Full wwPDB EM Validation Report ⓘ

Nov 3, 2026 – 04:14 pm GMT

PDB ID	:	31LI / pdb_000031li
EMDB ID	:	EMD-58505
Title	:	Yersinia entomophaga holotoxin in its prepore state
Authors	:	Ng'ang'a, P.N.; Raunser, S.; Bader, R.; Sitsel, O.
Deposited on	:	2026-06-11
Resolution	:	3.13 Å(reported)
Based on initial models	:	4DWS, 6OGD, 3OA5, 6H6E

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

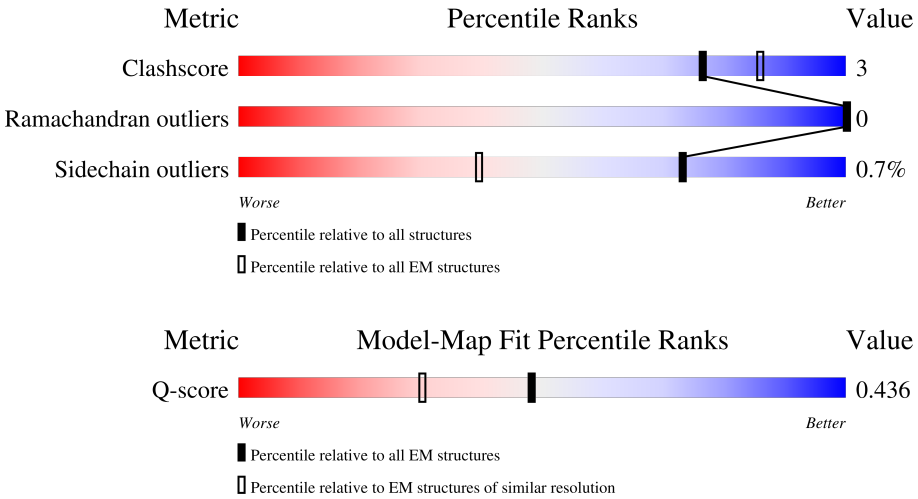
EMDB validation analysis	:	0.0.1.dev133
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.13 Å.

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



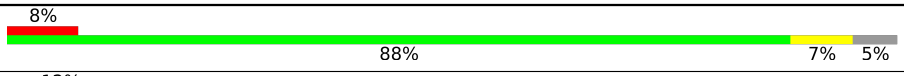
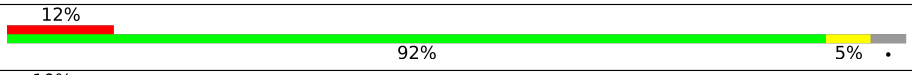
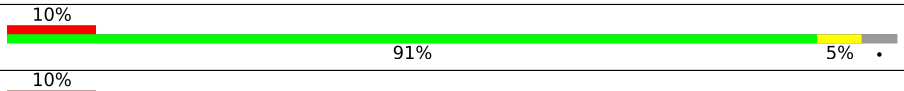
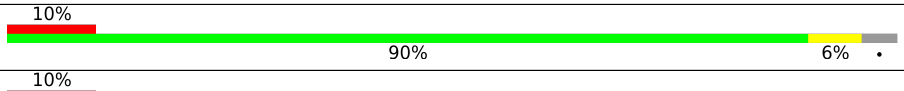
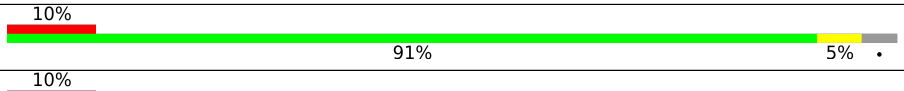
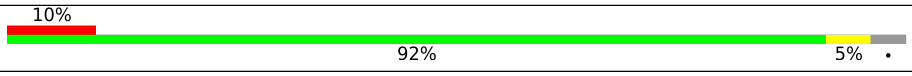
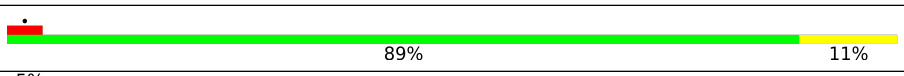
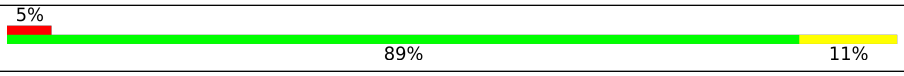
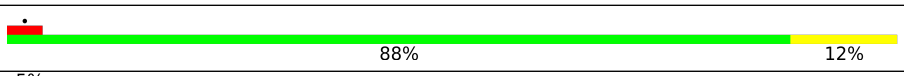
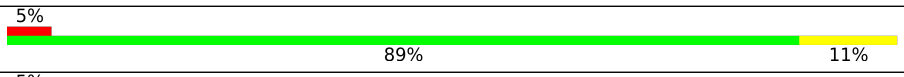
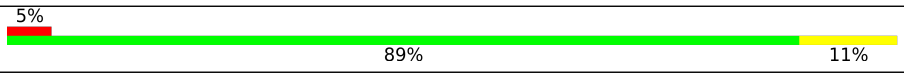
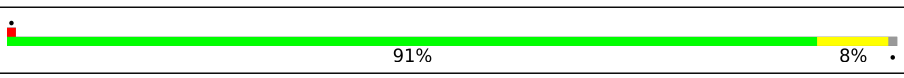
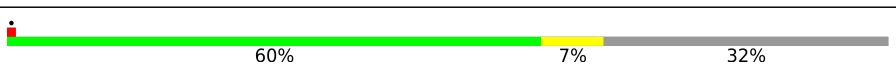
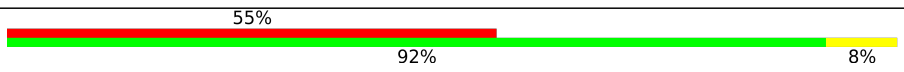
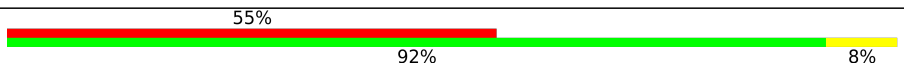
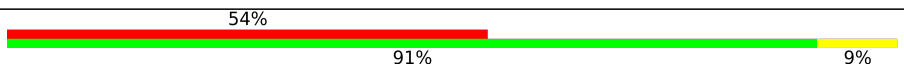
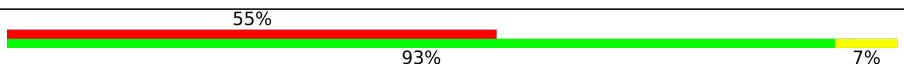
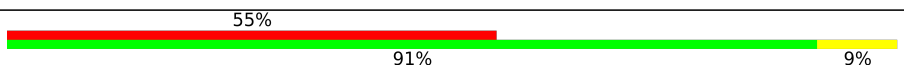
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 (2.63 - 3.63)

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

Mol	Chain	Length	Quality of chain
1	A	1164	8% 90% 5% 5%
1	F	1164	8% 88% 6% 5%
1	I	1164	8% 88% 6% 5%
1	L	1164	8% 89% 6% 5%

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Mol	Chain	Length	Quality of chain
1	O	1164	
2	B	1364	
2	G	1364	
2	J	1364	
2	M	1364	
2	P	1364	
3	C	633	
3	H	633	
3	K	633	
3	N	633	
3	Q	633	
4	D	1487	
5	E	970	
6	R	542	
6	S	542	
6	T	542	
6	U	542	
6	V	542	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 159282 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 Toxin subunit YenA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1104	Total 8691	C 5545	N 1440	O 1682	S 24	0	0
1	F	1104	Total 8691	C 5545	N 1440	O 1682	S 24	0	0
1	I	1104	Total 8691	C 5545	N 1440	O 1682	S 24	0	0
1	L	1104	Total 8691	C 5545	N 1440	O 1682	S 24	0	0
1	O	1104	Total 8691	C 5545	N 1440	O 1682	S 24	0	0

- Molecule 2 is a protein called Toxin subunit YenA2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1316	Total 10631	C 6739	N 1786	O 2068	S 38	0	0
2	G	1316	Total 10631	C 6739	N 1786	O 2068	S 38	0	0
2	J	1316	Total 10631	C 6739	N 1786	O 2068	S 38	0	0
2	M	1316	Total 10631	C 6739	N 1786	O 2068	S 38	0	0
2	P	1316	Total 10631	C 6739	N 1786	O 2068	S 38	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	351	THR	-	insertion	UNP B6A878
B	?	-	PRO	deletion	UNP B6A878
G	351	THR	-	insertion	UNP B6A878
G	?	-	PRO	deletion	UNP B6A878
J	351	THR	-	insertion	UNP B6A878
J	?	-	PRO	deletion	UNP B6A878

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Chain	Residue	Modelled	Actual	Comment	Reference
M	351	THR	-	insertion	UNP B6A878
M	?	-	PRO	deletion	UNP B6A878
P	351	THR	-	insertion	UNP B6A878
P	?	-	PRO	deletion	UNP B6A878

- Molecule 3 is a protein called Chitinase 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	H	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	K	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	N	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		
3	Q	633	Total	C	N	O	S	0	0
			4914	3107	824	964	19		

- Molecule 4 is a protein called Toxin subunit YenB.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	1474	Total	C	N	O	S	0	0
			11696	7381	2021	2258	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1484	ASP	ASN	conflict	UNP B6A880

- Molecule 5 is a protein called Toxin subunit YenC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	658	Total	C	N	O	S	0	0
			5111	3187	895	1017	12		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	109	SER	LYS	conflict	UNP B6A882

- Molecule 6 is a protein called Chitinase 1.

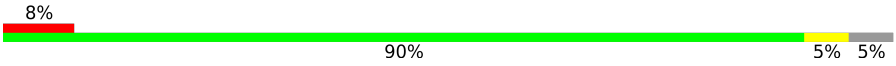
Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	542	Total	C	N	O	S	0	0
			4259	2691	706	849	13		
6	S	542	Total	C	N	O	S	0	0
			4259	2691	706	849	13		
6	T	542	Total	C	N	O	S	0	0
			4259	2691	706	849	13		
6	U	542	Total	C	N	O	S	0	0
			4259	2691	706	849	13		
6	V	542	Total	C	N	O	S	0	0
			4259	2691	706	849	13		

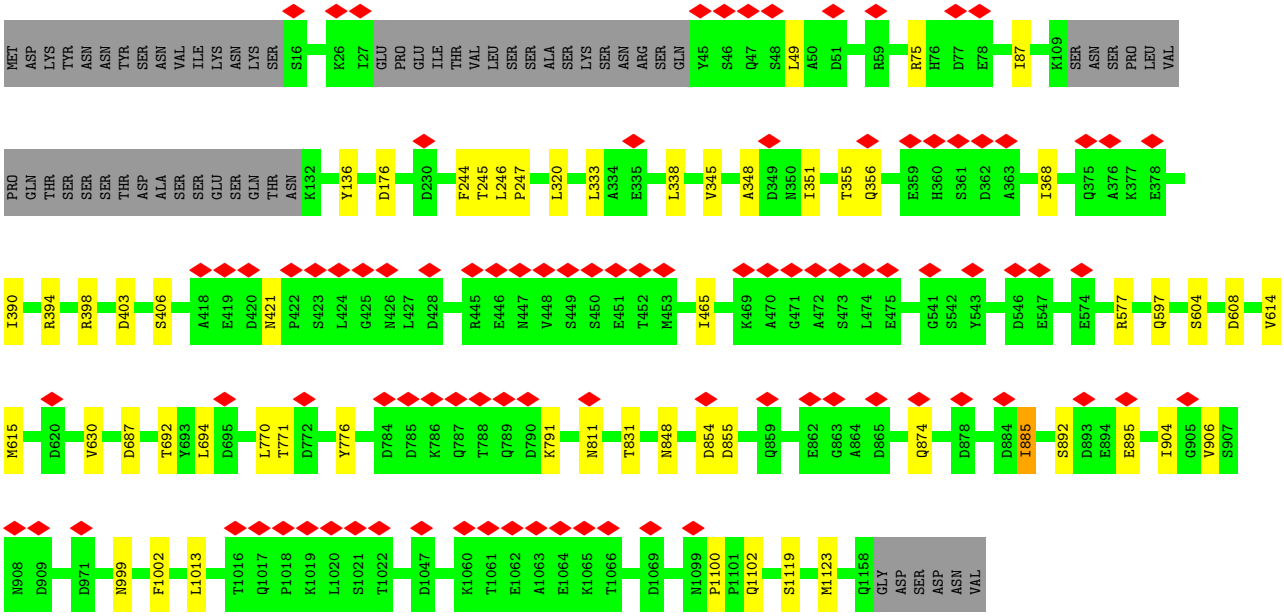
3 Residue-property plots (i)

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

• Molecule 1: Toxin subunit YenA1

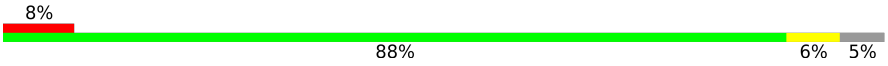
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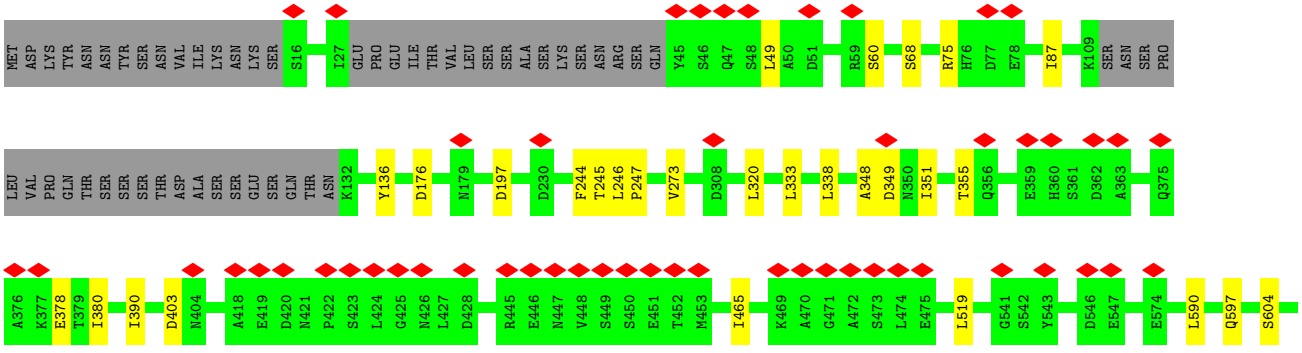


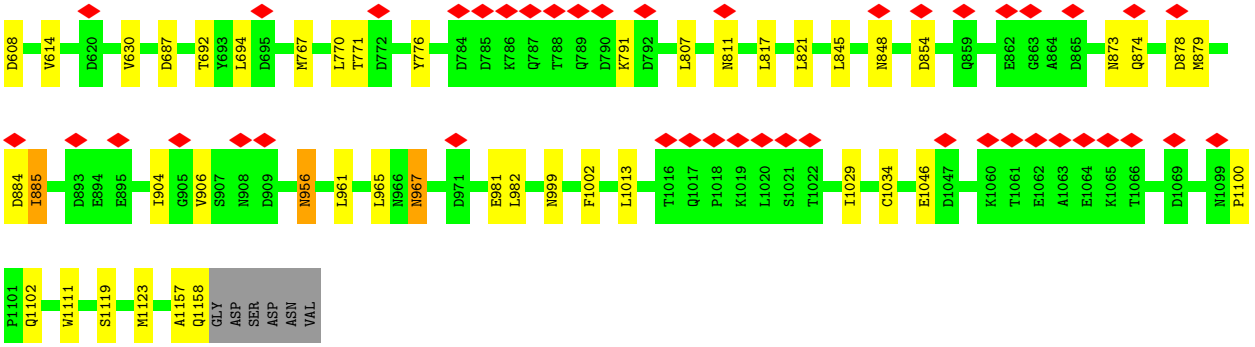


• Molecule 1: Toxin subunit YenA1

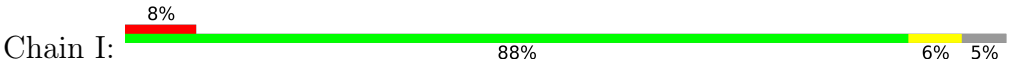
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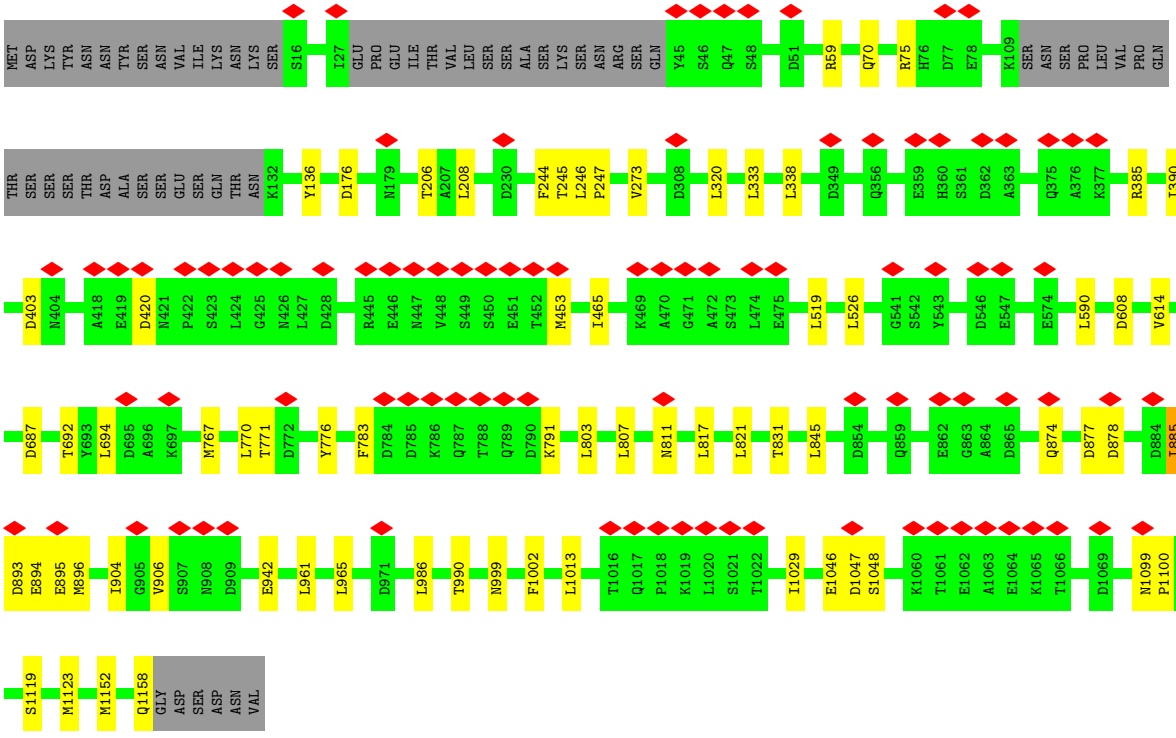




