	1.85	0.41
2:B:516:PRO:O	2:B:521:GLU:HB2	2.21	0.41
2:B:585:GLN:HG2	2:X:584:ALA:HB2	2.02	0.41
2:D:18:ASP:O	2:D:21:ARG:HG2	2.20	0.41
2:D:440:ILE:O	2:D:444:ILE:HG12	2.21	0.41
1:E:60:ASP:OD1	1:E:60:ASP:N	2.53	0.41
2:H:131:SER:O	2:H:131:SER:OG	2.27	0.41
2:H:183:ALA:HA	2:H:188:LEU:HB2	2.03	0.41
2:J:587:VAL:HG11	2:L:588:LEU:HB3	2.02	0.41
2:L:405:SER:O	2:L:409:GLU:HG3	2.20	0.41
2:N:357:MET:HE1	2:N:368:LEU:HG	2.01	0.41
2:N:483:ILE:HG13	2:N:485:GLY:N	2.33	0.41
1:Q:14:LYS:HD3	1:Q:14:LYS:HA	1.82	0.41
2:R:145:HIS:CD2	2:T:304:PHE:HB2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:HD11	2:D:302:TRP:HZ3	1.85	0.41
2:B:196:PHE:O	2:B:213:GLN:NE2	2.53	0.41
2:B:269:ARG:HB2	2:B:291:GLU:HG2	2.02	0.41
2:B:594:GLU:CD	2:D:596:ALA:HB2	2.46	0.41
1:C:12:LEU:HB3	1:C:17:VAL:O	2.21	0.41
2:F:204:PHE:HB3	2:F:206:TRP:NE1	2.35	0.41
1:G:139:ALA:HB1	1:G:144:TRP:CZ3	2.55	0.41
1:G:144:TRP:CE2	2:J:26:ASN:ND2	2.89	0.41
2:H:366:TYR:HE1	2:J:358:TYR:HB2	1.86	0.41
2:J:141:ARG:NH2	2:J:433:ASP:OD2	2.53	0.41
2:P:440:ILE:O	2:P:444:ILE:HG12	2.20	0.41
2:R:53:ASP:O	2:T:410:VAL:HG22	2.21	0.41
1:S:139:ALA:HB1	1:S:144:TRP:CZ3	2.56	0.41
2:T:122:ARG:NH2	2:T:142:GLU:OE1	2.53	0.41
2:T:431:ARG:HA	2:T:491:THR:HG21	2.02	0.41
1:U:44:GLU:O	1:U:47:GLN:HG2	2.21	0.41
1:W:60:ASP:N	1:W:60:ASP:OD1	2.53	0.41
2:B:112:GLU:O	2:B:116:ALA:N	2.52	0.41
2:B:523:GLN:HE22	2:B:554:VAL:HG11	1.86	0.41
1:C:60:ASP:N	1:C:60:ASP:OD1	2.53	0.41
2:F:503:GLN:O	2:F:507:GLU:HG3	2.21	0.41
2:H:359:ASP:HB3	1:I:124:ALA:HB2	2.02	0.41
2:H:441:VAL:HG22	2:H:445:TYR:CD2	2.56	0.41
2:H:550:ILE:HD13	2:H:562:GLU:HB3	2.03	0.41
1:I:12:LEU:HB3	1:I:17:VAL:O	2.21	0.41
1:M:2:LYS:HE3	1:M:2:LYS:HB2	1.89	0.41
2:P:141:ARG:NH2	2:P:433:ASP:OD2	2.54	0.41
2:T:389:ASN:HB3	2:V:393:PRO:HB3	2.02	0.41
2:V:60:ARG:NH2	2:X:312:GLU:OE2	2.53	0.41
2:V:110:VAL:O	2:V:114:ILE:HG12	2.21	0.41
2:V:590:GLN:O	2:V:594:GLU:HG3	2.20	0.41
2:X:327:MET:HE3	2:X:327:MET:HB3	1.86	0.41
2:D:61:LYS:HE2	2:D:61:LYS:HB3	1.94	0.41
2:D:161:ASP:O	2:D:432:ARG:NH1	2.53	0.41
1:G:135:GLY:O	2:H:42:GLN:NE2	2.54	0.41
2:L:237:GLU:N	2:L:238:PRO:HD3	2.36	0.41
2:N:456:GLU:HB2	2:N:459:SER:HB3	2.02	0.41
2:P:317:LEU:HB3	2:P:410:VAL:HG11	2.03	0.41
2:P:329:MET:HE3	2:P:329:MET:HB3	1.86	0.41
2:P:590:GLN:O	2:P:594:GLU:HG3	2.20	0.41
2:R:516:PRO:O	2:R:521:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:332:ASN:O	2:T:336:VAL:HG23	2.20	0.41
2:V:252:ASP:OD1	2:V:253:LEU:N	2.54	0.41
2:B:237:GLU:N	2:B:238:PRO:HD3	2.36	0.41
2:B:431:ARG:HA	2:B:491:THR:HG21	2.01	0.41
2:D:46:LEU:HD12	2:D:46:LEU:HA	1.88	0.41
2:D:252:ASP:OD1	2:D:253:LEU:HD12	2.21	0.41
2:D:532:LEU:HD12	2:D:532:LEU:HA	1.81	0.41
2:F:594:GLU:CD	2:H:596:ALA:HB2	2.46	0.41
2:H:252:ASP:OD1	2:H:253:LEU:N	2.54	0.41
2:H:413:LEU:HD23	2:H:413:LEU:HA	1.95	0.41
2:H:456:GLU:HB2	2:H:459:SER:HB3	2.03	0.41
2:J:35:GLN:H	2:J:51:GLN:HE22	1.68	0.41
2:J:56:ARG:NH2	2:L:312:GLU:OE1	2.54	0.41
2:J:252:ASP:OD1	2:J:253:LEU:N	2.54	0.41
2:J:420:TYR:C	2:J:421:VAL:O	2.62	0.41
2:L:162:LYS:NZ	2:L:309:GLU:OE2	2.50	0.41
2:L:318:THR:HB	2:L:407:VAL:HG13	2.02	0.41
2:L:329:MET:HE3	2:L:329:MET:HB3	1.89	0.41
2:L:441:VAL:HG22	2:L:445:TYR:CD2	2.56	0.41
1:M:129:ARG:O	2:P:327:MET:HG3	2.21	0.41
1:M:144:TRP:CE2	2:P:26:ASN:ND2	2.89	0.41
2:N:112:GLU:O	2:N:116:ALA:N	2.54	0.41
2:N:230:TYR:O	2:N:240:SER:N	2.54	0.41
2:N:540:MET:HE2	2:P:527:LEU:HD22	2.02	0.41
1:O:12:LEU:HB3	1:O:17:VAL:O	2.21	0.41
1:O:44:GLU:O	1:O:47:GLN:HG2	2.21	0.41
2:P:18:ASP:O	2:P:21:ARG:HG2	2.20	0.41
2:P:252:ASP:OD1	2:P:253:LEU:HD12	2.21	0.41
2:P:413:LEU:HD21	2:P:422:PHE:CG	2.56	0.41
1:Q:129:ARG:O	2:T:327:MET:HG3	2.20	0.41
1:S:74:ARG:HH22	1:S:112:LEU:HD23	1.86	0.41
2:T:62:LEU:HD13	2:T:413:LEU:HD12	2.03	0.41
2:T:590:GLN:HG2	2:T:594:GLU:OE2	2.21	0.41
2:T:590:GLN:O	2:T:594:GLU:HG3	2.20	0.41
2:V:129:ASP:OD2	2:X:224:LYS:NZ	2.54	0.41
1:W:137:SER:OG	2:X:205:PRO:HG2	2.20	0.41
2:B:206:TRP:HA	2:D:19:GLU:OE2	2.21	0.41
2:B:207:LEU:HD22	2:D:15:THR:HG23	2.02	0.41
2:B:590:GLN:O	2:B:594:GLU:HG3	2.21	0.41
2:D:352:ALA:HB3	2:D:370:ASN:HD21	1.85	0.41
2:H:46:LEU:HD12	2:H:46:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:324:LEU:HD12	2:H:324:LEU:HA	1.97	0.41
2:J:456:GLU:HB2	2:J:459:SER:HB3	2.03	0.41
2:J:532:LEU:HD12	2:J:532:LEU:HA	1.83	0.41
2:L:96:ASP:OD2	2:L:437:TYR:OH	2.30	0.41
2:L:206:TRP:HA	2:N:19:GLU:OE2	2.21	0.41
2:N:504:ASN:O	2:N:508:ILE:HG12	2.21	0.41
2:V:305:VAL:HG13	2:V:306:GLU:N	2.36	0.41
2:X:112:GLU:O	2:X:116:ALA:N	2.52	0.41
2:L:253:LEU:HD22	2:L:473:ALA:HA	2.02	0.40
2:N:332:ASN:O	2:N:336:VAL:HG23	2.21	0.40
2:N:375:ASN:HB3	1:O:102:ILE:HG23	2.03	0.40
2:T:504:ASN:O	2:T:508:ILE:HG12	2.22	0.40
1:U:52:ILE:HD13	1:U:113:TYR:HA	2.02	0.40
2:X:66:MET:HE3	2:X:419:THR:HB	2.03	0.40
2:X:413:LEU:HD23	2:X:413:LEU:HA	1.84	0.40
2:D:185:LYS:HD2	2:D:186:TYR:CE2	2.56	0.40
2:D:456:GLU:HB2	2:D:459:SER:HB3	2.03	0.40
