



## Full wwPDB EM Validation Report ⓘ

May 6, 2023 – 11:20 am BST

PDB ID : 8ADL  
EMDB ID : EMD-15364  
Title : Cryo-EM structure of the SEA complex  
Authors : Tafur, L.; Loewith, R.  
Deposited on : 2022-07-08  
Resolution : 2.95 Å(reported)  
Based on initial models : 3MZK, 3F3F

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.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

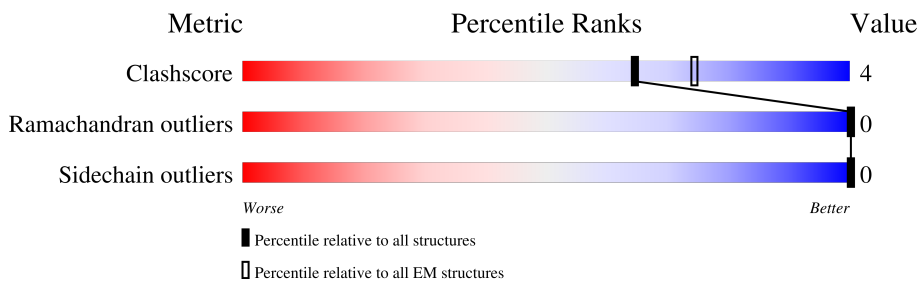
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	C	1148	
1	Q	1148	
2	D	349	
2	E	349	
2	F	349	
2	L	349	
2	M	349	
2	N	349	

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Mol	Chain	Length	Quality of chain
3	B	1038	 68% 9% 23%
3	G	1038	 67% 9% 24%
3	J	1038	 68% 9% 23%
3	O	1038	 66% 9% 24%
4	H	297	 85% 11% .
4	P	297	 84% 12% .
5	A	1341	 42% 5% 53%
5	I	1341	 42% 5% 53%
6	U	1146	 14% 43% 6% 51%
6	V	1146	 14% 45% . 51%
7	W	1584	 42% 52% 7% 41%
7	X	1584	 43% 52% 7% 41%
8	S	615	 18% 56% 9% 35%
8	T	615	 20% 58% 7% 35%

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 98972 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 Maintenance of telomere capping protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	C	782	Total	C	N	O	S	0	0
			6344	4048	1076	1182	38		
1	Q	782	Total	C	N	O	S	0	0
			6344	4048	1076	1182	38		

- Molecule 2 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		
2	D	310	Total	C	N	O	S	0	0
			2457	1554	425	467	11		
2	F	311	Total	C	N	O	S	0	0
			2469	1562	427	469	11		
2	M	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		
2	L	310	Total	C	N	O	S	0	0
			2457	1554	425	467	11		
2	N	311	Total	C	N	O	S	0	0
			2469	1562	427	469	11		

- Molecule 3 is a protein called SEH-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	786	Total	C	N	O	S	0	0
			6332	3997	1105	1188	42		
3	B	801	Total	C	N	O	S	0	0
			6450	4071	1128	1209	42		
3	O	786	Total	C	N	O	S	0	0
			6332	3997	1105	1188	42		
3	J	801	Total	C	N	O	S	0	0
			6450	4071	1128	1209	42		

- Molecule 4 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	286	Total	C	N	O	S	0	0
			2252	1437	385	427	3		
4	P	286	Total	C	N	O	S	0	0
			2252	1437	385	427	3		

- Molecule 5 is a protein called Restriction of telomere capping protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	633	Total	C	N	O	S	0	0
			5039	3224	835	952	28		
5	I	633	Total	C	N	O	S	0	0
			5039	3224	835	952	28		

- Molecule 6 is a protein called Nitrogen permease regulator 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	U	563	Total	C	N	O	S	0	0
			4641	2995	769	851	26		
6	V	563	Total	C	N	O	S	0	0
			4641	2995	769	851	26		

- Molecule 7 is a protein called Vacuolar membrane-associated protein IML1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	W	938	Total	C	N	O	S	0	0
			7762	5008	1302	1415	37		
7	X	938	Total	C	N	O	S	0	0
			7762	5008	1302	1415	37		

- Molecule 8 is a protein called Nitrogen permease regulator 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	402	Total	C	N	O	S	0	0
			3288	2149	520	600	19		
8	T	402	Total	C	N	O	S	0	0
			3288	2149	520	600	19		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	C	3	Total	Zn	0
			3	3	

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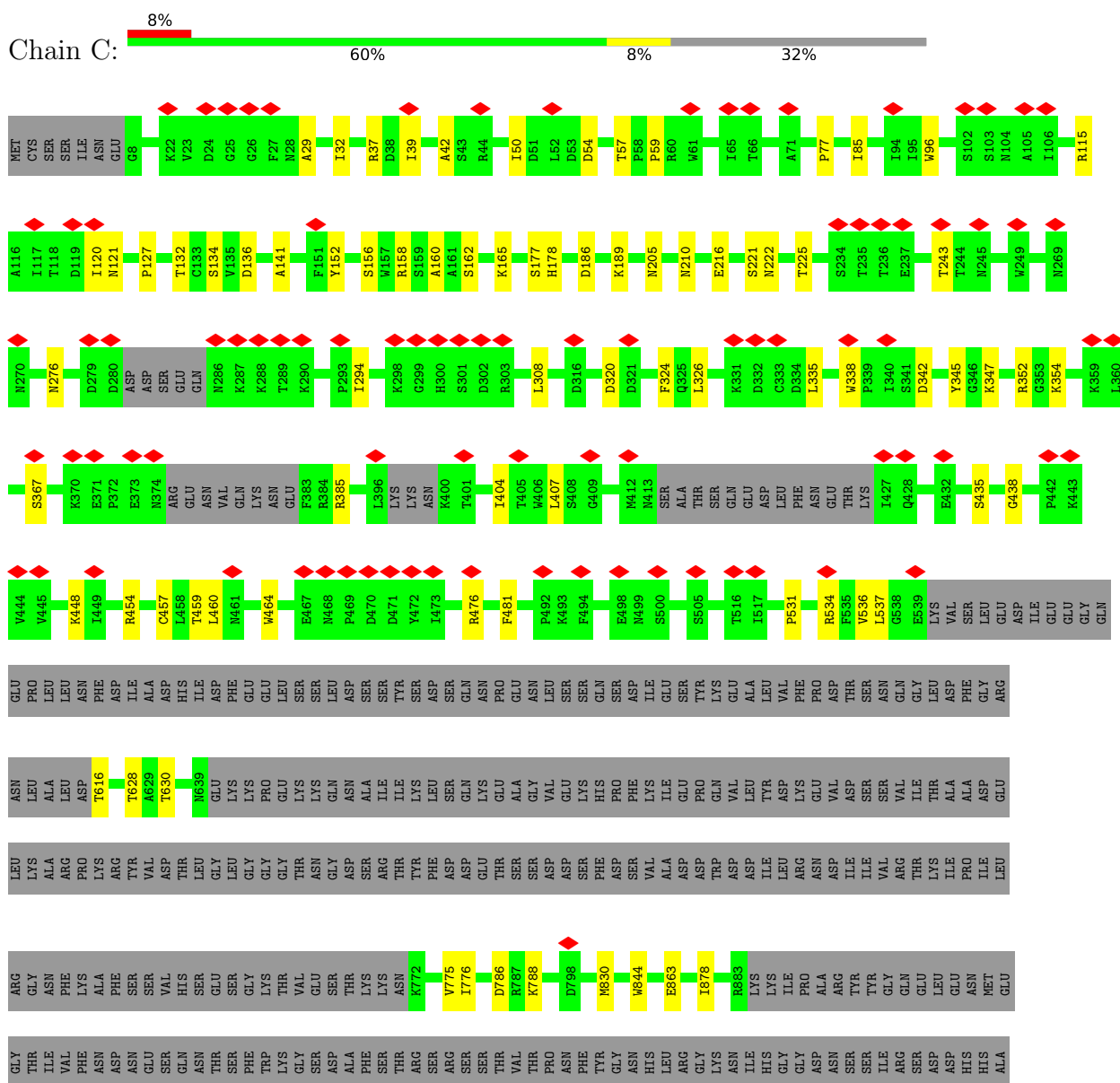
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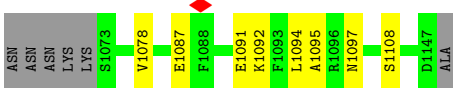
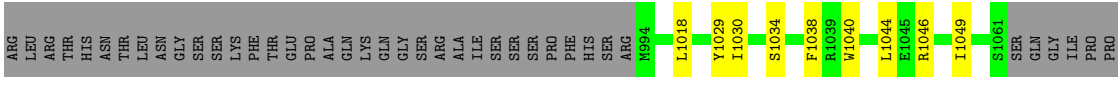
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
9	G	4	Total 4	Zn 4	0
9	A	3	Total 3	Zn 3	0
9	B	4	Total 4	Zn 4	0
9	Q	3	Total 3	Zn 3	0
9	O	4	Total 4	Zn 4	0
9	I	3	Total 3	Zn 3	0
9	J	4	Total 4	Zn 4	0

### 3 Residue-property plots

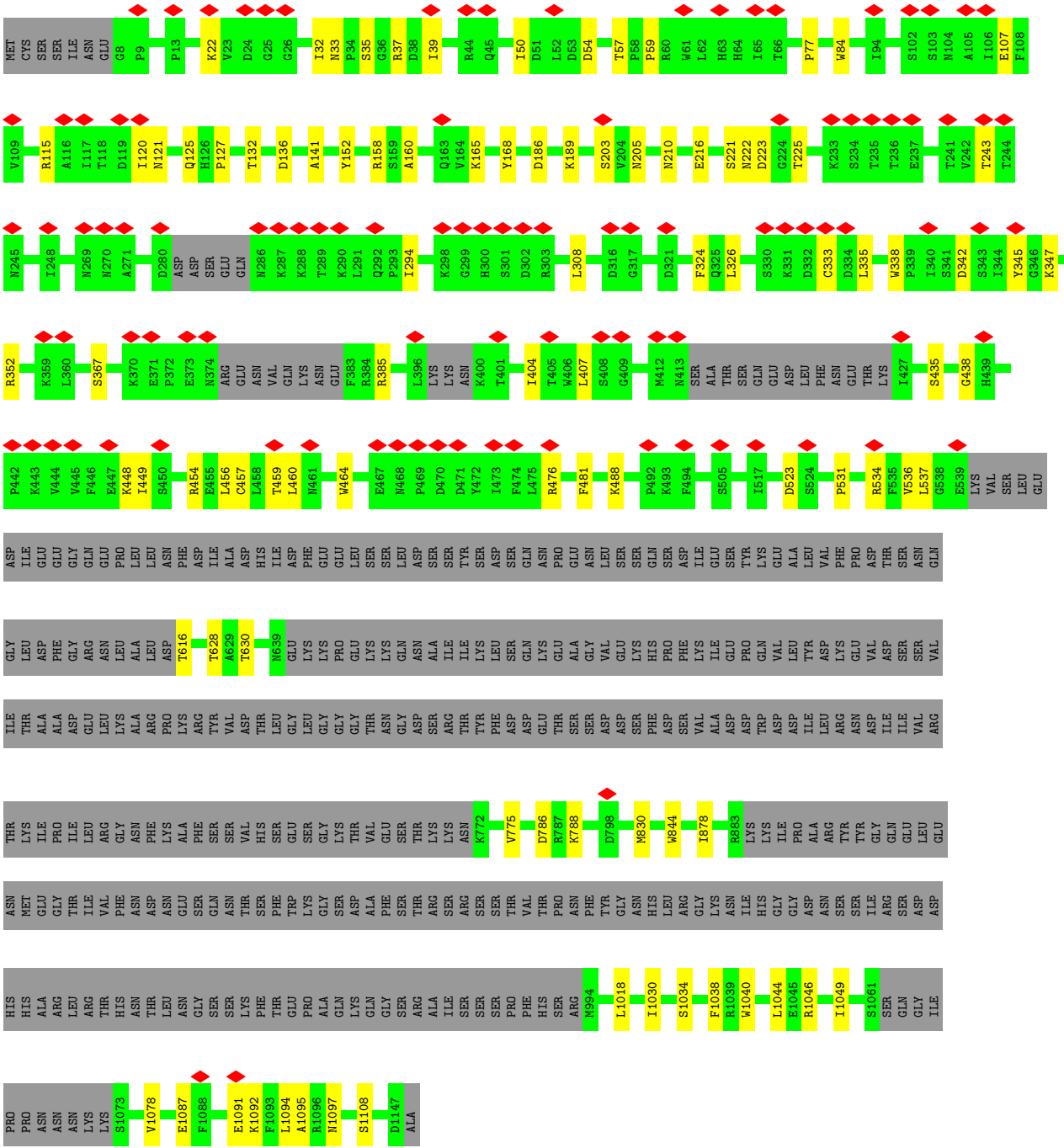
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Maintenance of telomere capping protein 5



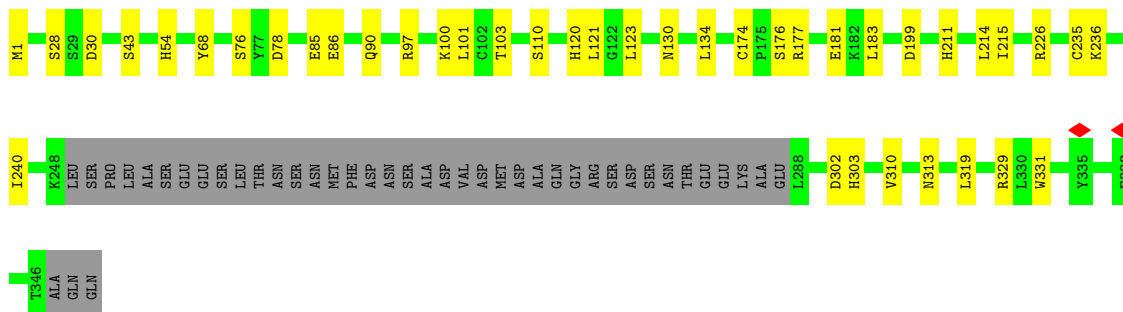
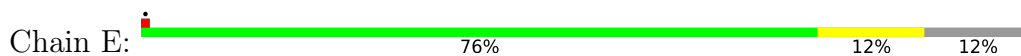


● Molecule 1: Maintenance of telomere capping protein 5

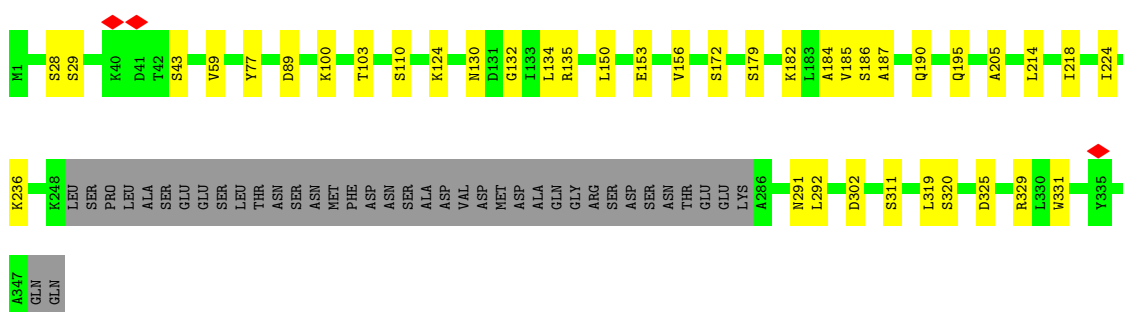
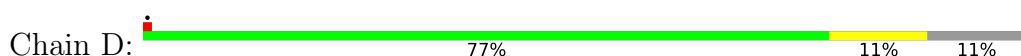




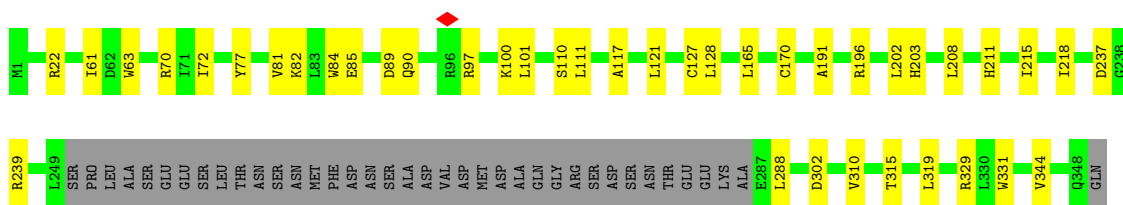
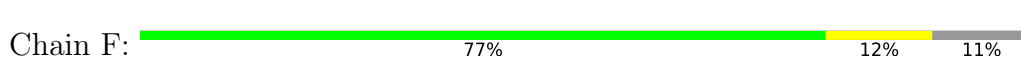
• Molecule 2: Nucleoporin SEH1



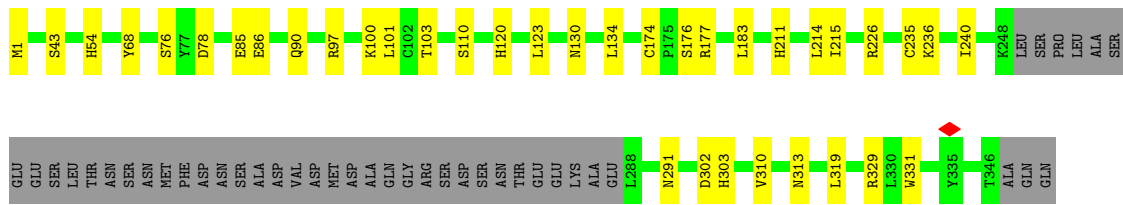
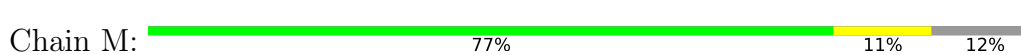
• Molecule 2: Nucleoporin SEH1




• Molecule 2: Nucleoporin SEH1

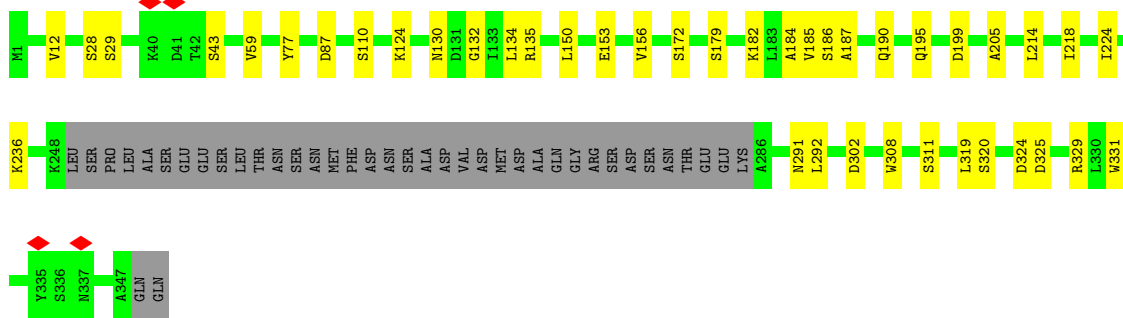


• Molecule 2: Nucleoporin SEH1




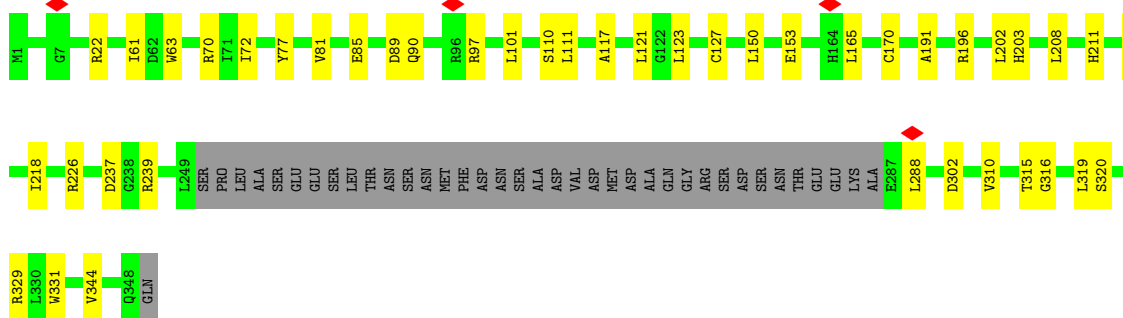
• Molecule 2: Nucleoporin SEH1

Chain L: 