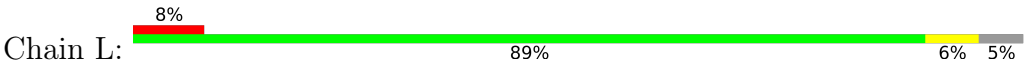


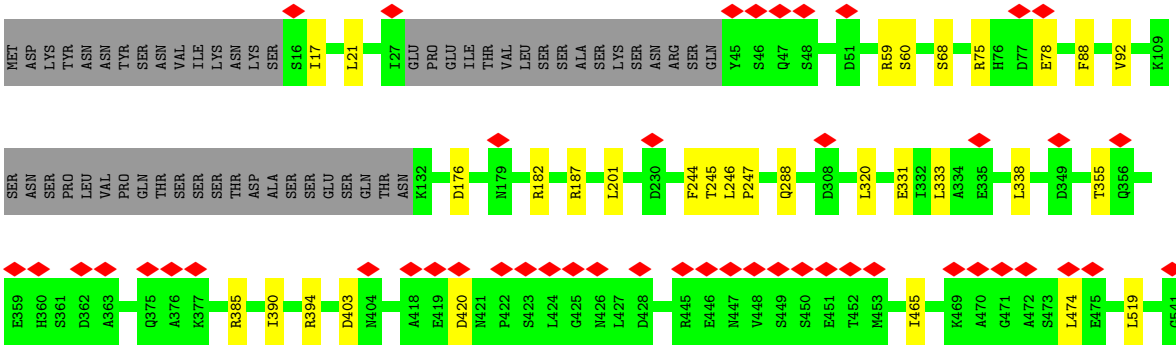
• Molecule 1: Toxin subunit YenA1

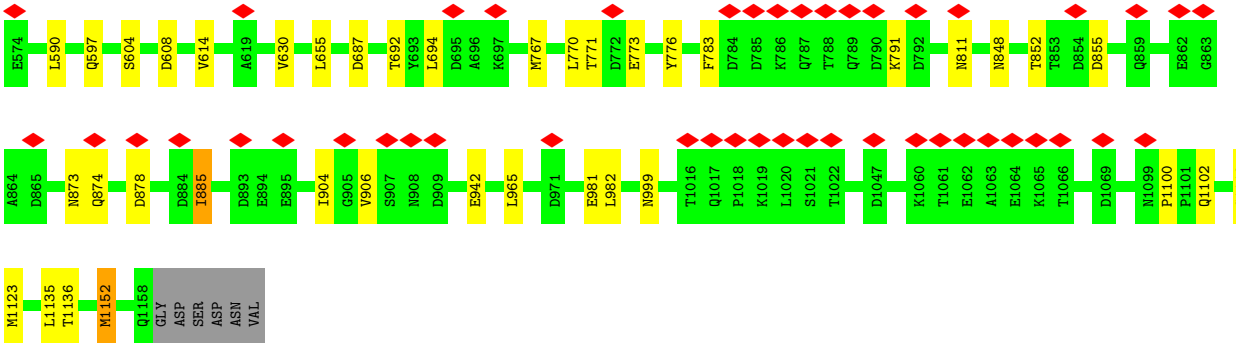




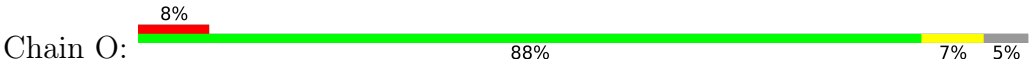
• Molecule 1: Toxin subunit YenA1

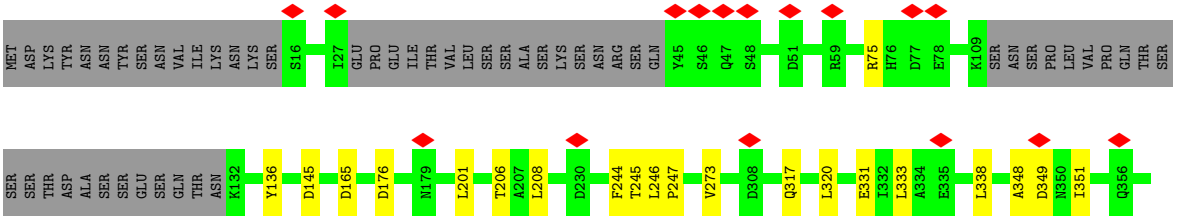


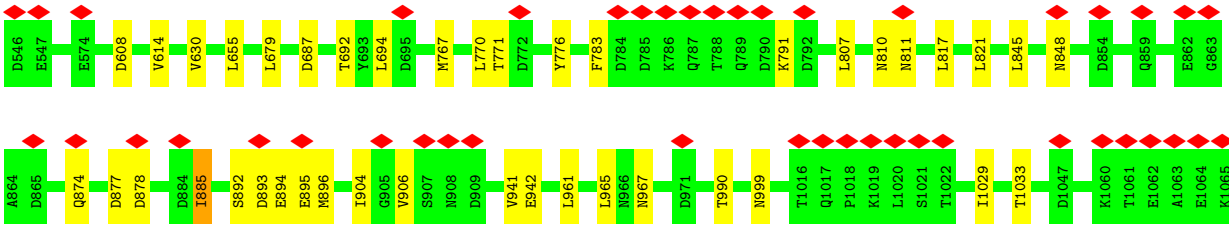




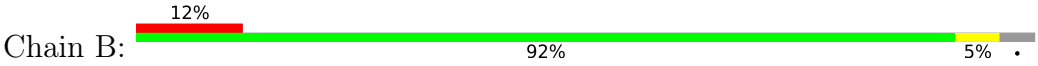
• Molecule 1: Toxin subunit YenA1

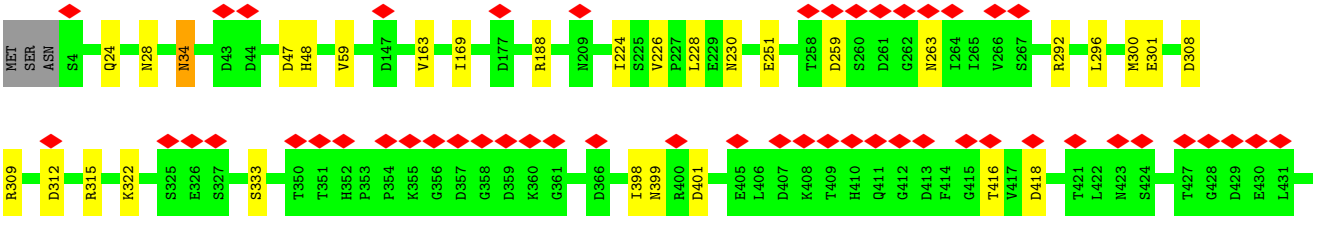


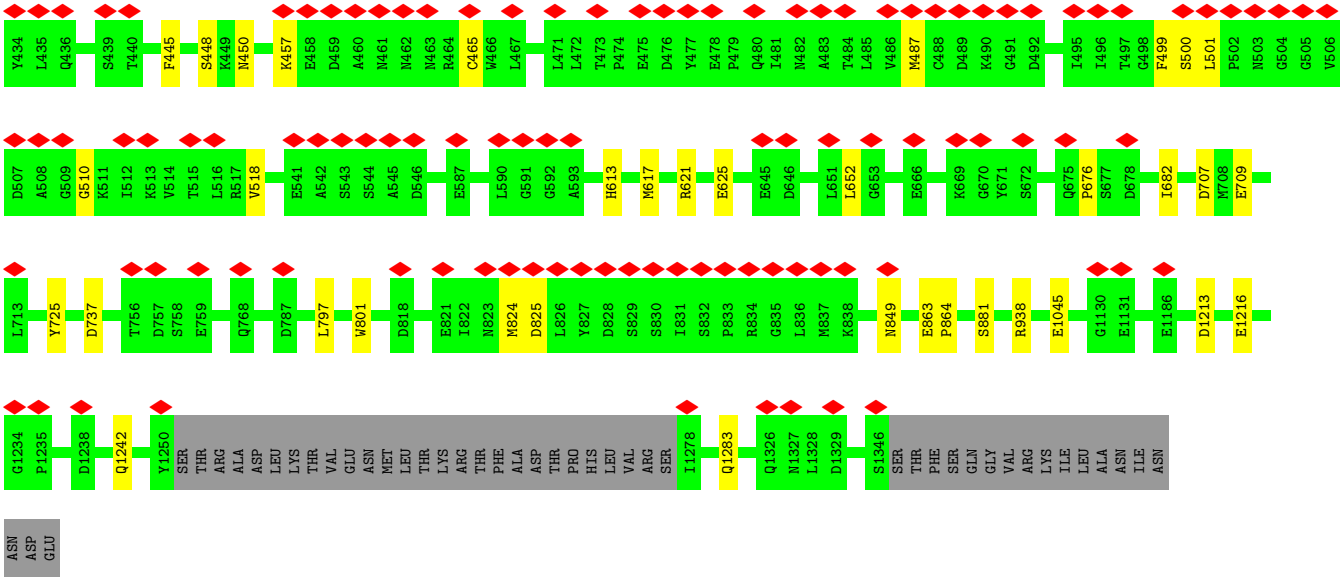




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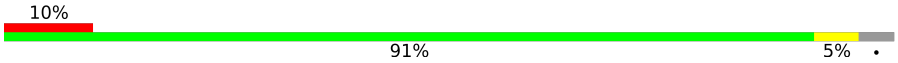


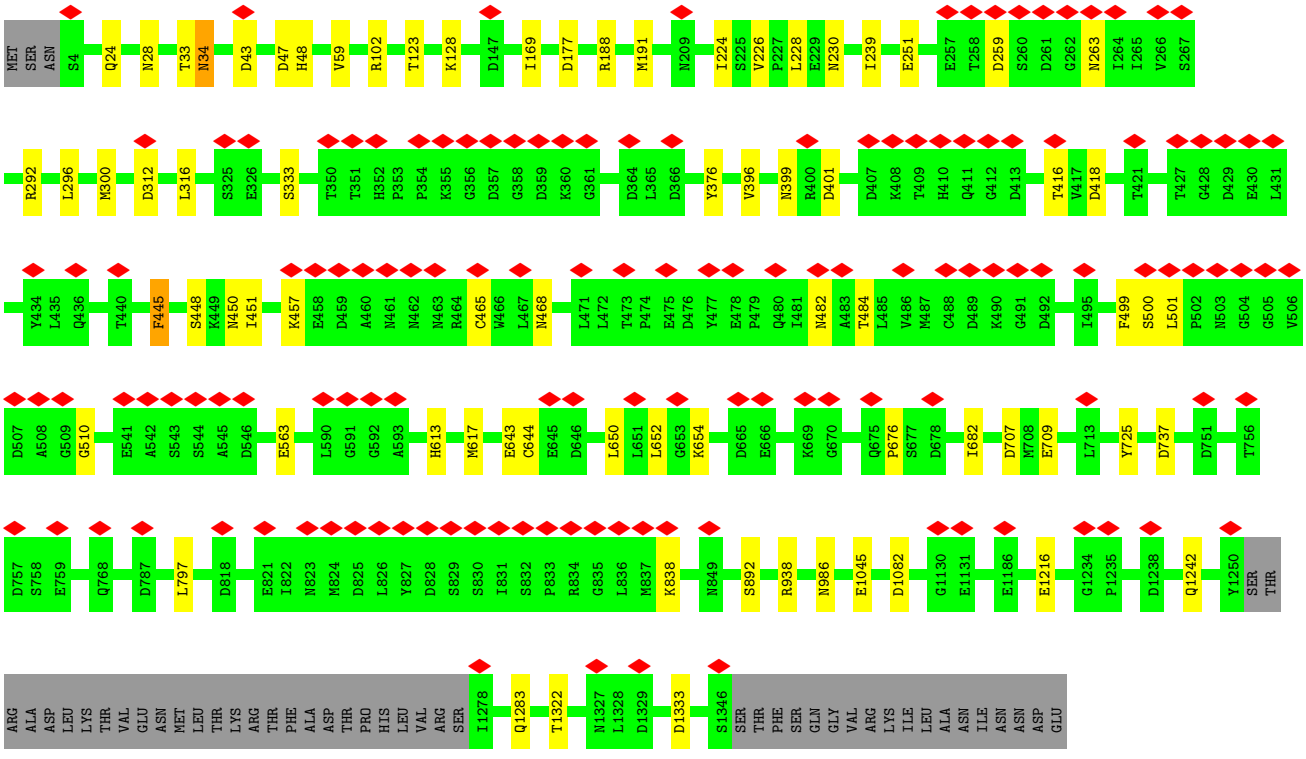




• Molecule 2: Toxin subunit YenA2

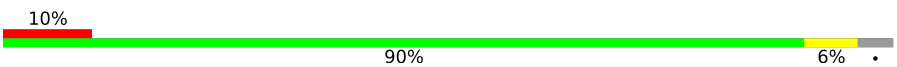
Chain G:

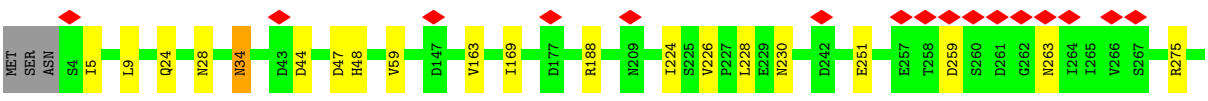


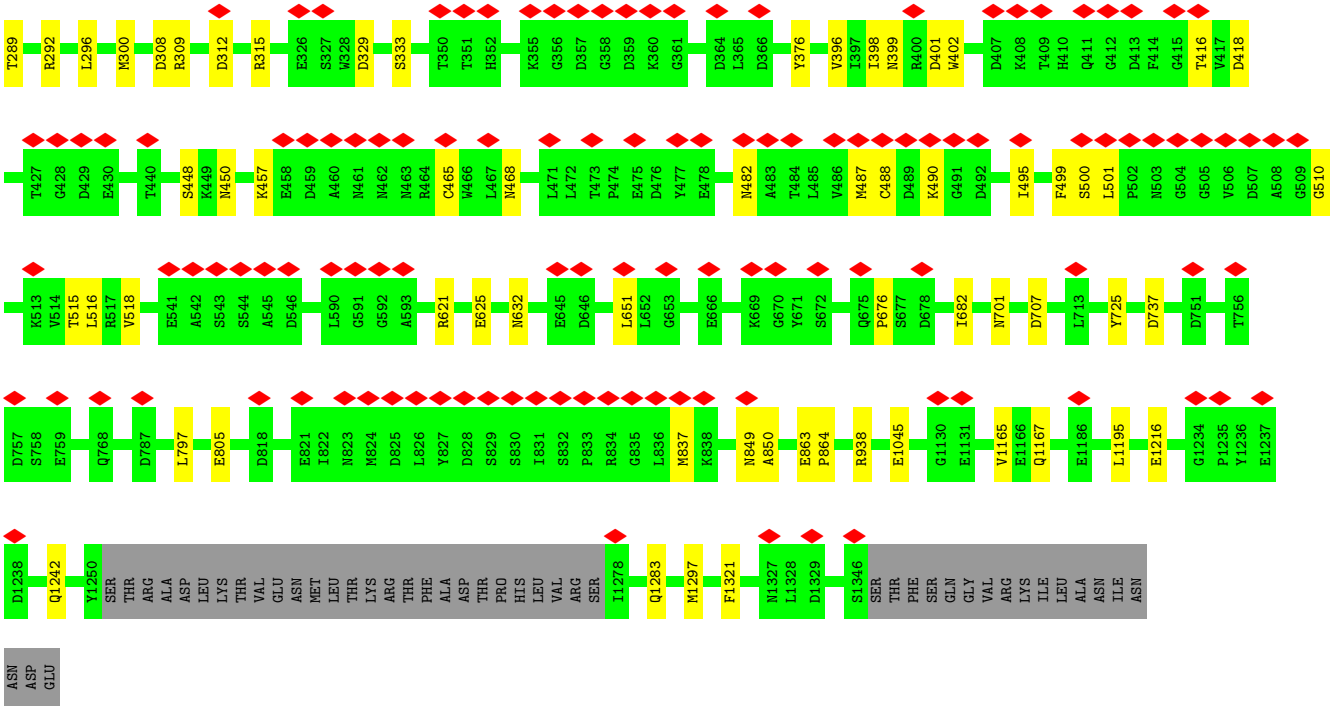


• Molecule 2: Toxin subunit YenA2

Chain J:

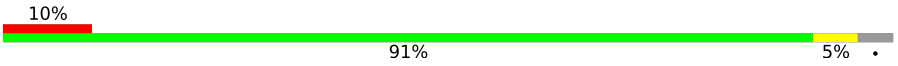


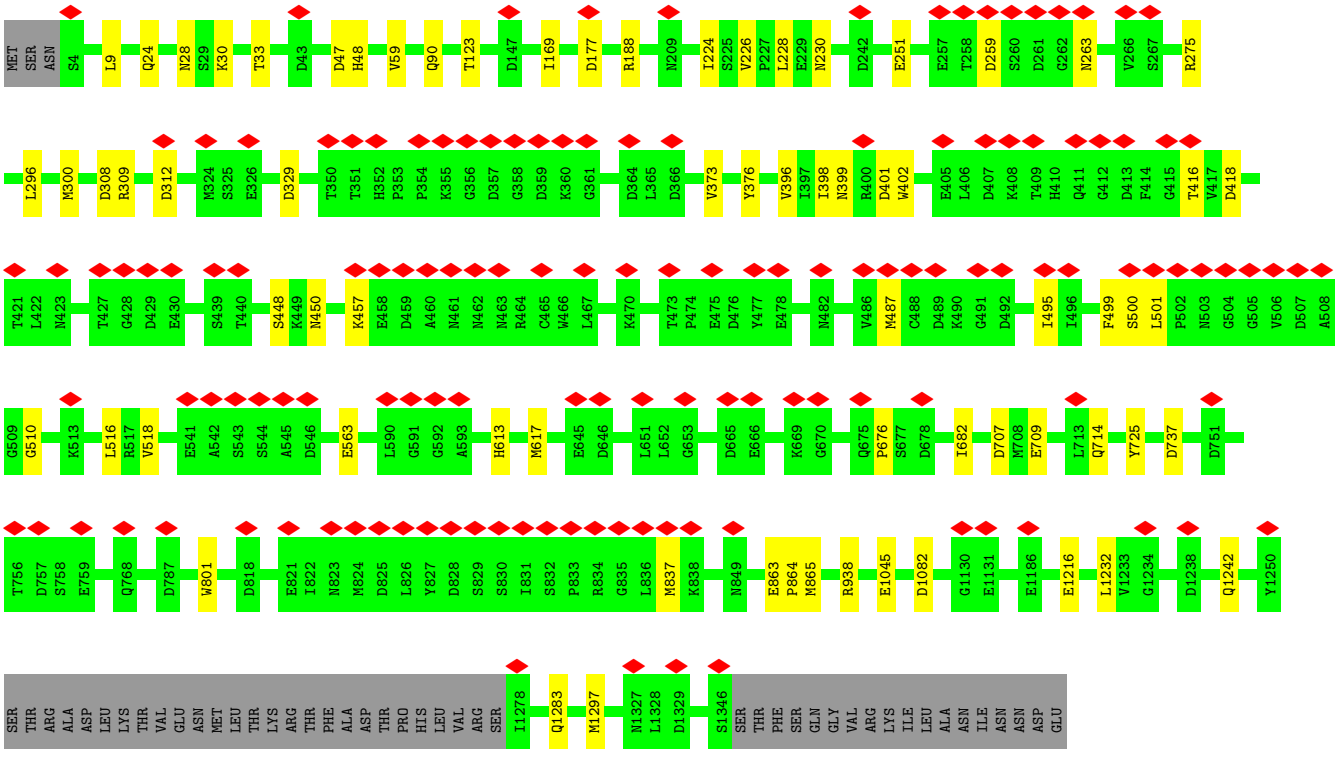




• Molecule 2: Toxin subunit YenA2

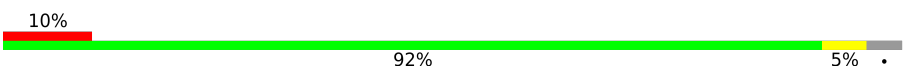
Chain M:

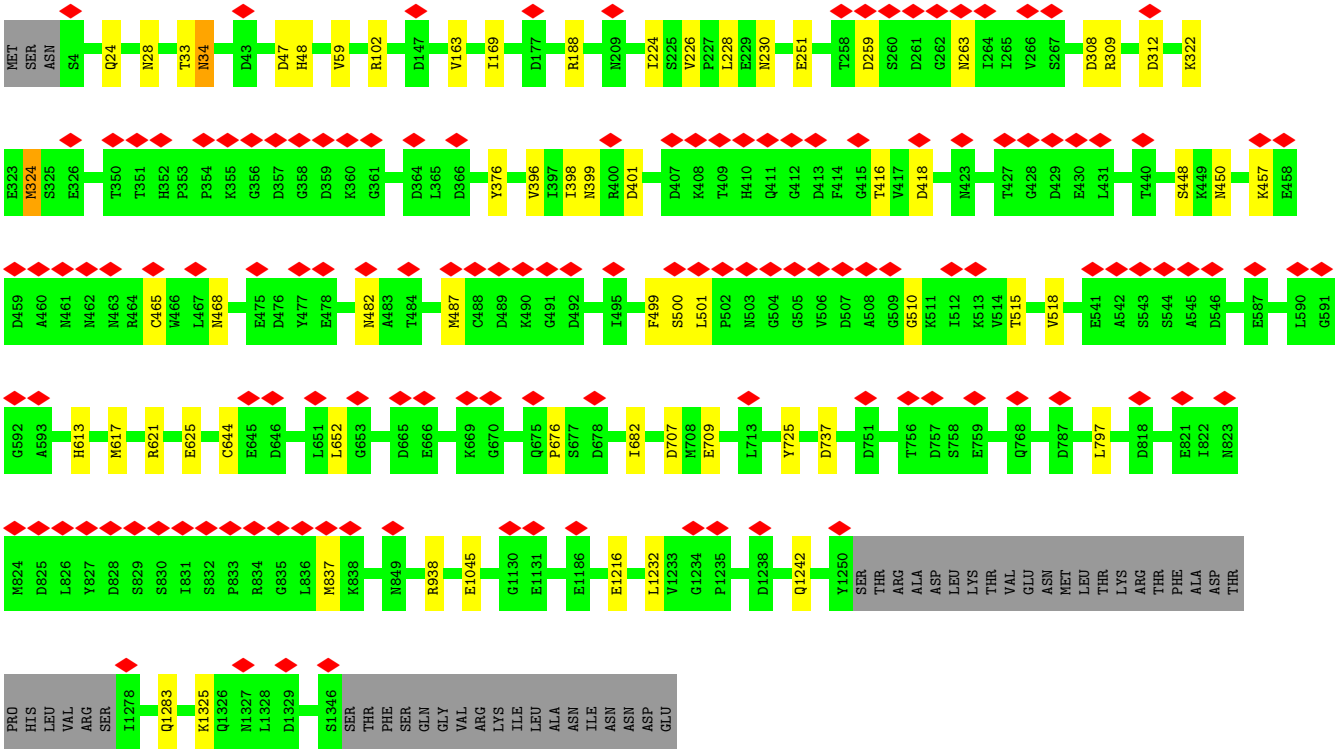




• Molecule 2: Toxin subunit YenA2

Chain P:

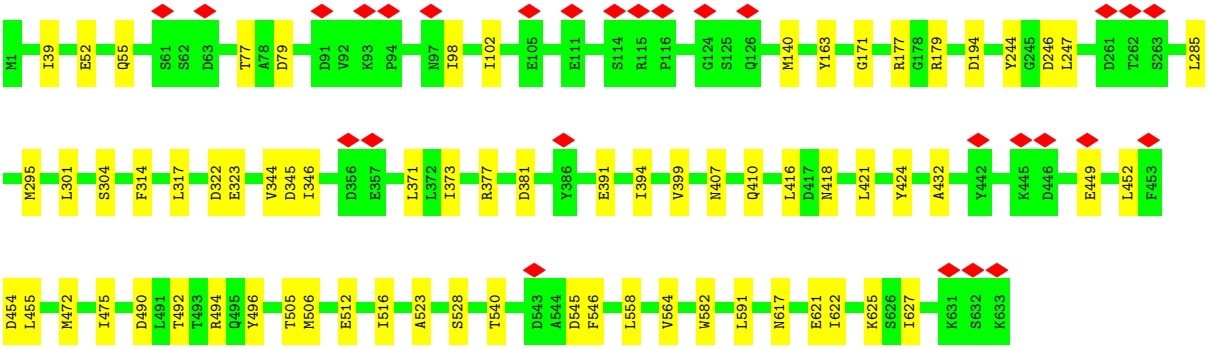




• Molecule 3: Chitinase 2

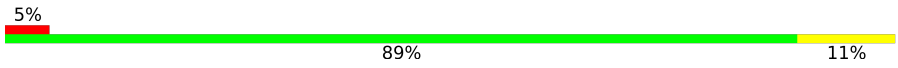
Chain C:

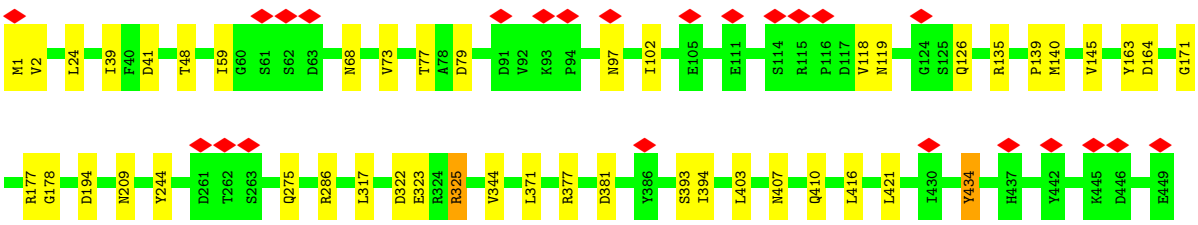


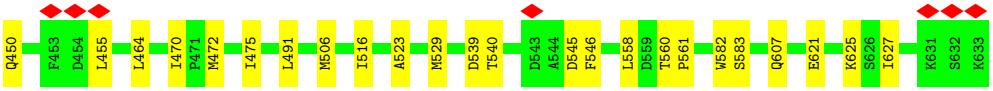


• Molecule 3: Chitinase 2

Chain H:



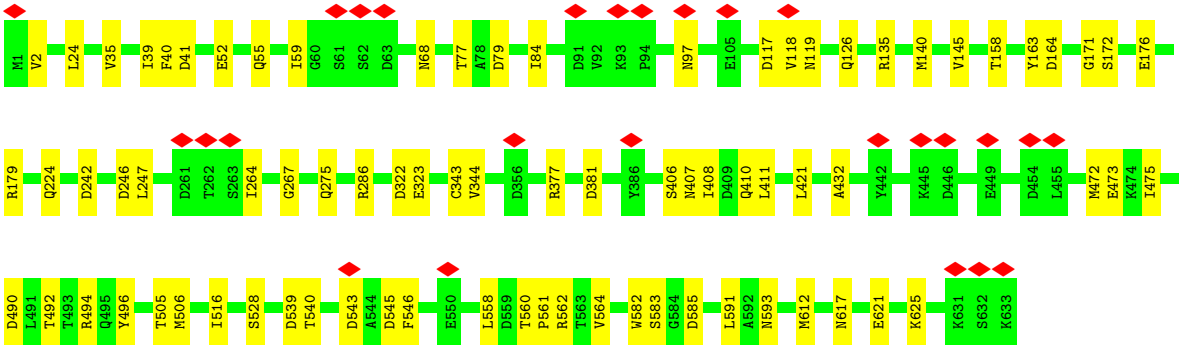




• Molecule 3: Chitinase 2

Chain K:

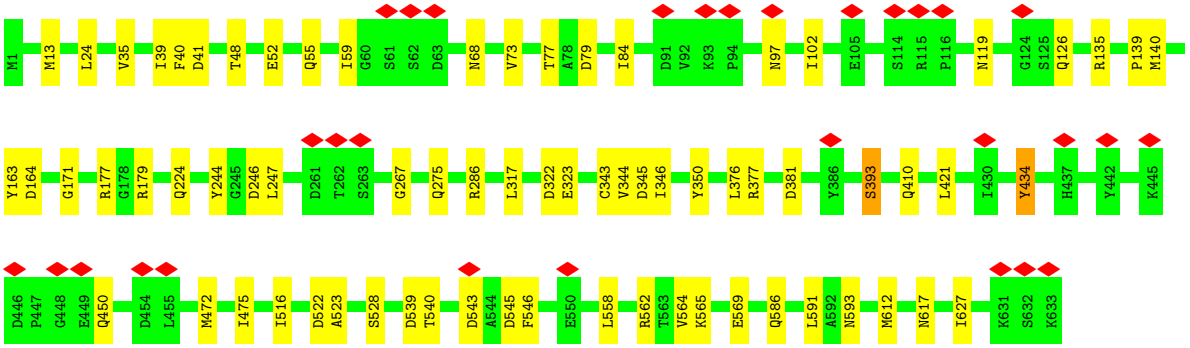




• Molecule 3: Chitinase 2

Chain N:

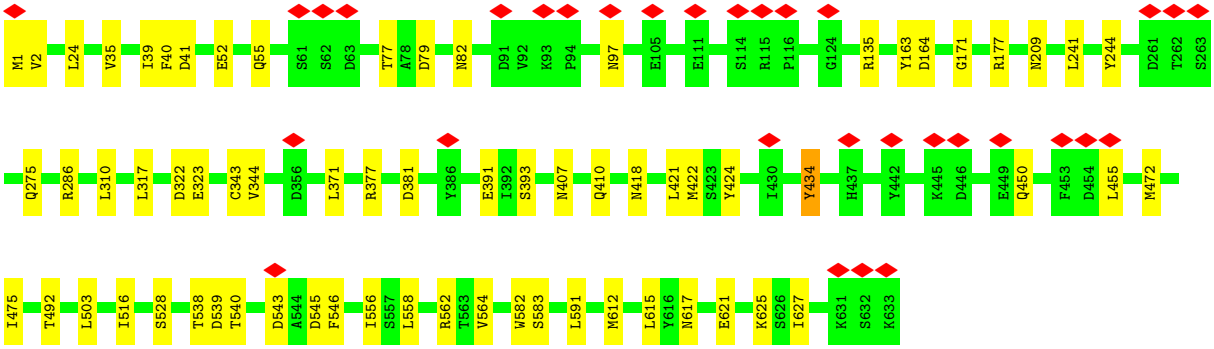




• Molecule 3: Chitinase 2

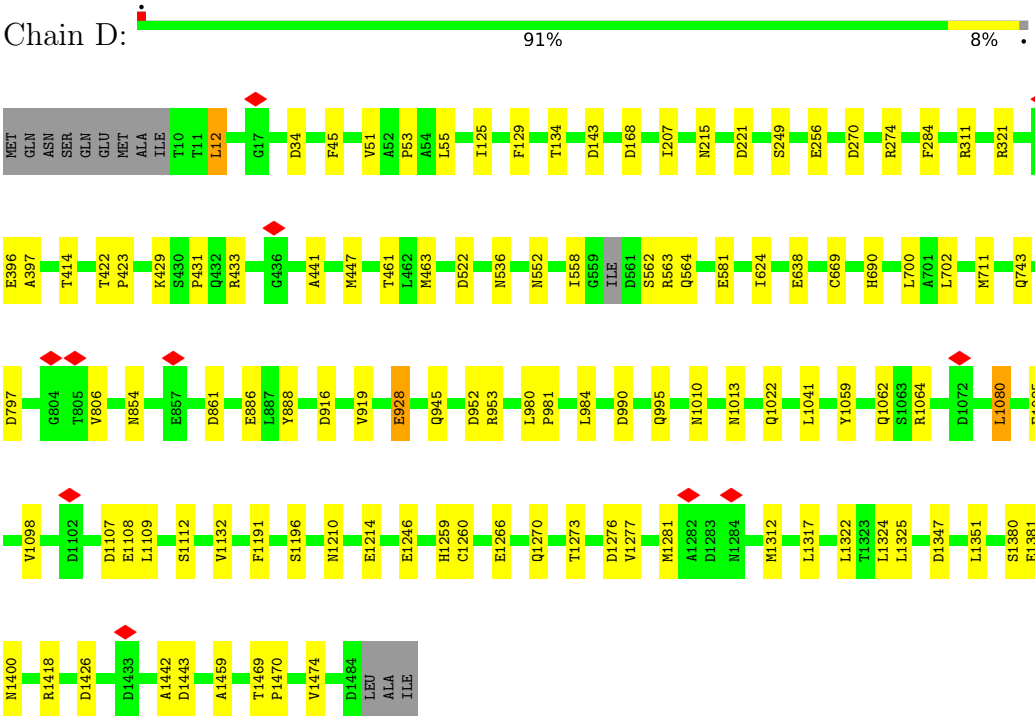
Chain Q:





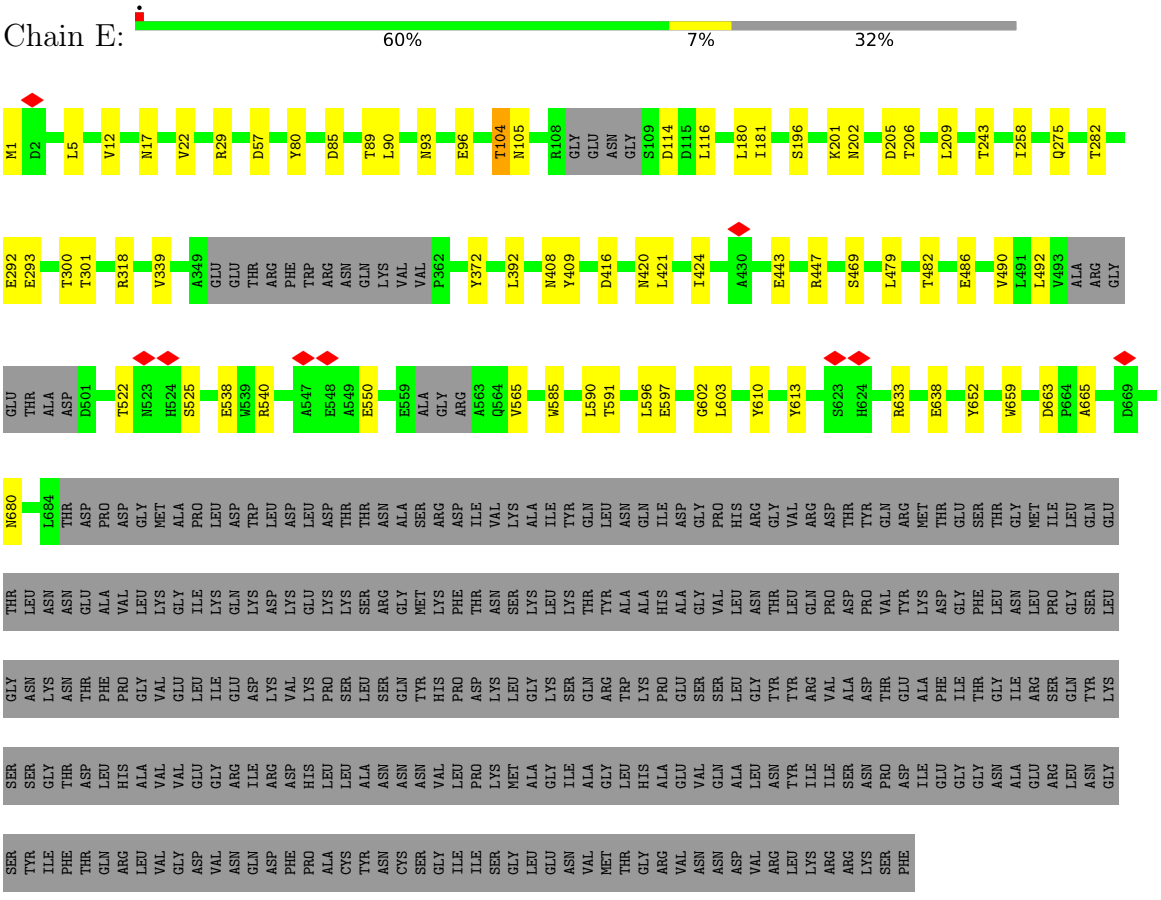
• Molecule 4: Toxin subunit YenB

Chain D:



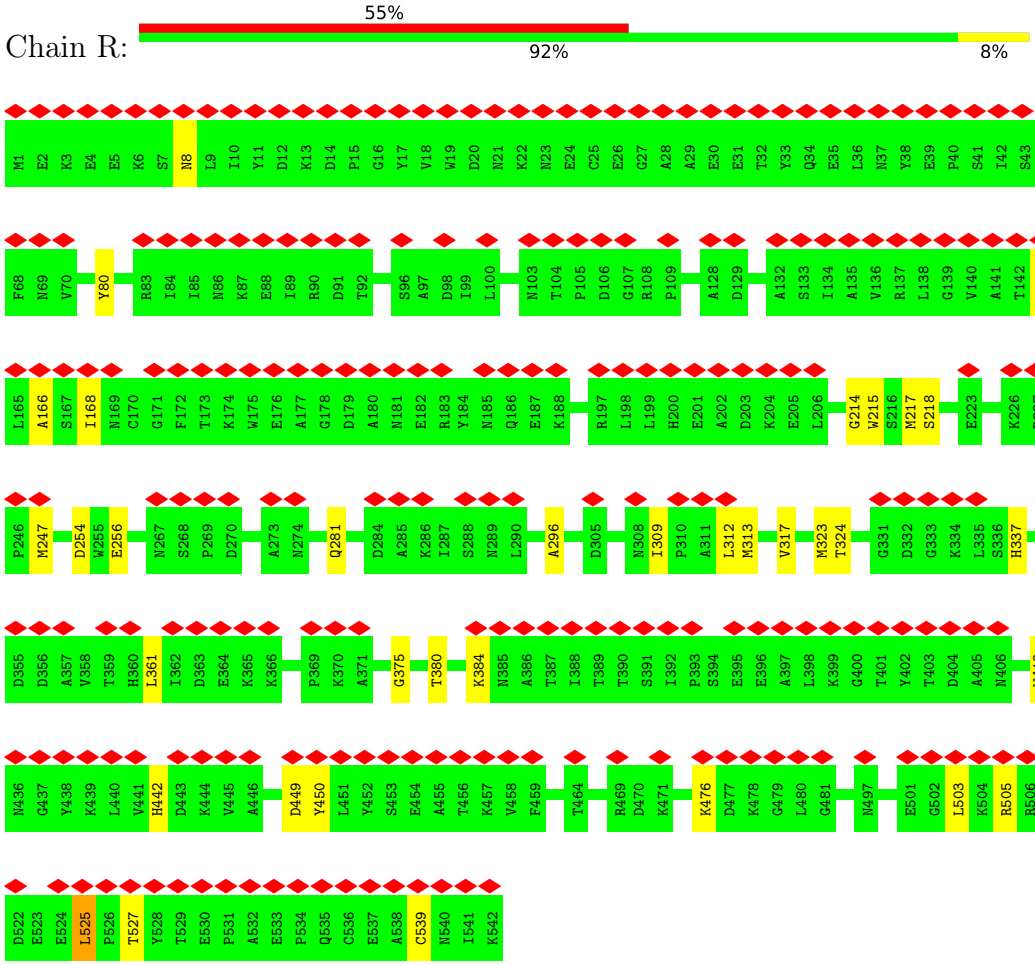
• Molecule 5: Toxin subunit YenC2

Chain E:



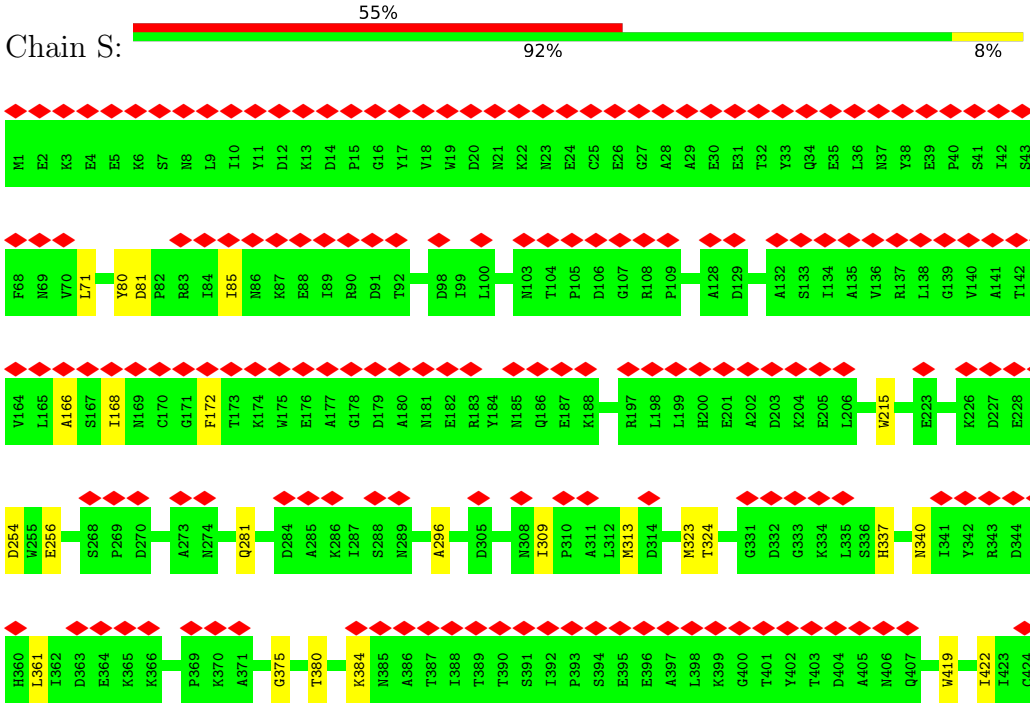
• Molecule 6: Chitinase 1

Chain R:



• Molecule 6: Chitinase 1

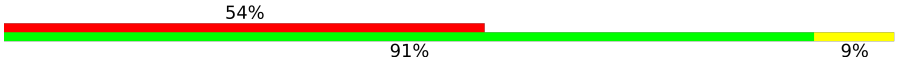
Chain S:

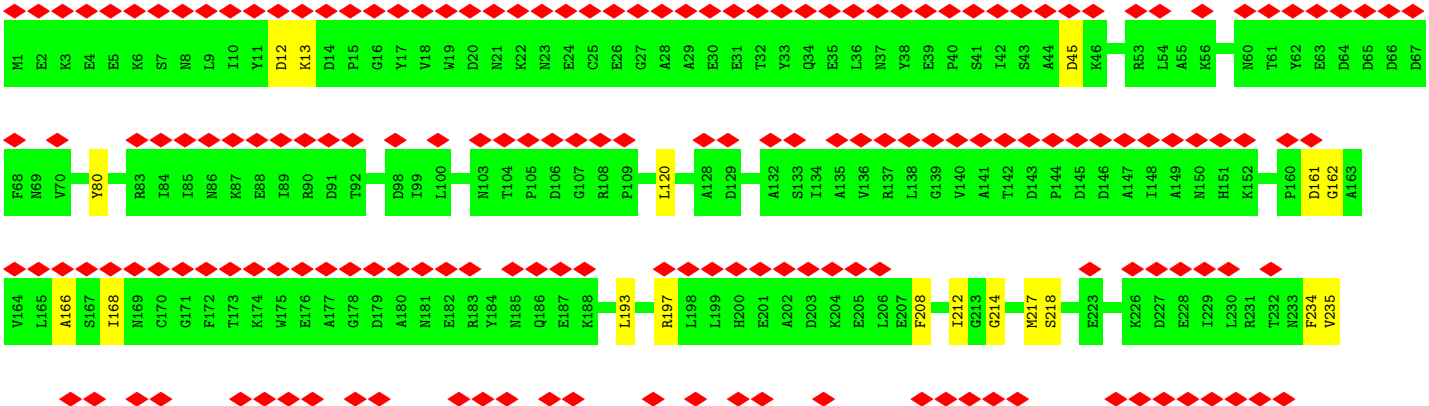




• Molecule 6: Chitinase 1

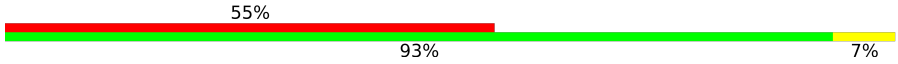
Chain T:

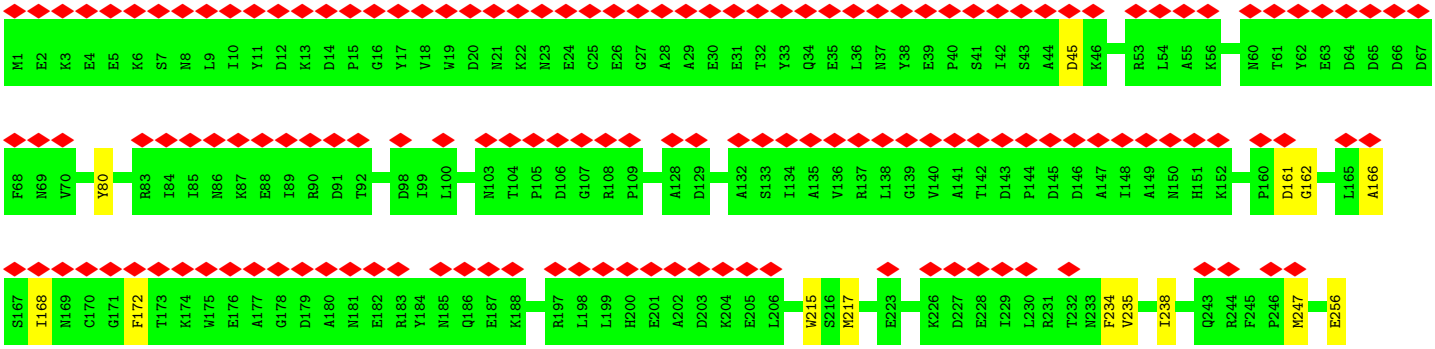


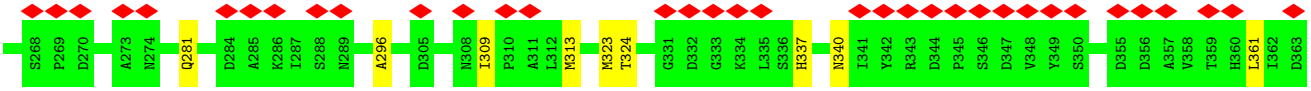


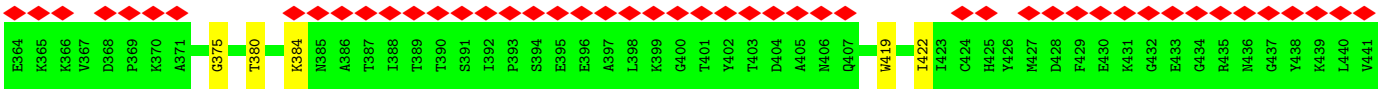
• Molecule 6: Chitinase 1

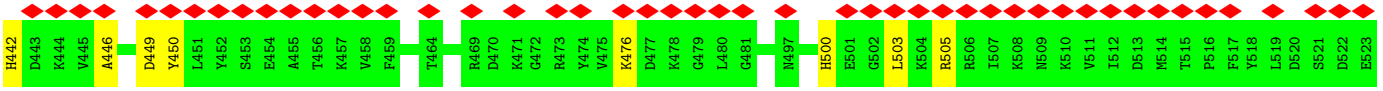
Chain U:

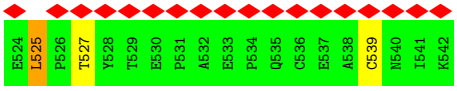




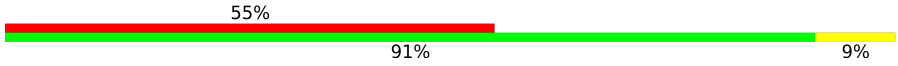


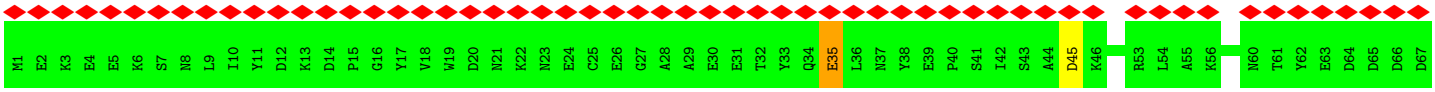


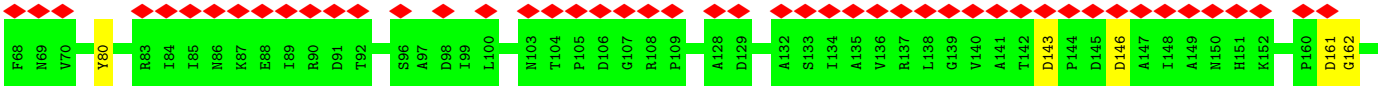


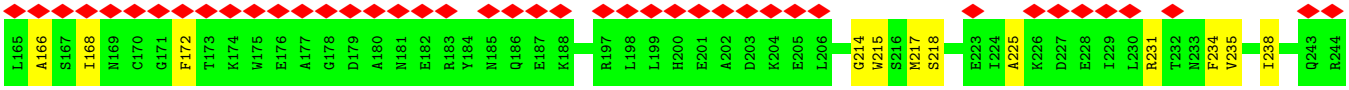


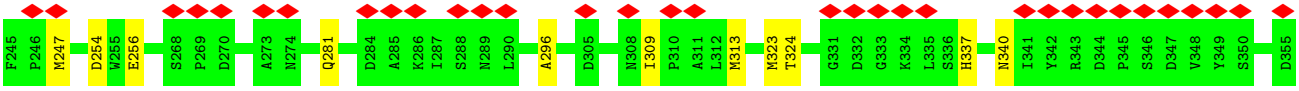
• Molecule 6: Chitinase 1

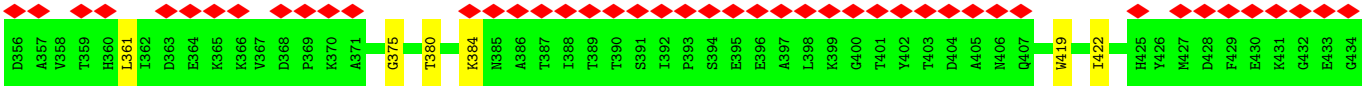


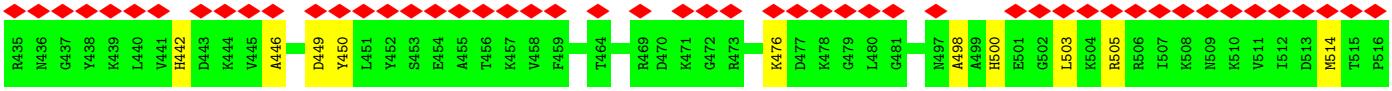


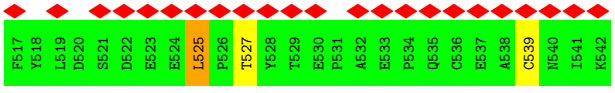












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	837287	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	64.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.923	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0969	Depositor
Map size (Å)	563.2, 563.2, 563.2	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.09	0/8856	0.21	0/12030
1	F	0.09	0/8856	0.21	0/12030
1	I	0.09	0/8856	0.21	0/12030
1	L	0.09	0/8856	0.22	0/12030
1	O	0.09	0/8856	0.21	0/12030
2	B	0.09	0/10854	0.23	0/14712
2	G	0.09	0/10854	0.23	0/14712
2	J	0.09	0/10854	0.23	0/14712
2	M	0.09	0/10854	0.23	0/14712
2	P	0.09	0/10854	0.22	0/14712
3	C	0.11	0/5033	0.25	0/6818
3	H	0.12	0/5033	0.27	0/6818
3	K	0.11	0/5033	0.26	0/6818
3	N	0.11	0/5033	0.26	0/6818
3	Q	0.11	0/5033	0.26	0/6818
4	D	0.11	0/12010	0.25	0/16371
5	E	0.12	0/5207	0.27	0/7086
6	R	0.10	0/4355	0.27	0/5900
6	S	0.10	0/4355	0.27	0/5900
6	T	0.10	0/4355	0.28	0/5900
6	U	0.10	0/4355	0.27	0/5900
6	V	0.10	0/4355	0.27	0/5900
All	All	0.10	0/162707	0.24	0/220757

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	325	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8691	0	8677	37	0
1	F	8691	0	8677	47	0
1	I	8691	0	8677	51	0
1	L	8691	0	8677	43	0
1	O	8691	0	8677	58	0
2	B	10631	0	10373	42	0
2	G	10631	0	10373	46	0
2	J	10631	0	10373	56	0
2	M	10631	0	10373	50	0
2	P	10631	0	10373	38	0
3	C	4914	0	4716	41	0
3	H	4914	0	4716	47	0
3	K	4914	0	4716	47	0
3	N	4914	0	4716	47	0
3	Q	4914	0	4716	46	0
4	D	11696	0	11142	80	0
5	E	5111	0	4959	47	0
6	R	4259	0	4098	32	0
6	S	4259	0	4098	34	0
6	T	4259	0	4098	38	0
6	U	4259	0	4098	28	0
6	V	4259	0	4098	34	0
All	All	159282	0	155421	936	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 3.