2:D:594:GLU:CD	2:F:596:ALA:HB2	2.46	0.40
2:F:18:ASP:O	2:F:22:ARG:HG3	2.21	0.40
2:F:29:PHE:CE2	2:F:204:PHE:HB2	2.55	0.40
2:F:366:TYR:CE1	2:H:358:TYR:HB2	2.56	0.40
2:L:534:ASP:HB2	2:N:77:PRO:HD3	2.04	0.40
2:N:29:PHE:CE2	2:N:204:PHE:HB2	2.56	0.40
2:N:66:MET:HG3	2:N:423:GLN:NE2	2.37	0.40
2:N:594:GLU:CD	2:P:596:ALA:HB2	2.46	0.40
2:P:66:MET:HE1	2:P:422:PHE:HB3	2.02	0.40
2:P:112:GLU:O	2:P:116:ALA:N	2.53	0.40
2:R:207:LEU:HD23	2:R:208:THR:HG23	2.03	0.40
2:R:329:MET:HE3	2:R:329:MET:HB3	1.89	0.40
2:R:358:TYR:HD1	2:T:387:TYR:HH	1.70	0.40
2:T:207:LEU:HD22	2:V:15:THR:HG23	2.03	0.40
2:X:18:ASP:O	2:X:22:ARG:HG3	2.22	0.40
2:X:96:ASP:OD2	2:X:437:TYR:OH	2.31	0.40
2:D:366:TYR:CE1	2:F:358:TYR:HB2	2.52	0.40
1:E:52:ILE:HD13	1:E:113:TYR:HA	2.03	0.40
2:H:108:ILE:HD11	2:J:302:TRP:HZ3	1.85	0.40
2:H:237:GLU:N	2:H:238:PRO:HD3	2.36	0.40
2:J:440:ILE:O	2:J:444:ILE:HG12	2.21	0.40
2:P:71:ILE:HD11	2:P:423:GLN:HG2	2.03	0.40
2:R:71:ILE:HD11	2:R:423:GLN:CG	2.50	0.40
2:B:366:TYR:HE1	2:D:358:TYR:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:583:GLN:HE22	2:F:585:GLN:C	2.29	0.40
2:H:174:MET:HE1	2:H:182:PHE:CD2	2.57	0.40
2:L:112:GLU:O	2:L:116:ALA:N	2.53	0.40
2:N:159:LEU:HD23	2:N:159:LEU:HA	1.93	0.40
2:R:206:TRP:HA	2:T:19:GLU:OE2	2.21	0.40
2:R:237:GLU:N	2:R:238:PRO:HD3	2.37	0.40
2:T:228:PHE:N	2:T:242:PHE:O	2.52	0.40
2:T:248:ASP:OD1	2:T:249:VAL:N	2.55	0.40
2:T:533:LEU:HD12	2:V:507:GLU:OE2	2.21	0.40
2:T:594:GLU:CD	2:V:596:ALA:HB2	2.46	0.40
1:U:60:ASP:OD1	1:U:60:ASP:N	2.53	0.40
2:V:18:ASP:O	2:V:22:ARG:HG3	2.22	0.40
2:V:431:ARG:HA	2:V:491:THR:HG21	2.03	0.40
2:X:35:GLN:H	2:X:51:GLN:HE22	1.69	0.40
2:B:35:GLN:H	2:B:51:GLN:HE22	1.69	0.40
2:B:423:GLN:HB2	2:B:423:GLN:HE21	1.61	0.40
2:B:456:GLU:HB2	2:B:459:SER:HB3	2.03	0.40
2:B:533:LEU:HD22	2:D:76:ARG:HH12	1.87	0.40
2:D:591:GLY:HA2	2:D:594:GLU:OE1	2.21	0.40
1:E:14:LYS:HD3	1:E:14:LYS:HA	1.90	0.40
2:H:523:GLN:NE2	2:H:554:VAL:HG21	2.37	0.40
2:J:457:ASP:OD1	2:J:457:ASP:N	2.49	0.40
2:J:504:ASN:O	2:J:508:ILE:HG12	2.21	0.40
2:L:53:ASP:O	2:N:410:VAL:HG22	2.21	0.40
2:L:456:GLU:HB2	2:L:459:SER:HB3	2.04	0.40
2:N:237:GLU:N	2:N:238:PRO:HD3	2.36	0.40
2:P:204:PHE:HB3	2:P:206:TRP:NE1	2.36	0.40
2:P:587:VAL:HG11	2:R:588:LEU:HB3	2.03	0.40
2:T:441:VAL:HG22	2:T:445:TYR:CD2	2.56	0.40
2:T:523:GLN:NE2	2:T:554:VAL:HG21	2.37	0.40
2:X:511:LEU:HB3	2:X:524:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	C	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	E	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	G	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	I	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
1	K	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	M	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
1	O	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
1	Q	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	S	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	U	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
1	W	147/149 (99%)	146 (99%)	1 (1%)	0	100	100
2	B	594/621 (96%)	568 (96%)	26 (4%)	0	100	100
2	D	594/621 (96%)	569 (96%)	25 (4%)	0	100	100
2	F	594/621 (96%)	569 (96%)	25 (4%)	0	100	100
2	H	594/621 (96%)	570 (96%)	24 (4%)	0	100	100
2	J	594/621 (96%)	569 (96%)	25 (4%)	0	100	100
2	L	594/621 (96%)	562 (95%)	32 (5%)	0	100	100
2	N	594/621 (96%)	572 (96%)	22 (4%)	0	100	100
2	P	594/621 (96%)	569 (96%)	25 (4%)	0	100	100
2	R	594/621 (96%)	564 (95%)	30 (5%)	0	100	100
2	T	594/621 (96%)	573 (96%)	21 (4%)	0	100	100
2	V	594/621 (96%)	572 (96%)	22 (4%)	0	100	100
2	X	594/621 (96%)	569 (96%)	25 (4%)	0	100	100
All	All	8892/9240 (96%)	8575 (96%)	317 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/117 (100%)	117 (100%)	0	100	100
1	C	117/117 (100%)	117 (100%)	0	100	100
1	E	117/117 (100%)	117 (100%)	0	100	100
1	G	117/117 (100%)	117 (100%)	0	100	100
1	I	117/117 (100%)	117 (100%)	0	100	100
1	K	117/117 (100%)	117 (100%)	0	100	100
1	M	117/117 (100%)	117 (100%)	0	100	100
1	O	117/117 (100%)	117 (100%)	0	100	100
1	Q	117/117 (100%)	117 (100%)	0	100	100
1	S	117/117 (100%)	117 (100%)	0	100	100
1	U	117/117 (100%)	117 (100%)	0	100	100
1	W	117/117 (100%)	117 (100%)	0	100	100
2	B	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	D	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	F	523/541 (97%)	523 (100%)	0	100	100
2	H	523/541 (97%)	523 (100%)	0	100	100
2	J	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	L	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	N	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	P	523/541 (97%)	521 (100%)	2 (0%)	89	94
2	R	523/541 (97%)	522 (100%)	1 (0%)	92	97
2	T	523/541 (97%)	523 (100%)	0	100	100
2	V	523/541 (97%)	523 (100%)	0	100	100
2	X	523/541 (97%)	523 (100%)	0	100	100
All	All	7680/7896 (97%)	7672 (100%)	8 (0%)	92	98