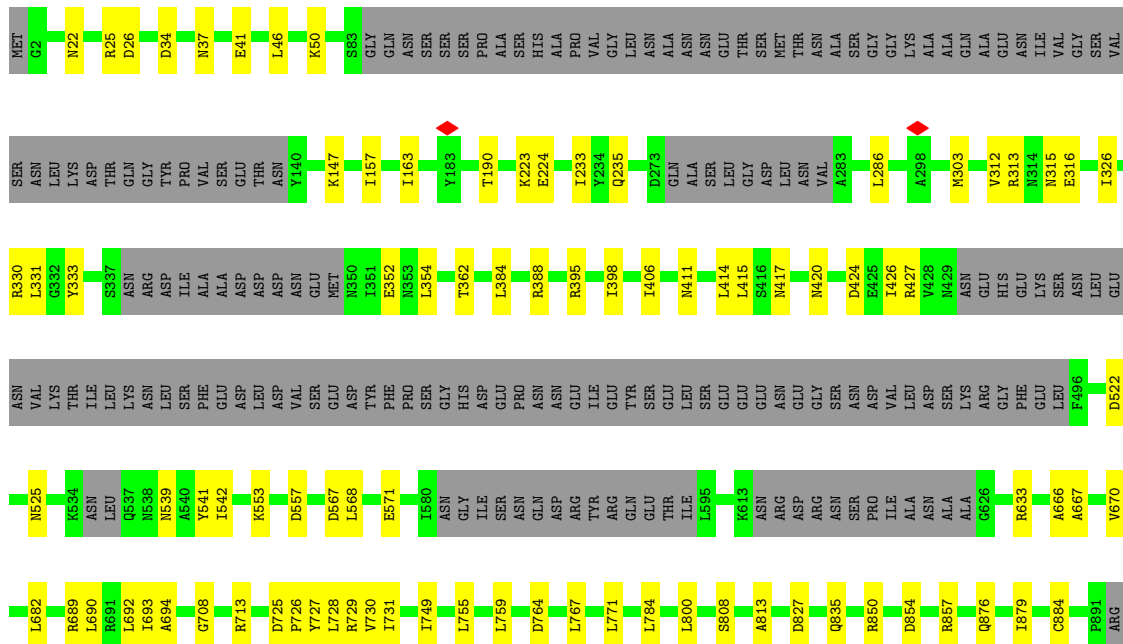
• Molecule 2: Nucleoporin SEH1

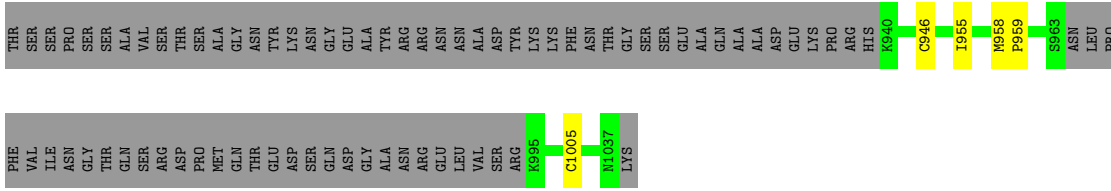
Chain N: 



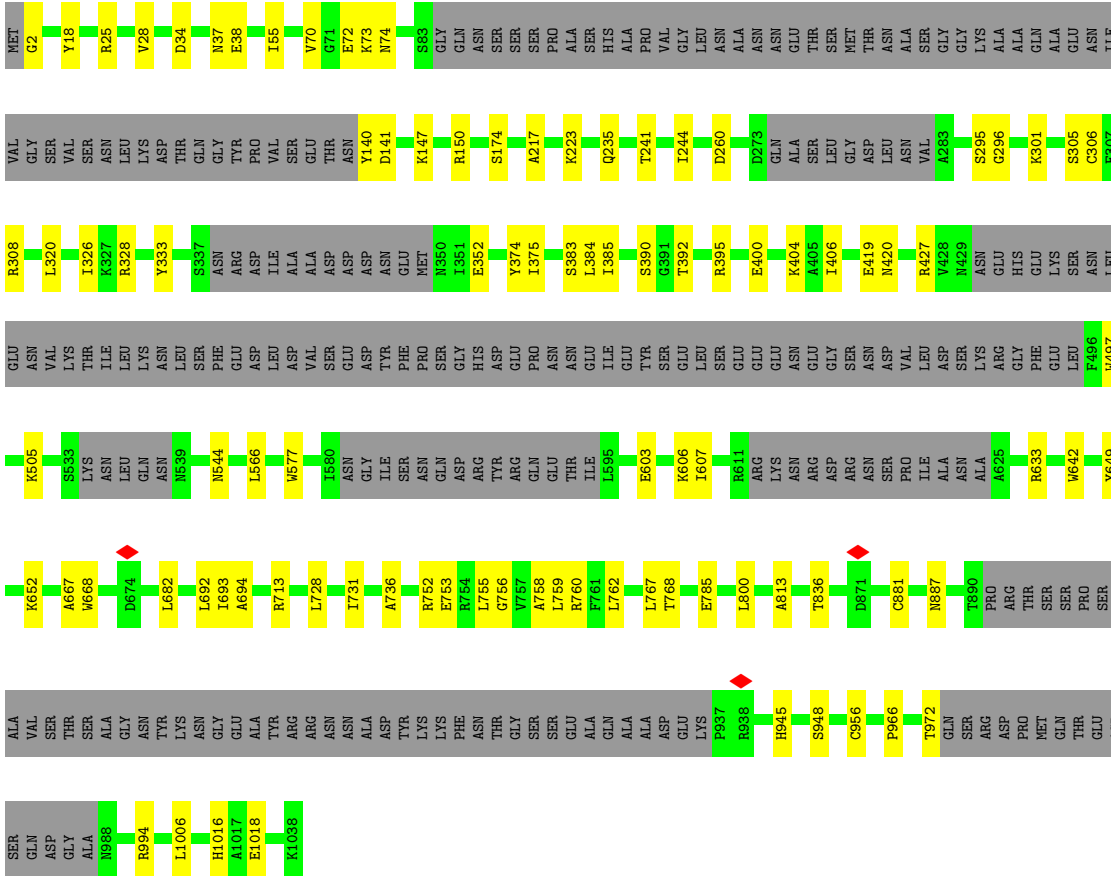
• Molecule 3: SEH-associated protein 4

Chain G: 

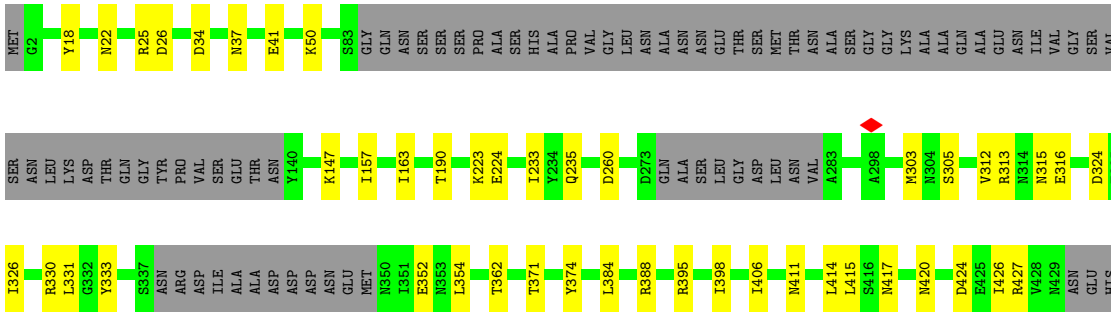
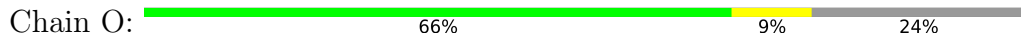


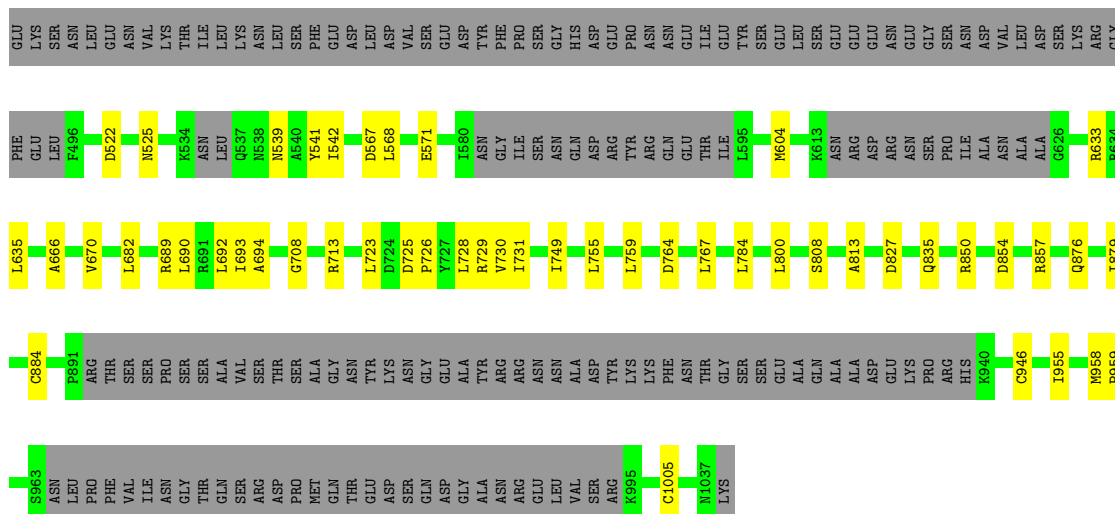


• Molecule 3: SEH-associated protein 4

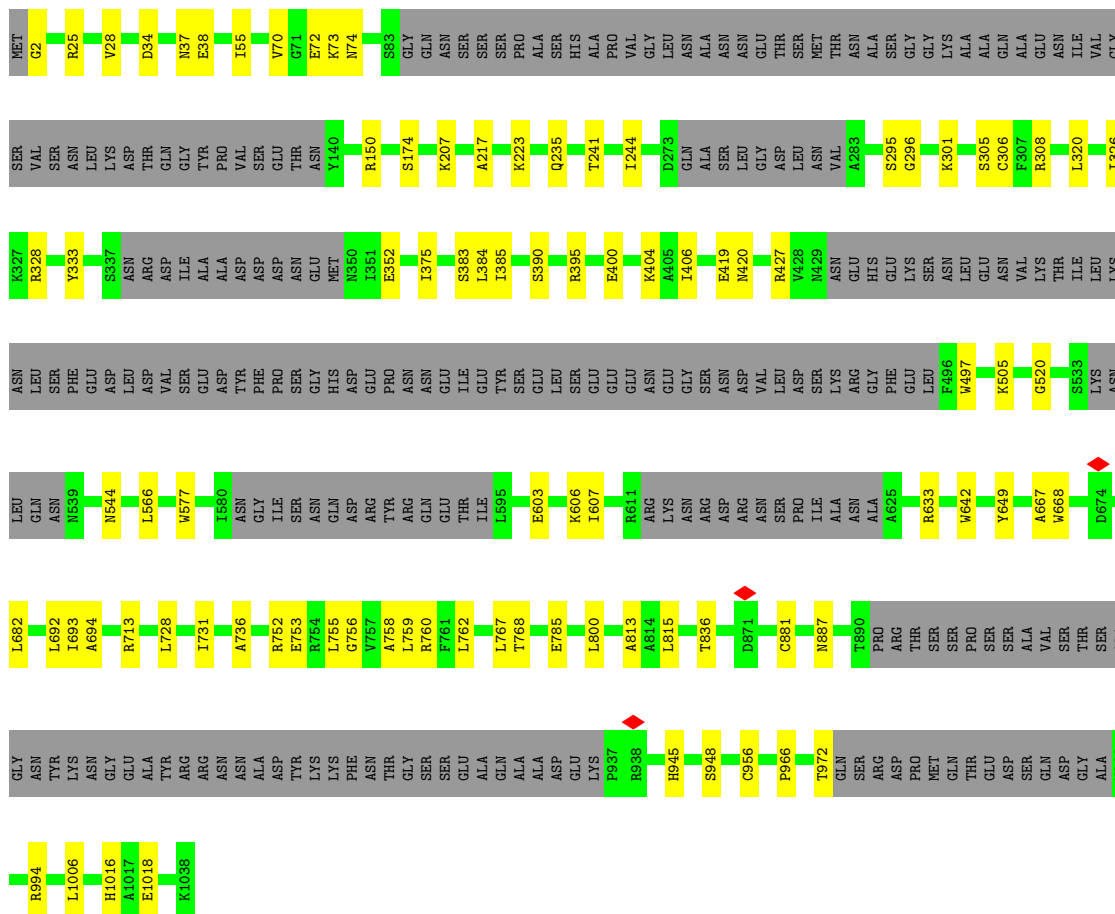


• Molecule 3: SEH-associated protein 4

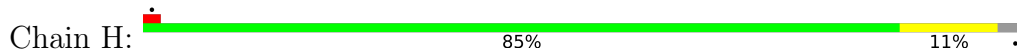




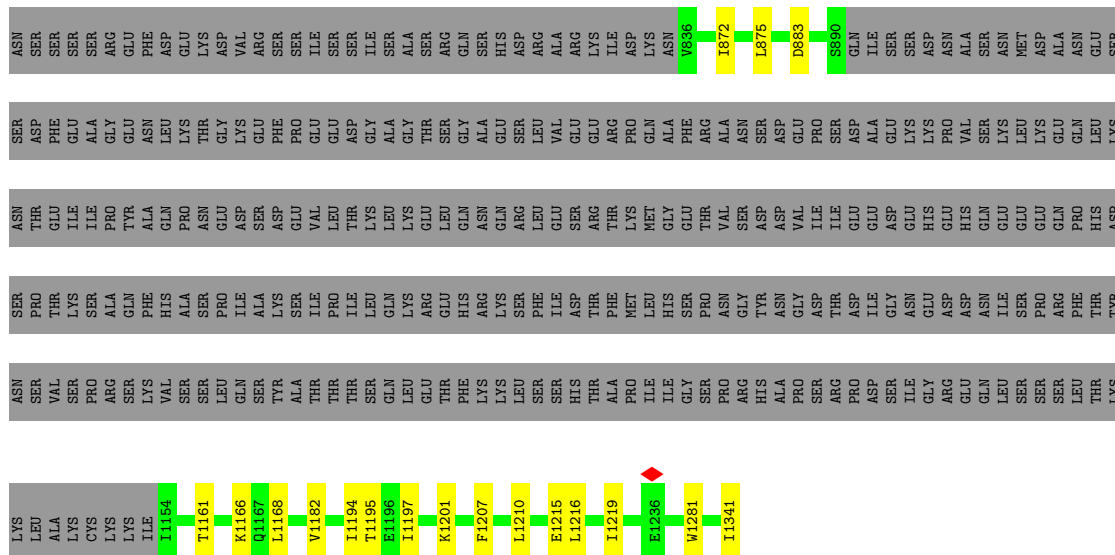
- Molecule 3: SEH-associated protein 4



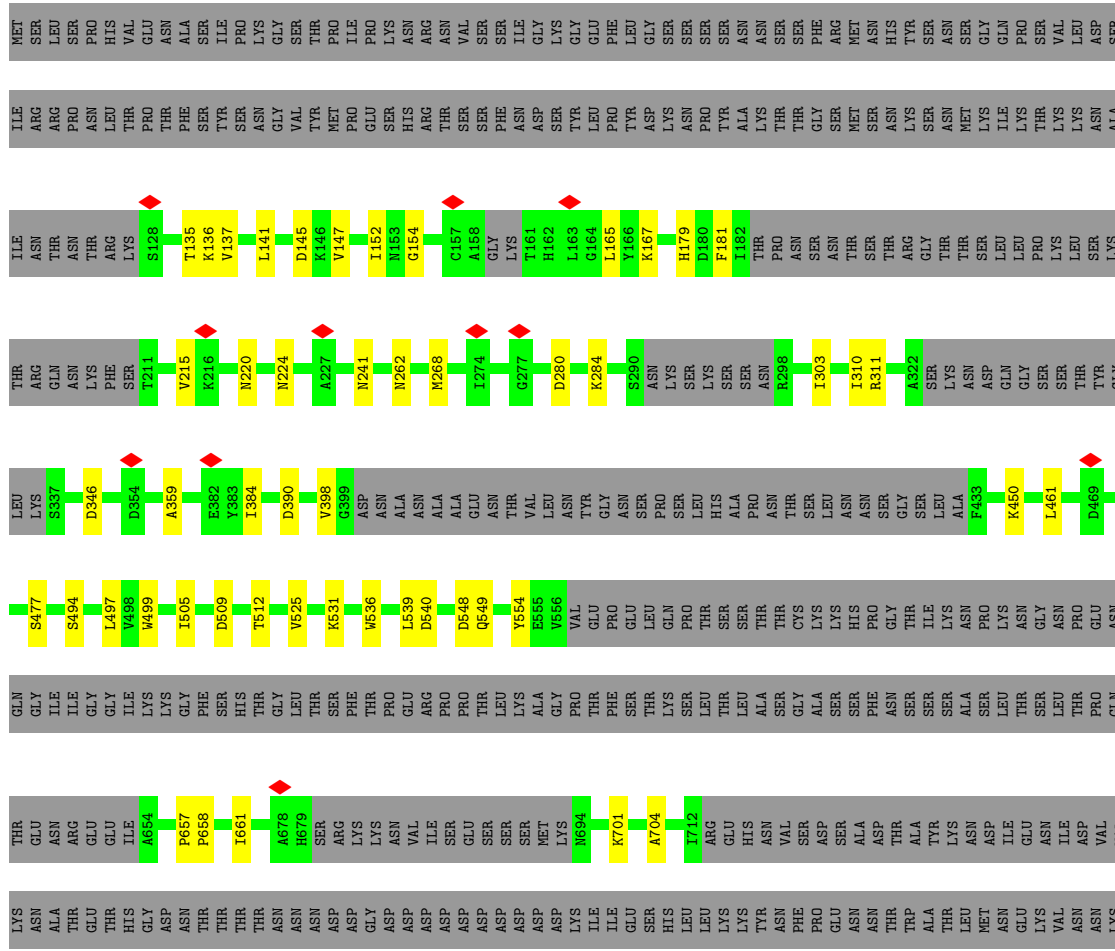
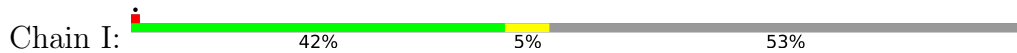
- Molecule 4: Protein transport protein SEC13