All (936) 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)
5:E:96:GLU:OE1	5:E:96:GLU:N	2.05	0.89
5:E:522:THR:OG1	5:E:525:SER:O	1.93	0.84
5:E:610:TYR:OH	5:E:633:ARG:O	1.95	0.84
2:M:399:ASN:ND2	2:M:401:ASP:O	2.12	0.83
3:C:179:ARG:NH1	3:C:512:GLU:OE2	2.12	0.83
1:I:942:GLU:N	1:I:942:GLU:OE1	2.11	0.82
1:L:942:GLU:OE1	1:L:942:GLU:N	2.12	0.82
4:D:690:HIS:O	4:D:690:HIS:ND1	2.14	0.81
1:F:884:ASP:OD2	1:F:956:ASN:ND2	2.15	0.80
2:B:399:ASN:ND2	2:B:401:ASP:O	2.15	0.79
1:O:893:ASP:OD1	1:O:894:GLU:N	2.15	0.79
2:P:399:ASN:ND2	2:P:401:ASP:O	2.16	0.78
3:C:39:ILE:O	3:C:39:ILE:HD12	1.84	0.77
3:N:179:ARG:NH1	3:N:586:GLN:OE1	2.19	0.76
4:D:256:GLU:OE1	4:D:256:GLU:N	2.19	0.76
4:D:624:ILE:HG23	4:D:700:LEU:HD11	1.67	0.76
2:G:399:ASN:ND2	2:G:401:ASP:O	2.18	0.75
2:J:399:ASN:ND2	2:J:401:ASP:O	2.20	0.75
6:V:313:MET:HE3	6:V:313:MET:O	1.87	0.75
4:D:1381:GLU:OE2	4:D:1381:GLU:N	2.19	0.75
1:L:770:LEU:HD12	1:L:771:THR:HG23	1.69	0.75
4:D:984:LEU:CD1	5:E:12:VAL:HG21	2.17	0.75
1:A:892:SER:OG	1:A:895:GLU:OE1	2.04	0.74
2:P:47:ASP:OD2	2:P:48:HIS:N	2.20	0.74
4:D:928:GLU:OE1	4:D:945:GLN:NE2	2.20	0.74
3:N:224:GLN:NE2	3:N:267:GLY:O	2.20	0.74
3:H:119:ASN:O	3:H:126:GLN:NE2	2.21	0.74
4:D:1312:MET:SD	4:D:1312:MET:N	2.61	0.74
4:D:270:ASP:OD1	4:D:274:ARG:NH1	2.20	0.74
5:E:482:THR:HG22	5:E:486:GLU:O	1.88	0.74
2:G:47:ASP:OD2	2:G:48:HIS:N	2.21	0.73
5:E:590:LEU:O	5:E:591:THR:OG1	2.07	0.73
3:C:472:MET:HE2	3:C:472:MET:HA	1.69	0.73
2:M:47:ASP:OD1	2:M:48:HIS:N	2.22	0.73
6:V:35:GLU:OE2	6:V:35:GLU:N	2.20	0.73
2:B:47:ASP:OD1	2:B:48:HIS:N	2.21	0.72
2:J:487:MET:HE3	2:J:488:CYS:N	2.03	0.72
4:D:125:ILE:HD11	4:D:249:SER:HB2	1.71	0.72
2:J:47:ASP:OD1	2:J:48:HIS:N	2.22	0.72
3:K:140:MET:HA	3:K:140:MET:HE2	1.72	0.72
3:Q:422:MET:SD	3:Q:424:TYR:OH	2.46	0.72
1:I:770:LEU:HD12	1:I:771:THR:HG23	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:457:LYS:NZ	6:S:539:CYS:SG	2.61	0.71
3:H:119:ASN:OD1	3:H:126:GLN:NE2	2.24	0.71
1:I:767:MET:O	1:I:771:THR:OG1	2.08	0.71
5:E:80:TYR:OH	5:E:114:ASP:OD2	2.09	0.71
3:N:545:ASP:OD2	3:N:546:PHE:N	2.23	0.71
5:E:372:TYR:O	5:E:680:ASN:ND2	2.25	0.70
3:N:140:MET:HE2	3:N:140:MET:HA	1.72	0.70
3:C:516:ILE:HD13	3:C:558:LEU:HD13	1.73	0.70
1:O:770:LEU:HD12	1:O:771:THR:HG23	1.72	0.70
3:N:119:ASN:O	3:N:126:GLN:NE2	2.24	0.70
1:O:453:MET:HE3	1:O:453:MET:HA	1.72	0.70
3:K:410:GLN:N	3:K:410:GLN:OE1	2.24	0.70
2:J:1216:GLU:OE2	2:M:1242:GLN:NE2	2.25	0.69
2:B:1216:GLU:OE2	2:G:1242:GLN:NE2	2.25	0.69
3:Q:540:THR:OG1	3:Q:621:GLU:OE2	2.10	0.69
3:H:472:MET:HE2	3:H:472:MET:HA	1.74	0.69
3:H:410:GLN:OE1	3:H:410:GLN:N	2.25	0.69
2:M:714:GLN:N	2:M:714:GLN:OE1	2.25	0.69
2:M:1216:GLU:OE2	2:P:1242:GLN:NE2	2.25	0.69
2:P:837:MET:HA	2:P:837:MET:HE3	1.75	0.69
1:A:885:ILE:HD12	1:A:885:ILE:O	1.93	0.69
1:F:767:MET:O	1:F:771:THR:OG1	2.09	0.69
1:A:597:GLN:OE1	1:A:604:SER:OG	2.07	0.68
2:G:1216:GLU:OE2	2:J:1242:GLN:NE2	2.27	0.68
1:F:244:PHE:O	1:F:245:THR:OG1	2.10	0.68
3:Q:410:GLN:N	3:Q:410:GLN:OE1	2.24	0.68
4:D:1281:MET:SD	4:D:1281:MET:N	2.67	0.68
3:C:140:MET:HE2	3:C:140:MET:HA	1.74	0.68
3:N:516:ILE:HD13	3:N:558:LEU:HD13	1.76	0.67
2:B:1242:GLN:NE2	2:P:1216:GLU:OE2	2.27	0.67
3:N:410:GLN:N	3:N:410:GLN:OE1	2.27	0.67
5:E:275:GLN:N	5:E:275:GLN:OE1	2.27	0.67
3:K:171:GLY:N	3:K:176:GLU:OE1	2.27	0.67
3:K:472:MET:HE2	3:K:472:MET:HA	1.76	0.67
3:C:52:GLU:OE1	3:C:55:GLN:NE2	2.27	0.67
2:P:938:ARG:NH1	2:P:1045:GLU:OE1	2.28	0.67
1:F:597:GLN:OE1	1:F:604:SER:OG	2.08	0.66
2:P:676:PRO:O	2:P:682:ILE:HD11	1.96	0.66
1:F:967:ASN:O	1:F:967:ASN:ND2	2.24	0.66
2:G:938:ARG:NH1	2:G:1045:GLU:OE1	2.27	0.66
4:D:522:ASP:OD1	4:D:536:ASN:N	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:938:ARG:NH1	2:M:1045:GLU:OE1	2.28	0.66
3:N:135:ARG:NH1	3:N:164:ASP:OD2	2.29	0.65
3:K:52:GLU:OE1	3:K:55:GLN:NE2	2.30	0.65
3:H:434:TYR:CD2	3:H:627:ILE:HD11	2.32	0.65
6:S:296:ALA:HB1	6:S:323:MET:HE3	1.79	0.65
2:J:676:PRO:O	2:J:682:ILE:HD11	1.97	0.65
3:N:246:ASP:C	3:N:247:LEU:HD12	2.22	0.65
3:C:407:ASN:O	3:C:410:GLN:NE2	2.29	0.65
2:J:938:ARG:NH1	2:J:1045:GLU:OE1	2.28	0.65
6:S:215:TRP:N	6:S:256:GLU:OE2	2.29	0.64
1:F:904:ILE:CG2	1:F:906:VAL:HG23	2.28	0.64
1:A:49:LEU:HD13	1:A:87:ILE:HD11	1.79	0.64
1:A:244:PHE:O	1:A:245:THR:OG1	2.10	0.64
2:B:938:ARG:NH1	2:B:1045:GLU:OE1	2.30	0.64
2:G:676:PRO:O	2:G:682:ILE:HD11	1.97	0.64
4:D:1064:ARG:NE	4:D:1085:GLU:OE2	2.30	0.64
3:N:52:GLU:OE1	3:N:55:GLN:NE2	2.31	0.64
3:N:77:THR:OG1	3:N:79:ASP:OD1	2.13	0.64
5:E:292:GLU:OE2	5:E:293:GLU:N	2.31	0.63
3:K:545:ASP:OD1	3:K:546:PHE:N	2.30	0.63
3:H:539:ASP:OD1	3:H:540:THR:N	2.31	0.63
3:K:246:ASP:C	3:K:247:LEU:HD12	2.22	0.63
2:M:676:PRO:O	2:M:682:ILE:HD11	1.97	0.63
3:H:39:ILE:O	3:H:39:ILE:HD12	1.99	0.63
3:N:39:ILE:HD12	3:N:39:ILE:O	1.99	0.63
3:K:59:ILE:O	3:K:68:ASN:ND2	2.31	0.62
2:B:457:LYS:NZ	6:R:539:CYS:SG	2.64	0.62
2:B:676:PRO:O	2:B:682:ILE:HD11	1.98	0.62
3:N:472:MET:HE2	3:N:472:MET:HA	1.82	0.62
3:Q:322:ASP:OD1	3:Q:323:GLU:N	2.33	0.62
3:C:432:ALA:O	3:C:496:TYR:OH	2.08	0.62
4:D:1107:ASP:OD1	4:D:1108:GLU:N	2.31	0.62
3:N:322:ASP:OD1	3:N:323:GLU:N	2.32	0.62
1:O:244:PHE:O	1:O:245:THR:OG1	2.11	0.62
3:Q:39:ILE:HD12	3:Q:39:ILE:O	1.99	0.62
3:H:275:GLN:O	3:H:286:ARG:NH1	2.33	0.62
1:O:810:ASN:HD21	1:O:1033:THR:HG21	1.65	0.62
1:L:597:GLN:OE1	1:L:604:SER:OG	2.09	0.62
3:N:564:VAL:HG21	3:N:591:LEU:HG	1.82	0.61
3:H:140:MET:HE2	3:H:140:MET:HA	1.82	0.61
3:N:13:MET:HE1	1:O:368:ILE:HD11	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:45:ASP:OD2	6:S:384:LYS:NZ	2.28	0.61
3:C:77:THR:OG1	3:C:79:ASP:OD1	2.18	0.61
5:E:486:GLU:N	5:E:486:GLU:OE1	2.34	0.61
4:D:433:ARG:NH1	4:D:441:ALA:O	2.34	0.61
3:H:322:ASP:OD1	3:H:323:GLU:N	2.33	0.61
6:T:214:GLY:O	6:T:218:SER:OG	2.12	0.61
3:C:322:ASP:OD1	3:C:323:GLU:N	2.34	0.60
1:I:244:PHE:O	1:I:245:THR:OG1	2.12	0.60
3:Q:135:ARG:NH1	3:Q:164:ASP:OD2	2.34	0.60
1:A:776:TYR:OH	1:A:791:LYS:O	2.17	0.60
3:C:346:ILE:HD11	3:C:373:ILE:HD11	1.83	0.60
2:G:123:THR:O	2:G:128:LYS:NZ	2.32	0.60
3:H:77:THR:OG1	3:H:79:ASP:OD1	2.13	0.60
1:L:244:PHE:O	1:L:245:THR:OG1	2.11	0.60
1:O:845:LEU:HD11	1:O:961:LEU:HD22	1.83	0.60
3:Q:450:GLN:OE1	3:Q:450:GLN:N	2.35	0.60
3:N:434:TYR:CD1	3:N:627:ILE:HD11	2.36	0.60
3:C:246:ASP:C	3:C:247:LEU:HD12	2.26	0.60
5:E:565:VAL:HG22	5:E:585:TRP:HD1	1.67	0.60
1:L:885:ILE:HD12	1:L:885:ILE:O	2.01	0.60
1:F:49:LEU:HD13	1:F:87:ILE:HD11	1.81	0.60
6:R:215:TRP:N	6:R:256:GLU:OE2	2.35	0.60
1:F:378:GLU:OE1	1:F:378:GLU:N	2.35	0.60
3:Q:52:GLU:OE1	3:Q:55:GLN:NE2	2.35	0.60
5:E:443:GLU:N	5:E:443:GLU:OE1	2.35	0.59
1:O:942:GLU:OE1	1:O:942:GLU:N	2.33	0.59
4:D:215:ASN:O	4:D:311:ARG:NH2	2.34	0.59
6:U:215:TRP:N	6:U:256:GLU:OE2	2.35	0.59
4:D:564:GLN:NE2	4:D:581:GLU:OE2	2.36	0.59
3:K:2:VAL:HG12	3:K:145:VAL:HG21	1.85	0.59
5:E:421:LEU:HD12	5:E:424:ILE:HD11	1.84	0.59
6:V:45:ASP:OD2	6:V:384:LYS:NZ	2.28	0.59
1:I:1152:MET:HE3	2:J:9:LEU:HD11	1.85	0.59
2:P:448:SER:HB3	6:V:525:LEU:HD12	1.85	0.59
4:D:1351:LEU:O	5:E:258:ILE:HD11	2.03	0.59
3:H:450:GLN:N	3:H:450:GLN:OE1	2.35	0.59
1:L:75:ARG:NH2	1:L:176:ASP:OD1	2.36	0.59
3:C:98:ILE:HG22	3:C:98:ILE:O	2.01	0.59
4:D:1443:ASP:OD1	4:D:1459:ALA:N	2.36	0.58
1:F:770:LEU:HD12	1:F:771:THR:HG23	1.85	0.58
1:I:614:VAL:HG11	1:I:630:VAL:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:776:TYR:OH	1:O:791:LYS:O	2.20	0.58
2:B:448:SER:HB3	6:R:525:LEU:HD12	1.85	0.58
3:K:322:ASP:OD1	3:K:323:GLU:N	2.36	0.58
6:T:168:ILE:HD12	6:T:168:ILE:O	2.03	0.58
6:U:313:MET:HE3	6:U:313:MET:O	2.03	0.58
5:E:479:LEU:HD22	5:E:490:VAL:HG22	1.85	0.58
5:E:638:GLU:C	5:E:638:GLU:OE1	2.47	0.58
3:H:59:ILE:O	3:H:68:ASN:ND2	2.37	0.58
2:J:448:SER:HB3	6:T:525:LEU:HD12	1.84	0.58
6:T:217:MET:HE3	6:T:217:MET:O	2.03	0.58
3:C:545:ASP:OD1	3:C:546:PHE:N	2.37	0.58
5:E:292:GLU:O	5:E:300:THR:N	2.36	0.58
1:O:967:ASN:ND2	1:O:967:ASN:O	2.37	0.58
3:Q:545:ASP:OD1	3:Q:546:PHE:N	2.37	0.58
6:T:390:THR:HG23	6:T:396:GLU:OE1	2.04	0.58
2:G:448:SER:HB3	6:S:525:LEU:HD12	1.86	0.58
3:K:39:ILE:HD12	3:K:39:ILE:O	2.03	0.58
3:C:449:GLU:OE1	3:C:452:LEU:HD23	2.04	0.57
3:H:516:ILE:HD13	3:H:558:LEU:HD13	1.84	0.57
1:O:614:VAL:HG11	1:O:630:VAL:HA	1.85	0.57
1:A:614:VAL:HG11	1:A:630:VAL:HA	1.87	0.57
1:O:398:ARG:HB2	1:O:399:MET:HE2	1.85	0.57
6:R:168:ILE:O	6:R:168:ILE:HD12	2.05	0.57
2:B:169:ILE:HD11	2:B:188:ARG:HE	1.70	0.57
1:A:904:ILE:CG2	1:A:906:VAL:HG23	2.35	0.57
4:D:1010:ASN:O	4:D:1013:ASN:ND2	2.38	0.57
3:H:135:ARG:NH1	3:H:164:ASP:OD2	2.37	0.57
1:L:614:VAL:HG11	1:L:630:VAL:HA	1.85	0.57
6:T:217:MET:HE3	6:T:217:MET:C	2.30	0.57
6:U:476:LYS:HB2	6:U:503:LEU:HD23	1.87	0.57
1:A:770:LEU:HD12	1:A:771:THR:HG23	1.87	0.57
1:F:75:ARG:NH2	1:F:176:ASP:OD1	2.37	0.57
1:I:75:ARG:NH2	1:I:176:ASP:OD1	2.38	0.57
2:J:487:MET:HE3	2:J:487:MET:C	2.30	0.57
5:E:104:THR:HG22	5:E:105:ASN:H	1.70	0.56
2:G:838:LYS:HE2	2:G:838:LYS:N	2.19	0.56
3:Q:472:MET:HA	3:Q:472:MET:HE2	1.86	0.56
2:M:448:SER:HB3	6:U:525:LEU:HD12	1.85	0.56
1:O:810:ASN:ND2	1:O:1033:THR:HG21	2.19	0.56
6:T:45:ASP:OD2	6:T:384:LYS:NZ	2.29	0.56
4:D:919:VAL:HG23	4:D:919:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:U:380:THR:CG2	6:U:422:ILE:HD11	2.36	0.56
1:O:1119:SER:O	1:O:1123:MET:N	2.39	0.56
2:B:308:ASP:OD1	2:B:309:ARG:N	2.39	0.56
4:D:321:ARG:NH1	4:D:333:GLU:OE1	2.39	0.56
4:D:397:ALA:HB3	2:M:1232:LEU:HD13	1.88	0.56
1:I:70:GLN:OE1	1:I:70:GLN:C	2.49	0.56
2:M:308:ASP:OD1	2:M:309:ARG:N	2.39	0.56
6:T:476:LYS:HB2	6:T:503:LEU:HD23	1.88	0.56
3:N:59:ILE:O	3:N:68:ASN:ND2	2.38	0.56
1:L:776:TYR:OH	1:L:791:LYS:O	2.20	0.56
1:O:885:ILE:HD12	1:O:885:ILE:O	2.05	0.56
6:U:168:ILE:O	6:U:168:ILE:HD12	2.06	0.56
6:V:168:ILE:HD12	6:V:168:ILE:O	2.06	0.56
4:D:1095:GLN:O	4:D:1098:VAL:HG22	2.06	0.56
1:I:1047:ASP:OD1	1:I:1048:SER:N	2.39	0.56
2:J:416:THR:OG1	2:J:418:ASP:OD1	2.23	0.56
2:J:1165:VAL:HG11	2:M:865:MET:HE1	1.87	0.56
6:R:380:THR:CG2	6:R:422:ILE:HD11	2.36	0.56
6:S:476:LYS:HB2	6:S:503:LEU:HD23	1.88	0.56
6:V:380:THR:CG2	6:V:422:ILE:HD11	2.36	0.56
4:D:1347:ASP:C	4:D:1347:ASP:OD1	2.49	0.56
1:L:1152:MET:HE2	2:M:9:LEU:HD11	1.88	0.56
3:N:171:GLY:O	3:N:177:ARG:NH2	2.39	0.56
1:O:75:ARG:NH2	1:O:176:ASP:OD1	2.37	0.56
2:P:169:ILE:HD11	2:P:188:ARG:HE	1.71	0.56
6:R:45:ASP:OD2	6:R:384:LYS:NZ	2.27	0.56
2:J:1297:MET:HE2	2:J:1297:MET:C	2.31	0.55
1:L:852:THR:OG1	1:L:855:ASP:OD1	2.23	0.55
3:Q:564:VAL:HG21	3:Q:591:LEU:HG	1.89	0.55
4:D:1400:ASN:ND2	4:D:1426:ASP:O	2.39	0.55
1:L:1152:MET:HE3	1:O:679:LEU:HD22	1.87	0.55
2:J:457:LYS:NZ	6:T:539:CYS:SG	2.71	0.55
6:V:476:LYS:HB2	6:V:503:LEU:HD23	1.88	0.55
1:F:614:VAL:HG11	1:F:630:VAL:HA	1.89	0.55
3:H:421:LEU:HD23	3:H:475:ILE:HG23	1.88	0.55
1:L:182:ARG:O	1:L:187:ARG:NH1	2.39	0.55
3:N:24:LEU:HD12	3:N:39:ILE:HG23	1.89	0.55
1:I:776:TYR:OH	1:I:791:LYS:O	2.23	0.55
3:Q:421:LEU:HD23	3:Q:475:ILE:HG23	1.89	0.55
6:T:380:THR:CG2	6:T:422:ILE:HD11	2.36	0.55
6:R:476:LYS:HB2	6:R:503:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:453:MET:HE2	1:I:453:MET:HA	1.88	0.55
2:M:169:ILE:HD11	2:M:188:ARG:HE	1.72	0.55
6:S:168:ILE:HD12	6:S:168:ILE:O	2.06	0.55
3:K:135:ARG:NH1	3:K:164:ASP:OD2	2.36	0.55
3:K:492:THR:O	3:K:625:LYS:NZ	2.36	0.55
1:F:1119:SER:O	1:F:1123:MET:N	2.37	0.55
2:J:308:ASP:OD1	2:J:309:ARG:N	2.39	0.55
6:S:296:ALA:HB1	6:S:323:MET:CE	2.37	0.55
1:A:1119:SER:O	1:A:1123:MET:N	2.37	0.54
5:E:416:ASP:OD1	5:E:420:ASN:N	2.40	0.54
2:G:563:GLU:C	2:G:563:GLU:OE1	2.50	0.54
2:P:308:ASP:OD1	2:P:309:ARG:N	2.40	0.54
2:G:416:THR:OG1	2:G:418:ASP:OD1	2.24	0.54
1:I:1119:SER:O	1:I:1123:MET:N	2.37	0.54
5:E:85:ASP:O	5:E:447:ARG:NH2	2.39	0.54
2:G:224:ILE:HG22	2:G:226:VAL:HG12	1.90	0.54
1:I:885:ILE:HD12	1:I:885:ILE:O	2.07	0.54
6:T:254:ASP:HA	6:T:296:ALA:HB2	1.89	0.54
3:Q:1:MET:HE2	3:Q:1:MET:C	2.32	0.54
2:M:416:THR:OG1	2:M:418:ASP:OD1	2.26	0.54
2:G:169:ILE:HD11	2:G:188:ARG:HE	1.72	0.54
3:K:539:ASP:OD1	3:K:540:THR:N	2.40	0.54
1:O:845:LEU:HD13	1:O:965:LEU:HD13	1.88	0.54
6:S:380:THR:CG2	6:S:422:ILE:HD11	2.37	0.54
1:A:348:ALA:HB3	1:A:351:ILE:HG22	1.89	0.54
1:F:776:TYR:OH	1:F:791:LYS:O	2.25	0.54
3:K:24:LEU:HD12	3:K:39:ILE:HG23	1.90	0.54
3:H:1:MET:HE2	3:H:1:MET:C	2.32	0.54
1:I:385:ARG:NH1	1:I:420:ASP:OD2	2.41	0.54
1:I:877:ASP:OD1	1:I:878:ASP:N	2.41	0.54
3:N:539:ASP:OD1	3:N:540:THR:N	2.41	0.54
3:Q:77:THR:OG1	3:Q:79:ASP:OD1	2.14	0.54
4:D:53:PRO:HB2	4:D:55:LEU:HD23	1.90	0.53
2:J:169:ILE:HD11	2:J:188:ARG:HE	1.72	0.53
1:L:767:MET:HA	1:L:767:MET:HE3	1.89	0.53
3:Q:539:ASP:OD1	3:Q:540:THR:N	2.41	0.53
6:R:419:TRP:HA	6:R:422:ILE:HD12	1.90	0.53
6:U:419:TRP:HA	6:U:422:ILE:HD12	1.90	0.53
1:A:904:ILE:HG22	1:A:906:VAL:HG23	1.88	0.53
3:C:540:THR:OG1	3:C:621:GLU:OE1	2.26	0.53
3:K:77:THR:OG1	3:K:79:ASP:OD1	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:419:TRP:HA	6:V:422:ILE:HD12	1.90	0.53
3:Q:516:ILE:HD13	3:Q:558:LEU:HD13	1.89	0.53
6:R:8:ASN:OD1	6:R:8:ASN:O	2.25	0.53
6:U:45:ASP:OD2	6:U:384:LYS:NZ	2.28	0.53
6:S:419:TRP:HA	6:S:422:ILE:HD12	1.90	0.53
2:M:47:ASP:OD1	2:M:47:ASP:C	2.51	0.53
6:R:296:ALA:HB1	6:R:323:MET:HE3	1.90	0.53
2:B:621:ARG:NH1	2:B:625:GLU:OE2	2.40	0.53
4:D:396:GLU:HB2	2:M:1232:LEU:HD12	1.89	0.53
1:L:385:ARG:NH1	1:L:420:ASP:OD2	2.41	0.53
5:E:180:LEU:HD23	5:E:181:ILE:N	2.24	0.53
5:E:408:ASN:OD1	5:E:409:TYR:N	2.42	0.53
6:T:296:ALA:HB1	6:T:323:MET:HE2	1.89	0.53
2:M:1082:ASP:OD1	2:M:1082:ASP:C	2.52	0.53
3:N:377:ARG:NH2	3:N:381:ASP:OD1	2.42	0.53
1:O:385:ARG:NH1	1:O:420:ASP:OD2	2.40	0.53
5:E:89:THR:HB	5:E:104:THR:HG23	1.90	0.53
3:H:325:ARG:NH1	3:H:325:ARG:HA	2.24	0.53
2:M:224:ILE:HG22	2:M:226:VAL:HG12	1.90	0.53
6:S:313:MET:HE3	6:S:313:MET:O	2.09	0.53
6:T:419:TRP:HA	6:T:422:ILE:HD12	1.91	0.53
1:F:854:ASP:OD2	1:F:854:ASP:C	2.52	0.52
3:H:403:LEU:HD21	3:H:464:LEU:HD21	1.91	0.52
4:D:980:LEU:HD11	4:D:984:LEU:HD22	1.91	0.52
3:N:163:TYR:OH	3:N:244:TYR:O	2.27	0.52
2:P:224:ILE:HG22	2:P:226:VAL:HG12	1.90	0.52
6:T:313:MET:HE3	6:T:313:MET:O	2.09	0.52
4:D:429:LYS:CD	4:D:447:MET:HE2	2.39	0.52
3:H:171:GLY:O	3:H:177:ARG:NH2	2.42	0.52
6:V:296:ALA:HB1	6:V:323:MET:HE3	1.90	0.52
3:C:391:GLU:OE2	3:C:418:ASN:ND2	2.42	0.52
5:E:205:ASP:OD1	5:E:206:THR:N	2.42	0.52
1:F:874:GLN:OE1	1:F:874:GLN:HA	2.09	0.52
1:I:811:ASN:ND2	1:I:811:ASN:O	2.43	0.52
1:I:1158:GLN:OE1	1:I:1158:GLN:HA	2.08	0.52
1:O:877:ASP:OD1	1:O:878:ASP:N	2.42	0.52
1:F:981:GLU:OE1	1:F:981:GLU:C	2.52	0.52
3:Q:171:GLY:O	3:Q:177:ARG:NH2	2.42	0.52
2:G:468:ASN:ND2	2:G:482:ASN:O	2.41	0.52
3:H:393:SER:C	3:H:394:ILE:HD12	2.33	0.52
1:I:893:ASP:OD1	1:I:894:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:811:ASN:O	1:L:811:ASN:ND2	2.43	0.52
1:O:941:VAL:HG11	1:O:990:THR:HG22	1.91	0.52
6:S:150:ASN:C	6:S:150:ASN:OD1	2.53	0.52
6:V:215:TRP:N	6:V:256:GLU:OE2	2.42	0.52
2:G:47:ASP:OD2	2:G:47:ASP:C	2.51	0.52
1:F:885:ILE:HD12	1:F:885:ILE:O	2.09	0.52
3:H:24:LEU:HD12	3:H:39:ILE:HG23	1.92	0.52
2:J:44:ASP:OD1	2:J:44:ASP:C	2.53	0.52
4:D:1276:ASP:OD1	4:D:1277:VAL:N	2.43	0.52
1:F:811:ASN:O	1:F:811:ASN:ND2	2.43	0.52
1:I:874:GLN:OE1	1:I:874:GLN:HA	2.10	0.52
2:B:47:ASP:OD1	2:B:47:ASP:C	2.52	0.51
4:D:45:PHE:C	4:D:45:PHE:CD2	2.88	0.51
4:D:552:ASN:C	4:D:552:ASN:OD1	2.53	0.51
2:J:47:ASP:OD1	2:J:47:ASP:C	2.54	0.51
3:K:224:GLN:NE2	3:K:267:GLY:O	2.40	0.51
3:K:516:ILE:HD13	3:K:558:LEU:HD13	1.92	0.51
6:S:254:ASP:HA	6:S:296:ALA:HB2	1.91	0.51
6:T:296:ALA:HB1	6:T:323:MET:CE	2.39	0.51
2:B:224:ILE:HG22	2:B:226:VAL:HG12	1.91	0.51
1:O:892:SER:O	1:O:896:MET:HE2	2.10	0.51
3:C:399:VAL:HG22	3:C:455:LEU:HD11	1.90	0.51
3:C:421:LEU:HD23	3:C:475:ILE:HG23	1.93	0.51
2:G:1082:ASP:C	2:G:1082:ASP:OD1	2.52	0.51
2:J:224:ILE:HG22	2:J:226:VAL:HG12	1.91	0.51
1:O:811:ASN:O	1:O:811:ASN:ND2	2.43	0.51
5:E:1:MET:HE3	5:E:1:MET:N	2.24	0.51
1:A:874:GLN:OE1	1:A:874:GLN:HA	2.10	0.51
1:I:608:ASP:OD1	1:I:608:ASP:C	2.54	0.51
3:K:179:ARG:HG3	3:K:506:MET:HE1	1.92	0.51
1:A:811:ASN:O	1:A:811:ASN:ND2	2.44	0.51
2:B:499:PHE:N	2:B:510:GLY:O	2.43	0.51
4:D:952:ASP:OD1	4:D:953:ARG:N	2.39	0.51
4:D:1469:THR:HG23	4:D:1470:PRO:HD2	1.92	0.51
1:F:879:MET:SD	1:F:965:LEU:HD22	2.50	0.51
2:P:259:ASP:OD1	2:P:263:ASN:N	2.44	0.51
4:D:990:ASP:OD2	5:E:22:VAL:HG11	2.10	0.51
4:D:1270:GLN:NE2	4:D:1325:LEU:O	2.42	0.51
4:D:1380:SER:OG	4:D:1381:GLU:OE2	2.26	0.51
1:F:608:ASP:OD1	1:F:608:ASP:C	2.54	0.51
3:K:421:LEU:HD23	3:K:475:ILE:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:596:LEU:HD13	5:E:597:GLU:N	2.26	0.51
1:O:608:ASP:C	1:O:608:ASP:OD1	2.54	0.51
1:A:394:ARG:HH12	3:Q:35:VAL:HG23	1.76	0.51
4:D:702:LEU:H	4:D:702:LEU:HD23	1.76	0.50
2:J:312:ASP:N	2:J:312:ASP:OD1	2.44	0.50
6:U:247:MET:SD	6:U:247:MET:C	2.94	0.50
2:J:737:ASP:OD1	2:J:737:ASP:N	2.44	0.50
2:M:837:MET:HE3	2:M:837:MET:HA	1.92	0.50
2:M:1297:MET:C	2:M:1297:MET:HE2	2.35	0.50
2:P:47:ASP:OD2	2:P:47:ASP:C	2.55	0.50
6:V:247:MET:SD	6:V:247:MET:C	2.95	0.50
1:O:165:ASP:C	1:O:165:ASP:OD2	2.54	0.50
3:Q:24:LEU:HD12	3:Q:39:ILE:HG23	1.92	0.50
3:H:178:GLY:C	3:H:506:MET:HE1	2.36	0.50
1:I:333:LEU:HB2	1:I:338:LEU:HD11	1.93	0.50
3:K:275:GLN:O	3:K:286:ARG:NH1	2.43	0.50
1:L:1119:SER:O	1:L:1123:MET:N	2.39	0.50
4:D:1246:GLU:N	4:D:1246:GLU:OE1	2.42	0.50
2:G:312:ASP:OD1	2:G:312:ASP:N	2.44	0.50
1:O:892:SER:OG	1:O:895:GLU:OE1	2.29	0.50
3:Q:407:ASN:O	3:Q:410:GLN:NE2	2.43	0.50
6:T:12:ASP:OD1	6:T:13:LYS:N	2.45	0.50
1:I:845:LEU:HD11	1:I:961:LEU:HD22	1.93	0.50
1:I:1046:GLU:OE1	1:I:1046:GLU:N	2.44	0.50
3:K:540:THR:OG1	3:K:621:GLU:OE1	2.25	0.50
2:M:259:ASP:OD1	2:M:263:ASN:N	2.44	0.50
4:D:396:GLU:CB	2:M:1232:LEU:HD12	2.42	0.50
1:A:333:LEU:HB2	1:A:338:LEU:HD11	1.94	0.50
1:A:770:LEU:HD12	1:A:771:THR:CG2	2.41	0.50
2:B:312:ASP:OD1	2:B:312:ASP:N	2.44	0.50
4:D:1059:TYR:OH	4:D:1062:GLN:OE1	2.30	0.50
3:H:464:LEU:HD12	3:H:470:ILE:HD12	1.94	0.50
1:L:608:ASP:C	1:L:608:ASP:OD1	2.54	0.50
2:P:487:MET:N	2:P:487:MET:HE3	2.26	0.50
2:B:259:ASP:OD1	2:B:263:ASN:N	2.45	0.49
6:R:8:ASN:ND2	6:R:512:ILE:HG23	2.27	0.49
1:L:78:GLU:OE1	1:L:78:GLU:N	2.39	0.49
6:S:309:ILE:HD12	6:S:361:LEU:HD21	1.94	0.49
3:H:118:VAL:HG12	3:H:118:VAL:O	2.12	0.49
3:K:593:ASN:HB2	3:K:612:MET:HE3	1.95	0.49
2:M:737:ASP:OD1	2:M:737:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:230:ASN:ND2	2:P:251:GLU:OE1	2.45	0.49
2:B:445:PHE:C	2:B:445:PHE:CD2	2.90	0.49
2:G:43:ASP:OD2	2:G:43:ASP:C	2.54	0.49
2:G:259:ASP:OD1	2:G:263:ASN:N	2.46	0.49
1:I:1152:MET:HE1	2:J:5:ILE:HG21	1.93	0.49
3:C:494:ARG:NH1	3:C:625:LYS:O	2.46	0.49
1:F:1046:GLU:N	1:F:1046:GLU:OE1	2.44	0.49
3:K:543:ASP:O	3:K:562:ARG:NH2	2.46	0.49
6:V:161:ASP:O	6:V:166:ALA:N	2.46	0.49
3:C:394:ILE:HD13	3:C:416:LEU:HD11	1.93	0.49
1:L:874:GLN:OE1	1:L:874:GLN:HA	2.13	0.49
2:M:312:ASP:N	2:M:312:ASP:OD1	2.44	0.49
6:S:53:ARG:NH1	6:S:81:ASP:OD2	2.42	0.49
6:S:161:ASP:O	6:S:166:ALA:N	2.45	0.49
4:D:995:GLN:O	5:E:17:ASN:ND2	2.45	0.49
4:D:563:ARG:NH2	2:G:1333:ASP:OD2	2.46	0.49
1:F:767:MET:HE3	1:F:767:MET:HA	1.95	0.49
2:P:737:ASP:OD1	2:P:737:ASP:N	2.45	0.49
6:T:161:ASP:O	6:T:166:ALA:N	2.46	0.49
2:B:487:MET:N	2:B:487:MET:HE3	2.27	0.49
4:D:854:ASN:N	4:D:854:ASN:OD1	2.44	0.49
1:F:348:ALA:HB3	1:F:351:ILE:HG22	1.95	0.49
3:N:450:GLN:H	3:N:450:GLN:CD	2.21	0.49
2:P:416:THR:OG1	2:P:418:ASP:OD1	2.31	0.49
1:A:608:ASP:OD1	1:A:608:ASP:C	2.56	0.49
4:D:711:MET:SD	4:D:711:MET:C	2.96	0.49
1:F:320:LEU:HD11	1:F:465:ILE:HD12	1.95	0.49
1:O:874:GLN:HA	1:O:874:GLN:OE1	2.13	0.49
1:A:1002:PHE:HE1	1:A:1013:LEU:HD11	1.78	0.48
2:B:34:ASN:OD1	2:B:34:ASN:N	2.46	0.48
3:C:490:ASP:CG	3:C:492:THR:HG1	2.21	0.48
4:D:34:ASP:OD1	4:D:34:ASP:N	2.44	0.48
4:D:429:LYS:HD2	4:D:447:MET:HE2	1.94	0.48
3:H:194:ASP:C	3:H:194:ASP:OD2	2.56	0.48
3:N:421:LEU:HD23	3:N:475:ILE:HG23	1.95	0.48
3:C:163:TYR:OH	3:C:244:TYR:O	2.30	0.48
2:G:707:ASP:OD1	2:G:725:TYR:OH	2.30	0.48
3:H:540:THR:OG1	3:H:621:GLU:OE2	2.25	0.48
3:N:346:ILE:HD11	3:N:376:LEU:HD23	1.96	0.48
6:R:309:ILE:HD12	6:R:361:LEU:HD21	1.95	0.48
6:T:309:ILE:HD12	6:T:361:LEU:HD21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ASN:ND2	2:B:251:GLU:OE1	2.46	0.48
2:B:737:ASP:OD1	2:B:737:ASP:N	2.46	0.48
5:E:538:GLU:OE2	5:E:540:ARG:NH2	2.39	0.48
3:H:394:ILE:HD13	3:H:416:LEU:HD11	1.96	0.48
2:J:621:ARG:NH1	2:J:625:GLU:OE2	2.45	0.48
6:S:65:ASP:OD1	6:S:65:ASP:C	2.56	0.48
1:A:403:ASP:OD1	1:A:403:ASP:N	2.46	0.48
3:H:407:ASN:O	3:H:410:GLN:NE2	2.47	0.48
4:D:221:ASP:OD1	4:D:221:ASP:N	2.46	0.48
2:G:484:THR:HG22	6:S:542:LYS:HZ3	1.78	0.48
2:J:259:ASP:OD1	2:J:263:ASN:N	2.46	0.48
4:D:984:LEU:HD11	5:E:12:VAL:HG21	1.94	0.48
2:G:24:GLN:O	2:G:28:ASN:ND2	2.45	0.48
1:I:403:ASP:N	1:I:403:ASP:OD1	2.46	0.48
1:L:403:ASP:N	1:L:403:ASP:OD1	2.47	0.48
2:G:737:ASP:OD1	2:G:737:ASP:N	2.46	0.48
1:O:333:LEU:HB2	1:O:338:LEU:HD11	1.95	0.48
3:Q:209:ASN:C	3:Q:209:ASN:OD1	2.56	0.48
6:U:161:ASP:O	6:U:166:ALA:N	2.46	0.48
2:B:24:GLN:O	2:B:28:ASN:ND2	2.46	0.48
4:D:143:ASP:OD1	4:D:143:ASP:N	2.46	0.48
2:G:34:ASN:OD1	2:G:34:ASN:N	2.46	0.48
2:J:837:MET:HE3	2:J:837:MET:HA	1.94	0.48
2:P:34:ASN:OD1	2:P:34:ASN:N	2.46	0.48
3:Q:434:TYR:CD2	3:Q:627:ILE:HD11	2.48	0.48
6:U:309:ILE:HD12	6:U:361:LEU:HD21	1.95	0.48
6:V:309:ILE:HD12	6:V:361:LEU:HD21	1.94	0.48
5:E:613:TYR:O	5:E:652:TYR:OH	2.30	0.48
2:J:34:ASN:OD1	2:J:34:ASN:N	2.46	0.48
3:K:172:SER:N	3:K:176:GLU:OE1	2.47	0.48
3:K:158:THR:OG1	3:K:585:ASP:OD2	2.32	0.48
3:K:407:ASN:O	3:K:410:GLN:NE2	2.45	0.48
1:L:331:GLU:OE1	1:L:331:GLU:N	2.47	0.48
2:M:709:GLU:OE1	2:M:709:GLU:HA	2.14	0.48
3:H:582:TRP:O	3:H:583:SER:OG	2.31	0.47
3:Q:163:TYR:OH	3:Q:244:TYR:O	2.31	0.47
1:I:273:VAL:O	1:I:1111:TRP:NE1	2.43	0.47
3:K:377:ARG:NH2	3:K:381:ASP:OD1	2.46	0.47
3:N:516:ILE:CD1	3:N:558:LEU:HD13	2.43	0.47
3:Q:275:GLN:O	3:Q:286:ARG:NH1	2.47	0.47