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	362	ASP

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Mol	Chain	Res	Type
2	D	423	GLN
2	J	423	GLN
2	L	417	LEU
2	N	423	GLN
2	P	417	LEU
2	P	423	GLN
2	R	423	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	47	GLN
2	B	26	ASN
2	B	145	HIS
2	B	150	HIS
2	B	177	ASN
2	B	209	GLN
2	B	356	HIS
2	B	375	ASN
2	B	423	GLN
2	B	450	ASN
2	B	464	GLN
2	B	498	GLN
2	B	583	GLN
1	C	47	GLN
1	C	136	ASN
2	D	26	ASN
2	D	145	HIS
2	D	150	HIS
2	D	370	ASN
2	D	423	GLN
2	D	438	GLN
2	D	442	ASN
2	D	450	ASN
2	D	478	GLN
2	D	523	GLN
2	D	548	GLN
2	D	563	GLN
2	D	564	GLN
2	F	26	ASN
2	F	69	ASN

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Mol	Chain	Res	Type
2	F	145	HIS
2	F	177	ASN
2	F	356	HIS
2	F	375	ASN
2	F	523	GLN
2	F	564	GLN
2	F	583	GLN
1	G	32	GLN
1	G	47	GLN
2	H	145	HIS
2	H	150	HIS
2	H	156	ASN
2	H	177	ASN
2	H	231	GLN
2	H	332	ASN
2	H	375	ASN
2	H	423	GLN
2	H	425	ASN
2	H	464	GLN
2	H	583	GLN
1	I	32	GLN
1	I	47	GLN
1	I	136	ASN
2	J	145	HIS
2	J	370	ASN
2	J	438	GLN
2	J	442	ASN
2	J	478	GLN
2	J	523	GLN
2	J	548	GLN
2	J	564	GLN
2	L	26	ASN
2	L	69	ASN
2	L	145	HIS
2	L	375	ASN
2	L	450	ASN
2	L	523	GLN
2	L	564	GLN
2	L	570	GLN
2	L	583	GLN
1	M	32	GLN
2	N	26	ASN

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Mol	Chain	Res	Type
2	N	145	HIS
2	N	150	HIS
2	N	209	GLN
2	N	231	GLN
2	N	375	ASN
2	N	423	GLN
2	N	464	GLN
2	N	498	GLN
2	N	570	GLN
2	N	583	GLN
1	O	32	GLN
1	O	47	GLN
2	P	145	HIS
2	P	150	HIS
2	P	370	ASN
2	P	375	ASN
2	P	423	GLN
2	P	425	ASN
2	P	498	GLN
2	P	523	GLN
2	P	564	GLN
2	R	26	ASN
2	R	375	ASN
2	R	423	GLN
2	R	450	ASN
2	R	478	GLN
2	R	523	GLN
2	R	570	GLN
2	R	583	GLN
1	S	32	GLN
1	S	47	GLN
2	T	26	ASN
2	T	145	HIS
2	T	150	HIS
2	T	375	ASN
2	T	425	ASN
2	T	450	ASN
2	T	498	GLN
2	T	583	GLN
1	U	32	GLN
1	U	47	GLN
1	U	136	ASN

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Mol	Chain	Res	Type
2	V	26	ASN
2	V	145	HIS
2	V	150	HIS
2	V	370	ASN
2	V	478	GLN
2	V	523	GLN
2	V	548	GLN
2	V	564	GLN
2	V	570	GLN
1	W	47	GLN
1	W	136	ASN
1	W	145	HIS
2	X	69	ASN
2	X	150	HIS
2	X	356	HIS
2	X	370	ASN
2	X	375	ASN
2	X	523	GLN
2	X	548	GLN
2	X	564	GLN
2	X	570	GLN
2	X	583	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

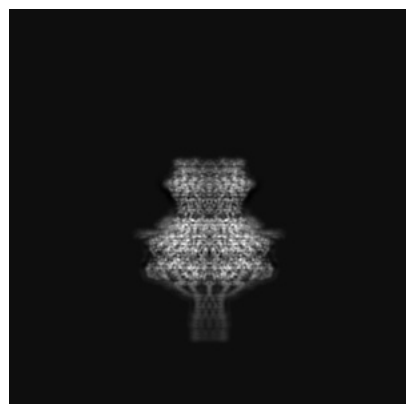
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27792. These allow visual inspection of the internal detail of the map and identification of artifacts.

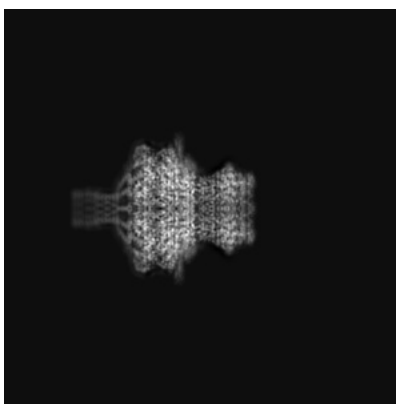
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