• Molecule 5: Restriction of telomere capping protein 1



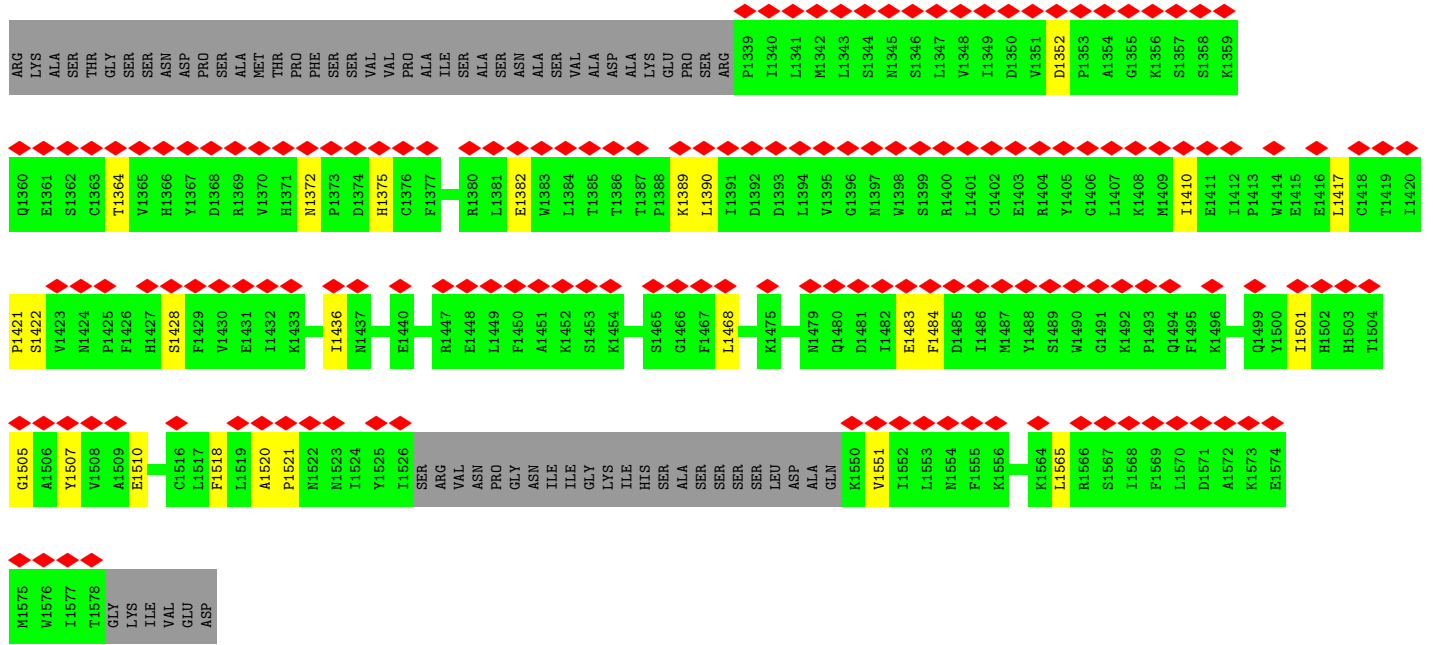




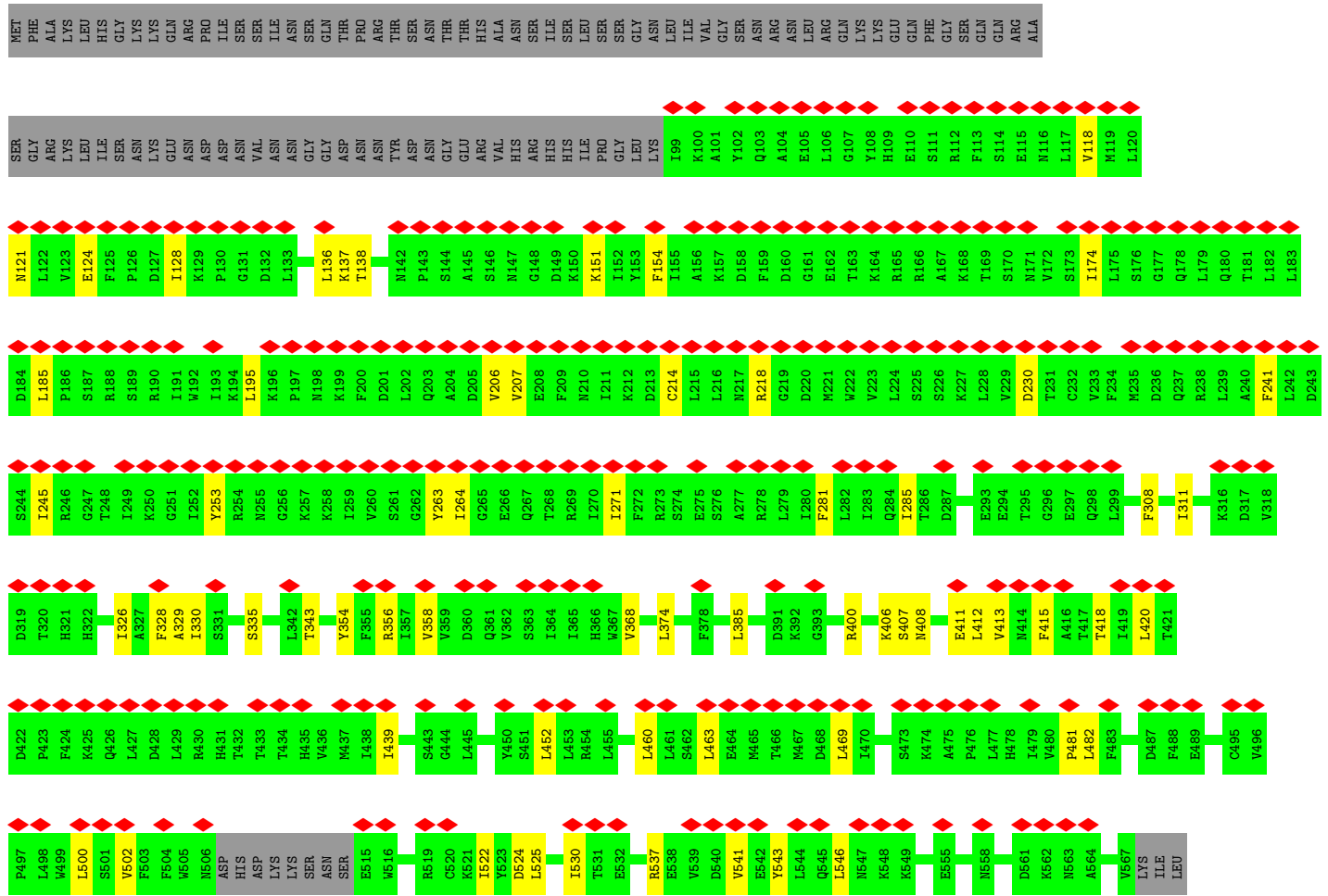




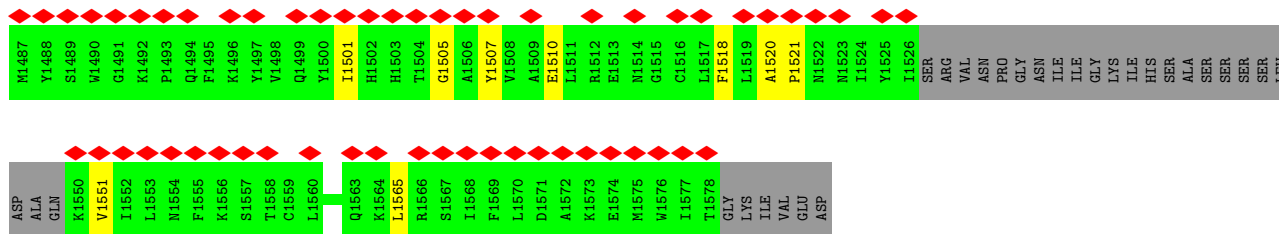




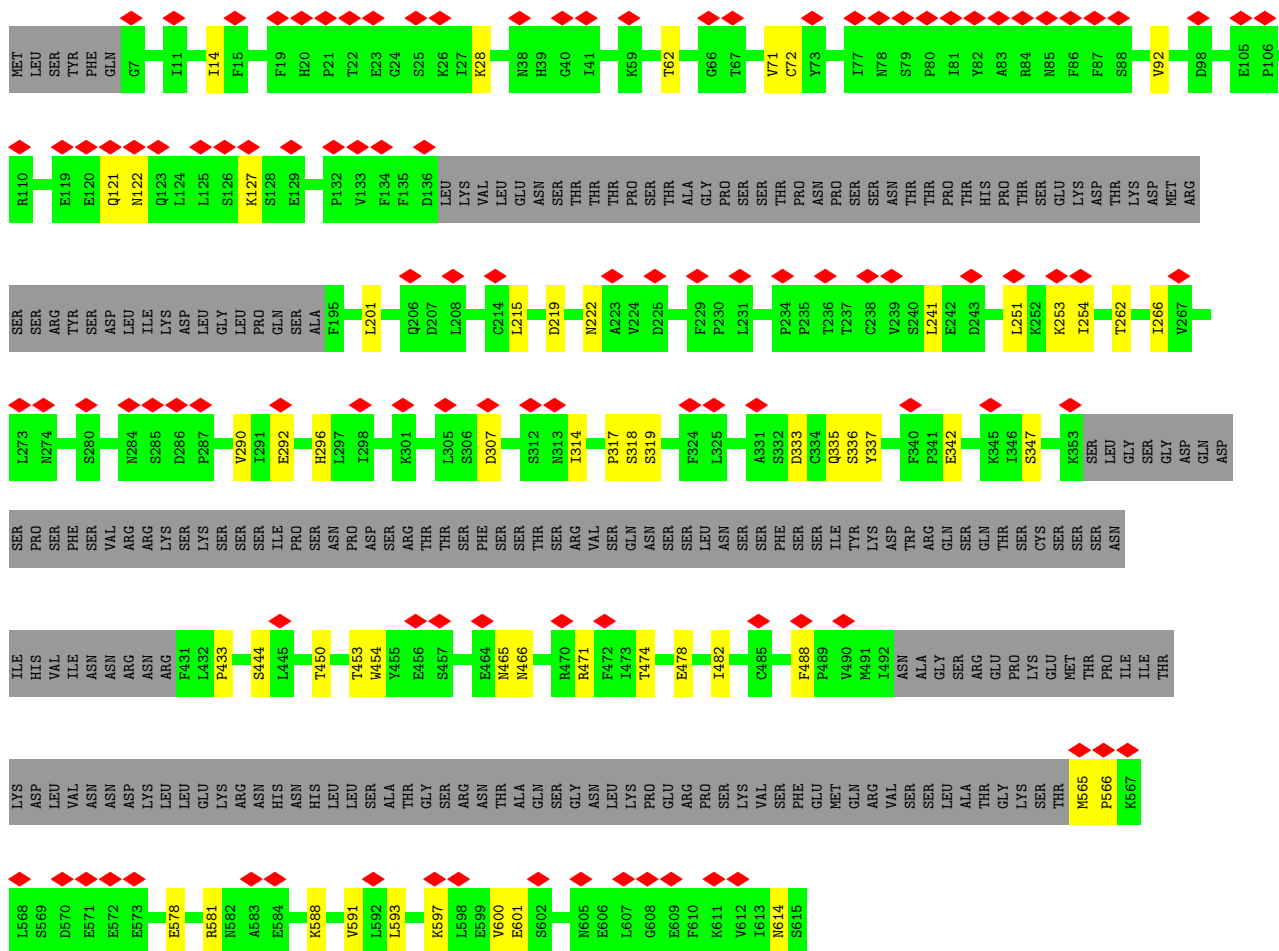
● Molecule 7: Vacuolar membrane-associated protein IML1



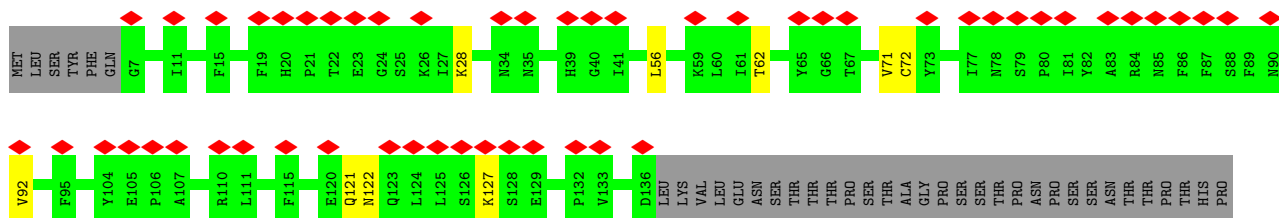


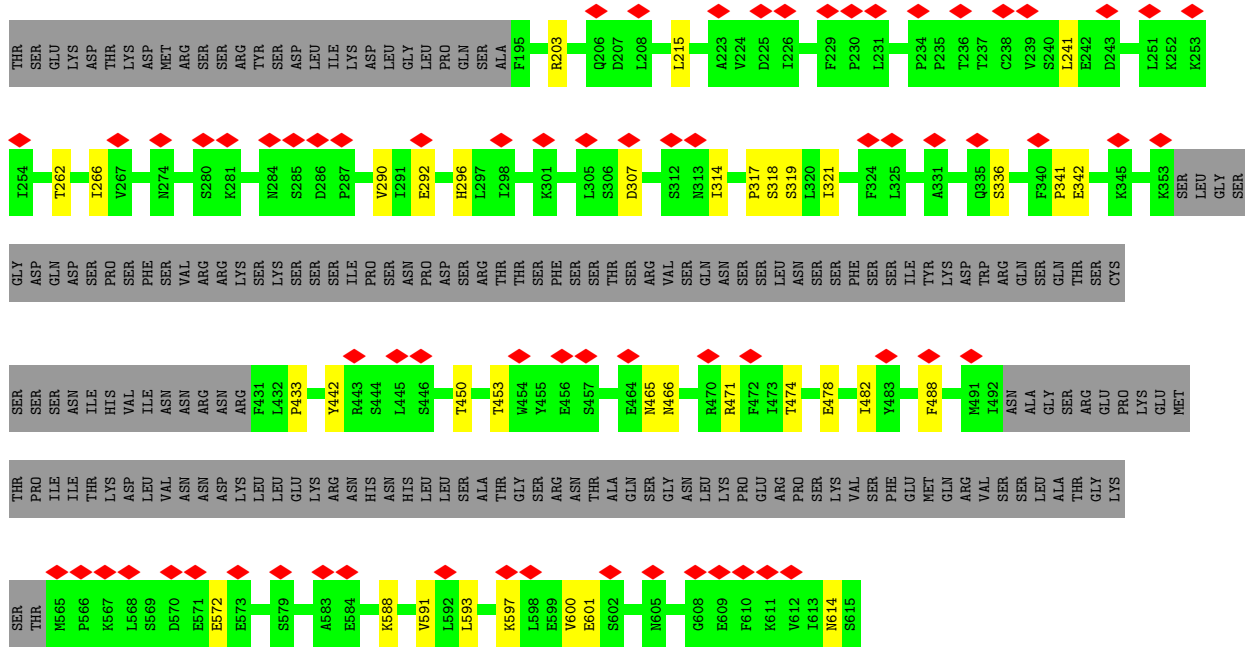


• Molecule 8: Nitrogen permease regulator 2



• Molecule 8: Nitrogen permease regulator 2





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	208379	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 ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.417	Depositor
Minimum map value	-0.004	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.05	Depositor
Map size ( $\text{\AA}$ )	464.64, 464.64, 464.64	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.726, 0.726, 0.726	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:  
ZN

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	C	0.25	0/6518	0.49	0/8846
1	Q	0.25	0/6518	0.49	0/8846
2	D	0.25	0/2518	0.51	0/3414
2	E	0.25	0/2499	0.52	0/3388
2	F	0.26	0/2530	0.52	0/3430
2	L	0.25	0/2518	0.51	0/3414
2	M	0.25	0/2499	0.52	0/3388
2	N	0.26	0/2530	0.52	0/3430
3	B	0.25	0/6583	0.52	0/8895
3	G	0.25	0/6462	0.52	0/8731
3	J	0.25	0/6583	0.52	0/8895
3	O	0.25	0/6462	0.52	0/8731
4	H	0.24	0/2313	0.49	0/3156
4	P	0.24	0/2313	0.49	0/3156
5	A	0.25	0/5144	0.49	0/6963
5	I	0.25	0/5144	0.49	0/6963
6	U	0.25	0/4743	0.49	0/6413
6	V	0.25	0/4743	0.49	0/6413
7	W	0.24	0/7941	0.49	0/10726
7	X	0.24	0/7941	0.49	0/10726
8	S	0.26	0/3372	0.48	0/4570
8	T	0.26	0/3372	0.49	0/4570
All	All	0.25	0/101246	0.50	0/137064

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.



## 5.2 Too-close contacts

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	C	6344	0	6100	60	0
1	Q	6344	0	6100	59	0
2	D	2457	0	2394	24	0
2	E	2438	0	2378	27	0
2	F	2469	0	2408	25	0
2	L	2457	0	2394	26	0
2	M	2438	0	2378	25	0
2	N	2469	0	2408	26	0
3	B	6450	0	6336	57	0
3	G	6332	0	6218	59	0
3	J	6450	0	6336	52	0
3	O	6332	0	6218	60	0
4	H	2252	0	2188	22	0
4	P	2252	0	2188	23	0
5	A	5039	0	4990	44	0
5	I	5039	0	4990	46	0
6	U	4641	0	4661	39	0
6	V	4641	0	4661	28	0
7	W	7762	0	7747	65	0
7	X	7762	0	7747	67	0
8	S	3288	0	3304	36	0
8	T	3288	0	3304	31	0
9	A	3	0	0	0	0
9	B	4	0	0	0	0
9	C	3	0	0	0	0
9	G	4	0	0	0	0
9	I	3	0	0	0	0
9	J	4	0	0	0	0
9	O	4	0	0	0	0
9	Q	3	0	0	0	0
All	All	98972	0	97448	829	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 4.