2:P:312:ASP:OD1	2:P:312:ASP:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLN:HA	1:A:356:GLN:OE1	2.14	0.47
1:I:655:LEU:HD22	1:I:783:PHE:HZ	1.79	0.47
2:J:376:TYR:OH	2:J:396:VAL:HG13	2.14	0.47
2:P:457:LYS:NZ	6:V:539:CYS:SG	2.70	0.47
2:B:707:ASP:OD1	2:B:725:TYR:OH	2.30	0.47
3:H:545:ASP:OD1	3:H:546:PHE:N	2.47	0.47
1:I:320:LEU:HD11	1:I:465:ILE:HD12	1.95	0.47
2:J:1195:LEU:HD21	2:J:1321:PHE:CE1	2.49	0.47
1:L:655:LEU:HD22	1:L:783:PHE:HZ	1.78	0.47
3:C:194:ASP:OD1	3:C:194:ASP:C	2.58	0.47
4:D:1418:ARG:HE	4:D:1442:ALA:HB3	1.79	0.47
1:F:807:LEU:HD21	1:F:817:LEU:HD22	1.97	0.47
3:H:163:TYR:OH	3:H:244:TYR:O	2.32	0.47
1:O:893:ASP:OD1	1:O:893:ASP:C	2.57	0.47
6:V:313:MET:HE3	6:V:313:MET:C	2.40	0.47
2:B:709:GLU:OE1	2:G:102:ARG:NH2	2.48	0.47
4:D:861:ASP:OD1	4:D:861:ASP:N	2.46	0.47
3:C:455:LEU:HD23	3:C:455:LEU:H	1.79	0.47
1:F:904:ILE:HG22	1:F:906:VAL:HG23	1.97	0.47
3:Q:434:TYR:CE2	3:Q:627:ILE:HD11	2.50	0.47
2:J:308:ASP:OD2	2:J:315:ARG:NE	2.37	0.47
3:N:350:TYR:CD2	3:N:350:TYR:N	2.83	0.47
3:C:424:TYR:HH	3:C:582:TRP:CG	2.32	0.46
3:C:516:ILE:CD1	3:C:558:LEU:HD13	2.42	0.46
1:L:873:ASN:HB3	1:L:904:ILE:HD11	1.98	0.46
3:N:543:ASP:O	3:N:562:ARG:NH2	2.48	0.46
2:B:301:GLU:OE2	2:B:322:LYS:NZ	2.47	0.46
3:H:209:ASN:OD1	3:H:209:ASN:C	2.58	0.46
2:M:450:ASN:C	6:U:525:LEU:HD13	2.40	0.46
3:H:371:LEU:H	3:H:371:LEU:HD22	1.79	0.46
1:O:821:LEU:HD21	1:O:1029:ILE:HD12	1.97	0.46
6:S:168:ILE:HD12	6:S:168:ILE:C	2.41	0.46
6:T:442:HIS:ND1	6:T:449:ASP:OD1	2.44	0.46
3:C:377:ARG:NH2	3:C:381:ASP:OD1	2.44	0.46
2:J:230:ASN:ND2	2:J:251:GLU:OE1	2.48	0.46
3:K:41:ASP:C	3:K:41:ASP:OD1	2.59	0.46
3:K:163:TYR:OH	3:K:242:ASP:OD2	2.22	0.46
1:O:273:VAL:O	1:O:1111:TRP:NE1	2.43	0.46
3:Q:241:LEU:HD11	3:Q:310:LEU:HD11	1.97	0.46
2:B:450:ASN:C	6:R:525:LEU:HD13	2.40	0.46
1:F:333:LEU:HB2	1:F:338:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:120:LEU:HD11	6:T:212:ILE:HG22	1.97	0.46
6:U:168:ILE:HD12	6:U:168:ILE:C	2.41	0.46
6:V:168:ILE:HD12	6:V:168:ILE:C	2.41	0.46
4:D:422:THR:OG1	4:D:423:PRO:HD3	2.15	0.46
1:F:821:LEU:HD21	1:F:1029:ILE:HD12	1.96	0.46
3:K:432:ALA:O	3:K:496:TYR:OH	2.32	0.46
1:L:320:LEU:HD11	1:L:465:ILE:HD12	1.97	0.46
6:R:143:ASP:OD1	6:R:146:ASP:N	2.46	0.46
6:T:80:TYR:OH	6:T:162:GLY:N	2.49	0.46
6:T:168:ILE:HD12	6:T:168:ILE:C	2.41	0.46
1:I:965:LEU:C	1:I:965:LEU:HD12	2.41	0.46
3:K:118:VAL:HG12	3:K:118:VAL:O	2.16	0.46
6:T:324:THR:OG1	6:T:375:GLY:N	2.49	0.46
6:U:80:TYR:OH	6:U:162:GLY:N	2.49	0.46
4:D:797:ASP:N	4:D:797:ASP:OD1	2.49	0.46
5:E:116:LEU:HD23	5:E:116:LEU:H	1.79	0.46
1:I:821:LEU:HD21	1:I:1029:ILE:HD12	1.97	0.46
2:J:24:GLN:O	2:J:28:ASN:ND2	2.49	0.46
2:J:849:ASN:OD1	2:J:849:ASN:C	2.59	0.46
3:N:41:ASP:C	3:N:41:ASP:OD1	2.59	0.46
2:P:376:TYR:OH	2:P:396:VAL:HG13	2.16	0.46
3:Q:41:ASP:OD1	3:Q:41:ASP:C	2.59	0.46
6:U:324:THR:OG1	6:U:375:GLY:N	2.49	0.46
6:V:324:THR:OG1	6:V:375:GLY:N	2.49	0.46
1:A:854:ASP:OD1	1:A:855:ASP:N	2.49	0.46
4:D:274:ARG:NH2	4:D:284:PHE:O	2.42	0.46
4:D:1080:LEU:HD12	4:D:1080:LEU:O	2.15	0.46
1:I:1100:PRO:O	1:I:1102:GLN:N	2.48	0.46
6:S:80:TYR:OH	6:S:162:GLY:N	2.49	0.46
1:L:474:LEU:HD12	1:L:474:LEU:C	2.41	0.45
2:M:402:TRP:CD1	2:M:402:TRP:C	2.94	0.45
2:P:450:ASN:C	6:V:525:LEU:HD13	2.41	0.45
3:H:41:ASP:OD1	3:H:41:ASP:C	2.59	0.45
1:O:474:LEU:C	1:O:474:LEU:HD12	2.42	0.45
1:O:904:ILE:HG22	1:O:906:VAL:HG23	1.98	0.45
2:M:487:MET:HE3	2:M:487:MET:N	2.32	0.45
6:R:168:ILE:HD12	6:R:168:ILE:C	2.41	0.45
6:R:254:ASP:HA	6:R:296:ALA:HB2	1.97	0.45
6:S:247:MET:SD	6:S:247:MET:C	2.99	0.45
6:S:503:LEU:HD12	6:S:505:ARG:NH2	2.32	0.45
5:E:318:ARG:NE	5:E:602:GLY:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:450:ASN:C	6:T:525:LEU:HD13	2.41	0.45
1:L:333:LEU:HB2	1:L:338:LEU:HD11	1.98	0.45
2:P:1242:GLN:OE1	2:P:1283:GLN:NE2	2.50	0.45
6:S:324:THR:OG1	6:S:375:GLY:O	2.31	0.45
1:I:1152:MET:HE1	2:J:5:ILE:CG2	2.46	0.45
2:J:296:LEU:HD13	2:J:300:MET:HE2	1.99	0.45
1:O:320:LEU:HD11	1:O:465:ILE:HD12	1.97	0.45
6:R:80:TYR:OH	6:R:162:GLY:N	2.49	0.45
6:R:324:THR:OG1	6:R:375:GLY:N	2.50	0.45
6:U:503:LEU:HD12	6:U:505:ARG:NH2	2.32	0.45
1:A:577:ARG:NH1	1:O:145:ASP:O	2.50	0.45
3:C:317:LEU:C	3:C:317:LEU:HD13	2.42	0.45
1:I:904:ILE:CG2	1:I:906:VAL:HG23	2.46	0.45
2:M:499:PHE:N	2:M:510:GLY:O	2.50	0.45
1:O:331:GLU:OE1	1:O:331:GLU:N	2.50	0.45
1:A:320:LEU:HD11	1:A:465:ILE:HD12	1.98	0.45
5:E:89:THR:OG1	5:E:90:LEU:N	2.49	0.45
5:E:663:ASP:OD1	5:E:665:ALA:N	2.45	0.45
1:F:403:ASP:OD1	1:F:403:ASP:N	2.47	0.45
2:G:1242:GLN:OE1	2:G:1283:GLN:NE2	2.50	0.45
3:H:139:PRO:O	3:H:140:MET:HE2	2.17	0.45
6:R:247:MET:C	6:R:247:MET:SD	3.00	0.45
1:L:244:PHE:C	1:L:245:THR:HG1	2.17	0.45
1:L:288:GLN:NE2	1:L:1135:LEU:O	2.50	0.45
1:L:981:GLU:OE2	1:L:981:GLU:C	2.59	0.45
2:M:123:THR:HG22	2:M:617:MET:HE1	1.99	0.45
3:N:39:ILE:HD12	3:N:39:ILE:C	2.42	0.45
3:Q:39:ILE:HD12	3:Q:39:ILE:C	2.42	0.45
3:Q:528:SER:N	3:Q:617:ASN:OD1	2.46	0.45
6:T:503:LEU:HD12	6:T:505:ARG:NH2	2.32	0.45
4:D:414:THR:HG23	4:D:431:PRO:HG2	1.99	0.45
5:E:180:LEU:HD23	5:E:180:LEU:C	2.42	0.45
1:F:197:ASP:OD1	1:F:197:ASP:C	2.60	0.45
2:M:24:GLN:O	2:M:28:ASN:ND2	2.50	0.45
3:N:545:ASP:OD2	3:N:545:ASP:C	2.59	0.45
1:O:403:ASP:OD1	1:O:403:ASP:N	2.46	0.45
1:O:807:LEU:HD21	1:O:817:LEU:HD22	1.99	0.45
2:P:499:PHE:N	2:P:510:GLY:O	2.50	0.45
2:B:308:ASP:OD2	2:B:315:ARG:NE	2.38	0.45
3:N:102:ILE:HD12	3:N:523:ALA:HB3	1.99	0.45
3:Q:97:ASN:OD1	3:Q:97:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:235:VAL:HG23	6:R:281:GLN:NE2	2.32	0.45
6:S:442:HIS:ND1	6:S:449:ASP:OD1	2.46	0.44
6:V:80:TYR:OH	6:V:162:GLY:N	2.50	0.44
6:V:235:VAL:HG23	6:V:281:GLN:NE2	2.33	0.44
2:J:707:ASP:OD1	2:J:725:TYR:OH	2.31	0.44
2:M:402:TRP:CD1	2:M:402:TRP:O	2.71	0.44
1:A:345:VAL:HG21	1:A:368:ILE:HD11	1.99	0.44
1:A:1100:PRO:O	1:A:1102:GLN:N	2.49	0.44
3:H:377:ARG:NH2	3:H:381:ASP:OD1	2.48	0.44
3:K:35:VAL:HG23	1:L:394:ARG:HH12	1.82	0.44
2:M:457:LYS:NZ	6:U:539:CYS:SG	2.73	0.44
1:O:655:LEU:HD22	1:O:783:PHE:HZ	1.81	0.44
6:R:217:MET:O	6:R:217:MET:SD	2.76	0.44
6:T:525:LEU:O	6:T:527:THR:N	2.50	0.44
6:U:235:VAL:HG23	6:U:281:GLN:NE2	2.32	0.44
3:C:454:ASP:OD2	3:C:627:ILE:HG22	2.17	0.44
1:F:519:LEU:HD21	1:F:590:LEU:HD22	2.00	0.44
1:F:878:ASP:OD2	1:F:878:ASP:N	2.49	0.44
2:M:177:ASP:OD1	2:M:177:ASP:N	2.50	0.44
3:N:275:GLN:O	3:N:286:ARG:NH1	2.51	0.44
6:S:525:LEU:O	6:S:527:THR:N	2.51	0.44
3:K:582:TRP:O	3:K:583:SER:OG	2.35	0.44
2:M:230:ASN:ND2	2:M:251:GLU:OE1	2.47	0.44
6:S:542:LYS:N	6:S:542:LYS:HD3	2.32	0.44
6:V:503:LEU:HD12	6:V:505:ARG:NH2	2.32	0.44
5:E:339:VAL:HG21	5:E:372:TYR:CE2	2.53	0.44
5:E:392:LEU:HD23	5:E:392:LEU:H	1.83	0.44
1:F:965:LEU:HD23	1:F:965:LEU:C	2.42	0.44
2:J:487:MET:HE2	2:J:490:LYS:H	1.83	0.44
2:M:707:ASP:OD1	2:M:725:TYR:OH	2.30	0.44
6:R:503:LEU:HD12	6:R:505:ARG:NH2	2.32	0.44
6:V:143:ASP:OD1	6:V:146:ASP:N	2.46	0.44
6:V:172:PHE:N	6:V:172:PHE:CD1	2.85	0.44
1:A:75:ARG:NH1	1:A:176:ASP:OD1	2.51	0.44
2:J:500:SER:C	2:J:501:LEU:HD22	2.43	0.44
2:M:563:GLU:C	2:M:563:GLU:OE2	2.61	0.44
1:O:904:ILE:CG2	1:O:906:VAL:HG23	2.47	0.44
1:O:1100:PRO:O	1:O:1102:GLN:N	2.48	0.44
6:R:234:PHE:CE2	6:R:238:ILE:HD11	2.53	0.44
6:R:525:LEU:O	6:R:527:THR:N	2.50	0.44
6:U:442:HIS:ND1	6:U:449:ASP:OD1	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:217:MET:O	6:V:217:MET:SD	2.76	0.44
1:F:848:ASN:OD1	1:F:848:ASN:N	2.51	0.44
2:J:402:TRP:CG	2:J:402:TRP:O	2.70	0.44
2:M:1242:GLN:OE1	2:M:1283:GLN:NE2	2.50	0.44
6:R:312:LEU:HB3	6:R:317:VAL:HG21	2.00	0.44
5:E:565:VAL:HG22	5:E:585:TRP:CD1	2.50	0.44
3:N:97:ASN:OD1	3:N:97:ASN:N	2.50	0.44
3:Q:317:LEU:C	3:Q:317:LEU:HD13	2.43	0.44
2:B:457:LYS:O	2:B:465:CYS:N	2.51	0.43
3:K:119:ASN:O	3:K:126:GLN:NE2	2.51	0.43
3:K:406:SER:HB3	3:K:408:ILE:HD11	2.00	0.43
1:O:848:ASN:OD1	1:O:848:ASN:N	2.51	0.43
6:R:161:ASP:O	6:R:166:ALA:N	2.51	0.43
6:V:214:GLY:O	6:V:218:SER:OG	2.35	0.43
5:E:201:LYS:O	5:E:202:ASN:OD1	2.35	0.43
1:F:273:VAL:O	1:F:1111:TRP:NE1	2.43	0.43
2:J:499:PHE:N	2:J:510:GLY:O	2.51	0.43
1:L:904:ILE:CG2	1:L:906:VAL:HG23	2.48	0.43
3:Q:582:TRP:O	3:Q:583:SER:OG	2.31	0.43
1:A:136:TYR:CZ	2:B:797:LEU:HD11	2.54	0.43
1:A:692:THR:HG22	1:A:694:LEU:H	1.83	0.43
4:D:51:VAL:HG12	4:D:207:ILE:HD11	1.99	0.43
3:H:194:ASP:OD2	3:H:194:ASP:O	2.35	0.43
2:J:1242:GLN:OE1	2:J:1283:GLN:NE2	2.50	0.43
2:P:24:GLN:O	2:P:28:ASN:ND2	2.50	0.43
2:P:500:SER:C	2:P:501:LEU:HD22	2.43	0.43
6:V:442:HIS:ND1	6:V:449:ASP:OD1	2.45	0.43
6:V:525:LEU:O	6:V:527:THR:N	2.51	0.43
4:D:12:LEU:H	4:D:12:LEU:HD22	1.84	0.43
1:L:965:LEU:C	1:L:965:LEU:HD12	2.42	0.43
1:O:767:MET:O	1:O:771:THR:OG1	2.21	0.43
2:G:292:ARG:NH1	2:G:333:SER:O	2.49	0.43
3:K:97:ASN:OD1	3:K:97:ASN:N	2.49	0.43
6:S:235:VAL:HG23	6:S:281:GLN:NE2	2.33	0.43
6:T:208:PHE:CG	6:T:247:MET:HE1	2.54	0.43
6:T:247:MET:SD	6:T:247:MET:C	3.01	0.43
2:B:296:LEU:HD13	2:B:300:MET:HE3	2.00	0.43
5:E:550:GLU:OE1	5:E:550:GLU:N	2.51	0.43
1:F:136:TYR:CZ	2:G:797:LEU:HD11	2.54	0.43
2:G:230:ASN:ND2	2:G:251:GLU:OE1	2.49	0.43
3:H:607:GLN:OE1	3:H:607:GLN:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:692:THR:HG22	1:I:694:LEU:H	1.83	0.43
3:K:505:THR:HG23	3:K:506:MET:N	2.33	0.43
1:O:348:ALA:HB3	1:O:351:ILE:HG22	2.00	0.43
1:O:351:ILE:HD12	1:O:436:MET:HG3	2.00	0.43
6:T:247:MET:SD	6:T:247:MET:O	2.77	0.43
6:U:525:LEU:O	6:U:527:THR:N	2.51	0.43
1:F:1100:PRO:O	1:F:1102:GLN:N	2.48	0.43
3:K:528:SER:N	3:K:617:ASN:OD1	2.49	0.43
2:M:613:HIS:O	2:M:617:MET:N	2.46	0.43
1:I:519:LEU:HD21	1:I:590:LEU:HD22	2.01	0.43
2:B:613:HIS:O	2:B:617:MET:N	2.48	0.43
3:C:171:GLY:O	3:C:177:ARG:NH2	2.51	0.43
4:D:168:ASP:OD2	4:D:168:ASP:C	2.61	0.43
4:D:1324:LEU:HD12	4:D:1325:LEU:HD22	2.01	0.43
3:H:317:LEU:C	3:H:317:LEU:HD13	2.44	0.43
1:L:687:ASP:OD1	1:L:687:ASP:N	2.52	0.43
6:T:450:TYR:CD1	6:T:450:TYR:C	2.97	0.43
5:E:492:LEU:HD12	5:E:492:LEU:H	1.84	0.43
2:G:239:ILE:HD12	2:G:316:LEU:HD22	2.01	0.43
2:G:709:GLU:OE1	2:G:709:GLU:HA	2.19	0.43
1:L:692:THR:HG22	1:L:694:LEU:H	1.84	0.43
1:O:317:GLN:C	1:O:317:GLN:OE1	2.62	0.43
3:Q:371:LEU:H	3:Q:371:LEU:HD22	1.83	0.43
6:V:450:TYR:CD1	6:V:450:TYR:C	2.97	0.43
4:D:980:LEU:HD13	4:D:981:PRO:HD2	2.01	0.42
4:D:1088:ILE:HD12	4:D:1089:LEU:N	2.33	0.42
1:F:687:ASP:OD1	1:F:687:ASP:N	2.52	0.42
2:G:450:ASN:C	6:S:525:LEU:HD13	2.44	0.42
3:H:491:LEU:O	3:H:625:LYS:NZ	2.52	0.42
1:I:807:LEU:HD21	1:I:817:LEU:HD22	2.01	0.42
1:I:892:SER:OG	1:I:895:GLU:OE1	2.32	0.42
3:K:343:CYS:SG	3:K:344:VAL:N	2.92	0.42
6:T:246:PRO:O	6:T:289:ASN:ND2	2.50	0.42
2:B:416:THR:OG1	2:B:418:ASP:OD1	2.35	0.42
3:N:139:PRO:O	3:N:140:MET:HE2	2.19	0.42
3:Q:377:ARG:NH2	3:Q:381:ASP:OD1	2.47	0.42
6:V:234:PHE:CE2	6:V:238:ILE:HD11	2.54	0.42
3:C:247:LEU:HD12	3:C:247:LEU:N	2.34	0.42
4:D:1351:LEU:N	4:D:1351:LEU:HD22	2.34	0.42
1:F:349:ASP:OD1	1:F:349:ASP:N	2.50	0.42
2:G:499:PHE:N	2:G:510:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:560:THR:OG1	3:H:561:PRO:HD2	2.19	0.42
1:I:1099:ASN:HB3	1:I:1100:PRO:HD3	2.01	0.42
2:J:457:LYS:O	2:J:465:CYS:N	2.52	0.42
3:K:473:GLU:O	3:K:473:GLU:OE1	2.37	0.42
3:N:52:GLU:OE2	1:O:398:ARG:NH1	2.52	0.42
1:O:349:ASP:OD1	1:O:349:ASP:N	2.52	0.42
2:P:707:ASP:OD1	2:P:725:TYR:OH	2.31	0.42
3:Q:503:LEU:HD11	3:Q:556:ILE:HD11	2.00	0.42
3:Q:543:ASP:O	3:Q:562:ARG:NH2	2.53	0.42
6:R:442:HIS:ND1	6:R:449:ASP:OD1	2.46	0.42
6:U:500:HIS:O	6:U:505:ARG:NE	2.48	0.42
6:V:254:ASP:HA	6:V:296:ALA:HB2	2.01	0.42
3:C:505:THR:HG23	3:C:506:MET:N	2.35	0.42
4:D:916:ASP:OD1	4:D:916:ASP:N	2.52	0.42
4:D:984:LEU:HD11	5:E:12:VAL:HG11	2.02	0.42
1:L:1100:PRO:O	1:L:1102:GLN:N	2.48	0.42
3:N:35:VAL:HG23	1:O:394:ARG:HH12	1.84	0.42
6:U:172:PHE:N	6:U:172:PHE:CD1	2.86	0.42
6:V:498:ALA:HA	6:V:514:MET:HE1	2.00	0.42
1:F:246:LEU:N	1:F:247:PRO:HD2	2.35	0.42
1:F:873:ASN:HB3	1:F:904:ILE:HD11	2.01	0.42
1:I:767:MET:HE3	1:I:767:MET:HA	2.01	0.42
1:I:904:ILE:HG22	1:I:906:VAL:HG23	2.00	0.42
2:J:651:LEU:N	2:J:651:LEU:HD22	2.35	0.42
2:M:500:SER:C	2:M:501:LEU:HD22	2.44	0.42
6:U:450:TYR:CD1	6:U:450:TYR:C	2.98	0.42
1:F:1002:PHE:HE1	1:F:1013:LEU:HD11	1.83	0.42
2:G:500:SER:C	2:G:501:LEU:HD22	2.45	0.42
1:O:692:THR:HG22	1:O:694:LEU:H	1.84	0.42
6:R:450:TYR:C	6:R:450:TYR:CD2	2.97	0.42
6:S:172:PHE:CD1	6:S:172:PHE:N	2.86	0.42
6:V:500:HIS:O	6:V:505:ARG:NE	2.50	0.42
2:B:709:GLU:OE2	2:B:709:GLU:HA	2.18	0.42
2:B:1242:GLN:OE1	2:B:1283:GLN:NE2	2.53	0.42
3:C:304:SER:OG	3:C:345:ASP:OD1	2.38	0.42
4:D:125:ILE:HD11	4:D:249:SER:CB	2.46	0.42
4:D:1109:LEU:HD13	4:D:1109:LEU:C	2.44	0.42
2:J:251:GLU:OE2	2:J:275:ARG:NH1	2.47	0.42
1:L:17:ILE:HD11	1:L:21:LEU:HD23	2.02	0.42
6:T:235:VAL:HG23	6:T:281:GLN:NE2	2.33	0.42
6:T:340:ASN:HB2	6:T:446:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:LEU:N	1:A:247:PRO:HD2	2.35	0.42
1:A:687:ASP:OD1	1:A:687:ASP:N	2.51	0.42
1:L:878:ASP:OD1	1:L:878:ASP:N	2.51	0.42
2:M:398:ILE:HD11	2:M:518:VAL:HG21	2.01	0.42
1:O:206:THR:HG22	1:O:208:LEU:H	1.85	0.42
3:Q:1:MET:O	3:Q:1:MET:SD	2.78	0.42
4:D:638:GLU:N	4:D:638:GLU:OE1	2.52	0.42
1:I:687:ASP:OD1	1:I:687:ASP:N	2.52	0.42
1:I:892:SER:O	1:I:896:MET:HE2	2.20	0.42
3:N:522:ASP:N	3:N:522:ASP:OD1	2.52	0.42
3:Q:343:CYS:SG	3:Q:344:VAL:N	2.92	0.42
6:S:234:PHE:CE2	6:S:238:ILE:HD11	2.54	0.42
6:U:217:MET:O	6:U:217:MET:SD	2.78	0.42
6:U:234:PHE:CE2	6:U:238:ILE:HD11	2.55	0.42
1:A:848:ASN:OD1	1:A:848:ASN:N	2.52	0.42
4:D:1041:LEU:HD23	4:D:1041:LEU:O	2.20	0.42
5:E:1:MET:HE3	5:E:1:MET:H1	1.85	0.42
5:E:603:LEU:H	5:E:603:LEU:HD23	1.84	0.42
1:F:981:GLU:OE1	1:F:982:LEU:N	2.53	0.42
1:O:687:ASP:N	1:O:687:ASP:OD1	2.51	0.42
2:P:468:ASN:ND2	2:P:482:ASN:O	2.46	0.42
2:P:709:GLU:OE1	2:P:709:GLU:HA	2.19	0.42
6:T:208:PHE:CD1	6:T:247:MET:HE1	2.55	0.42
3:C:528:SER:N	3:C:617:ASN:OD1	2.48	0.41
3:H:102:ILE:HD12	3:H:523:ALA:HB3	2.02	0.41
2:J:329:ASP:OD2	2:J:329:ASP:N	2.52	0.41
3:K:117:ASP:OD1	3:K:117:ASP:N	2.53	0.41
2:M:329:ASP:OD1	2:M:373:VAL:HG11	2.19	0.41
2:M:495:ILE:HD12	2:M:516:LEU:HD12	2.01	0.41
3:Q:82:ASN:OD1	3:Q:82:ASN:N	2.52	0.41
6:R:324:THR:OG1	6:R:375:GLY:O	2.34	0.41
6:S:71:LEU:N	6:S:71:LEU:HD12	2.35	0.41
1:F:845:LEU:HD11	1:F:961:LEU:HD22	2.02	0.41
2:G:296:LEU:HD13	2:G:300:MET:HE3	2.02	0.41
1:I:136:TYR:CZ	2:J:797:LEU:HD11	2.55	0.41
2:J:805:GLU:OE2	2:J:805:GLU:HA	2.20	0.41
3:K:490:ASP:O	3:K:494:ARG:N	2.51	0.41
1:L:999:ASN:OD1	1:L:999:ASN:N	2.52	0.41
2:M:251:GLU:OE2	2:M:275:ARG:NH1	2.47	0.41
3:N:40:PHE:O	3:N:41:ASP:OD1	2.38	0.41
3:N:343:CYS:SG	3:N:344:VAL:N	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:244:PHE:C	1:O:245:THR:HG1	2.19	0.41
1:O:246:LEU:N	1:O:247:PRO:HD2	2.35	0.41
3:Q:472:MET:HE2	3:Q:472:MET:CA	2.50	0.41
3:Q:612:MET:HE3	3:Q:615:LEU:HD12	2.02	0.41
6:S:340:ASN:HB2	6:S:446:ALA:HB1	2.02	0.41
1:A:421:ASN:OD1	1:A:421:ASN:N	2.53	0.41
2:B:1213:ASP:O	2:G:1322:THR:OG1	2.36	0.41
3:C:285:LEU:HB3	3:C:301:LEU:HD21	2.01	0.41
3:C:371:LEU:H	3:C:371:LEU:HD22	1.85	0.41
4:D:1317:LEU:HD23	4:D:1322:LEU:HB3	2.01	0.41
2:M:226:VAL:HG13	2:M:228:LEU:HG	2.03	0.41
2:M:863:GLU:HB2	2:M:864:PRO:HD3	2.03	0.41
3:N:565:LYS:NZ	3:N:569:GLU:OE2	2.49	0.41
1:O:999:ASN:OD1	1:O:999:ASN:N	2.52	0.41
1:A:398:ARG:NH1	3:Q:52:GLU:OE2	2.54	0.41
4:D:743:GLN:OE1	4:D:743:GLN:O	2.37	0.41
4:D:886:GLU:OE1	4:D:888:TYR:OH	2.23	0.41
1:F:692:THR:HG22	1:F:694:LEU:H	1.85	0.41
1:I:206:THR:HG22	1:I:208:LEU:H	1.84	0.41
3:K:494:ARG:NH1	3:K:625:LYS:O	2.54	0.41
3:Q:492:THR:O	3:Q:625:LYS:NZ	2.45	0.41
2:G:613:HIS:O	2:G:617:MET:N	2.48	0.41
1:I:244:PHE:C	1:I:245:THR:HG1	2.19	0.41
1:I:246:LEU:N	1:I:247:PRO:HD2	2.35	0.41
1:I:986:LEU:O	1:I:990:THR:HG23	2.20	0.41
2:J:632:ASN:OD1	2:J:701:ASN:ND2	2.52	0.41
2:J:1195:LEU:HD23	2:J:1195:LEU:C	2.45	0.41
1:L:59:ARG:HB3	1:L:59:ARG:CZ	2.51	0.41
2:P:613:HIS:O	2:P:617:MET:N	2.51	0.41
6:T:193:LEU:O	6:T:197:ARG:NH2	2.53	0.41
6:V:225:ALA:O	6:V:231:ARG:NH1	2.53	0.41
2:B:824:MET:SD	2:B:825:ASP:N	2.94	0.41
3:C:564:VAL:HG21	3:C:591:LEU:HG	2.02	0.41
4:D:461:THR:HG23	4:D:463:MET:HE3	2.03	0.41
4:D:1085:GLU:OE1	4:D:1132:VAL:HG21	2.21	0.41
4:D:1210:ASN:OD1	4:D:1214:GLU:N	2.44	0.41
2:G:226:VAL:HG13	2:G:228:LEU:HG	2.03	0.41
2:G:643:GLU:OE2	2:G:654:LYS:NZ	2.46	0.41
1:I:59:ARG:CZ	1:I:59:ARG:HB3	2.50	0.41
2:J:226:VAL:HG13	2:J:228:LEU:HG	2.03	0.41
6:R:247:MET:SD	6:R:247:MET:O	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:217:MET:O	6:T:217:MET:CE	2.69	0.41
6:T:234:PHE:CE2	6:T:238:ILE:HD11	2.55	0.41
6:V:340:ASN:HB2	6:V:446:ALA:HB1	2.02	0.41
1:F:999:ASN:OD1	1:F:999:ASN:N	2.54	0.41
2:G:177:ASP:OD2	2:G:177:ASP:N	2.51	0.41
3:K:40:PHE:O	3:K:41:ASP:OD1	2.39	0.41
1:L:246:LEU:N	1:L:247:PRO:HD2	2.35	0.41
3:N:345:ASP:OD1	3:N:393:SER:OG	2.39	0.41
1:O:878:ASP:N	1:O:878:ASP:OD2	2.53	0.41
2:P:1325:LYS:HD2	2:P:1325:LYS:O	2.20	0.41
3:Q:1:MET:HE2	3:Q:2:VAL:N	2.35	0.41
6:S:85:ILE:HD12	6:S:85:ILE:O	2.21	0.41
6:U:296:ALA:HB1	6:U:323:MET:HE3	2.03	0.41
1:A:355:THR:O	1:A:355:THR:OG1	2.38	0.41
2:B:226:VAL:HG13	2:B:228:LEU:HG	2.02	0.41
2:G:445:PHE:CE2	2:G:451:ILE:HD12	2.56	0.41
3:H:516:ILE:CD1	3:H:558:LEU:HD13	2.51	0.41
1:L:519:LEU:HD21	1:L:590:LEU:HD22	2.03	0.41
1:O:136:TYR:CZ	2:P:797:LEU:HD11	2.56	0.41
3:Q:40:PHE:O	3:Q:41:ASP:OD1	2.38	0.41
4:D:980:LEU:HD21	4:D:1474:VAL:HG21	2.03	0.41
2:G:986:ASN:O	2:G:986:ASN:ND2	2.53	0.41
1:I:999:ASN:OD1	1:I:999:ASN:N	2.54	0.41
2:J:292:ARG:NH1	2:J:333:SER:O	2.50	0.41
2:M:30:LYS:O	2:M:33:THR:HG23	2.20	0.41
2:M:296:LEU:HD13	2:M:300:MET:HE2	2.02	0.41
2:M:376:TYR:OH	2:M:396:VAL:HG13	2.21	0.41
3:N:317:LEU:HD13	3:N:317:LEU:C	2.46	0.41
2:P:621:ARG:NH1	2:P:625:GLU:OE1	2.47	0.41
6:U:313:MET:HE3	6:U:313:MET:C	2.45	0.41
3:H:394:ILE:HD13	3:H:416:LEU:CD1	2.51	0.41
2:J:398:ILE:HD11	2:J:518:VAL:HG21	2.02	0.41
3:N:13:MET:CE	1:O:368:ILE:HD11	2.47	0.41
2:P:322:LYS:HG2	2:P:324:MET:HE2	2.03	0.41
2:B:500:SER:C	2:B:501:LEU:HD22	2.46	0.40
3:C:102:ILE:HD12	3:C:523:ALA:HB3	2.03	0.40
1:F:1157:ALA:O	1:F:1158:GLN:NE2	2.49	0.40
2:G:376:TYR:OH	2:G:396:VAL:HG13	2.21	0.40
2:M:709:GLU:OE2	2:P:102:ARG:NH2	2.54	0.40
2:P:226:VAL:HG13	2:P:228:LEU:HG	2.03	0.40
6:R:214:GLY:O	6:R:218:SER:OG	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.98	0.40
2:B:292:ARG:NH1	2:B:333:SER:O	2.50	0.40
2:B:863:GLU:HB2	2:B:864:PRO:HD3	2.03	0.40
2:G:484:THR:HG22	6:S:542:LYS:NZ	2.37	0.40
3:H:2:VAL:HG12	3:H:145:VAL:HG21	2.02	0.40
3:H:97:ASN:OD1	3:H:97:ASN:N	2.50	0.40
3:N:593:ASN:HB2	3:N:612:MET:CE	2.52	0.40
3:Q:391:GLU:OE2	3:Q:418:ASN:ND2	2.53	0.40
6:R:313:MET:C	6:R:313:MET:SD	3.05	0.40
6:T:324:THR:OG1	6:T:375:GLY:O	2.31	0.40
6:U:340:ASN:HB2	6:U:446:ALA:HB1	2.02	0.40
2:B:398:ILE:HD11	2:B:518:VAL:HG21	2.03	0.40
2:B:849:ASN:OD1	2:B:849:ASN:C	2.64	0.40
4:D:1266:GLU:OE2	4:D:1266:GLU:C	2.65	0.40
1:I:526:LEU:HD12	1:I:526:LEU:HA	1.99	0.40
1:I:1002:PHE:HE1	1:I:1013:LEU:HD11	1.85	0.40
2:J:468:ASN:ND2	2:J:482:ASN:O	2.48	0.40
2:J:495:ILE:HD12	2:J:516:LEU:HD12	2.02	0.40
2:J:849:ASN:OD1	2:J:850:ALA:N	2.55	0.40
3:K:560:THR:OG1	3:K:561:PRO:HD2	2.21	0.40
3:C:621:GLU:OE1	3:C:622:ILE:N	2.54	0.40
4:D:1266:GLU:OE2	4:D:1266:GLU:O	2.39	0.40
5:E:5:LEU:O	5:E:29:ARG:NE	2.54	0.40
2:J:863:GLU:HB2	2:J:864:PRO:HD3	2.03	0.40
1:L:88:PHE:CE2	1:L:92:VAL:HG21	2.56	0.40
3:N:528:SER:N	3:N:617:ASN:OD1	2.48	0.40
2:P:457:LYS:O	2:P:465:CYS:N	2.54	0.40
1:A:999:ASN:OD1	1:A:999:ASN:N	2.55	0.40
3:C:39:ILE:HD12	3:C:39:ILE:C	2.44	0.40
4:D:624:ILE:HD12	4:D:700:LEU:HD11	2.02	0.40
3:K:564:VAL:HG21	3:K:591:LEU:HG	2.04	0.40
1:L:981:GLU:OE2	1:L:982:LEU:N	2.55	0.40
2:P:398:ILE:HD11	2:P:518:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1098/1164 (94%)	1086 (99%)	12 (1%)	0	100	100
1	F	1098/1164 (94%)	1085 (99%)	13 (1%)	0	100	100
1	I	1098/1164 (94%)	1087 (99%)	11 (1%)	0	100	100
1	L	1098/1164 (94%)	1087 (99%)	11 (1%)	0	100	100
1	O	1098/1164 (94%)	1087 (99%)	11 (1%)	0	100	100
2	B	1312/1364 (96%)	1293 (99%)	19 (1%)	0	100	100
2	G	1312/1364 (96%)	1292 (98%)	20 (2%)	0	100	100
2	J	1312/1364 (96%)	1289 (98%)	23 (2%)	0	100	100
2	M	1312/1364 (96%)	1289 (98%)	23 (2%)	0	100	100
2	P	1312/1364 (96%)	1290 (98%)	22 (2%)	0	100	100
3	C	631/633 (100%)	617 (98%)	14 (2%)	0	100	100
3	H	631/633 (100%)	619 (98%)	12 (2%)	0	100	100
3	K	631/633 (100%)	618 (98%)	13 (2%)	0	100	100
3	N	631/633 (100%)	616 (98%)	15 (2%)	0	100	100
3	Q	631/633 (100%)	616 (98%)	15 (2%)	0	100	100
4	D	1472/1487 (99%)	1441 (98%)	31 (2%)	0	100	100
5	E	648/970 (67%)	630 (97%)	18 (3%)	0	100	100
6	R	540/542 (100%)	531 (98%)	9 (2%)	0	100	100
6	S	540/542 (100%)	531 (98%)	9 (2%)	0	100	100
6	T	540/542 (100%)	527 (98%)	13 (2%)	0	100	100
6	U	540/542 (100%)	529 (98%)	11 (2%)	0	100	100
6	V	540/542 (100%)	531 (98%)	9 (2%)	0	100	100
All	All	20025/20972 (96%)	19691 (98%)	334 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	962/1022 (94%)	957 (100%)	5 (0%)	81	82
1	F	962/1022 (94%)	953 (99%)	9 (1%)	70	77
1	I	962/1022 (94%)	958 (100%)	4 (0%)	84	84
1	L	962/1022 (94%)	952 (99%)	10 (1%)	68	76
1	O	962/1022 (94%)	960 (100%)	2 (0%)	87	87
2	B	1165/1209 (96%)	1159 (100%)	6 (0%)	81	82
2	G	1165/1209 (96%)	1155 (99%)	10 (1%)	70	77
2	J	1165/1209 (96%)	1159 (100%)	6 (0%)	81	82
2	M	1165/1209 (96%)	1162 (100%)	3 (0%)	86	85
2	P	1165/1209 (96%)	1156 (99%)	9 (1%)	73	78
3	C	520/520 (100%)	517 (99%)	3 (1%)	78	80
3	H	520/520 (100%)	514 (99%)	6 (1%)	63	74
3	K	520/520 (100%)	517 (99%)	3 (1%)	78	80
3	N	520/520 (100%)	515 (99%)	5 (1%)	68	76
3	Q	520/520 (100%)	516 (99%)	4 (1%)	73	78
4	D	1255/1266 (99%)	1236 (98%)	19 (2%)	57	71
5	E	551/818 (67%)	541 (98%)	10 (2%)	51	69
6	R	455/455 (100%)	453 (100%)	2 (0%)	84	84
6	S	455/455 (100%)	453 (100%)	2 (0%)	84	84
6	T	455/455 (100%)	453 (100%)	2 (0%)	84	84
6	U	455/455 (100%)	453 (100%)	2 (0%)	84	84
6	V	455/455 (100%)	452 (99%)	3 (1%)	76	79
All	All	17316/18114 (96%)	17191 (99%)	125 (1%)	73	79