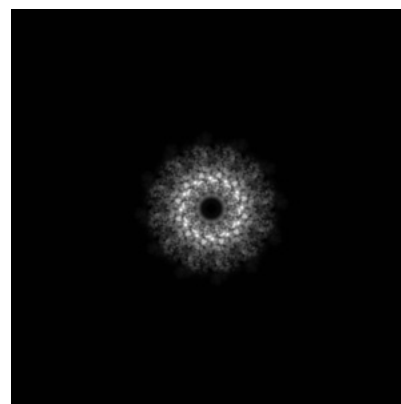
#### 6.1.1 Primary map



X

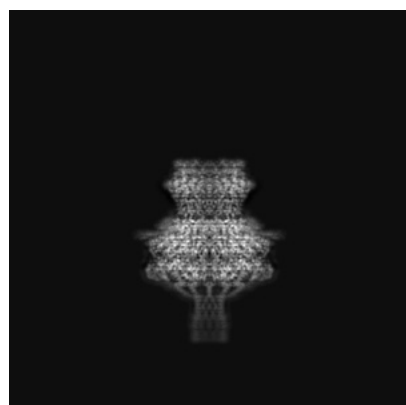


Y

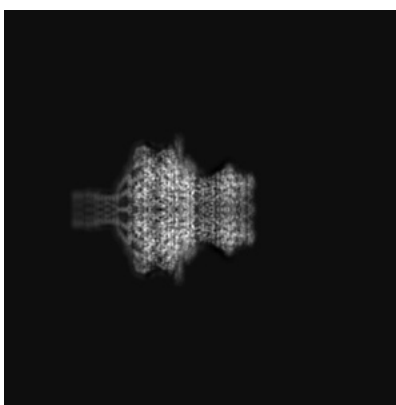


Z

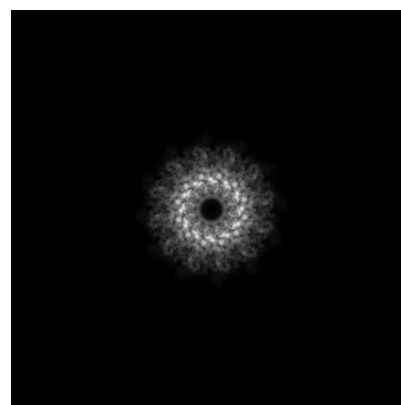
#### 6.1.2 Raw map



X



Y



Z

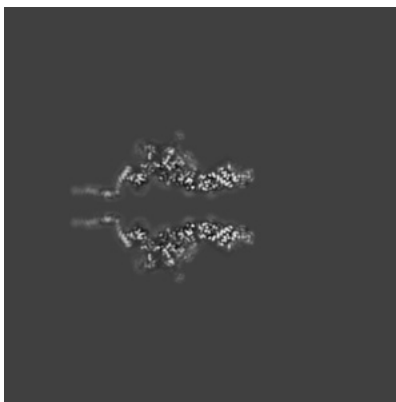
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

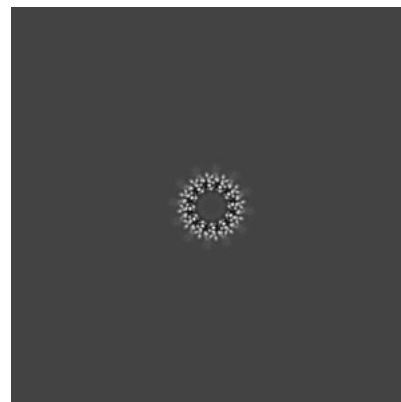
### 6.2.1 Primary map



X Index: 240



Y Index: 240

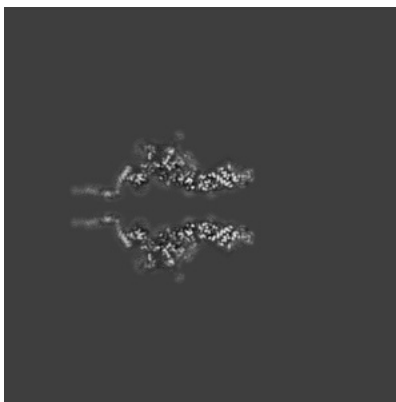


Z Index: 240

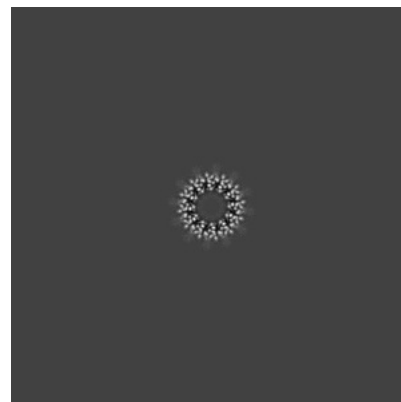
### 6.2.2 Raw map



X Index: 240



Y Index: 240

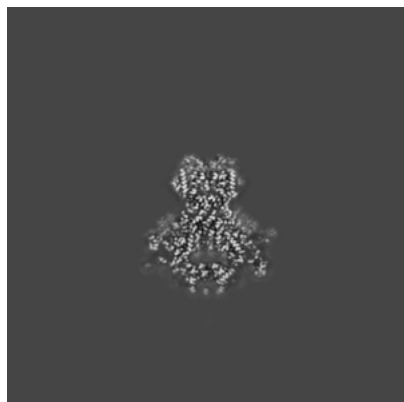


Z Index: 240

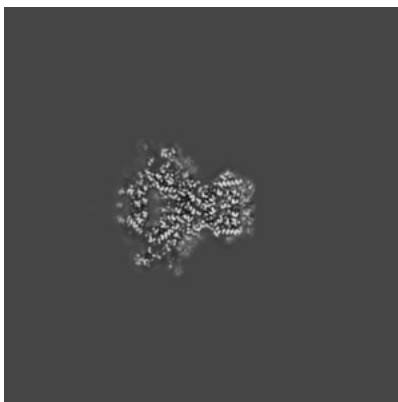
The images above show central slices of the map in three orthogonal directions.

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

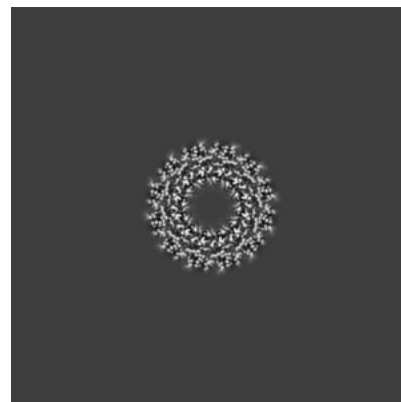
### 6.3.1 Primary map



X Index: 269

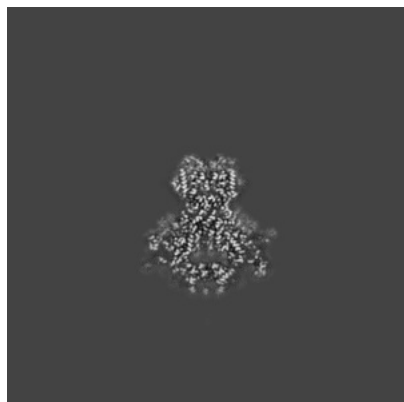


Y Index: 269

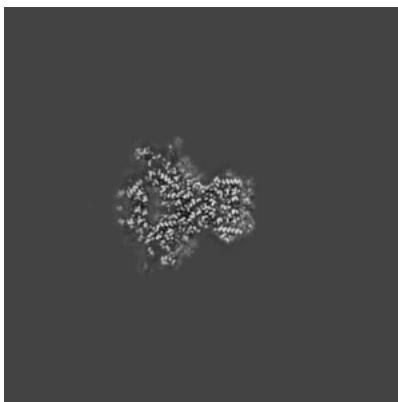


Z Index: 198

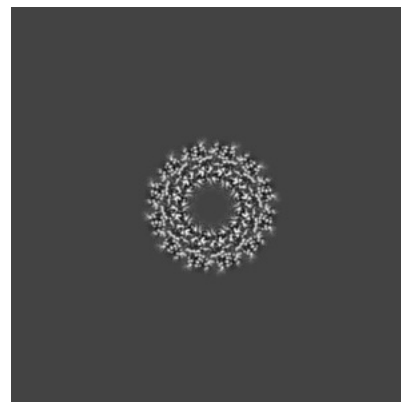
### 6.3.2 Raw map



X Index: 269



Y Index: 211

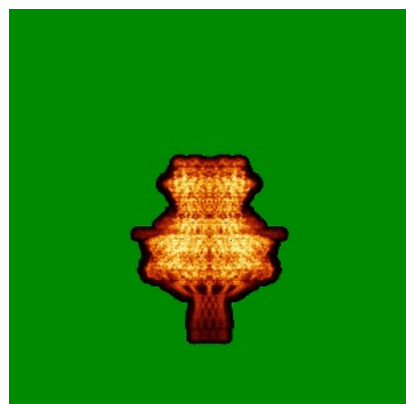


Z Index: 198

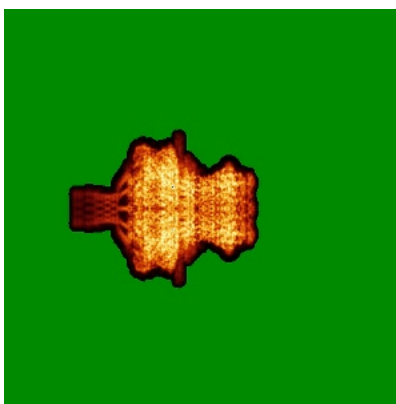
The images above show the largest variance slices of the map in three orthogonal directions.