All (829) 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:A:1341:ILE:HG12	3:B:994:ARG:HG2	1.75	0.69
5:I:1341:ILE:HG12	3:J:994:ARG:HG2	1.74	0.68
8:T:72:CYS:HB3	8:T:92:VAL:HG13	1.76	0.67
2:L:319:LEU:HB3	2:L:331:TRP:HB2	1.77	0.66
8:S:72:CYS:HB3	8:S:92:VAL:HG13	1.78	0.66
2:L:182:LYS:HE3	2:L:195:GLN:HE21	1.61	0.66
2:D:319:LEU:HB3	2:D:331:TRP:HB2	1.77	0.65
2:D:182:LYS:HE3	2:D:195:GLN:HE21	1.62	0.65
1:C:121:ASN:HD22	1:C:165:LYS:HA	1.63	0.64
2:D:179:SER:OG	2:D:182:LYS:NZ	2.32	0.63
3:B:223:LYS:HG2	3:B:235:GLN:HG2	1.81	0.63
2:L:179:SER:OG	2:L:182:LYS:NZ	2.32	0.62
1:Q:121:ASN:HD22	1:Q:165:LYS:HA	1.64	0.62
1:Q:448:LYS:HB3	1:Q:457:CYS:HB3	1.80	0.62
3:B:2:GLY:N	6:V:1063:ASP:OD2	2.33	0.62
1:C:160:ALA:HB2	8:S:215:LEU:HB3	1.82	0.61
3:J:2:GLY:N	6:U:1063:ASP:OD2	2.32	0.61
6:V:11:LEU:HD22	6:V:37:LEU:HB3	1.83	0.61
3:G:522:ASP:HB3	3:G:525:ASN:HB2	1.82	0.61
3:O:730:VAL:HG11	3:O:749:ILE:HD13	1.83	0.61
3:O:522:ASP:HB3	3:O:525:ASN:HB2	1.82	0.61
3:J:34:ASP:O	3:J:395:ARG:NH1	2.32	0.60
6:U:557:VAL:HG13	6:U:648:LEU:HD13	1.83	0.60
7:X:343:THR:O	7:X:406:LYS:NZ	2.34	0.60
5:A:548:ASP:HB2	5:A:661:ILE:HD11	1.83	0.60
3:J:223:LYS:HG2	3:J:235:GLN:HG2	1.83	0.60
1:Q:1087:GLU:HB2	1:Q:1092:LYS:HG3	1.84	0.60
3:G:730:VAL:HG11	3:G:749:ILE:HD13	1.83	0.60
5:I:548:ASP:HB2	5:I:661:ILE:HD11	1.84	0.60
1:C:448:LYS:HB3	1:C:457:CYS:HB3	1.82	0.59
1:Q:141:ALA:HB3	1:Q:152:TYR:HB3	1.83	0.59
1:Q:454:ARG:HB3	1:Q:481:PHE:HB2	1.85	0.59
6:V:557:VAL:HG13	6:V:648:LEU:HD13	1.83	0.59
1:C:1087:GLU:HB2	1:C:1092:LYS:HG3	1.85	0.58
6:U:650:ILE:O	6:U:832:ARG:NH2	2.36	0.58
2:E:90:GLN:HB3	2:E:97:ARG:HD2	1.85	0.58
3:B:217:ALA:HB1	3:B:241:THR:HB	1.86	0.58
7:W:356:ARG:NH1	7:W:1031:THR:O	2.37	0.58
6:V:968:VAL:HG21	6:V:1086:TRP:HD1	1.69	0.58
1:C:32:ILE:HB	1:C:308:LEU:HD13	1.86	0.58
7:W:1417:LEU:HD11	7:W:1520:ALA:HB3	1.84	0.58
3:B:34:ASP:O	3:B:395:ARG:NH1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:90:GLN:HB3	2:M:97:ARG:HD2	1.86	0.58
7:W:368:VAL:HG13	8:S:121:GLN:HG2	1.86	0.58
3:B:693:ILE:HD13	3:B:728:LEU:HD13	1.86	0.57
6:U:11:LEU:HD22	6:U:37:LEU:HB3	1.87	0.57
7:W:343:THR:O	7:W:406:LYS:NZ	2.36	0.57
7:X:1417:LEU:HD11	7:X:1520:ALA:HB3	1.85	0.57
3:G:25:ARG:NH2	3:G:303:MET:O	2.37	0.57
6:U:968:VAL:HG21	6:U:1086:TRP:HD1	1.70	0.57
1:C:141:ALA:HB3	1:C:152:TYR:HB3	1.85	0.57
3:O:25:ARG:NH2	3:O:303:MET:O	2.37	0.57
3:G:415:LEU:HB2	3:G:424:ASP:HB2	1.87	0.57
1:Q:160:ALA:HB2	8:T:215:LEU:HB3	1.86	0.57
7:X:356:ARG:NH1	7:X:1031:THR:O	2.37	0.57
1:C:454:ARG:HB3	1:C:481:PHE:HB2	1.87	0.57
3:J:693:ILE:HD13	3:J:728:LEU:HD13	1.86	0.57
6:V:419:ARG:HH21	6:V:550:ILE:HG22	1.69	0.57
3:B:756:GLY:O	3:B:760:ARG:NH1	2.38	0.56
1:Q:50:ILE:HG12	1:Q:59:PRO:HB3	1.85	0.56
7:X:541:VAL:O	8:T:471:ARG:NH2	2.37	0.56
3:O:415:LEU:HB2	3:O:424:ASP:HB2	1.87	0.56
1:C:326:LEU:HB3	1:C:338:TRP:HB2	1.87	0.56
1:C:460:LEU:HD13	1:C:537:LEU:HB3	1.86	0.56
2:E:240:ILE:HD11	2:E:303:HIS:HD2	1.71	0.56
3:J:217:ALA:HB1	3:J:241:THR:HB	1.87	0.56
1:C:85:ILE:HB	1:C:96:TRP:HB2	1.86	0.56
5:A:1197:ILE:HG22	5:A:1201:LYS:HE2	1.88	0.56
1:Q:342:ASP:OD1	1:Q:352:ARG:NH1	2.38	0.56
6:U:962:LYS:HE3	6:U:1068:HIS:HA	1.87	0.56
7:X:206:VAL:HB	7:X:253:TYR:HB2	1.87	0.56
3:G:633:ARG:NH2	3:G:759:LEU:O	2.39	0.56
3:J:667:ALA:HA	3:J:731:ILE:HD11	1.88	0.56
7:W:541:VAL:O	8:S:471:ARG:NH2	2.39	0.56
3:O:316:GLU:HG3	3:O:330:ARG:HG2	1.87	0.56
3:J:756:GLY:O	3:J:760:ARG:NH1	2.39	0.56
7:X:368:VAL:HG13	8:T:121:GLN:HG2	1.86	0.56
3:G:316:GLU:HG3	3:G:330:ARG:HG2	1.88	0.55
6:U:413:ARG:NH1	6:U:436:VAL:O	2.40	0.55
6:U:670:GLY:HA2	6:U:853:PRO:HD3	1.88	0.55
6:V:962:LYS:HE3	6:V:1068:HIS:HA	1.86	0.55
7:W:335:SER:O	7:W:400:ARG:NH2	2.37	0.55
3:B:667:ALA:HA	3:B:731:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:32:THR:HG22	4:H:50:THR:HG22	1.89	0.55
3:O:633:ARG:NH2	3:O:759:LEU:O	2.39	0.55
2:M:240:ILE:HD11	2:M:303:HIS:HD2	1.71	0.55
5:A:701:LYS:HG2	5:A:1216:LEU:HD11	1.88	0.55
3:J:966:PRO:HG3	2:N:70:ARG:HD3	1.89	0.55
7:W:214:CYS:HB2	7:W:1389:LYS:HD3	1.88	0.55
7:X:1124:ARG:NH1	7:X:1125:LEU:O	2.40	0.55
3:B:759:LEU:HD23	3:B:767:LEU:HD21	1.90	0.54
2:M:76:SER:OG	2:M:78:ASP:OD1	2.25	0.54
2:E:76:SER:OG	2:E:78:ASP:OD1	2.25	0.54
2:M:43:SER:O	3:O:427:ARG:NH2	2.40	0.54
4:P:32:THR:HG22	4:P:50:THR:HG22	1.90	0.54
5:I:1197:ILE:HG22	5:I:1201:LYS:HE2	1.88	0.54
2:L:302:ASP:O	2:L:329:ARG:NH2	2.41	0.54
2:E:43:SER:O	3:G:427:ARG:NH2	2.40	0.54
2:D:302:ASP:O	2:D:329:ARG:NH2	2.41	0.54
1:Q:460:LEU:HD13	1:Q:537:LEU:HB3	1.89	0.54
1:C:50:ILE:HG12	1:C:59:PRO:HB3	1.90	0.54
7:W:1124:ARG:NH1	7:W:1125:LEU:O	2.40	0.54
5:I:701:LYS:HG2	5:I:1216:LEU:HD11	1.89	0.54
2:N:81:VAL:HG23	2:N:111:LEU:HD13	1.89	0.54
1:C:1095:ALA:O	3:G:876:GLN:NE2	2.41	0.54
5:A:1281:TRP:HB3	3:B:1006:LEU:HD13	1.89	0.54
1:Q:1095:ALA:O	3:O:876:GLN:NE2	2.41	0.54
5:I:137:VAL:HB	5:I:512:THR:HB	1.90	0.54
4:H:227:GLN:HA	4:H:256:VAL:HG23	1.90	0.54
3:B:633:ARG:NH2	3:B:762:LEU:O	2.39	0.54
3:B:966:PRO:HG3	2:F:70:ARG:HD3	1.89	0.54
1:Q:788:LYS:HE3	1:Q:1040:TRP:HB3	1.89	0.53
4:P:227:GLN:HA	4:P:256:VAL:HG23	1.90	0.53
5:A:154:GLY:HA2	5:A:167:LYS:HA	1.91	0.53
5:I:450:LYS:HD2	5:I:461:LEU:HB2	1.91	0.53
6:V:670:GLY:HA2	6:V:853:PRO:HD3	1.90	0.53
3:G:708:GLY:HA2	3:G:713:ARG:HE	1.73	0.53
7:W:934:ASP:HA	7:W:937:ARG:HG2	1.90	0.53
5:I:872:ILE:HG23	5:I:1168:LEU:HD13	1.91	0.53
3:J:759:LEU:HD23	3:J:767:LEU:HD21	1.90	0.53
8:T:597:LYS:NZ	8:T:601:GLU:OE2	2.40	0.53
2:E:177:ARG:NH1	3:G:835:GLN:OE1	2.41	0.53
1:Q:1038:PHE:HB2	1:Q:1046:ARG:HD2	1.90	0.53
5:I:536:TRP:HE1	2:N:320:SER:HG	1.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:649:TYR:OH	3:J:760:ARG:NH2	2.42	0.53
8:S:597:LYS:NZ	8:S:601:GLU:OE2	2.40	0.53
7:X:934:ASP:HA	7:X:937:ARG:HG2	1.90	0.53
1:C:385:ARG:NH2	8:S:336:SER:OG	2.41	0.53
3:G:333:TYR:HB2	3:G:352:GLU:HB3	1.90	0.53
3:B:390:SER:HB3	6:V:966:MET:HB3	1.91	0.53
2:F:81:VAL:HG23	2:F:111:LEU:HD13	1.90	0.53
5:A:473:VAL:HG13	5:A:497:LEU:HD22	1.90	0.53
5:I:165:LEU:HB3	5:I:179:HIS:HB3	1.91	0.53
3:J:668:TRP:NE1	3:J:753:GLU:OE2	2.40	0.53
7:W:118:VAL:HG22	7:W:174:ILE:HG12	1.91	0.53
7:W:207:VAL:HG21	7:W:264:ILE:HG12	1.90	0.53
5:A:165:LEU:HB3	5:A:179:HIS:HB3	1.91	0.53
2:F:77:TYR:HA	2:F:110:SER:HB2	1.90	0.53
2:M:177:ARG:NH1	3:O:835:GLN:OE1	2.41	0.53
7:X:118:VAL:HG22	7:X:174:ILE:HG12	1.91	0.53
7:X:241:PHE:HB3	7:X:245:ILE:HB	1.91	0.53
5:I:224:ASN:ND2	5:I:241:ASN:OD1	2.38	0.53
7:X:214:CYS:HB2	7:X:1389:LYS:HD3	1.91	0.53
3:B:887:ASN:O	3:B:945:HIS:NE2	2.40	0.52
5:I:473:VAL:HG13	5:I:497:LEU:HD22	1.90	0.52
7:X:522:ILE:HG21	7:X:525:LEU:HD12	1.91	0.52
5:A:872:ILE:HG23	5:A:1168:LEU:HD13	1.90	0.52
3:B:37:ASN:O	3:B:395:ARG:NH1	2.42	0.52
5:I:1281:TRP:HB3	3:J:1006:LEU:HD13	1.91	0.52
3:B:649:TYR:OH	3:B:760:ARG:NH2	2.41	0.52
3:O:37:ASN:ND2	3:O:41:GLU:OE2	2.37	0.52
1:C:1038:PHE:HB2	1:C:1046:ARG:HD2	1.89	0.52
2:F:191:ALA:HB3	2:F:208:LEU:HB2	1.92	0.52
1:Q:385:ARG:NH2	8:T:336:SER:OG	2.39	0.52
1:Q:786:ASP:OD2	4:P:265:SER:OG	2.28	0.52
2:N:77:TYR:HA	2:N:110:SER:HB2	1.90	0.52
8:S:333:ASP:O	8:S:337:TYR:HB2	2.09	0.52
1:C:788:LYS:HE3	1:C:1040:TRP:HB3	1.90	0.52
1:C:342:ASP:OD1	1:C:352:ARG:NH1	2.42	0.52
5:A:450:LYS:HD2	5:A:461:LEU:HB2	1.91	0.52
1:Q:464:TRP:NE1	1:Q:536:VAL:O	2.37	0.52
7:X:128:ILE:HG12	7:X:195:LEU:HD22	1.91	0.52
1:C:205:ASN:ND2	1:C:222:ASN:OD1	2.43	0.52
3:B:400:GLU:OE2	3:B:420:ASN:ND2	2.43	0.52
5:I:494:SER:HA	5:I:509:ASP:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:V:650:ILE:O	6:V:832:ARG:NH2	2.43	0.52
2:M:174:CYS:HG	2:M:176:SER:HG	1.56	0.52
3:J:37:ASN:O	3:J:395:ARG:NH1	2.43	0.52
5:A:137:VAL:HB	5:A:512:THR:HB	1.90	0.52
2:N:191:ALA:HB3	2:N:208:LEU:HB2	1.91	0.52
3:B:642:TRP:NE1	3:B:752:ARG:O	2.43	0.52
2:F:63:TRP:HZ3	2:F:70:ARG:HE	1.59	0.52
7:W:218:ARG:NH2	7:W:948:PHE:O	2.43	0.52
3:O:333:TYR:HB2	3:O:352:GLU:HB3	1.91	0.51
5:I:549:GLN:HB3	5:I:658:PRO:HB3	1.92	0.51
3:J:305:SER:OG	3:J:308:ARG:NH2	2.44	0.51
8:S:62:THR:HG23	8:S:71:VAL:HG22	1.92	0.51
3:O:568:LEU:HD12	3:O:571:GLU:HG3	1.92	0.51
4:P:2:VAL:HG22	4:P:41:GLU:HA	1.92	0.51
7:W:241:PHE:HB3	7:W:245:ILE:HB	1.92	0.51
3:J:633:ARG:NH2	3:J:762:LEU:O	2.39	0.51
7:W:128:ILE:HG12	7:W:195:LEU:HD22	1.91	0.51
3:G:568:LEU:HD12	3:G:571:GLU:HG3	1.93	0.51
4:H:226:SER:OG	4:H:228:ASP:OD1	2.28	0.51
1:Q:32:ILE:HB	1:Q:308:LEU:HD13	1.93	0.51
7:X:469:LEU:HD23	7:X:502:VAL:HG22	1.93	0.51
3:B:150:ARG:NH2	3:B:174:SER:O	2.43	0.51
8:T:122:ASN:O	8:T:127:LYS:NZ	2.44	0.51
8:T:241:LEU:HB2	8:T:588:LYS:HE3	1.92	0.51
1:C:29:ALA:HB3	1:C:42:ALA:HB3	1.91	0.51
3:G:759:LEU:HD23	3:G:767:LEU:HD21	1.92	0.51
5:A:224:ASN:ND2	5:A:241:ASN:OD1	2.37	0.51
5:A:494:SER:HA	5:A:509:ASP:HA	1.93	0.51
5:I:154:GLY:HA2	5:I:167:LYS:HA	1.91	0.51
7:X:481:PRO:HG3	7:X:500:LEU:HB3	1.93	0.51
3:G:157:ILE:HG23	3:G:163:ILE:HG12	1.92	0.51
4:H:2:VAL:HG22	4:H:41:GLU:HA	1.93	0.51
4:P:79:VAL:HB	4:P:95:HIS:HB3	1.91	0.51
2:L:311:SER:HG	2:L:320:SER:HG	1.58	0.51
6:U:1084:LYS:HA	6:U:1087:LEU:HD12	1.93	0.51
1:Q:77:PRO:HG2	1:Q:127:PRO:HB3	1.91	0.51
6:U:916:SER:O	8:S:614:ASN:ND2	2.41	0.51
3:B:305:SER:OG	3:B:308:ARG:NH2	2.44	0.51
1:Q:115:ARG:HB2	1:Q:136:ASP:HB3	1.92	0.51
1:C:830:MET:HG2	1:C:844:TRP:HH2	1.76	0.51
3:J:881:CYS:SG	3:J:948:SER:OG	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:312:VAL:HG13	3:G:313:ARG:HG2	1.93	0.50
5:A:539:LEU:HD11	5:A:1210:LEU:HD21	1.93	0.50
2:D:100:LYS:HZ1	2:D:103:THR:HG1	1.56	0.50
1:Q:210:ASN:ND2	1:Q:216:GLU:OE1	2.44	0.50
7:W:522:ILE:HG21	7:W:525:LEU:HD12	1.93	0.50
7:X:218:ARG:NH2	7:X:948:PHE:O	2.44	0.50
5:A:311:ARG:NH2	5:A:346:ASP:OD1	2.43	0.50
1:Q:186:ASP:HB3	1:Q:189:LYS:HB2	1.92	0.50
4:P:226:SER:OG	4:P:228:ASP:OD1	2.28	0.50
4:H:79:VAL:HB	4:H:95:HIS:HB3	1.92	0.50
2:F:196:ARG:HD3	2:F:202:LEU:HD12	1.94	0.50
1:Q:225:THR:HG22	1:Q:243:THR:HG22	1.93	0.50
2:N:63:TRP:HZ3	2:N:70:ARG:HE	1.59	0.50
7:W:948:PHE:HB3	7:W:988:LEU:HB3	1.93	0.50
7:X:1410:ILE:HD13	7:X:1505:GLY:HA3	1.94	0.50
1:C:464:TRP:NE1	1:C:536:VAL:O	2.38	0.50
5:A:549:GLN:HB3	5:A:658:PRO:HB3	1.93	0.50
3:O:223:LYS:HG2	3:O:235:GLN:HG2	1.93	0.50
3:O:312:VAL:HG13	3:O:313:ARG:HG2	1.93	0.50
3:J:887:ASN:O	3:J:945:HIS:NE2	2.40	0.50
6:U:749:LEU:HG	6:U:789:LEU:HD11	1.93	0.50
7:X:411:GLU:HG3	7:X:1045:LEU:HD21	1.93	0.50
1:C:77:PRO:HG2	1:C:127:PRO:HB3	1.94	0.50
1:Q:221:SER:OG	1:Q:222:ASN:N	2.45	0.50
8:S:292:GLU:O	8:S:296:HIS:ND1	2.42	0.50
7:X:330:ILE:HG21	7:X:385:LEU:HD13	1.94	0.50
3:G:22:ASN:HD21	3:G:26:ASP:HB2	1.77	0.50
3:O:759:LEU:HD23	3:O:767:LEU:HD21	1.93	0.50
3:J:427:ARG:HH12	2:L:43:SER:HB3	1.77	0.50
6:U:596:TYR:O	6:U:605:LYS:NZ	2.43	0.50
3:G:693:ILE:HD13	3:G:728:LEU:HD13	1.94	0.50
4:H:205:ASP:HB3	4:H:227:GLN:HB2	1.93	0.50
3:O:157:ILE:HG23	3:O:163:ILE:HG12	1.92	0.50
3:O:708:GLY:HA2	3:O:713:ARG:HE	1.76	0.50
3:J:150:ARG:NH2	3:J:174:SER:O	2.44	0.50
7:X:989:MET:HG3	7:X:994:ILE:HG12	1.93	0.50
5:A:303:ILE:HG12	5:A:359:ALA:H	1.77	0.50
1:Q:830:MET:HG2	1:Q:844:TRP:HH2	1.77	0.50
5:I:303:ILE:HG12	5:I:359:ALA:H	1.76	0.50
5:I:311:ARG:NH2	5:I:346:ASP:OD1	2.45	0.50
2:N:196:ARG:HD3	2:N:202:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1194:ILE:HG22	5:A:1195:THR:HG23	1.94	0.50
7:W:340:LYS:NZ	8:S:253:LYS:O	2.40	0.50
7:X:948:PHE:HB3	7:X:988:LEU:HB3	1.94	0.50
1:C:786:ASP:OD2	4:H:265:SER:OG	2.28	0.49
2:E:226:ARG:NH1	3:G:808:SER:OG	2.45	0.49
3:B:668:TRP:NE1	3:B:753:GLU:OE2	2.39	0.49
6:V:855:GLN:HG3	8:T:488:PHE:HE2	1.77	0.49
7:X:207:VAL:HG21	7:X:264:ILE:HG12	1.94	0.49
3:B:328:ARG:NH2	3:B:419:GLU:OE2	2.45	0.49
2:F:203:HIS:HB2	2:F:288:LEU:HD21	1.94	0.49
1:Q:326:LEU:HB3	1:Q:338:TRP:HB2	1.93	0.49
5:I:539:LEU:HD11	5:I:1210:LEU:HD21	1.93	0.49
5:I:1194:ILE:HG22	5:I:1195:THR:HG23	1.95	0.49
2:N:203:HIS:HB2	2:N:288:LEU:HD21	1.94	0.49
7:W:328:PHE:HB2	7:W:356:ARG:HB3	1.94	0.49
3:J:642:TRP:NE1	3:J:752:ARG:O	2.43	0.49
3:J:972:THR:HB	3:J:1018:GLU:HG2	1.94	0.49
1:C:39:ILE:HD13	1:C:335:LEU:HD21	1.94	0.49
1:C:616:THR:HG21	4:H:146:ILE:HG13	1.93	0.49
3:B:881:CYS:SG	3:B:948:SER:OG	2.70	0.49
3:J:25:ARG:HB3	3:J:55:ILE:H	1.78	0.49
7:W:330:ILE:HG21	7:W:385:LEU:HD13	1.94	0.49
1:C:210:ASN:ND2	1:C:216:GLU:OE1	2.46	0.49
2:D:28:SER:OG	2:D:29:SER:N	2.45	0.49
3:O:693:ILE:HD13	3:O:728:LEU:HD13	1.93	0.49
2:N:61:ILE:HD11	2:N:72:ILE:HD12	1.95	0.49
8:S:241:LEU:HB2	8:S:588:LYS:HE3	1.94	0.49
8:T:307:ASP:OD1	8:T:307:ASP:N	2.44	0.49
3:G:223:LYS:HG2	3:G:235:GLN:HG2	1.94	0.49
3:G:326:ILE:HD13	3:G:384:LEU:HD13	1.95	0.49
3:G:670:VAL:HG21	3:G:731:ILE:HG12	1.95	0.49
5:A:540:ASP:OD1	5:A:540:ASP:N	2.44	0.49
2:M:226:ARG:NH1	3:O:808:SER:OG	2.45	0.49
4:P:74:SER:OG	4:P:76:ASP:OD1	2.31	0.49
6:U:860:ASP:OD1	6:U:860:ASP:N	2.45	0.49
7:W:989:MET:HG3	7:W:994:ILE:HG12	1.94	0.49
7:X:335:SER:O	7:X:400:ARG:NH2	2.44	0.49
2:D:186:SER:HB3	2:D:218:ILE:HG13	1.94	0.49
3:O:22:ASN:HD21	3:O:26:ASP:HB2	1.78	0.49
2:L:110:SER:N	2:L:130:ASN:OD1	2.46	0.49
2:L:186:SER:HB3	2:L:218:ILE:HG13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:544:ASN:ND2	3:B:785:GLU:OE2	2.45	0.49
1:C:221:SER:OG	1:C:222:ASN:N	2.46	0.49
3:B:25:ARG:HB3	3:B:55:ILE:H	1.77	0.49
1:Q:37:ARG:NE	1:Q:367:SER:OG	2.43	0.49
3:O:670:VAL:HG21	3:O:731:ILE:HG12	1.95	0.49
3:J:544:ASN:ND2	3:J:785:GLU:OE2	2.46	0.49