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	390	ILE
1	A	406	SER
1	A	615	MET
1	A	831	THR
1	A	885	ILE
2	B	34	ASN
2	B	59	VAL
2	B	163	VAL
2	B	652	LEU
2	B	801	TRP
2	B	881	SER
3	C	295	MET
3	C	314	PHE
3	C	344	VAL
4	D	12	LEU
4	D	129	PHE
4	D	134	THR
4	D	350	SER
4	D	558	ILE
4	D	562	SER
4	D	669	CYS
4	D	753	HIS
4	D	769	LEU
4	D	806	VAL
4	D	928	GLU
4	D	1022	GLN
4	D	1080	LEU
4	D	1112	SER
4	D	1191	PHE
4	D	1196	SER
4	D	1259	HIS
4	D	1260	CYS
4	D	1273	THR
5	E	57	ASP
5	E	93	ASN
5	E	104	THR
5	E	196	SER
5	E	209	LEU
5	E	243	THR
5	E	282	THR
5	E	301	THR
5	E	469	SER
5	E	659	TRP

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Mol	Chain	Res	Type
1	F	60	SER
1	F	68	SER
1	F	355	THR
1	F	380	ILE
1	F	390	ILE
1	F	885	ILE
1	F	956	ASN
1	F	967	ASN
1	F	1034	CYS
2	G	33	THR
2	G	34	ASN
2	G	59	VAL
2	G	191	MET
2	G	445	PHE
2	G	465	CYS
2	G	644	CYS
2	G	650	LEU
2	G	652	LEU
2	G	892	SER
3	H	48	THR
3	H	73	VAL
3	H	344	VAL
3	H	434	TYR
3	H	455	LEU
3	H	529	MET
1	I	390	ILE
1	I	803	LEU
1	I	831	THR
1	I	885	ILE
2	J	34	ASN
2	J	59	VAL
2	J	163	VAL
2	J	289	THR
2	J	515	THR
2	J	1167	GLN
3	K	84	ILE
3	K	264	ILE
3	K	411	LEU
1	L	60	SER
1	L	68	SER
1	L	201	LEU
1	L	355	THR