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

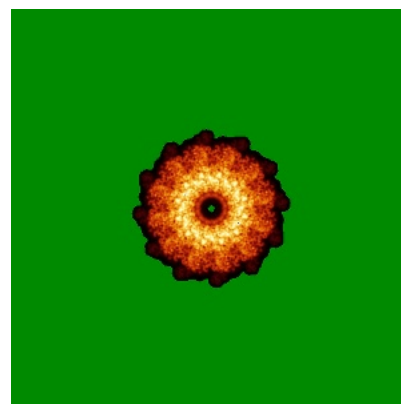
### 6.4.1 Primary map



X

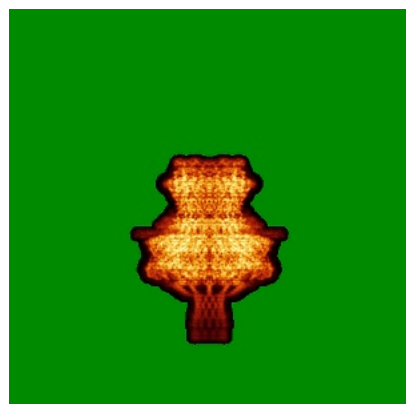


Y

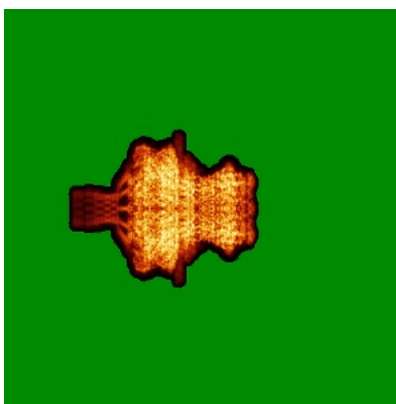


Z

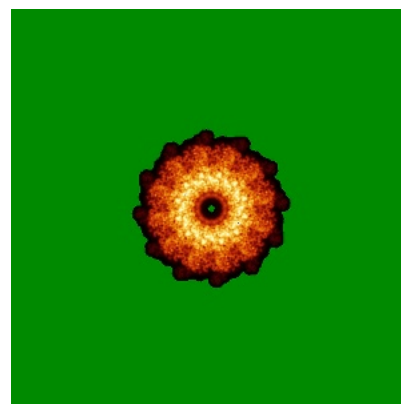
### 6.4.2 Raw map



X



Y

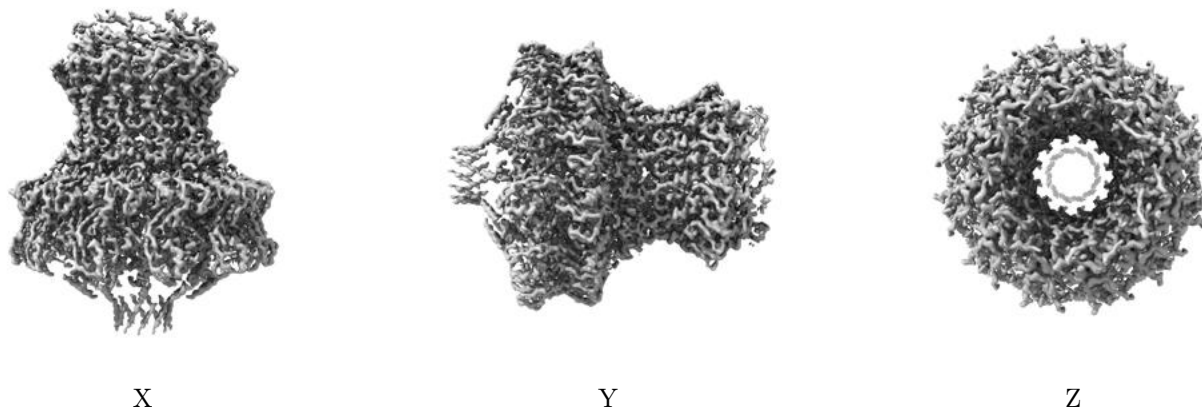


Z

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

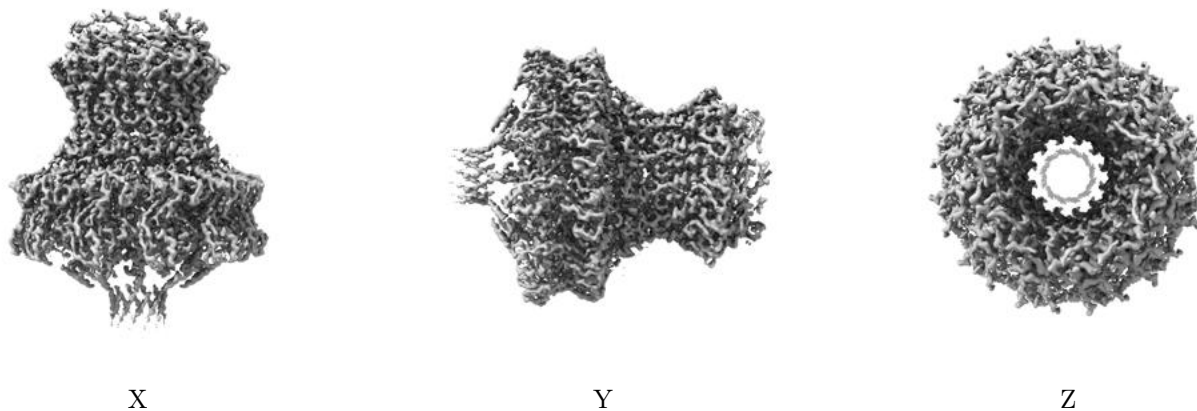
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

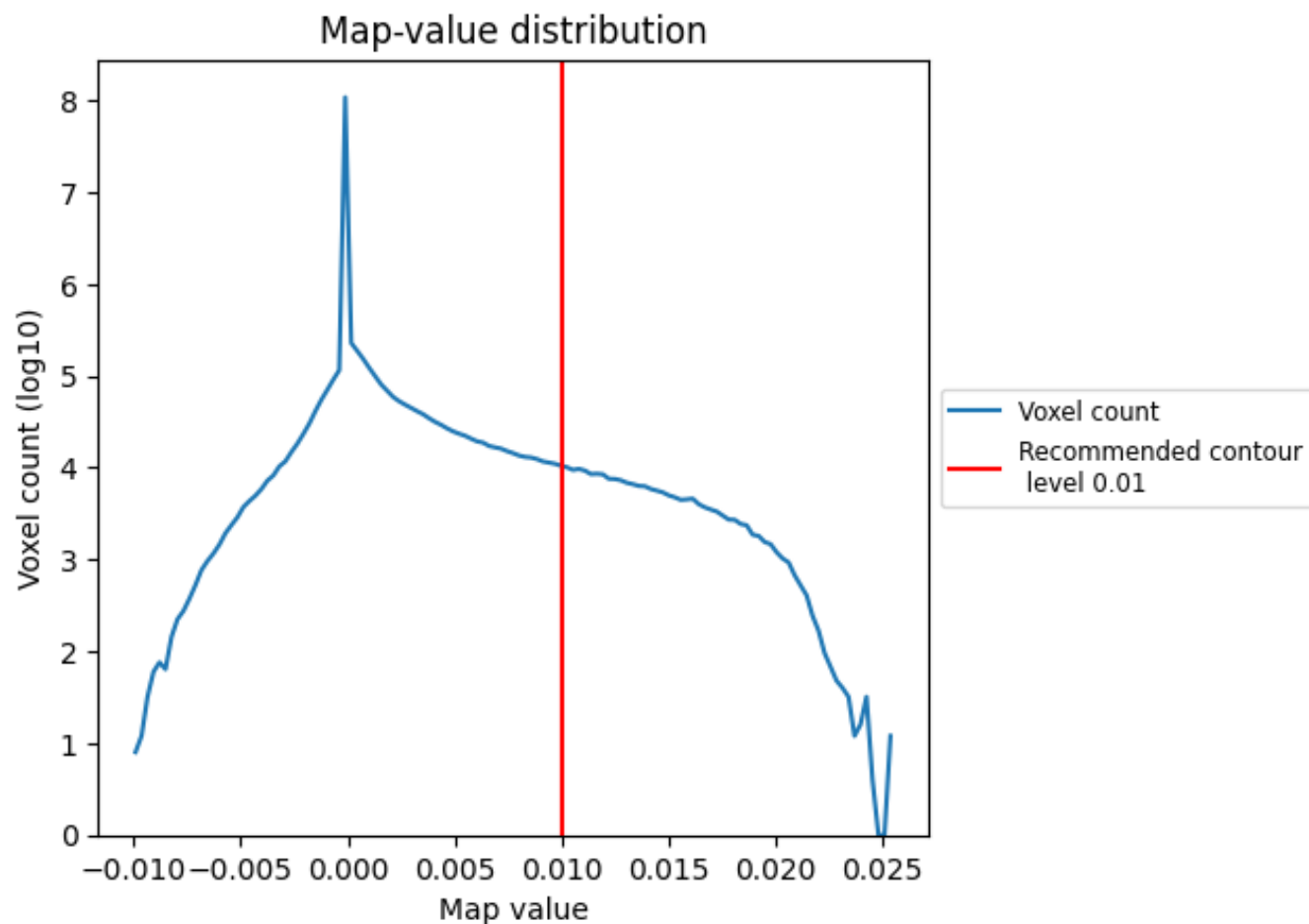
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