4:P:179:ASP:OD1	4:P:179:ASP:N	2.46	0.49
4:P:205:ASP:HB3	4:P:227:GLN:HB2	1.94	0.49
5:I:147:VAL:HG11	5:I:152:ILE:HD11	1.95	0.49
7:W:469:LEU:HD23	7:W:502:VAL:HG22	1.95	0.49
1:C:628:THR:HG23	1:C:630:THR:H	1.78	0.48
3:B:972:THR:HB	3:B:1018:GLU:HG2	1.94	0.48
2:D:110:SER:N	2:D:130:ASN:OD1	2.46	0.48
7:W:1410:ILE:HD13	7:W:1505:GLY:HA3	1.95	0.48
7:W:1436:ILE:H	7:W:1565:LEU:HD23	1.77	0.48
8:S:578:GLU:OE2	8:S:581:ARG:NH1	2.45	0.48
1:C:1030:ILE:HG23	1:C:1049:ILE:HG12	1.95	0.48
1:Q:616:THR:HG21	4:P:146:ILE:HG13	1.93	0.48
3:J:577:TRP:HE1	3:J:768:THR:HB	1.79	0.48
7:W:206:VAL:HB	7:W:253:TYR:HB2	1.95	0.48
6:V:667:VAL:O	6:V:862:TYR:OH	2.23	0.48
6:V:899:ARG:NH1	6:V:905:LEU:O	2.46	0.48
8:T:318:SER:OG	8:T:319:SER:N	2.46	0.48
1:Q:775:VAL:HB	4:P:4:ILE:HB	1.96	0.48
3:O:326:ILE:HD13	3:O:384:LEU:HD13	1.95	0.48
5:I:280:ASP:OD2	5:I:284:LYS:NZ	2.46	0.48
8:T:593:LEU:HD12	8:T:600:VAL:HG22	1.93	0.48
3:G:37:ASN:ND2	3:G:41:GLU:OE2	2.37	0.48
3:B:427:ARG:HH12	2:D:43:SER:HB3	1.77	0.48
1:Q:205:ASN:ND2	1:Q:222:ASN:OD1	2.46	0.48
3:J:400:GLU:OE2	3:J:420:ASN:ND2	2.43	0.48
7:W:121:ASN:HB3	7:W:124:GLU:HB2	1.94	0.48
3:G:633:ARG:NH1	3:G:764:ASP:OD1	2.46	0.48
1:Q:459:THR:HG22	1:Q:476:ARG:HG2	1.95	0.48
1:Q:628:THR:HG23	1:Q:630:THR:H	1.77	0.48
6:V:860:ASP:OD1	6:V:860:ASP:N	2.45	0.48
1:C:878:ILE:HG13	1:C:1018:LEU:HD11	1.96	0.48
2:E:100:LYS:HZ1	2:E:103:THR:HG1	1.56	0.48
4:H:128:VAL:HB	4:H:138:PRO:HB3	1.96	0.48
5:A:147:VAL:HG11	5:A:152:ILE:HD11	1.96	0.48
5:A:262:ASN:ND2	5:A:310:ILE:O	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:404:LYS:HG2	3:B:406:ILE:HG23	1.95	0.48
3:J:404:LYS:HG2	3:J:406:ILE:HG23	1.95	0.48
2:L:28:SER:OG	2:L:29:SER:N	2.45	0.48
2:L:150:LEU:HD21	2:L:153:GLU:HB2	1.96	0.48
2:L:199:ASP:OD1	2:L:199:ASP:N	2.42	0.48
8:S:318:SER:OG	8:S:319:SER:N	2.47	0.48
1:C:1078:VAL:HG13	3:G:879:ILE:HG23	1.96	0.48
4:H:23:ARG:NH1	4:H:84:GLU:OE1	2.46	0.48
7:W:329:ALA:HB1	7:W:412:LEU:HD22	1.96	0.48
8:S:122:ASN:O	8:S:127:LYS:NZ	2.47	0.48
6:V:1084:LYS:HA	6:V:1087:LEU:HD12	1.95	0.48
8:T:314:ILE:HG12	8:T:450:THR:HA	1.95	0.48
3:G:800:LEU:HD22	3:G:813:ALA:HA	1.96	0.48
8:T:342:GLU:O	8:T:466:ASN:ND2	2.39	0.48
2:E:235:CYS:SG	2:E:236:LYS:N	2.87	0.48
3:G:854:ASP:OD1	3:G:857:ARG:NH1	2.47	0.48
3:B:392:THR:HG21	6:V:970:GLU:OE2	2.14	0.48
2:D:311:SER:HG	2:D:320:SER:HG	1.61	0.48
1:Q:1078:VAL:HG13	3:O:879:ILE:HG23	1.95	0.48
5:I:220:ASN:ND2	5:I:268:MET:O	2.47	0.48
5:I:540:ASP:OD1	5:I:540:ASP:N	2.44	0.48
3:J:713:ARG:HH11	3:J:736:ALA:HA	1.79	0.48
3:O:723:LEU:O	3:O:729:ARG:NE	2.35	0.47
7:X:537:ARG:NH2	8:T:478:GLU:OE2	2.47	0.47
3:B:800:LEU:HD22	3:B:813:ALA:HA	1.96	0.47
2:M:235:CYS:SG	2:M:236:LYS:N	2.87	0.47
8:S:593:LEU:HD12	8:S:600:VAL:HG22	1.96	0.47
7:X:121:ASN:HB3	7:X:124:GLU:HB2	1.95	0.47
7:X:328:PHE:HB2	7:X:356:ARG:HB3	1.95	0.47
3:G:827:ASP:OD1	3:G:827:ASP:N	2.47	0.47
2:F:211:HIS:HB3	2:F:215:ILE:HD11	1.96	0.47
2:F:237:ASP:OD2	2:F:239:ARG:NH1	2.47	0.47
5:I:262:ASN:ND2	5:I:310:ILE:O	2.43	0.47
3:J:390:SER:HB3	6:U:966:MET:HB3	1.96	0.47
7:X:898:THR:HB	7:X:974:LYS:HE3	1.96	0.47
1:Q:531:PRO:HA	1:Q:534:ARG:HG2	1.95	0.47
8:T:292:GLU:O	8:T:296:HIS:ND1	2.42	0.47
3:G:567:ASP:OD1	3:G:567:ASP:N	2.47	0.47
2:F:61:ILE:HD11	2:F:72:ILE:HD12	1.96	0.47
4:P:23:ARG:NH1	4:P:84:GLU:OE1	2.48	0.47
1:C:115:ARG:HB2	1:C:136:ASP:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:SER:HG	1:C:178:HIS:CE1	2.33	0.47
1:C:186:ASP:HB3	1:C:189:LYS:HB2	1.96	0.47
1:C:459:THR:HG22	1:C:476:ARG:HG2	1.97	0.47
1:C:531:PRO:HA	1:C:534:ARG:HG2	1.96	0.47
2:E:1:MET:HG2	3:G:426:ILE:HG12	1.97	0.47
2:E:313:ASN:ND2	3:G:411:ASN:OD1	2.41	0.47
3:G:682:LEU:HB3	3:G:694:ALA:HB2	1.96	0.47
5:A:220:ASN:ND2	5:A:268:MET:O	2.47	0.47
3:B:577:TRP:HE1	3:B:768:THR:HB	1.80	0.47
4:P:128:VAL:HB	4:P:138:PRO:HB3	1.96	0.47
5:I:539:LEU:HD22	2:N:315:THR:HG23	1.96	0.47
2:N:237:ASP:OD2	2:N:239:ARG:NH1	2.48	0.47
7:W:898:THR:HB	7:W:974:LYS:HE3	1.97	0.47
8:T:266:ILE:HD11	8:T:290:VAL:HG22	1.97	0.47
2:E:86:GLU:OE2	2:E:97:ARG:NH2	2.48	0.47
2:M:100:LYS:HZ1	2:M:103:THR:HG1	1.59	0.47
3:J:328:ARG:NH2	3:J:419:GLU:OE2	2.48	0.47
7:W:413:VAL:HG11	7:W:460:LEU:HD11	1.97	0.47
1:C:830:MET:HG3	5:A:875:LEU:HD21	1.96	0.47
5:A:539:LEU:HD22	2:F:315:THR:HG23	1.96	0.47
2:D:135:ARG:HG2	2:D:150:LEU:HD11	1.97	0.47
3:O:854:ASP:OD1	3:O:857:ARG:NH1	2.47	0.47
7:W:1031:THR:HB	7:W:1428:SER:HA	1.97	0.47
7:X:420:LEU:HD23	7:X:463:LEU:HD13	1.97	0.47
1:C:460:LEU:HD11	1:C:536:VAL:HG12	1.95	0.47
3:G:388:ARG:HH11	3:O:50:LYS:HE2	1.80	0.47
5:A:137:VAL:HG11	5:A:141:LEU:HD21	1.97	0.47
5:A:303:ILE:HG23	5:A:359:ALA:HA	1.97	0.47
1:Q:830:MET:HG3	5:I:875:LEU:HD21	1.96	0.47
2:M:86:GLU:OE2	2:M:97:ARG:NH2	2.48	0.47
6:U:889:PRO:HD2	6:U:892:TYR:HD2	1.79	0.47
8:S:314:ILE:HG12	8:S:450:THR:HA	1.97	0.47
5:A:1215:GLU:OE2	2:F:22:ARG:NH1	2.48	0.46
1:Q:1030:ILE:HG23	1:Q:1049:ILE:HG12	1.96	0.46
7:X:413:VAL:HG11	7:X:460:LEU:HD11	1.96	0.46
3:G:884:CYS:HB3	3:G:946:CYS:HB3	1.97	0.46
4:H:74:SER:OG	4:H:76:ASP:OD1	2.31	0.46
3:B:692:LEU:HB3	3:O:692:LEU:HB3	1.97	0.46
2:D:150:LEU:HD21	2:D:153:GLU:HB2	1.98	0.46
1:Q:54:ASP:OD2	1:Q:57:THR:OG1	2.32	0.46
1:C:1094:LEU:HA	1:C:1097:ASN:HD22	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:280:ASP:OD2	5:A:284:LYS:NZ	2.48	0.46
3:O:682:LEU:HB3	3:O:694:ALA:HB2	1.96	0.46
2:L:87:ASP:OD1	2:L:87:ASP:N	2.48	0.46
6:V:916:SER:O	8:T:614:ASN:ND2	2.43	0.46
3:O:827:ASP:N	3:O:827:ASP:OD1	2.47	0.46
6:U:13:VAL:HG11	6:U:623:LEU:HB3	1.97	0.46
6:U:16:VAL:O	6:U:534:HIS:N	2.49	0.46
1:C:407:LEU:HB3	1:C:435:SER:HB2	1.97	0.46
3:G:689:ARG:NH2	3:G:725:ASP:OD2	2.48	0.46
3:O:800:LEU:HD22	3:O:813:ALA:HA	1.98	0.46
3:G:34:ASP:O	3:G:395:ARG:NH1	2.44	0.46
2:L:135:ARG:HG2	2:L:150:LEU:HD11	1.97	0.46
2:N:211:HIS:HB3	2:N:215:ILE:HD11	1.96	0.46
6:U:855:GLN:HG3	8:S:488:PHE:HE2	1.80	0.46
1:Q:878:ILE:HG13	1:Q:1018:LEU:HD11	1.97	0.46
2:M:1:MET:HG2	3:O:426:ILE:HG12	1.97	0.46
2:D:214:LEU:O	2:D:236:LYS:N	2.44	0.46
1:Q:1034:SER:HB2	1:Q:1046:ARG:HB2	1.98	0.46
7:W:358:VAL:HG11	7:W:374:LEU:HA	1.98	0.46
7:X:329:ALA:HB1	7:X:412:LEU:HD22	1.97	0.46
7:X:1372:ASN:HB2	7:X:1375:HIS:HB2	1.97	0.46
7:X:1468:LEU:N	7:X:1501:ILE:O	2.49	0.46
3:B:72:GLU:OE1	3:B:74:ASN:ND2	2.41	0.46
2:L:214:LEU:O	2:L:236:LYS:N	2.44	0.46
8:S:266:ILE:HD11	8:S:290:VAL:HG22	1.98	0.46
8:T:321:ILE:HD11	8:T:442:TYR:HB3	1.98	0.46
5:I:137:VAL:HG11	5:I:141:LEU:HD21	1.97	0.45
3:J:73:LYS:HE3	3:J:301:LYS:HD2	1.98	0.45
7:W:328:PHE:N	7:W:356:ARG:O	2.43	0.45
8:S:14:ILE:HG12	8:S:201:LEU:HD22	1.98	0.45
8:S:317:PRO:HA	8:S:482:ILE:HG22	1.97	0.45
8:S:444:SER:OG	8:S:454:TRP:NE1	2.42	0.45
3:B:375:ILE:HD11	3:B:385:ILE:HB	1.98	0.45
3:B:497:TRP:HZ3	3:B:505:LYS:HD3	1.81	0.45
3:B:713:ARG:HH11	3:B:736:ALA:HA	1.80	0.45
2:D:134:LEU:HD22	2:D:185:VAL:HG21	1.98	0.45
1:Q:460:LEU:HD11	1:Q:536:VAL:HG12	1.96	0.45
1:Q:1094:LEU:HA	1:Q:1097:ASN:HD22	1.80	0.45
3:O:541:TYR:HD2	3:O:784:LEU:HB2	1.81	0.45
8:S:342:GLU:O	8:S:466:ASN:ND2	2.42	0.45
7:X:285:ILE:HB	7:X:330:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:110:SER:N	2:E:130:ASN:OD1	2.50	0.45
3:G:755:LEU:HD23	3:G:755:LEU:HA	1.83	0.45
3:O:633:ARG:NH1	3:O:764:ASP:OD1	2.49	0.45
3:O:689:ARG:NH2	3:O:725:ASP:OD2	2.49	0.45
4:H:123:GLY:HA2	4:H:148:VAL:HG23	1.98	0.45
1:Q:294:ILE:HD13	1:Q:347:LYS:HB3	1.98	0.45
2:N:89:ASP:N	2:N:89:ASP:OD1	2.49	0.45
6:U:667:VAL:O	6:U:862:TYR:OH	2.23	0.45
7:W:951:CYS:HB3	7:W:956:VAL:HG21	1.98	0.45
7:W:1364:THR:HB	7:W:1382:GLU:HB2	1.98	0.45
7:X:138:THR:HG21	7:X:185:LEU:HD11	1.98	0.45
1:C:320:ASP:H	1:C:354:LYS:H	1.65	0.45
1:C:1034:SER:HB2	1:C:1046:ARG:HB2	1.98	0.45
2:E:214:LEU:O	2:E:236:LYS:N	2.48	0.45
3:G:682:LEU:HD22	3:G:690:LEU:HB3	1.98	0.45
3:O:224:GLU:HG2	3:O:233:ILE:HD12	1.99	0.45
4:P:8:HIS:CG	4:P:28:SER:HG	2.34	0.45
4:P:256:VAL:O	4:P:274:GLY:N	2.49	0.45
3:G:539:ASN:HB3	3:G:542:ILE:HD12	1.98	0.45
4:H:256:VAL:O	4:H:274:GLY:N	2.49	0.45
7:W:326:ILE:HD13	7:W:374:LEU:HD12	1.99	0.45
8:S:262:THR:O	8:S:266:ILE:HG12	2.17	0.45
8:S:335:GLN:NE2	8:S:433:PRO:O	2.39	0.45
1:C:1044:LEU:HD23	3:G:955:ILE:HD12	1.99	0.45
2:D:89:ASP:OD1	2:D:89:ASP:N	2.48	0.45
2:D:172:SER:HB3	2:D:184:ALA:HB3	1.99	0.45
1:Q:22:LYS:HE3	1:Q:333:CYS:HB2	1.98	0.45
3:J:326:ILE:HD13	3:J:384:LEU:HD13	1.99	0.45
3:J:375:ILE:HD11	3:J:385:ILE:HB	1.99	0.45
3:J:497:TRP:HZ3	3:J:505:LYS:HD3	1.82	0.45
7:W:150:LYS:NZ	7:W:182:LEU:O	2.44	0.45
7:W:230:ASP:OD1	7:W:263:TYR:OH	2.35	0.45
3:B:603:GLU:HA	3:B:606:LYS:HE3	1.99	0.45
3:B:755:LEU:HD23	3:B:758:ALA:HB3	1.99	0.45
1:Q:125:GLN:NE2	1:Q:168:TYR:O	2.50	0.45
3:O:567:ASP:OD1	3:O:567:ASP:N	2.47	0.45
5:I:390:ASP:OD1	5:I:390:ASP:N	2.50	0.45
3:J:682:LEU:HB3	3:J:694:ALA:HB2	1.99	0.45
7:W:1042:ILE:HB	7:W:1422:SER:HA	1.99	0.45
7:X:326:ILE:HD13	7:X:374:LEU:HD12	1.99	0.45
7:X:415:PHE:O	7:X:418:THR:OG1	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:1031:THR:HB	7:X:1428:SER:HA	1.99	0.45
4:P:129:GLU:HG2	4:P:131:LYS:HG2	1.99	0.45
3:J:956:CYS:SG	3:J:1016:HIS:HE1	2.40	0.45
6:U:28:HIS:O	6:U:610:TYR:OH	2.31	0.45
7:X:230:ASP:OD1	7:X:263:TYR:OH	2.35	0.45
4:P:52:HIS:HD1	4:P:74:SER:HG	1.58	0.45
5:I:303:ILE:HG23	5:I:359:ALA:HA	1.97	0.45
2:L:134:LEU:HD22	2:L:185:VAL:HG21	1.99	0.45
6:V:578:GLU:HG3	6:V:619:LEU:HB2	1.99	0.45
2:E:28:SER:OG	2:E:30:ASP:OD1	2.29	0.44
3:G:541:TYR:HD2	3:G:784:LEU:HB2	1.81	0.44
3:G:692:LEU:HB3	3:J:692:LEU:HB3	1.98	0.44
3:G:850:ARG:NH1	3:G:854:ASP:OD2	2.50	0.44
5:A:135:THR:OG1	5:A:136:LYS:N	2.51	0.44
3:B:147:LYS:HB3	3:B:147:LYS:HE2	1.69	0.44
2:M:110:SER:N	2:M:130:ASN:OD1	2.50	0.44
3:J:603:GLU:HA	3:J:606:LYS:HE3	1.99	0.44
7:W:420:LEU:HD23	7:W:463:LEU:HD13	1.98	0.44
7:X:408:ASN:HB2	7:X:411:GLU:HB2	1.99	0.44
7:X:541:VAL:HG21	8:T:474:THR:HG21	1.98	0.44
8:T:317:PRO:HA	8:T:482:ILE:HG22	1.99	0.44
1:C:37:ARG:NE	1:C:367:SER:OG	2.49	0.44
3:G:406:ILE:HD11	3:G:414:LEU:HD23	1.99	0.44
4:H:129:GLU:HG2	4:H:131:LYS:HG2	1.99	0.44
2:M:313:ASN:ND2	3:O:411:ASN:OD1	2.41	0.44
3:O:539:ASN:HB3	3:O:542:ILE:HD12	1.98	0.44
3:O:884:CYS:HB3	3:O:946:CYS:HB3	1.99	0.44
2:L:172:SER:HB3	2:L:184:ALA:HB3	1.99	0.44
2:L:205:ALA:HB1	2:L:292:LEU:HD21	1.99	0.44
5:A:390:ASP:OD1	5:A:390:ASP:N	2.50	0.44
3:O:850:ARG:NH1	3:O:854:ASP:OD2	2.51	0.44
3:J:333:TYR:HB2	3:J:352:GLU:HB3	1.98	0.44
7:W:408:ASN:HB2	7:W:411:GLU:HB2	1.99	0.44
7:W:541:VAL:HG21	8:S:474:THR:HG21	1.99	0.44
8:T:62:THR:HG23	8:T:71:VAL:HG22	2.00	0.44
1:Q:33:ASN:ND2	1:Q:35:SER:OG	2.50	0.44
1:Q:1044:LEU:HD23	3:O:955:ILE:HD12	2.00	0.44
1:Q:1091:GLU:HA	1:Q:1094:LEU:HB2	2.00	0.44
6:U:560:ARG:NH2	6:U:647:SER:O	2.51	0.44
2:E:54:HIS:ND1	2:E:76:SER:OG	2.43	0.44
2:E:120:HIS:HB3	2:E:177:ARG:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:77:GLY:HA2	4:H:102:VAL:HG23	2.00	0.44
1:Q:407:LEU:HB3	1:Q:435:SER:HB2	2.00	0.44
3:J:28:VAL:HG21	3:J:70:VAL:HG21	2.00	0.44
2:N:302:ASP:HB2	2:N:331:TRP:HH2	1.82	0.44
1:C:54:ASP:OD2	1:C:57:THR:OG1	2.32	0.44
2:F:302:ASP:HB2	2:F:331:TRP:HH2	1.83	0.44
7:W:308:PHE:HA	7:W:311:ILE:HG22	1.99	0.44
8:S:219:ASP:HB2	8:S:222:ASN:HB2	2.00	0.44
6:V:889:PRO:HD2	6:V:892:TYR:HD2	1.83	0.44
7:X:358:VAL:HG11	7:X:374:LEU:HA	1.99	0.44
7:X:1364:THR:HB	7:X:1382:GLU:HB2	2.00	0.44
8:T:262:THR:O	8:T:266:ILE:HG12	2.18	0.44
1:C:162:SER:OG	1:C:177:SER:OG	2.31	0.44
2:N:226:ARG:NH1	2:N:316:GLY:O	2.43	0.44
7:X:308:PHE:HA	7:X:311:ILE:HG22	1.99	0.44
7:X:951:CYS:HB3	7:X:956:VAL:HG21	2.00	0.44
3:G:50:LYS:HE2	3:O:388:ARG:HH11	1.81	0.44
2:F:90:GLN:O	2:F:97:ARG:NH1	2.51	0.44
5:I:525:VAL:HG22	2:N:165:LEU:HD11	2.00	0.44
5:I:531:LYS:O	5:I:549:GLN:NE2	2.51	0.44
5:I:1215:GLU:OE2	2:N:22:ARG:NH1	2.51	0.44
6:U:766:SER:HB2	6:U:773:THR:HG21	2.00	0.44
8:T:433:PRO:HB3	8:T:465:ASN:HB3	2.00	0.44
3:G:224:GLU:HG2	3:G:233:ILE:HD12	1.99	0.44
5:A:145:ASP:HB2	5:A:215:VAL:HG13	2.00	0.44
2:M:120:HIS:HB3	2:M:177:ARG:HG2	1.99	0.44
3:O:682:LEU:HD22	3:O:690:LEU:HB3	1.98	0.44
3:J:800:LEU:HD22	3:J:813:ALA:HA	1.99	0.44
6:V:430:LEU:HD22	6:V:550:ILE:HG23	1.99	0.44
3:O:18:TYR:OH	3:O:374:TYR:O	2.33	0.43
3:O:305:SER:HG	3:O:371:THR:HG1	1.65	0.43
7:W:415:PHE:O	7:W:418:THR:OG1	2.31	0.43
4:P:17:LEU:HD23	4:P:17:LEU:HA	1.89	0.43
6:U:1089:ARG:HD2	6:U:1089:ARG:HA	1.88	0.43
7:W:1507:TYR:HE2	7:W:1551:VAL:HB	1.82	0.43
6:V:560:ARG:NH2	6:V:647:SER:O	2.51	0.43
6:V:596:TYR:O	6:V:605:LYS:NZ	2.43	0.43
4:H:179:ASP:OD1	4:H:179:ASP:N	2.45	0.43
3:B:333:TYR:HB2	3:B:352:GLU:HB3	2.00	0.43
2:F:89:ASP:OD1	2:F:89:ASP:N	2.49	0.43
8:S:28:LYS:HA	8:S:28:LYS:HD2	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:X:1507:TYR:HE2	7:X:1551:VAL:HB	1.83	0.43
2:D:132:GLY:O	2:D:156:VAL:N	2.51	0.43
2:D:325:ASP:OD1	2:D:325:ASP:N	2.49	0.43
1:Q:324:PHE:N	1:Q:345:TYR:OH	2.48	0.43
5:I:1302:LYS:HA	5:I:1302:LYS:HD2	1.90	0.43
3:J:207:LYS:HA	3:J:207:LYS:HD3	1.83	0.43
7:X:328:PHE:N	7:X:356:ARG:O	2.43	0.43
1:C:1091:GLU:HA	1:C:1094:LEU:HB2	1.99	0.43
2:E:85:GLU:HB2	2:E:101:LEU:HD11	2.00	0.43
2:D:205:ALA:HB1	2:D:292:LEU:HD21	2.00	0.43
4:P:77:GLY:HA2	4:P:102:VAL:HG23	2.01	0.43
2:N:170:CYS:HB3	2:N:218:ILE:HG22	2.00	0.43
6:V:1091:ILE:HD11	6:V:1136:LEU:HD21	2.01	0.43
1:C:863:GLU:OE2	1:C:1029:TYR:OH	2.33	0.43
3:B:140:TYR:HB2	3:B:141:ASP:H	1.65	0.43