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Mol	Chain	Res	Type
1	L	390	ILE
1	L	773	GLU
1	L	848	ASN
1	L	885	ILE
1	L	1136	THR
1	L	1152	MET
2	M	59	VAL
2	M	90	GLN
2	M	801	TRP
3	N	48	THR
3	N	73	VAL
3	N	84	ILE
3	N	393	SER
3	N	434	TYR
1	O	201	LEU
1	O	885	ILE
2	P	33	THR
2	P	34	ASN
2	P	59	VAL
2	P	163	VAL
2	P	324	MET
2	P	515	THR
2	P	644	CYS
2	P	652	LEU
2	P	1232	LEU
3	Q	393	SER
3	Q	434	TYR
3	Q	455	LEU
3	Q	538	THR
6	R	337	HIS
6	R	525	LEU
6	S	337	HIS
6	S	525	LEU
6	T	337	HIS
6	T	525	LEU
6	U	337	HIS
6	U	525	LEU
6	V	35	GLU
6	V	337	HIS
6	V	525	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	180	GLN
1	A	212	ASN
1	A	580	GLN
1	A	639	HIS
1	A	682	GLN
1	A	712	ASN
1	A	843	ASN
1	A	1041	ASN
1	A	1045	ASN
2	B	90	GLN
2	B	158	ASN
2	B	205	GLN
2	B	538	GLN
2	B	553	GLN
2	B	582	ASN
2	B	1041	GLN
2	B	1100	GLN
2	B	1145	GLN
2	B	1245	GLN
3	C	162	GLN
3	C	297	HIS
3	C	508	ASN
3	C	519	ASN
3	C	586	GLN
4	D	89	GLN
4	D	499	ASN
4	D	577	GLN
4	D	630	ASN
4	D	636	HIS
4	D	677	GLN
4	D	777	HIS
4	D	1007	HIS
4	D	1145	GLN
4	D	1168	HIS
4	D	1176	GLN
4	D	1274	GLN
1	F	682	GLN
1	F	873	ASN
1	F	962	ASN
1	F	1041	ASN
2	G	69	GLN
2	G	76	ASN

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Mol	Chain	Res	Type
2	G	90	GLN
2	G	109	ASN
2	G	158	ASN
2	G	209	ASN
2	G	582	ASN
2	G	955	GLN
2	G	1041	GLN
2	G	1100	GLN
2	G	1245	GLN
3	H	162	GLN
3	H	519	ASN
1	I	256	ASN
1	I	682	GLN
1	I	967	ASN
1	I	1043	ASN
2	J	76	ASN
2	J	158	ASN
2	J	205	GLN
2	J	243	ASN
2	J	278	HIS
2	J	378	HIS
2	J	582	ASN
2	J	1041	GLN
2	J	1145	GLN
2	J	1245	GLN
3	K	438	HIS
1	L	96	ASN
1	L	682	GLN
1	L	768	ASN
1	L	933	GLN
1	L	1041	ASN
1	L	1043	ASN
1	L	1045	ASN
2	M	76	ASN
2	M	90	GLN
2	M	109	ASN
2	M	158	ASN
2	M	205	GLN
2	M	243	ASN
2	M	263	ASN
2	M	278	HIS
2	M	378	HIS

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Mol	Chain	Res	Type
2	M	582	ASN
2	M	623	ASN
2	M	701	ASN
2	M	1041	GLN
2	M	1100	GLN
2	M	1145	GLN
2	M	1245	GLN
3	N	162	GLN
3	N	209	ASN
3	N	297	HIS
3	N	519	ASN
1	O	682	GLN
1	O	810	ASN
1	O	1041	ASN
1	O	1045	ASN
2	P	69	GLN
2	P	90	GLN
2	P	109	ASN
2	P	158	ASN
2	P	205	GLN
2	P	243	ASN
2	P	378	HIS
2	P	582	ASN
2	P	623	ASN
2	P	701	ASN
2	P	1041	GLN
2	P	1100	GLN
2	P	1245	GLN
2	P	1327	ASN
2	P	1337	HIS
3	Q	119	ASN
3	Q	162	GLN
3	Q	297	HIS
3	Q	438	HIS
3	Q	495	GLN
3	Q	519	ASN
6	T	8	ASN
6	T	509	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
5	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	109:SER	C	114:ASP	N	5.41

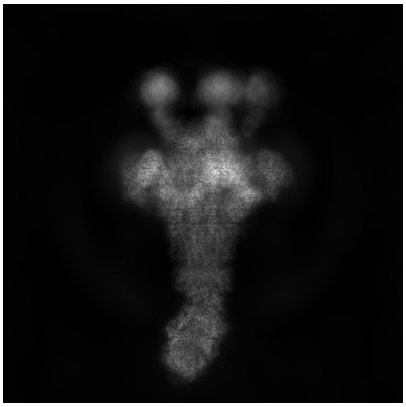
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-58505. These allow visual inspection of the internal detail of the map and identification of artifacts.

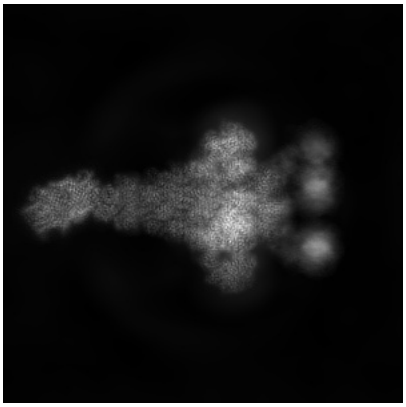
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

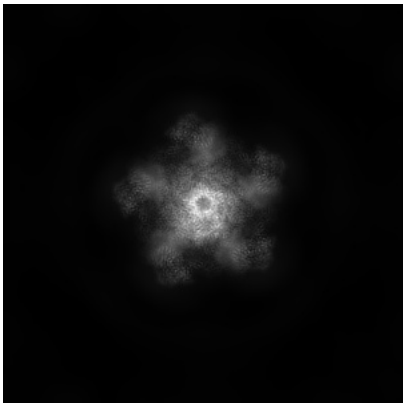
6.1.1 Primary map



X



Y



Z

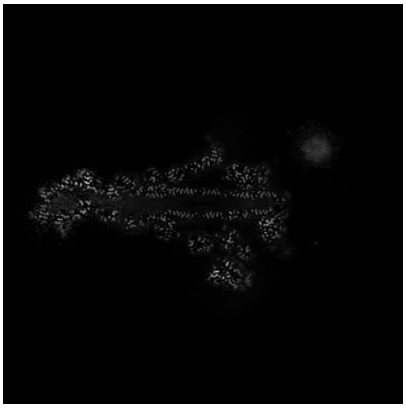
The images above show the map projected in three orthogonal directions.