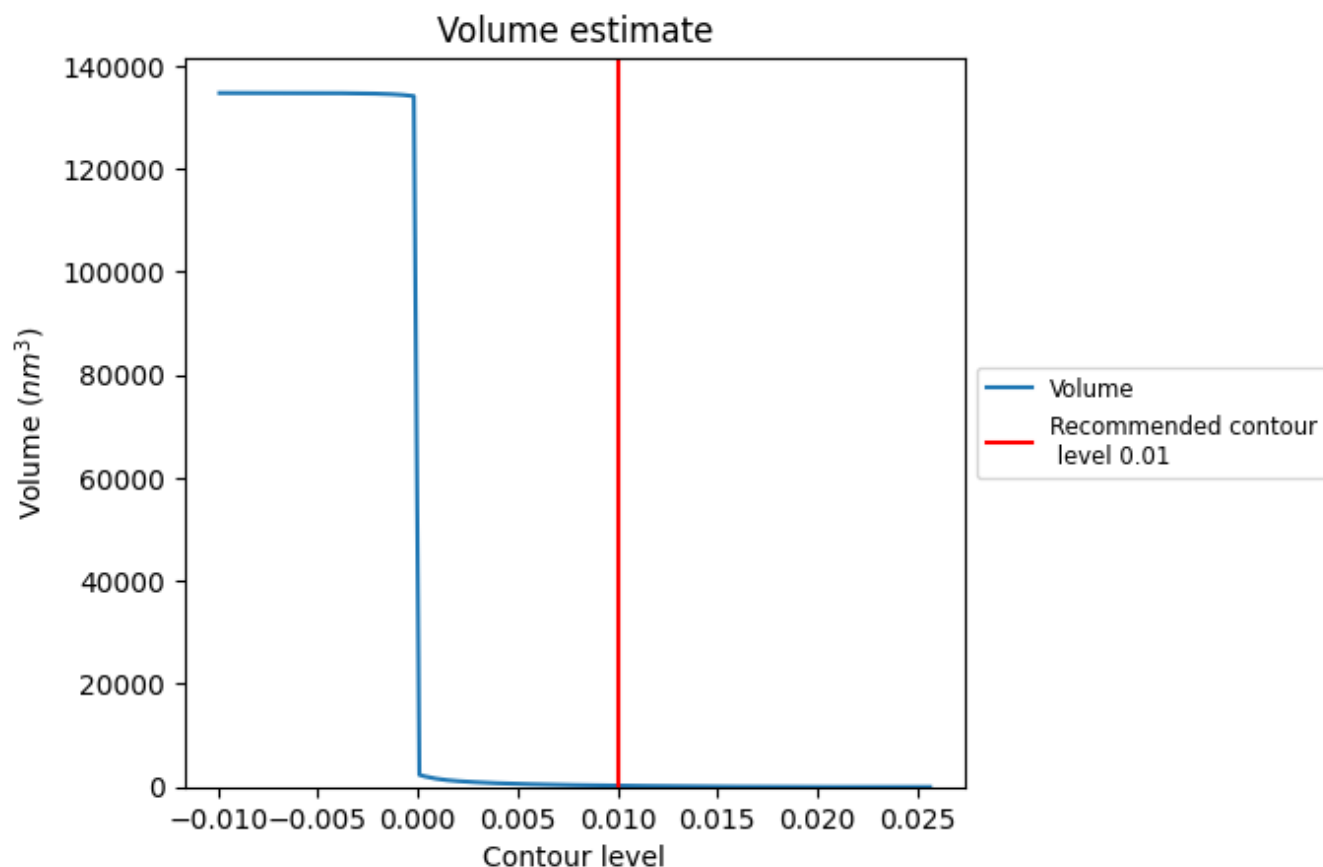
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

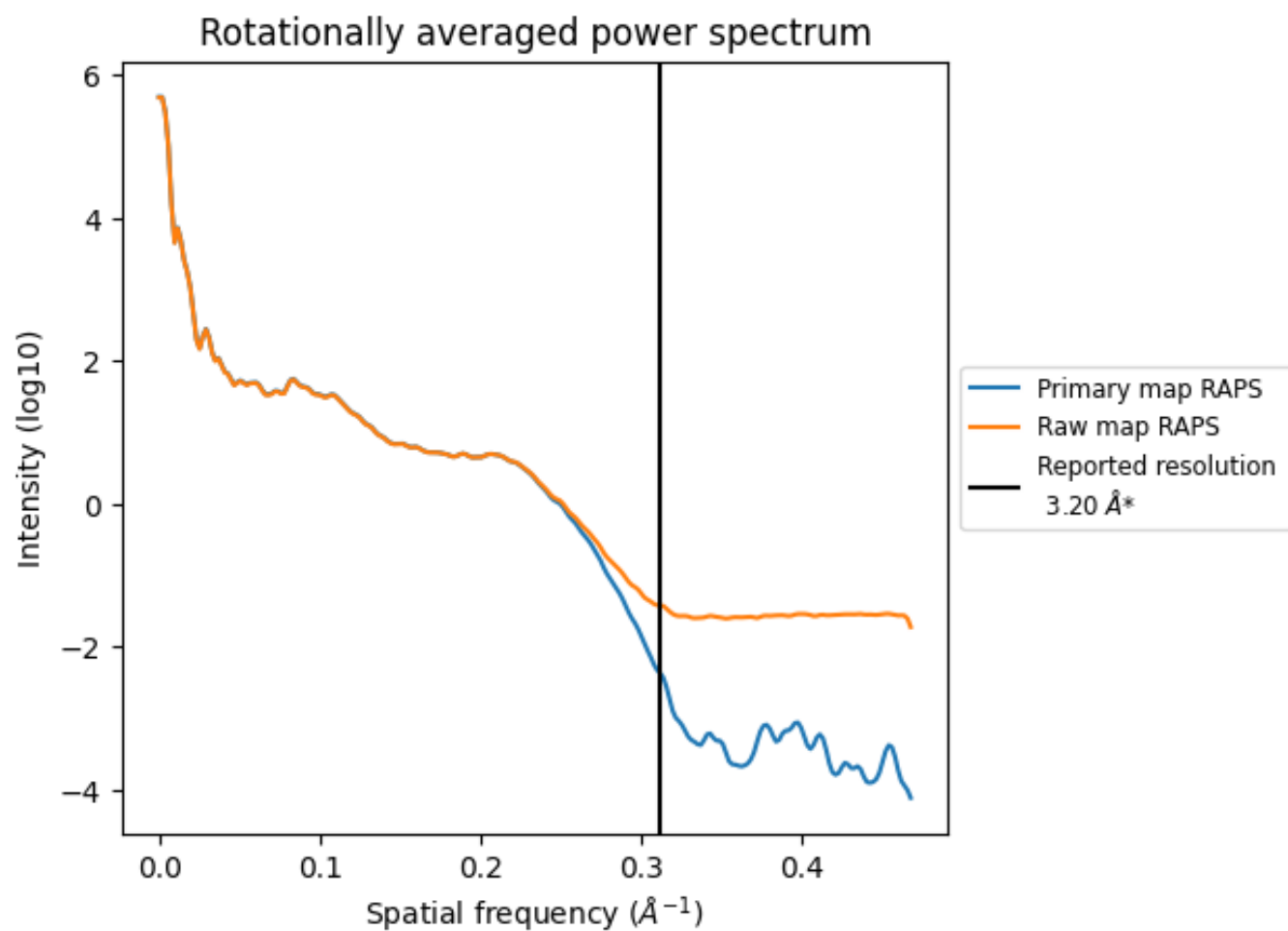
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 247  $\text{nm}^3$ ; this corresponds to an approximate mass of 223 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