2:F:85:GLU:HB2	2:F:101:LEU:HD11	2.01	0.43
2:M:134:LEU:HD21	2:M:183:LEU:HD23	2.00	0.43
5:I:135:THR:OG1	5:I:136:LYS:N	2.51	0.43
5:I:145:ASP:HB2	5:I:215:VAL:HG13	2.01	0.43
5:I:1185:LEU:HD23	5:I:1185:LEU:HA	1.88	0.43
3:J:755:LEU:HD23	3:J:758:ALA:HB3	1.99	0.43
7:X:1042:ILE:HB	7:X:1422:SER:HA	2.01	0.43
1:C:276:ASN:HB2	1:C:294:ILE:HD11	2.01	0.43
1:C:775:VAL:HB	4:H:4:ILE:HB	2.00	0.43
5:A:531:LYS:O	5:A:549:GLN:NE2	2.52	0.43
2:M:302:ASP:O	2:M:329:ARG:NE	2.52	0.43
7:W:1510:GLU:HB3	7:W:1518:PHE:HB2	2.01	0.43
3:G:147:LYS:HG2	3:G:190:THR:HB	1.99	0.43
4:H:17:LEU:HD23	4:H:17:LEU:HA	1.89	0.43
2:M:214:LEU:O	2:M:236:LYS:N	2.50	0.43
3:J:306:CYS:HB2	3:J:320:LEU:HB3	2.01	0.43
6:U:578:GLU:HG3	6:U:619:LEU:HB2	2.01	0.43
7:X:482:LEU:HD21	7:X:854:PRO:HB3	2.00	0.43
2:E:319:LEU:HB3	2:E:331:TRP:HB2	2.01	0.43
4:H:102:VAL:HA	4:H:120:SER:HA	2.00	0.43
3:B:306:CYS:HB2	3:B:320:LEU:HB3	2.00	0.43
2:F:128:LEU:HD12	2:F:128:LEU:HA	1.92	0.43
1:Q:39:ILE:HD13	1:Q:335:LEU:HD21	2.01	0.43
7:W:482:LEU:HD21	7:W:854:PRO:HB3	2.01	0.43
2:E:134:LEU:HD21	2:E:183:LEU:HD23	2.00	0.43
2:E:174:CYS:SG	2:E:176:SER:OG	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:295:SER:OG	3:B:296:GLY:N	2.52	0.43
3:B:836:THR:HG21	2:D:224:ILE:HA	2.00	0.43
6:V:373:MET:HB3	6:V:379:ILE:HG12	2.00	0.43
1:C:404:ILE:HG12	1:C:438:GLY:HA3	2.00	0.42
3:O:147:LYS:HG2	3:O:190:THR:HB	2.00	0.42
6:U:565:LEU:HA	6:U:568:VAL:HG12	2.01	0.42
7:W:1507:TYR:HA	7:W:1521:PRO:HA	2.01	0.42
3:B:260:ASP:OD1	3:B:260:ASP:N	2.45	0.42
3:B:326:ILE:HD13	3:B:384:LEU:HD13	2.00	0.42
2:N:329:ARG:HG2	2:N:344:VAL:HG22	2.00	0.42
7:W:281:PHE:HD2	7:W:439:ILE:HD11	1.84	0.42
7:W:1468:LEU:N	7:W:1501:ILE:O	2.52	0.42
3:B:566:LEU:HD21	3:B:607:ILE:HD11	2.01	0.42
3:O:406:ILE:HD11	3:O:414:LEU:HD23	1.99	0.42
3:O:417:ASN:ND2	3:O:420:ASN:OD1	2.38	0.42
5:I:657:PRO:HA	5:I:658:PRO:HD3	1.93	0.42
2:N:117:ALA:HB1	2:N:121:LEU:HD22	2.02	0.42
6:U:373:MET:HB3	6:U:379:ILE:HG12	2.00	0.42
6:U:858:THR:OG1	6:U:859:ILE:N	2.52	0.42
8:T:450:THR:HG23	8:T:453:THR:H	1.83	0.42
1:C:776:ILE:HG22	4:H:3:VAL:HG22	2.01	0.42
3:G:553:LYS:NZ	3:G:557:ASP:OD2	2.49	0.42
5:A:384:ILE:HD12	5:A:398:VAL:HG11	2.01	0.42
3:B:217:ALA:HB2	3:B:244:ILE:HD11	2.01	0.42
3:J:38:GLU:OE2	3:J:383:SER:OG	2.31	0.42
3:J:72:GLU:OE1	3:J:74:ASN:ND2	2.41	0.42
3:J:295:SER:OG	3:J:296:GLY:N	2.52	0.42
2:L:132:GLY:O	2:L:156:VAL:N	2.52	0.42
7:W:1372:ASN:HB2	7:W:1375:HIS:HB2	2.00	0.42
3:B:28:VAL:HG21	3:B:70:VAL:HG21	2.01	0.42
2:F:111:LEU:HD22	2:F:127:CYS:HB3	2.02	0.42
2:F:170:CYS:HB3	2:F:218:ILE:HG22	2.00	0.42
1:Q:203:SER:OG	8:T:203:ARG:NH1	2.50	0.42
2:M:291:ASN:OD1	2:M:291:ASN:N	2.53	0.42
4:P:102:VAL:HA	4:P:120:SER:HA	2.01	0.42
3:J:217:ALA:HB2	3:J:244:ILE:HD11	2.01	0.42
6:U:1059:PHE:HB3	6:U:1060:GLU:H	1.62	0.42
6:U:1079:ALA:HB3	6:U:1084:LYS:HG3	2.00	0.42
7:X:281:PHE:HD2	7:X:439:ILE:HD11	1.84	0.42
7:X:1483:GLU:O	7:X:1484:PHE:C	2.58	0.42
4:H:84:GLU:HB2	4:H:89:TRP:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1166:LYS:HG2	5:A:1194:ILE:HG23	2.01	0.42
1:Q:488:LYS:NZ	1:Q:523:ASP:O	2.45	0.42
7:W:206:VAL:HG13	7:W:271:ILE:HD12	2.02	0.42
8:S:433:PRO:HB3	8:S:465:ASN:HB3	2.00	0.42
8:S:565:MET:HA	8:S:566:PRO:HD3	1.92	0.42
6:V:858:THR:OG1	6:V:859:ILE:N	2.53	0.42
2:E:302:ASP:O	2:E:329:ARG:NE	2.52	0.42
2:F:329:ARG:HG2	2:F:344:VAL:HG22	2.01	0.42
3:O:324:ASP:OD1	3:O:324:ASP:N	2.52	0.42
5:I:450:LYS:HD2	5:I:461:LEU:HD12	2.02	0.42
5:I:704:ALA:HB1	5:I:1219:ILE:HG21	2.02	0.42
6:U:842:SER:O	6:U:924:SER:N	2.53	0.42
8:T:241:LEU:HB3	8:T:591:VAL:HG11	2.01	0.42
1:C:158:ARG:HD3	1:C:158:ARG:HA	1.82	0.42
1:C:342:ASP:HA	1:C:345:TYR:HB2	2.02	0.42
4:H:200:LEU:HD23	4:H:234:TRP:CD2	2.54	0.42
5:A:168:PHE:HB3	5:A:175:ILE:HG12	2.02	0.42
3:B:73:LYS:HE3	3:B:301:LYS:HD2	2.01	0.42
3:B:956:CYS:SG	3:B:1016:HIS:HE1	2.41	0.42
3:J:566:LEU:HD21	3:J:607:ILE:HD11	2.01	0.42
6:V:1079:ALA:HB3	6:V:1084:LYS:HG3	2.01	0.42
3:B:18:TYR:OH	3:B:374:TYR:O	2.29	0.42
3:B:682:LEU:HB3	3:B:694:ALA:HB2	2.00	0.42
3:O:34:ASP:O	3:O:395:ARG:NH1	2.43	0.42
3:O:726:PRO:HA	3:O:729:ARG:HB2	2.02	0.42
3:O:755:LEU:HD23	3:O:755:LEU:HA	1.83	0.42
2:L:187:ALA:HB3	2:L:190:GLN:HB2	2.02	0.42
7:W:136:LEU:HB2	7:W:154:PHE:HE1	1.85	0.42
7:W:407:SER:OG	7:W:408:ASN:N	2.53	0.42
7:W:411:GLU:HG3	7:W:1045:LEU:HD21	2.01	0.42
7:W:931:THR:OG1	7:W:932:TYR:N	2.53	0.42
7:X:136:LEU:HB2	7:X:154:PHE:HE1	1.85	0.42
7:X:206:VAL:HG13	7:X:271:ILE:HD12	2.02	0.42
1:C:324:PHE:N	1:C:345:TYR:OH	2.48	0.42
3:G:286:LEU:HD12	3:G:286:LEU:HA	1.95	0.42
2:D:187:ALA:HB3	2:D:190:GLN:HB2	2.02	0.42
5:I:477:SER:HB3	5:I:554:TYR:HD2	1.85	0.42
8:S:307:ASP:OD1	8:S:307:ASP:N	2.44	0.42
7:X:931:THR:OG1	7:X:932:TYR:N	2.53	0.42
3:G:331:LEU:HD13	3:G:354:LEU:HD13	2.02	0.41
3:G:417:ASN:ND2	3:G:420:ASN:OD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:666:ALA:HB2	3:G:682:LEU:HG	2.02	0.41
2:M:54:HIS:CG	2:M:76:SER:HG	2.33	0.41
3:O:260:ASP:OD1	3:O:260:ASP:N	2.44	0.41
3:O:958:MET:HA	3:O:959:PRO:HD3	1.90	0.41
6:U:419:ARG:HH22	6:U:551:ASP:HA	1.84	0.41
7:W:1041:MET:HB2	7:W:1421:PRO:HB2	2.02	0.41
6:V:565:LEU:HA	6:V:568:VAL:HG12	2.01	0.41
7:X:137:LYS:HE2	7:X:151:LYS:HG2	2.02	0.41
3:G:315:ASN:HB3	3:G:331:LEU:HB2	2.01	0.41
5:A:525:VAL:HG22	2:F:165:LEU:HD11	2.00	0.41
1:Q:84:TRP:NE1	1:Q:107:GLU:OE1	2.45	0.41
2:L:308:TRP:NE1	2:L:324:ASP:OD1	2.41	0.41
6:U:644:LYS:HE2	6:U:644:LYS:HB2	1.93	0.41
6:U:1091:ILE:HD11	6:U:1136:LEU:HD21	2.01	0.41
7:W:1352:ASP:HB2	7:W:1390:LEU:HD13	2.02	0.41
8:S:450:THR:HG23	8:S:453:THR:H	1.85	0.41
6:V:749:LEU:HG	6:V:789:LEU:HD11	2.01	0.41
2:D:124:LYS:HB3	2:D:124:LYS:HE3	1.91	0.41
1:Q:158:ARG:HA	1:Q:158:ARG:HD3	1.83	0.41
1:Q:404:ILE:HG12	1:Q:438:GLY:HA3	2.01	0.41
5:I:179:HIS:CE1	5:I:181:PHE:HB2	2.55	0.41
7:W:285:ILE:HB	7:W:330:ILE:HG13	2.01	0.41
7:W:481:PRO:HG3	7:W:500:LEU:HB3	2.01	0.41
7:X:407:SER:OG	7:X:408:ASN:N	2.54	0.41
7:X:917:HIS:HB2	7:X:1007:VAL:HB	2.01	0.41
1:C:225:THR:HG22	1:C:243:THR:HG22	2.01	0.41
5:A:450:LYS:HD2	5:A:461:LEU:HD12	2.02	0.41
3:B:38:GLU:OE2	3:B:383:SER:OG	2.31	0.41
2:F:117:ALA:HB1	2:F:121:LEU:HD22	2.01	0.41
1:Q:120:ILE:HG22	1:Q:132:THR:HG22	2.03	0.41
1:Q:1094:LEU:HD23	1:Q:1097:ASN:HD22	1.85	0.41
2:M:85:GLU:HB2	2:M:101:LEU:HD11	2.00	0.41
2:M:310:VAL:HG22	2:M:319:LEU:HD11	2.03	0.41
5:I:384:ILE:HD12	5:I:398:VAL:HG11	2.01	0.41
2:N:111:LEU:HD22	2:N:127:CYS:HB3	2.02	0.41
6:U:673:LEU:HD23	6:U:850:PRO:HD2	2.02	0.41
6:U:1087:LEU:HD22	6:U:1106:LEU:HD11	2.02	0.41
1:C:120:ILE:HG22	1:C:132:THR:HG22	2.01	0.41
1:C:294:ILE:HD13	1:C:347:LYS:HB3	2.02	0.41
5:A:182:ILE:HD13	5:A:182:ILE:HA	1.93	0.41
2:N:90:GLN:O	2:N:97:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:S:251:LEU:HD23	8:S:254:ILE:HD12	2.03	0.41
7:X:330:ILE:HB	7:X:354:TYR:HB2	2.01	0.41
7:X:546:LEU:HD23	7:X:546:LEU:HA	1.87	0.41
7:X:1436:ILE:H	7:X:1565:LEU:HD23	1.85	0.41
5:A:657:PRO:HA	5:A:658:PRO:HD3	1.93	0.41
3:B:682:LEU:HD23	3:B:682:LEU:HA	1.89	0.41
7:W:452:LEU:HD11	7:W:1045:LEU:HD22	2.03	0.41
8:S:347:SER:O	8:S:347:SER:OG	2.35	0.41
8:T:572:GLU:HG2	8:T:593:LEU:HD22	2.02	0.41
2:E:240:ILE:HD11	2:E:303:HIS:CD2	2.54	0.41
3:G:46:LEU:HD23	3:G:46:LEU:HA	1.91	0.41
3:G:726:PRO:HA	3:G:729:ARG:HB2	2.03	0.41
2:D:291:ASN:OD1	2:D:291:ASN:N	2.54	0.41
2:M:319:LEU:HB3	2:M:331:TRP:HB2	2.03	0.41
4:P:123:GLY:HA2	4:P:148:VAL:HG23	2.02	0.41
4:P:200:LEU:HD23	4:P:234:TRP:CD2	2.55	0.41
5:I:1166:LYS:HG2	5:I:1194:ILE:HG23	2.03	0.41
7:W:537:ARG:NH2	8:S:478:GLU:OE2	2.54	0.41
7:W:1087:ILE:HD13	7:W:1108:ILE:HD11	2.03	0.41
7:X:1507:TYR:HA	7:X:1521:PRO:HA	2.02	0.41
7:X:1510:GLU:HB3	7:X:1518:PHE:HB2	2.02	0.41
2:E:121:LEU:HD21	2:E:181:GLU:HB2	2.03	0.41
3:G:667:ALA:HB2	3:G:727:TYR:HB3	2.03	0.41
5:A:883:ASP:HB2	5:A:1161:THR:HG21	2.01	0.41
3:B:652:LYS:HD2	3:B:652:LYS:HA	1.84	0.41
2:D:59:VAL:HG11	2:D:77:TYR:CZ	2.56	0.41
1:Q:449:ILE:HA	1:Q:456:LEU:HD12	2.03	0.41
4:P:84:GLU:HB2	4:P:89:TRP:CE2	2.55	0.41
5:I:883:ASP:HB2	5:I:1161:THR:HG21	2.03	0.41
3:J:836:THR:HG21	2:L:224:ILE:HA	2.03	0.41
7:W:330:ILE:HB	7:W:354:TYR:HB2	2.01	0.41
7:W:544:LEU:HD23	7:W:544:LEU:HA	1.90	0.41
7:X:452:LEU:HD11	7:X:1045:LEU:HD22	2.03	0.41
1:C:1108:SER:H	3:G:1005:CYS:HA	1.86	0.41
2:E:310:VAL:HG22	2:E:319:LEU:HD11	2.03	0.41
5:A:280:ASP:OD1	5:A:280:ASP:N	2.54	0.41
5:A:1182:VAL:HG21	5:A:1207:PHE:HB2	2.03	0.41
2:F:82:LYS:HD3	2:F:100:LYS:HD2	2.03	0.41
2:M:211:HIS:HB3	2:M:215:ILE:HD11	2.02	0.41
2:M:240:ILE:HD11	2:M:303:HIS:CD2	2.54	0.41
3:O:331:LEU:HD13	3:O:354:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:280:ASP:OD1	5:I:280:ASP:N	2.54	0.41
5:I:499:TRP:CE2	5:I:505:ILE:HD12	2.56	0.41
2:L:12:VAL:HA	2:L:28:SER:HB2	2.03	0.41
2:L:325:ASP:N	2:L:325:ASP:OD1	2.50	0.41
2:N:310:VAL:HB	2:N:319:LEU:HD11	2.03	0.41
7:X:1054:TRP:HA	7:X:1057:ILE:HD12	2.03	0.41
8:T:56:LEU:HD23	8:T:56:LEU:HA	1.95	0.41
1:Q:223:ASP:OD1	1:Q:223:ASP:N	2.54	0.41
3:O:604:MET:HG2	3:O:635:LEU:HD21	2.02	0.41
3:J:755:LEU:HD23	3:J:755:LEU:HA	1.85	0.41
2:N:123:LEU:HD12	2:N:123:LEU:HA	1.88	0.41
6:U:923:TYR:CZ	6:U:940:LEU:HB2	2.56	0.41
7:W:868:PRO:HG2	7:W:871:TRP:HB2	2.02	0.41
8:S:241:LEU:HB3	8:S:591:VAL:HG11	2.03	0.41
7:X:408:ASN:N	7:X:408:ASN:OD1	2.53	0.41
2:E:68:TYR:CG	2:E:123:LEU:HD13	2.56	0.40
3:G:362:THR:HG21	3:G:398:ILE:HD13	2.04	0.40
5:A:179:HIS:CE1	5:A:181:PHE:HB2	2.56	0.40
3:B:505:LYS:HB3	3:B:505:LYS:HE3	1.93	0.40
2:L:59:VAL:HG11	2:L:77:TYR:CZ	2.56	0.40
2:L:124:LYS:HB3	2:L:124:LYS:HE3	1.91	0.40
7:W:1483:GLU:O	7:W:1484:PHE:C	2.58	0.40
7:X:1352:ASP:HB2	7:X:1390:LEU:HD13	2.03	0.40
1:C:134:SER:OG	1:C:136:ASP:OD1	2.28	0.40
3:G:958:MET:HA	3:G:959:PRO:HD3	1.90	0.40
2:F:72:ILE:HG12	2:F:84:TRP:HB2	2.03	0.40
3:O:315:ASN:HB3	3:O:331:LEU:HB2	2.02	0.40
2:N:85:GLU:HB2	2:N:101:LEU:HD11	2.01	0.40
2:E:199:ASP:OD1	2:E:199:ASP:N	2.46	0.40
2:E:211:HIS:HB3	2:E:215:ILE:HD11	2.03	0.40
5:A:704:ALA:HB1	5:A:1219:ILE:HG21	2.03	0.40
1:Q:342:ASP:HA	1:Q:345:TYR:HB2	2.03	0.40
3:O:666:ALA:HB2	3:O:682:LEU:HG	2.03	0.40
6:U:565:LEU:HD22	6:U:575:ILE:HD11	2.03	0.40
6:U:793:ARG:O	6:U:797:THR:OG1	2.34	0.40
7:X:524:ASP:HB3	7:X:530:ILE:HG12	2.04	0.40
7:X:543:TYR:CZ	8:T:341:PRO:HD3	2.56	0.40
1:C:1094:LEU:HD23	1:C:1097:ASN:HD22	1.86	0.40
2:N:150:LEU:HD21	2:N:153:GLU:HB2	2.04	0.40
3:G:771:LEU:HD23	3:G:771:LEU:HA	1.94	0.40
2:F:310:VAL:HB	2:F:319:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1108:SER:H	3:O:1005:CYS:HA	1.86	0.40
2:M:68:TYR:CG	2:M:123:LEU:HD13	2.56	0.40
3:O:362:THR:HG21	3:O:398:ILE:HD13	2.04	0.40
3:J:520:GLY:HA3	3:J:815:LEU:HG	2.03	0.40
2:L:291:ASN:N	2:L:291:ASN:OD1	2.54	0.40
6:U:411:PRO:HB2	6:U:415:MET:HB2	2.03	0.40
6:V:1114:PRO:HG2	6:V:1117:LEU:HG	2.04	0.40
8:T:28:LYS:HA	8:T:28:LYS:HD2	1.82	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	C	764/1148 (67%)	736 (96%)	28 (4%)	0	100	100
1	Q	764/1148 (67%)	734 (96%)	30 (4%)	0	100	100
2	D	306/349 (88%)	293 (96%)	13 (4%)	0	100	100
2	E	303/349 (87%)	289 (95%)	14 (5%)	0	100	100
2	F	307/349 (88%)	298 (97%)	9 (3%)	0	100	100
2	L	306/349 (88%)	293 (96%)	13 (4%)	0	100	100
2	M	303/349 (87%)	289 (95%)	14 (5%)	0	100	100
2	N	307/349 (88%)	298 (97%)	9 (3%)	0	100	100
3	B	781/1038 (75%)	758 (97%)	23 (3%)	0	100	100
3	G	766/1038 (74%)	740 (97%)	26 (3%)	0	100	100
3	J	781/1038 (75%)	758 (97%)	23 (3%)	0	100	100
3	O	766/1038 (74%)	741 (97%)	25 (3%)	0	100	100
4	H	282/297 (95%)	273 (97%)	9 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	P	282/297 (95%)	272 (96%)	10 (4%)	0	100	100
5	A	613/1341 (46%)	588 (96%)	25 (4%)	0	100	100
5	I	613/1341 (46%)	587 (96%)	26 (4%)	0	100	100
6	U	549/1146 (48%)	533 (97%)	16 (3%)	0	100	100
6	V	549/1146 (48%)	535 (97%)	14 (3%)	0	100	100
7	W	914/1584 (58%)	883 (97%)	31 (3%)	0	100	100
7	X	914/1584 (58%)	883 (97%)	31 (3%)	0	100	100
8	S	394/615 (64%)	383 (97%)	11 (3%)	0	100	100
8	T	394/615 (64%)	383 (97%)	11 (3%)	0	100	100
All	All	11958/18508 (65%)	11547 (97%)	411 (3%)	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	C	712/1040 (68%)	712 (100%)	0	100	100
1	Q	712/1040 (68%)	712 (100%)	0	100	100
2	D	270/305 (88%)	270 (100%)	0	100	100
2	E	269/305 (88%)	269 (100%)	0	100	100
2	F	272/305 (89%)	272 (100%)	0	100	100
2	L	270/305 (88%)	270 (100%)	0	100	100
2	M	269/305 (88%)	269 (100%)	0	100	100
2	N	272/305 (89%)	272 (100%)	0	100	100
3	B	717/919 (78%)	717 (100%)	0	100	100
3	G	704/919 (77%)	704 (100%)	0	100	100
3	J	717/919 (78%)	717 (100%)	0	100	100
3	O	704/919 (77%)	704 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	243/252 (96%)	243 (100%)	0	100	100
4	P	243/252 (96%)	243 (100%)	0	100	100
5	A	568/1207 (47%)	568 (100%)	0	100	100
5	I	568/1207 (47%)	568 (100%)	0	100	100
6	U	529/1060 (50%)	529 (100%)	0	100	100
6	V	529/1060 (50%)	529 (100%)	0	100	100
7	W	875/1458 (60%)	875 (100%)	0	100	100
7	X	875/1458 (60%)	875 (100%)	0	100	100
8	S	383/582 (66%)	383 (100%)	0	100	100
8	T	383/582 (66%)	383 (100%)	0	100	100
All	All	11084/16704 (66%)	11084 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	90	ASN
1	C	1097	ASN
2	D	195	GLN
1	Q	33	ASN
1	Q	90	ASN
1	Q	1097	ASN
2	L	195	GLN
7	W	291	ASN
7	X	291	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