6.2 Central slices

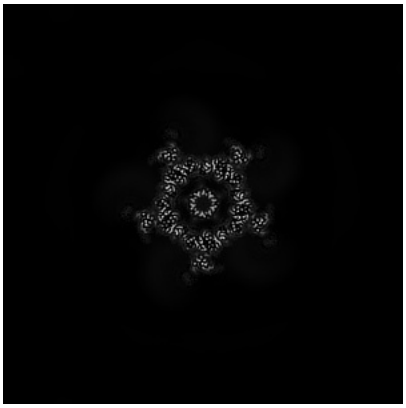
6.2.1 Primary map



X Index: 320



Y Index: 320



Z Index: 320

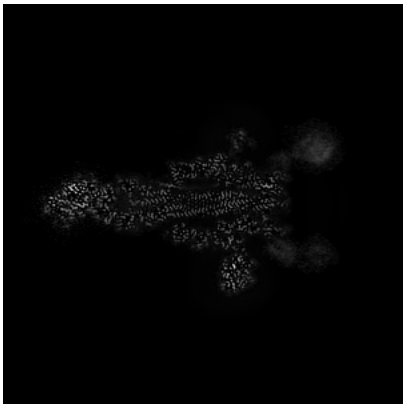
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

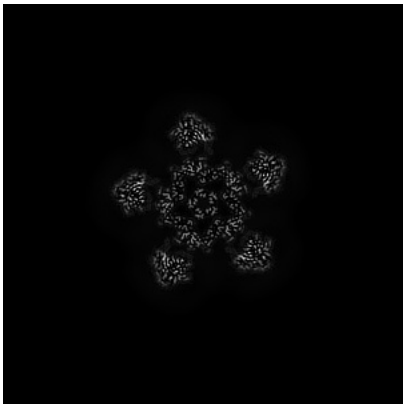
6.3.1 Primary map



X Index: 306



Y Index: 334

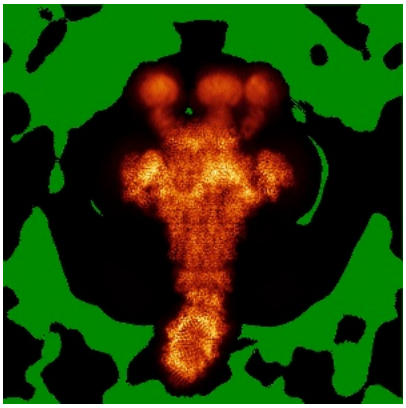


Z Index: 362

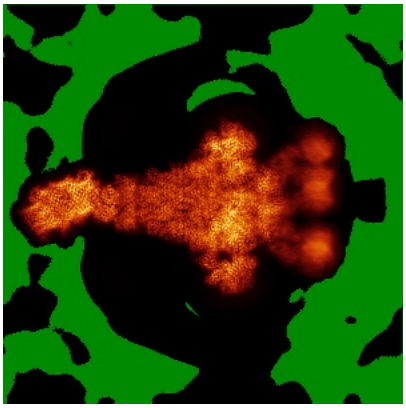
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

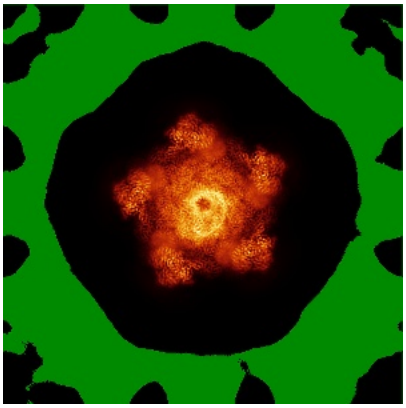
6.4.1 Primary map



X



Y



Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0969. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

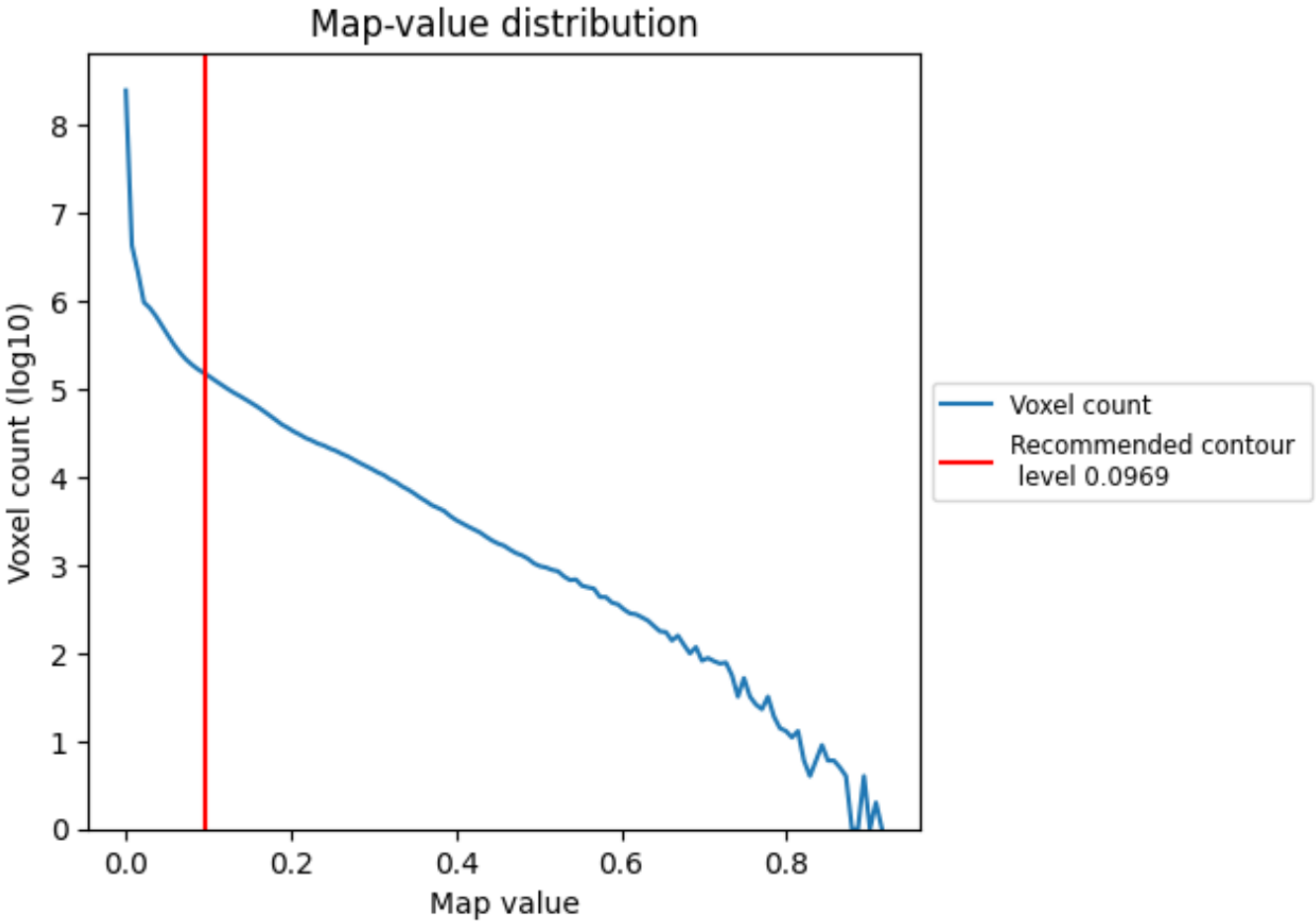
6.6 Mask visualisation (i)

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

7 Map analysis

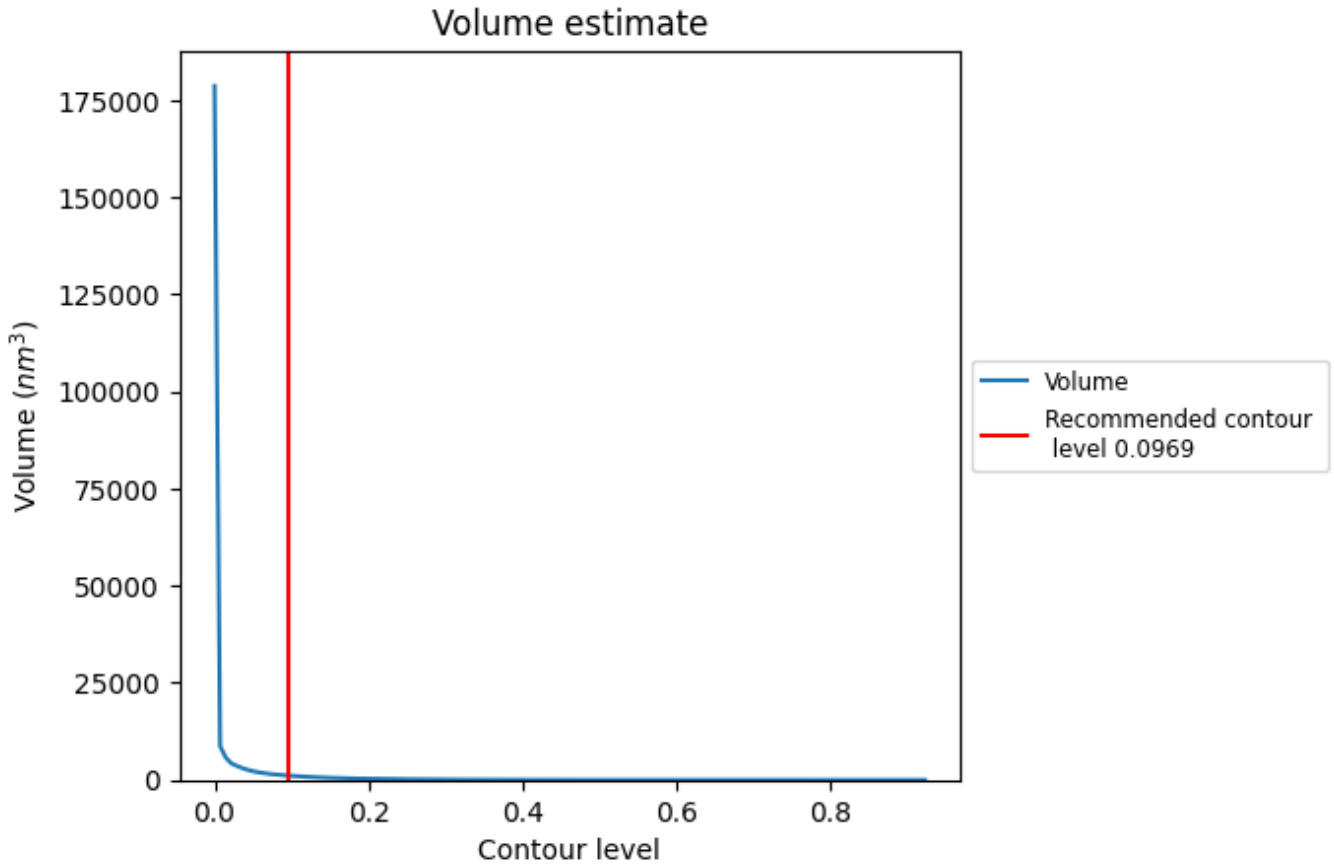
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

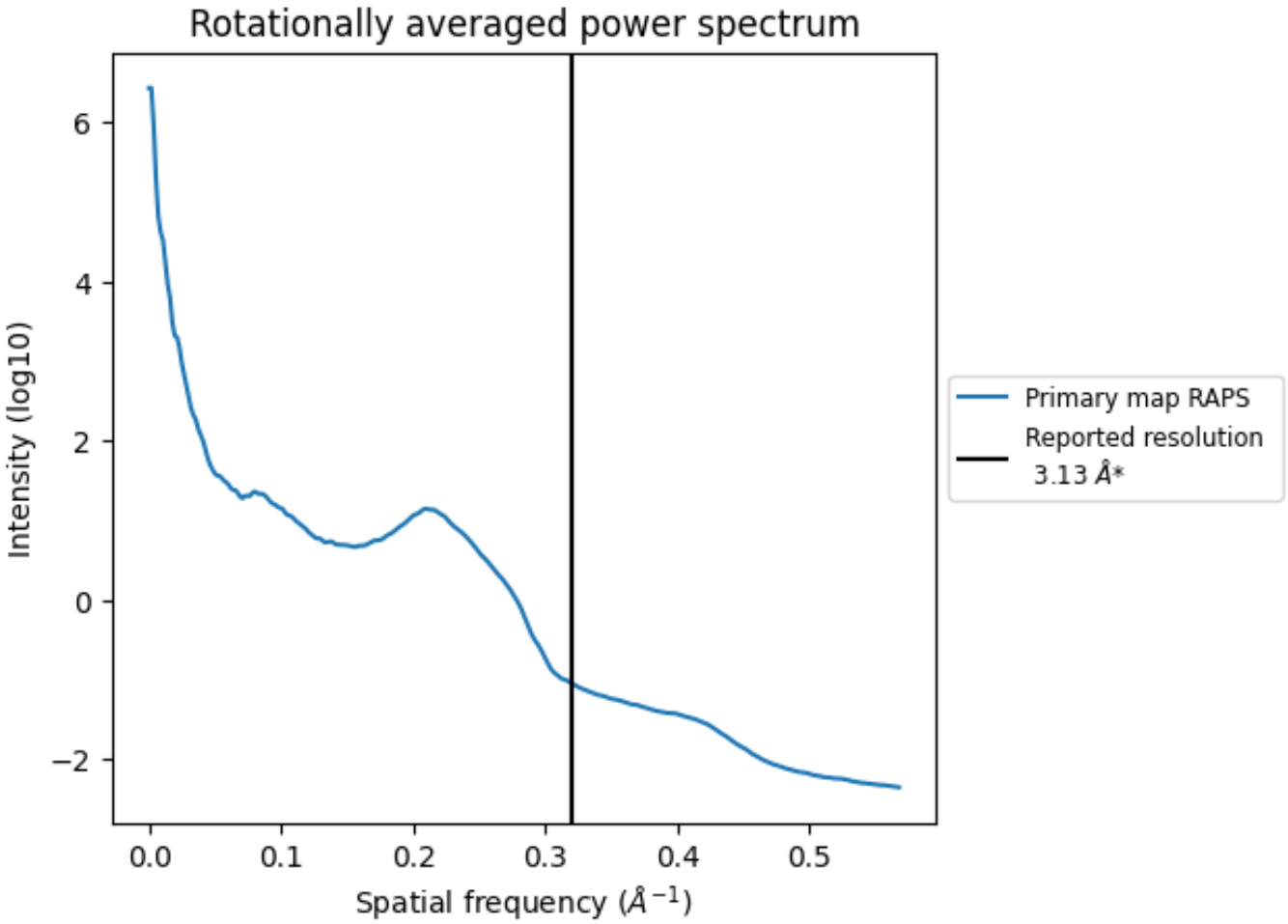
7.2 Volume estimate



The volume at the recommended contour level is 1100 nm^3; this corresponds to an approximate mass of 993 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.319 $Å^{-1}$

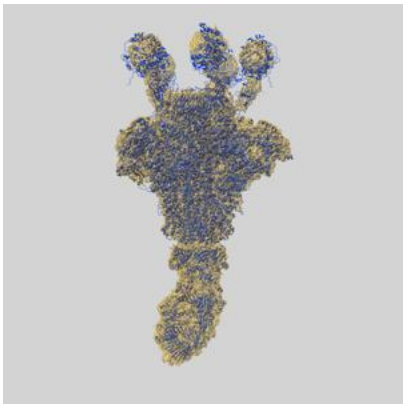
8 Fourier-Shell correlation

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

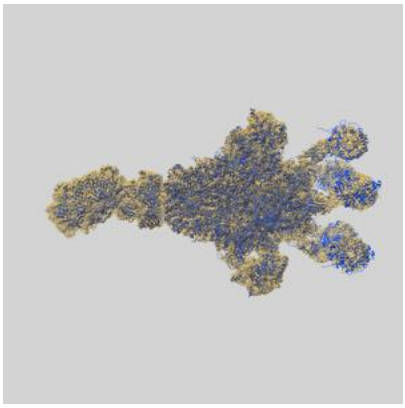
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-58505 and PDB model 31LI. Per-residue inclusion information can be found in section 3 on page 7.

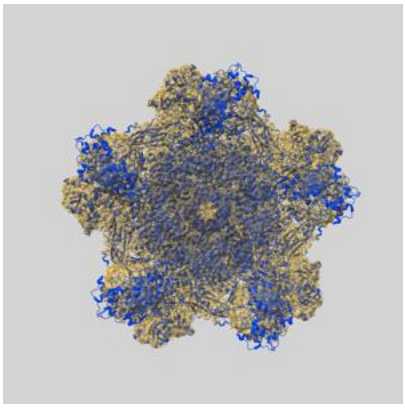
9.1 Map-model overlay



X



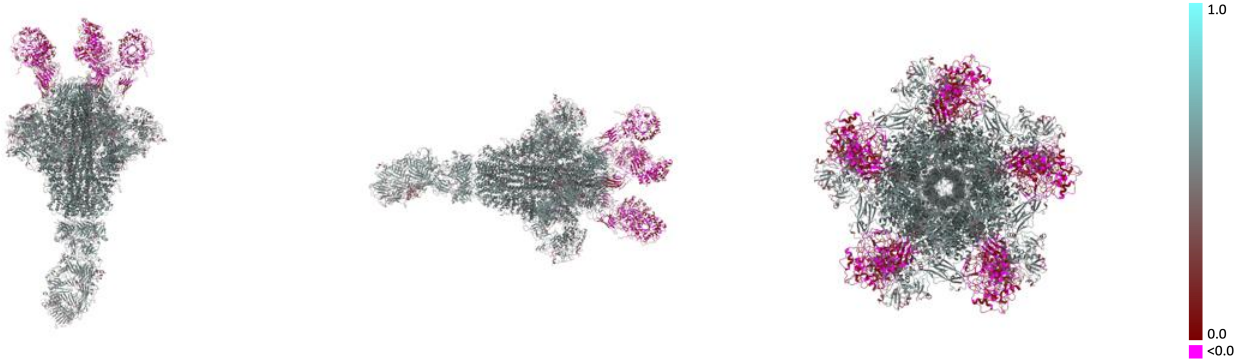
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0969 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

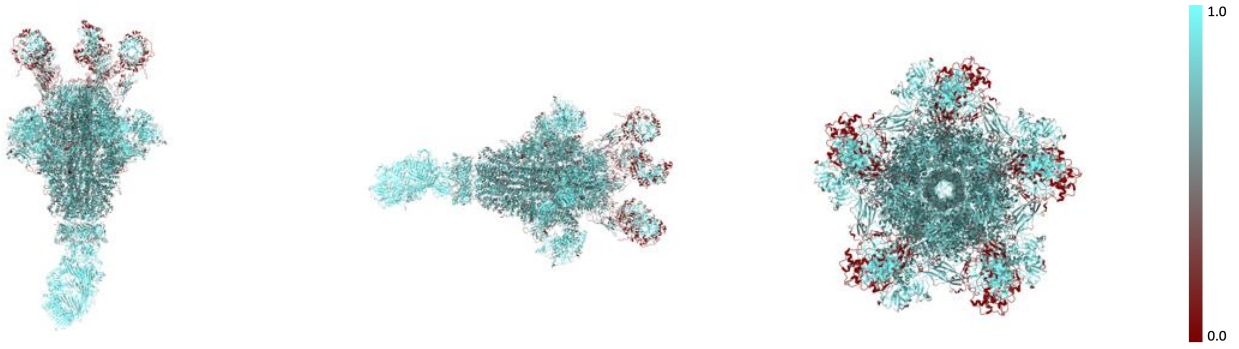
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

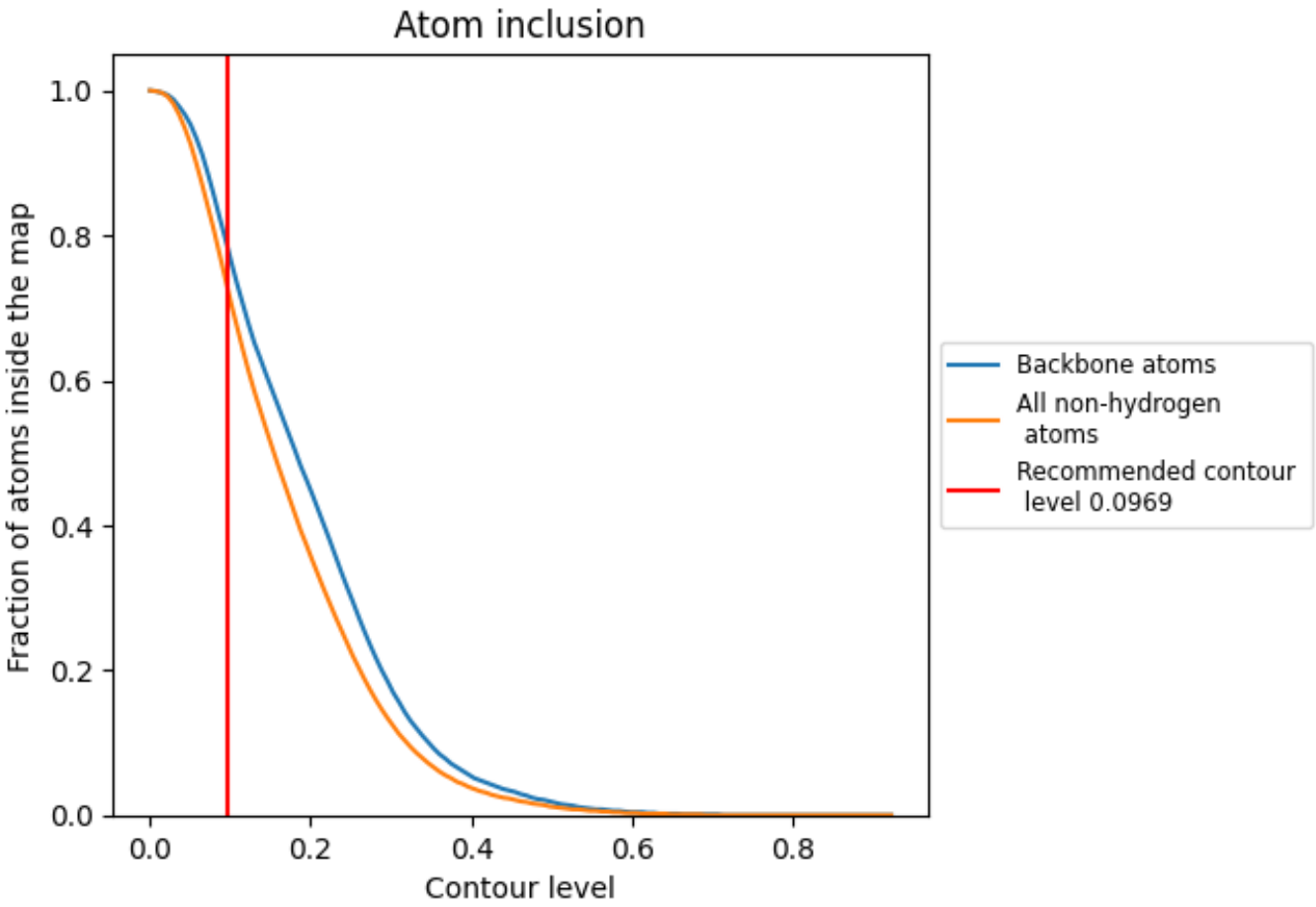
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0969).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 73% 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 (0.0969) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7260	0.4360
A	0.7320	0.5190
B	0.7170	0.4860
C	0.8490	0.4740
D	0.9220	0.4930
E	0.9070	0.4730
F	0.7330	0.5180
G	0.7270	0.4860
H	0.8430	0.4670
I	0.7300	0.5180
J	0.7290	0.4860
K	0.8480	0.4750
L	0.7320	0.5190
M	0.7270	0.4860
N	0.8440	0.4690
O	0.7330	0.5190
P	0.7280	0.4860
Q	0.8420	0.4690
R	0.4260	0.0650
S	0.4230	0.0580
T	0.4250	0.0610
U	0.4250	0.0620
V	0.4250	0.0620