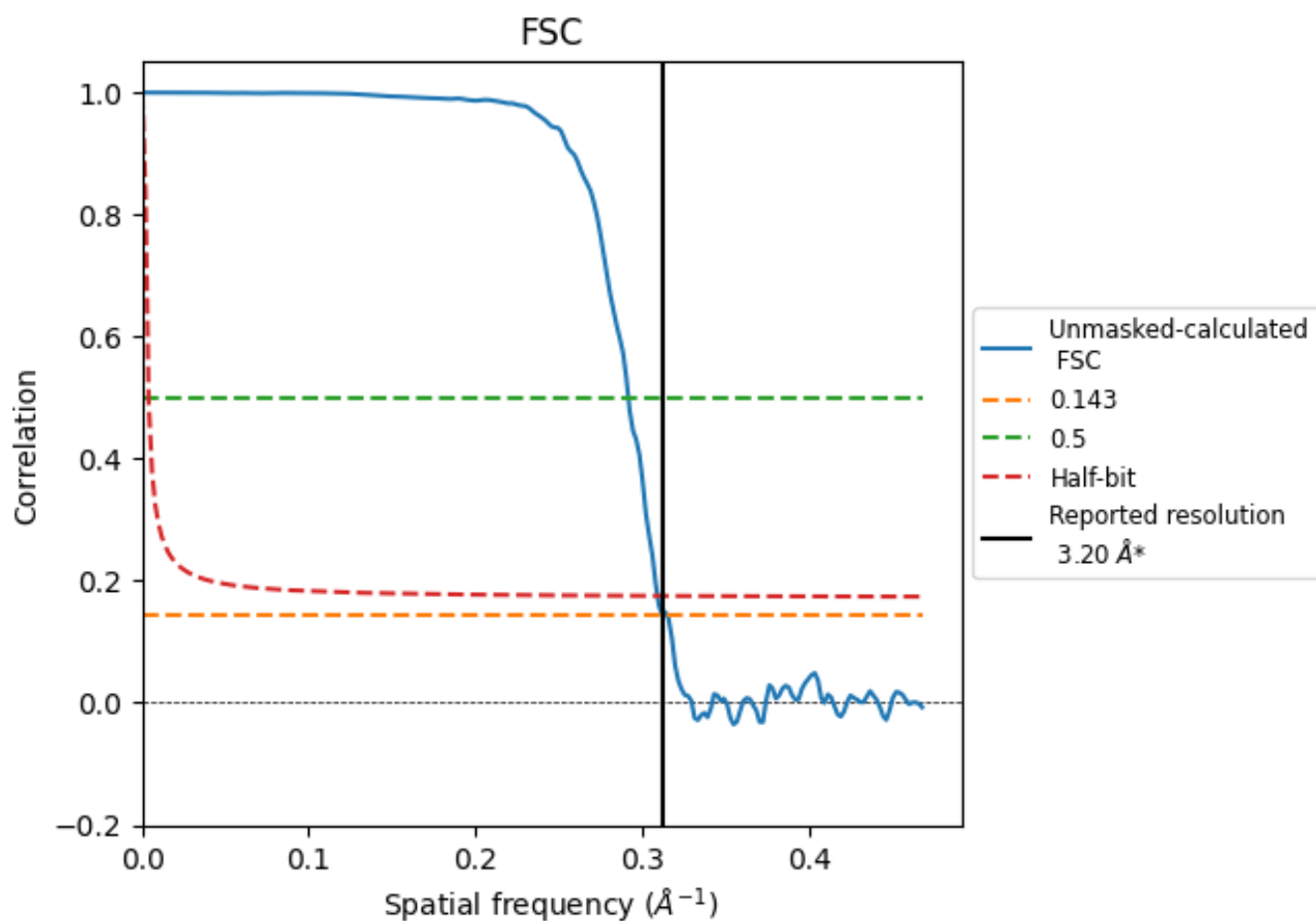


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.312  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

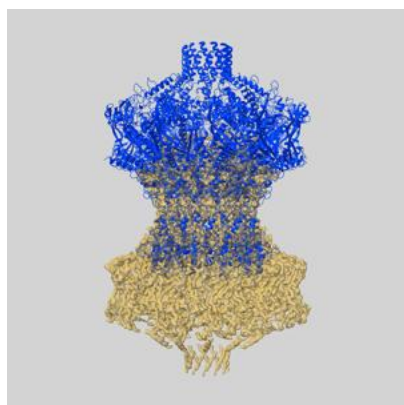
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.17	3.43	3.23

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

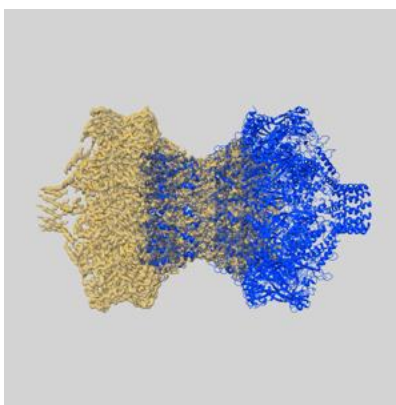
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27792 and PDB model 8EAO. Per-residue inclusion information can be found in section [3](#) on page [6](#).