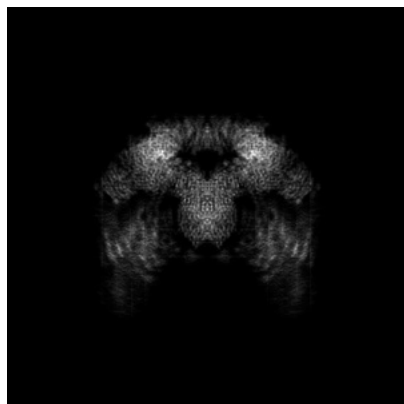
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15364. These allow visual inspection of the internal detail of the map and identification of artifacts.

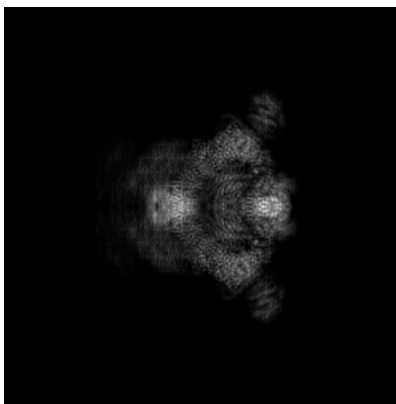
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

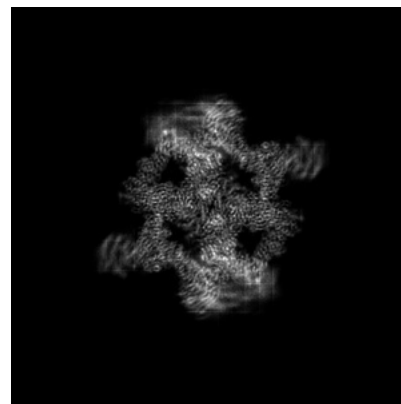
#### 6.1.1 Primary map



X

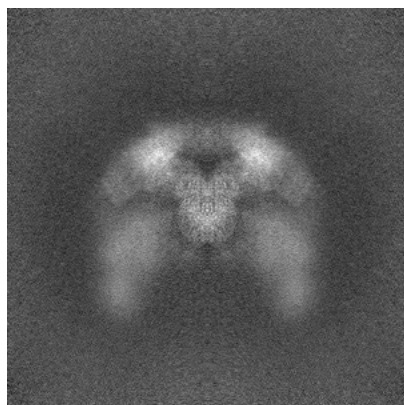


Y

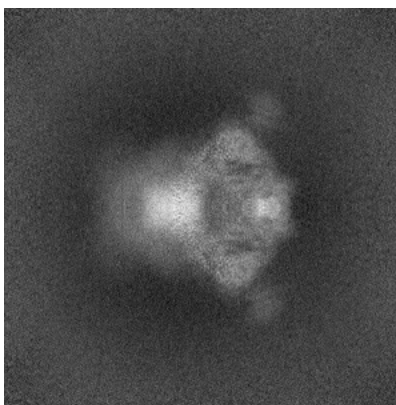


Z

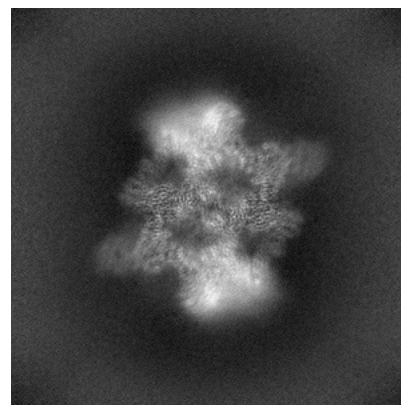
#### 6.1.2 Raw map



X



Y

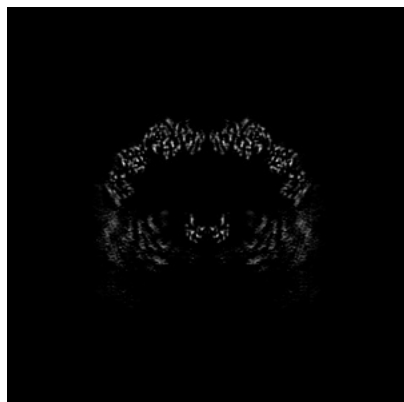


Z

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

## 6.2 Central slices [i](#)

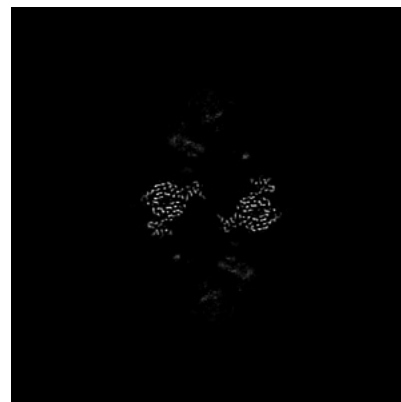
### 6.2.1 Primary map



X Index: 320

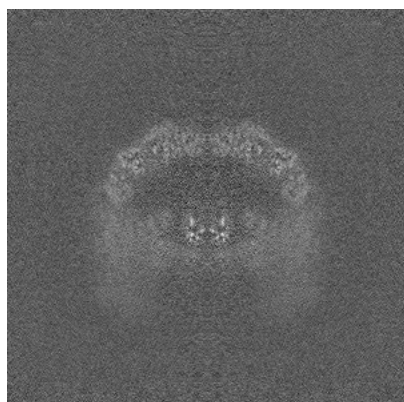


Y Index: 320

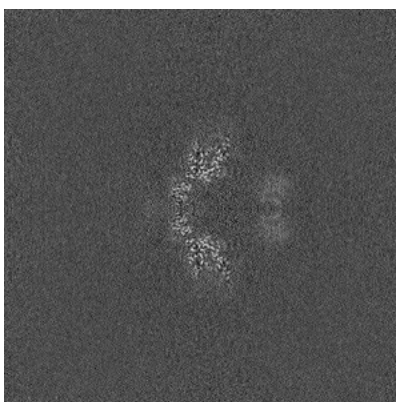


Z Index: 320

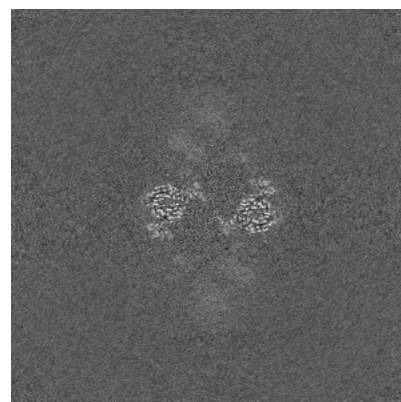
### 6.2.2 Raw map



X Index: 320



Y Index: 320

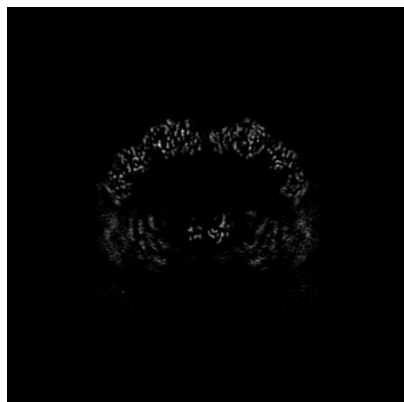


Z Index: 320

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: 318

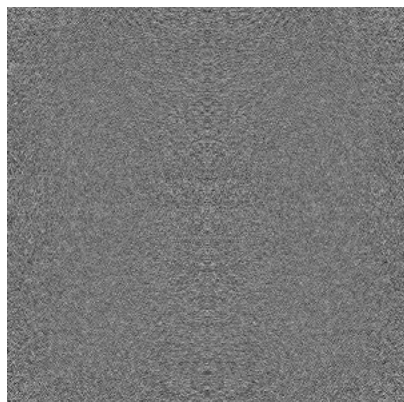


Y Index: 305

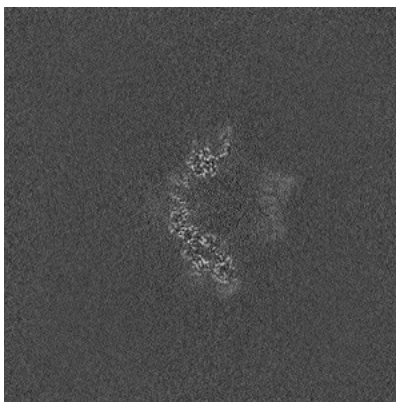


Z Index: 419

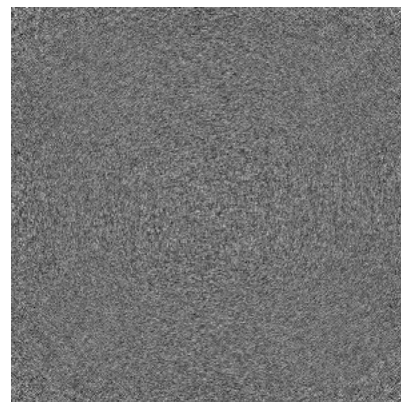
### 6.3.2 Raw map



X Index: 0



Y Index: 327

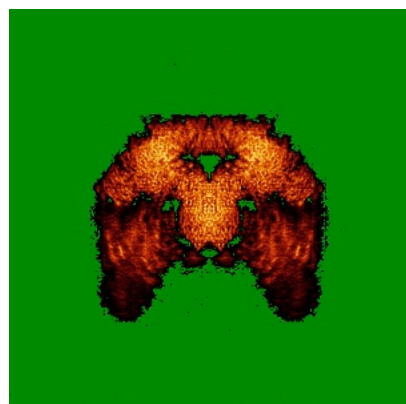


Z Index: 0

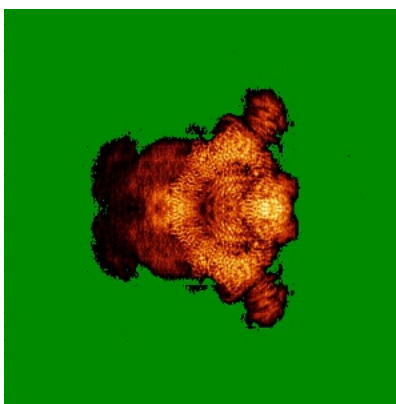
The images above show the largest variance slices of the map in three orthogonal directions.

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

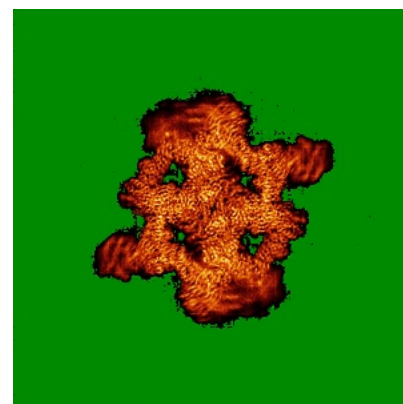
### 6.4.1 Primary map



X

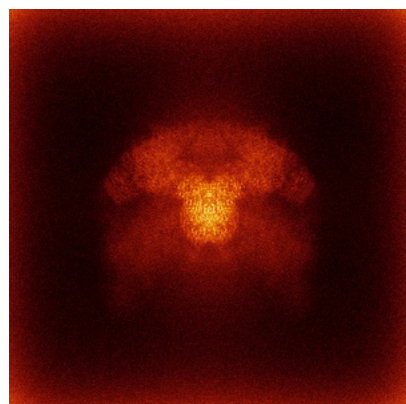


Y

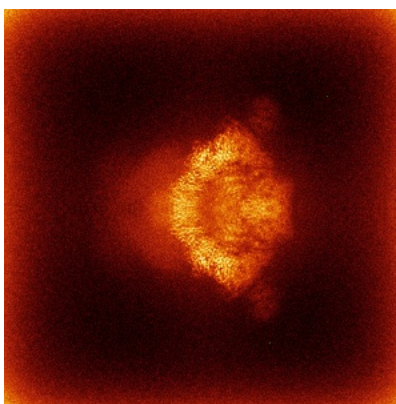


Z

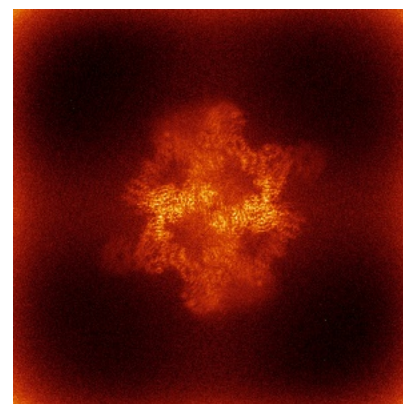
### 6.4.2 Raw map



X



Y

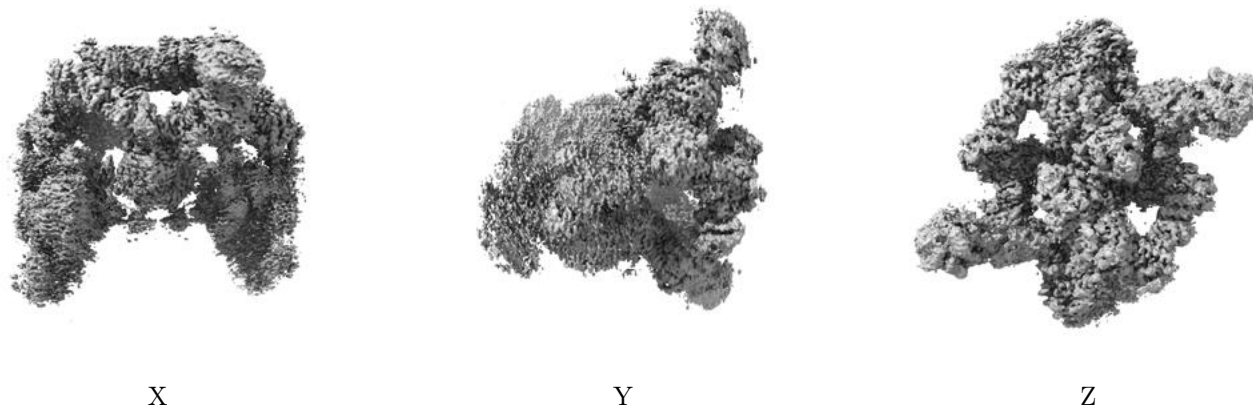


Z

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.