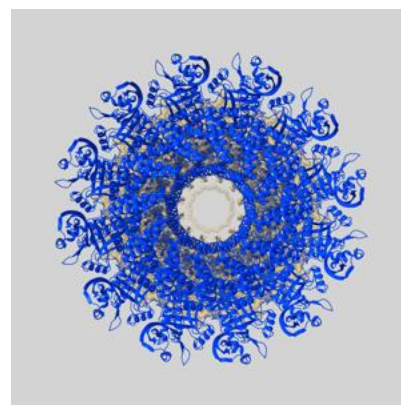
### 9.1 Map-model overlay [i](#)



X



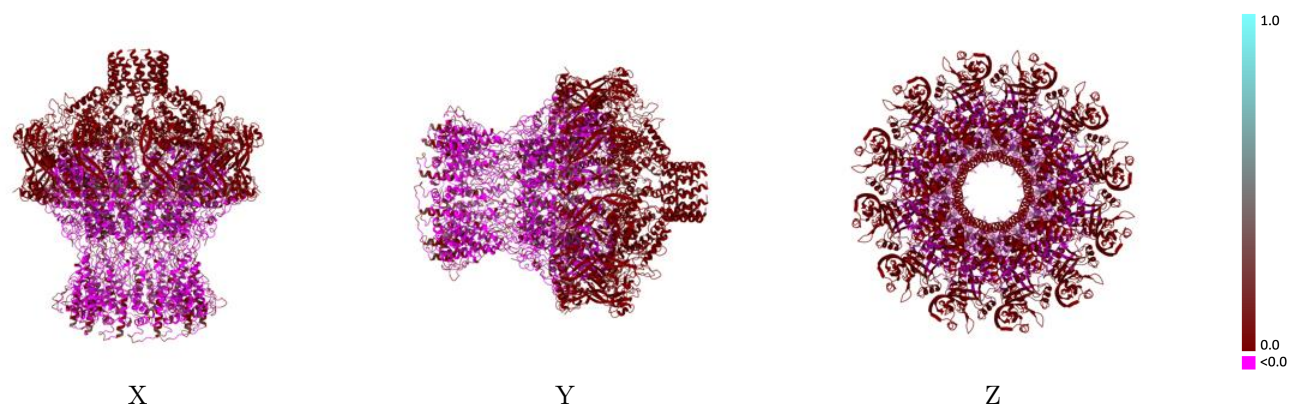
Y



Z

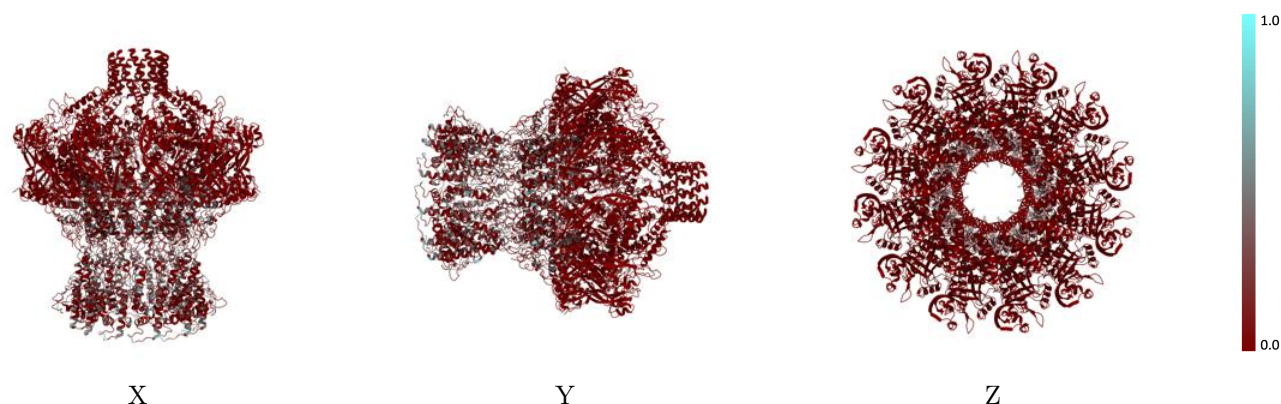
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



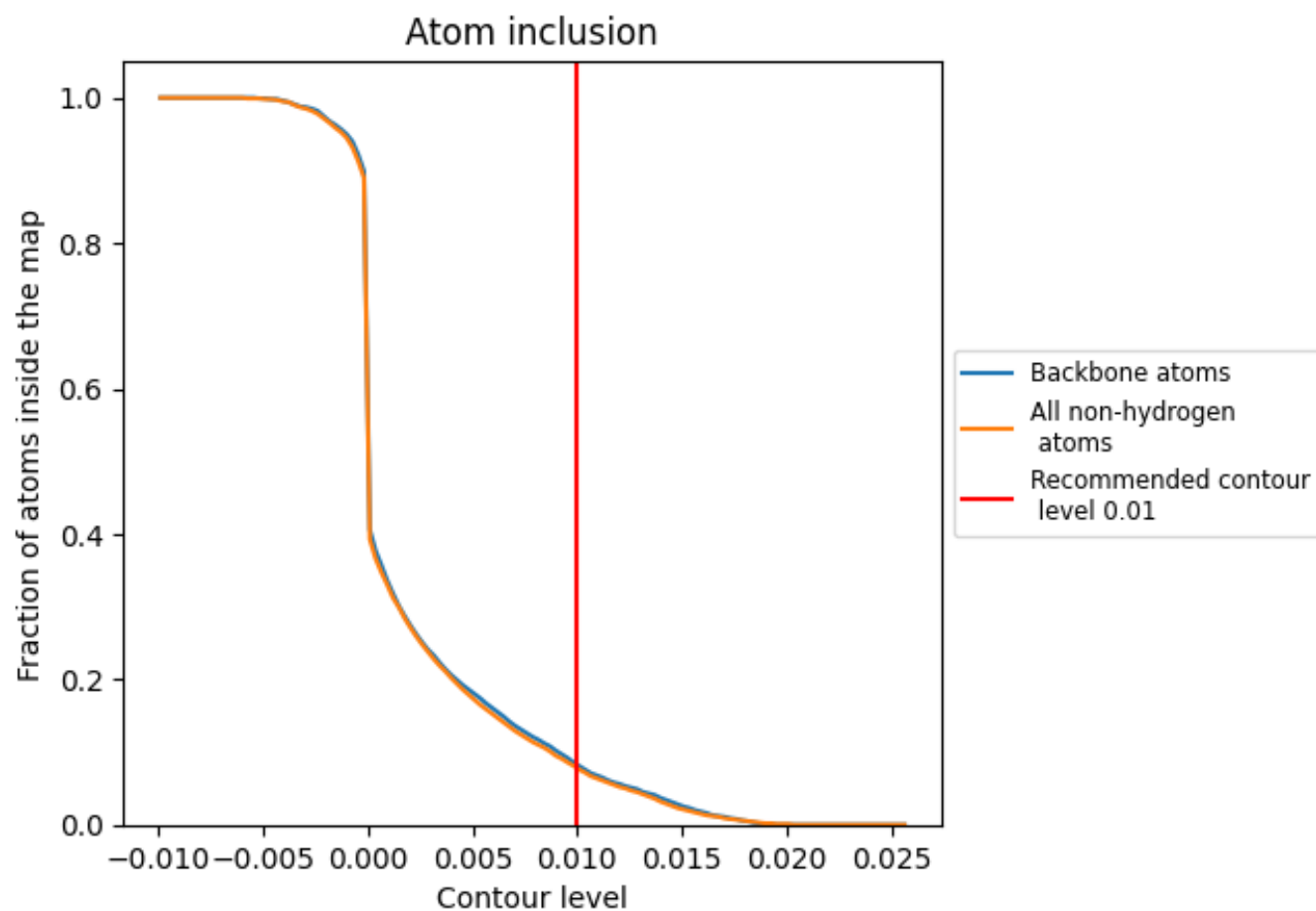
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

## 9.4 Atom inclusion [i](#)





















































At the recommended contour level, 8% of all backbone atoms, 8% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0780	 -0.0150
A	 0.1730	 -0.0300
B	 0.0550	 -0.0110
C	 0.1700	 -0.0350
D	 0.0560	 -0.0110
E	 0.1730	 -0.0320
F	 0.0570	 -0.0120
G	 0.1700	 -0.0280
H	 0.0560	 -0.0110
I	 0.1700	 -0.0360
J	 0.0560	 -0.0120
K	 0.1720	 -0.0310
L	 0.0550	 -0.0110
M	 0.1710	 -0.0270
N	 0.0550	 -0.0120
O	 0.1700	 -0.0350
P	 0.0560	 -0.0110
Q	 0.1750	 -0.0310
R	 0.0560	 -0.0110
S	 0.1710	 -0.0290
T	 0.0550	 -0.0110
U	 0.1730	 -0.0360
V	 0.0550	 -0.0110
W	 0.1690	 -0.0350
X	 0.0560	 -0.0110