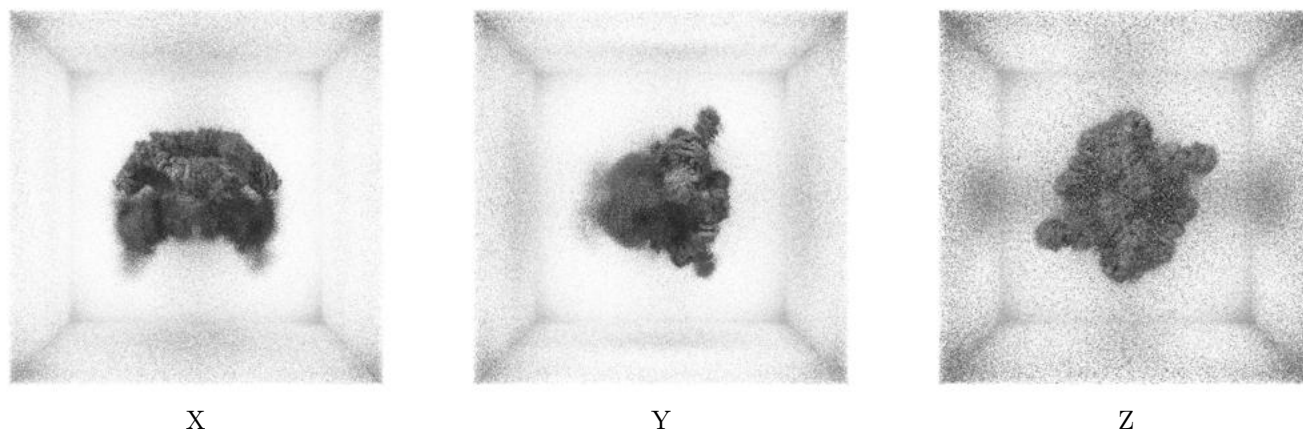
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. 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.

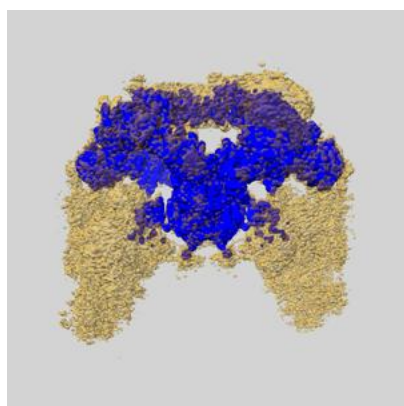
## 6.6 Mask visualisation [i](#)

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

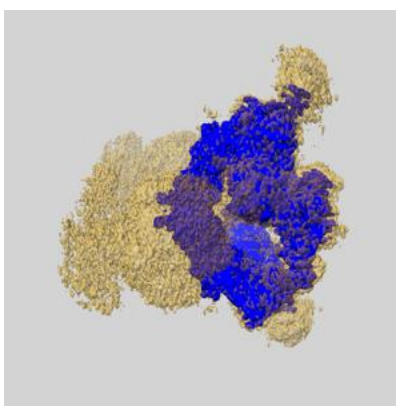
A mask typically either:

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

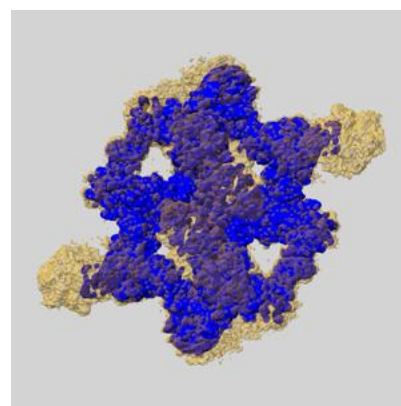
### 6.6.1 emd\_15364\_msk\_1.map [i](#)



X



Y

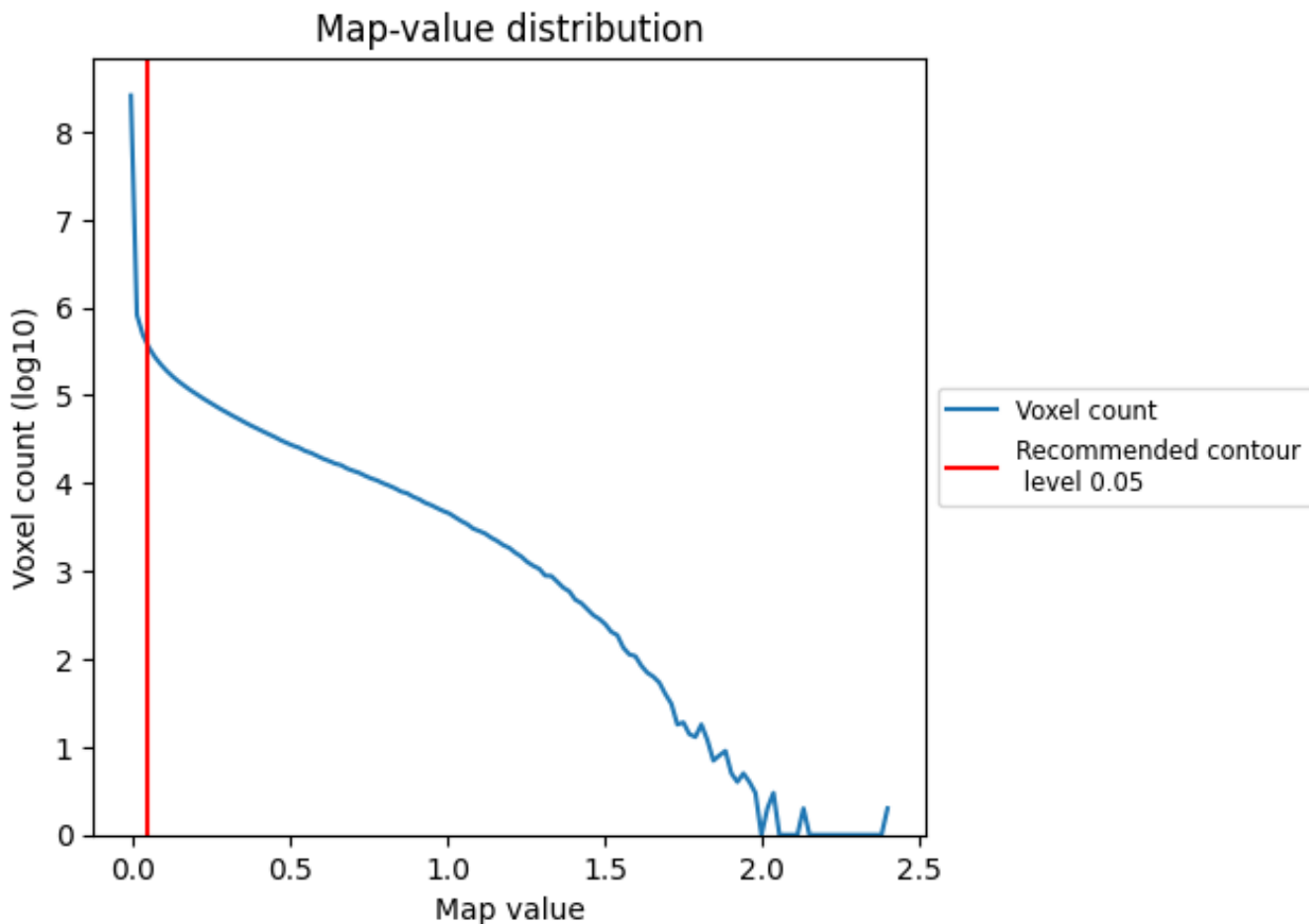


Z

## 7 Map analysis [i](#)

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

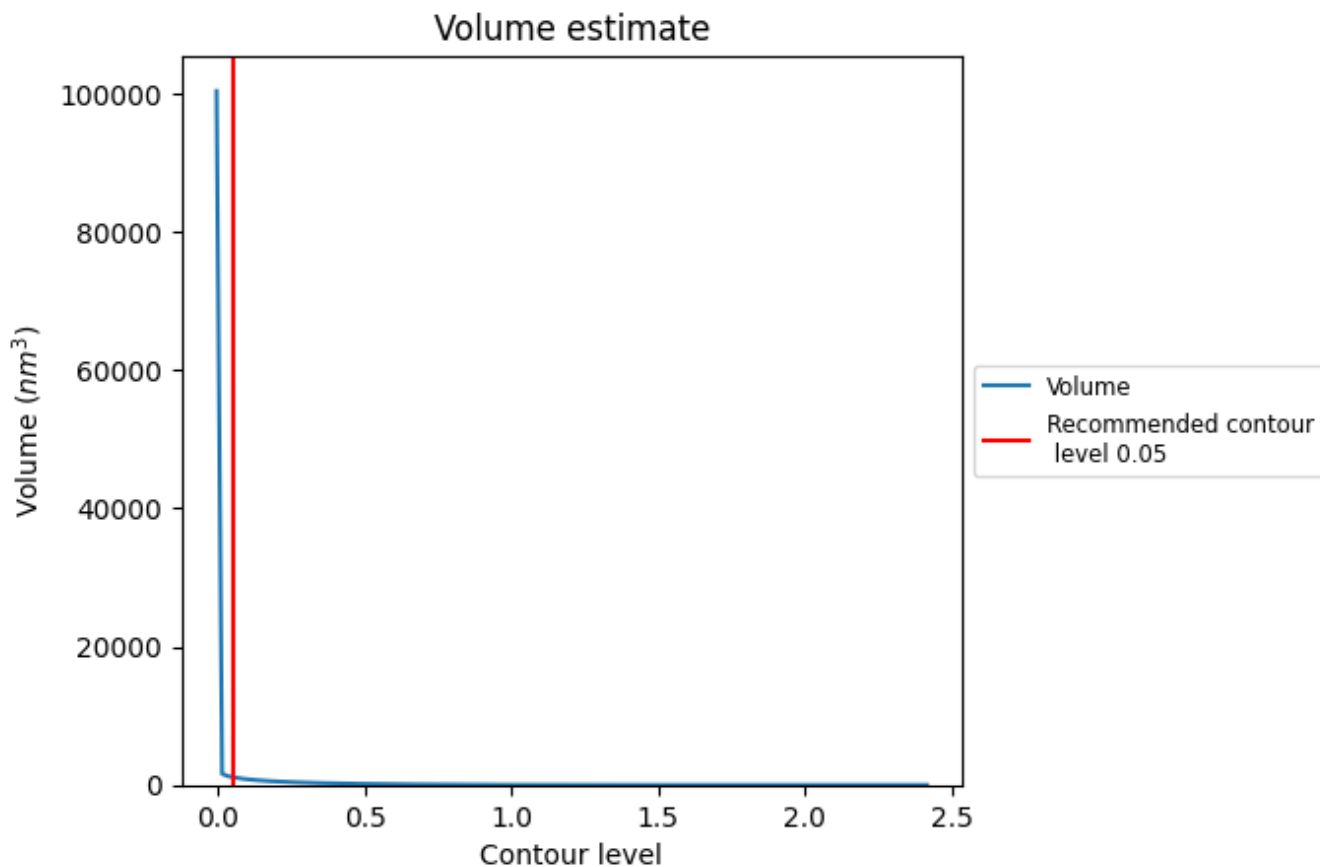
### 7.1 Map-value distribution [i](#)



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.



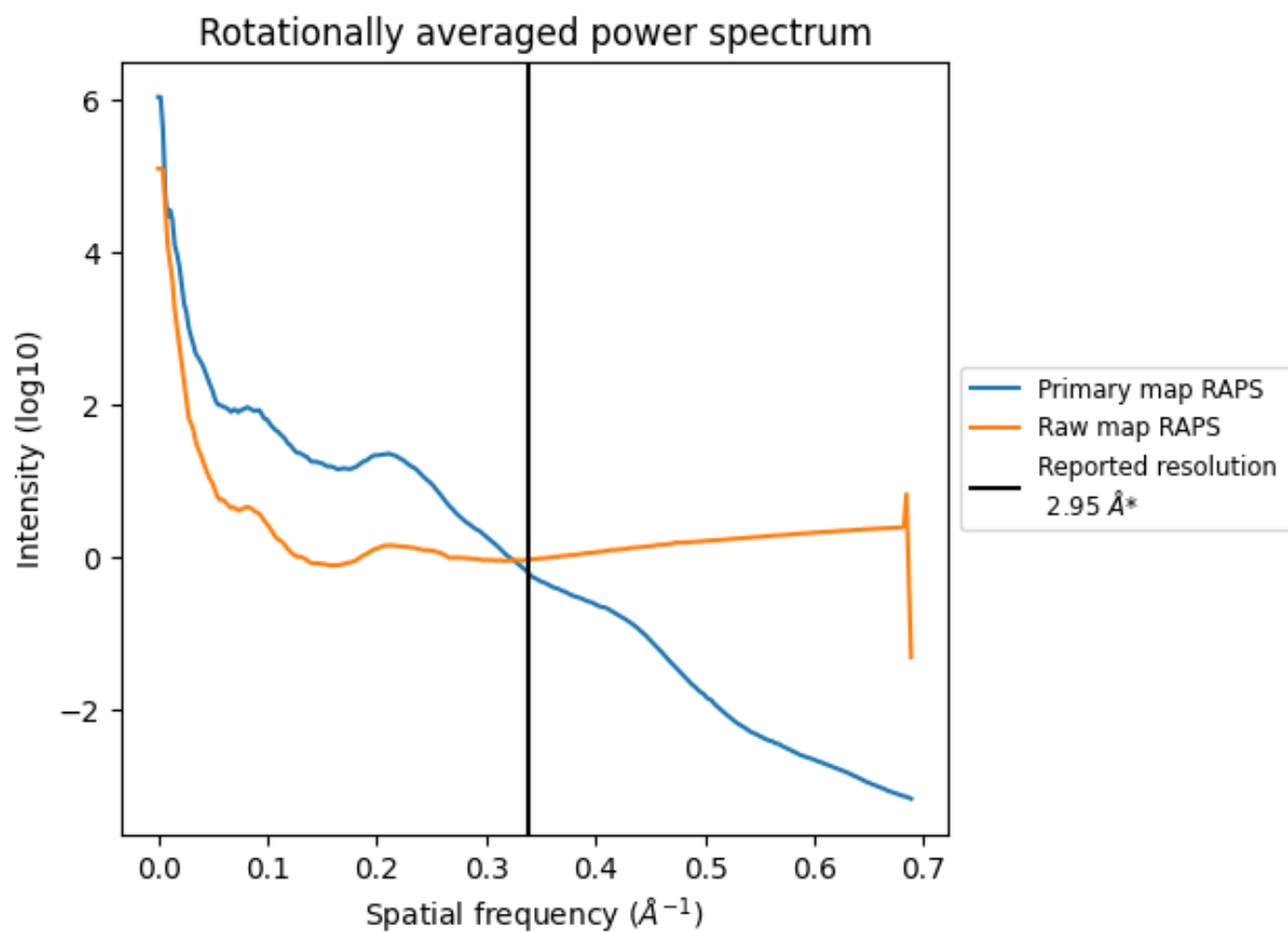
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1132 nm<sup>3</sup>; this corresponds to an approximate mass of 1023 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

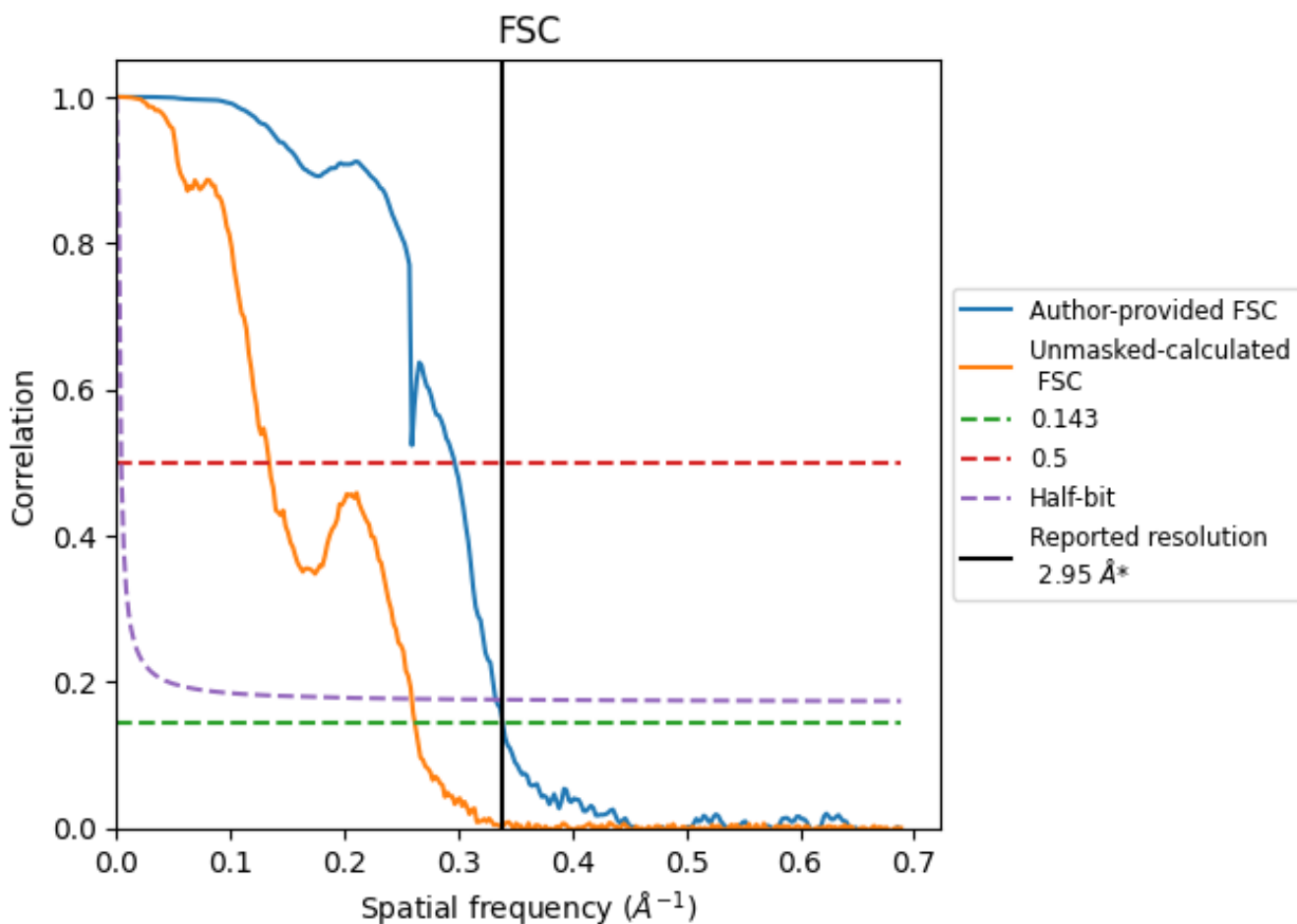


\*Reported resolution corresponds to spatial frequency of 0.339 Å<sup>-1</sup>

## 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 0.339 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

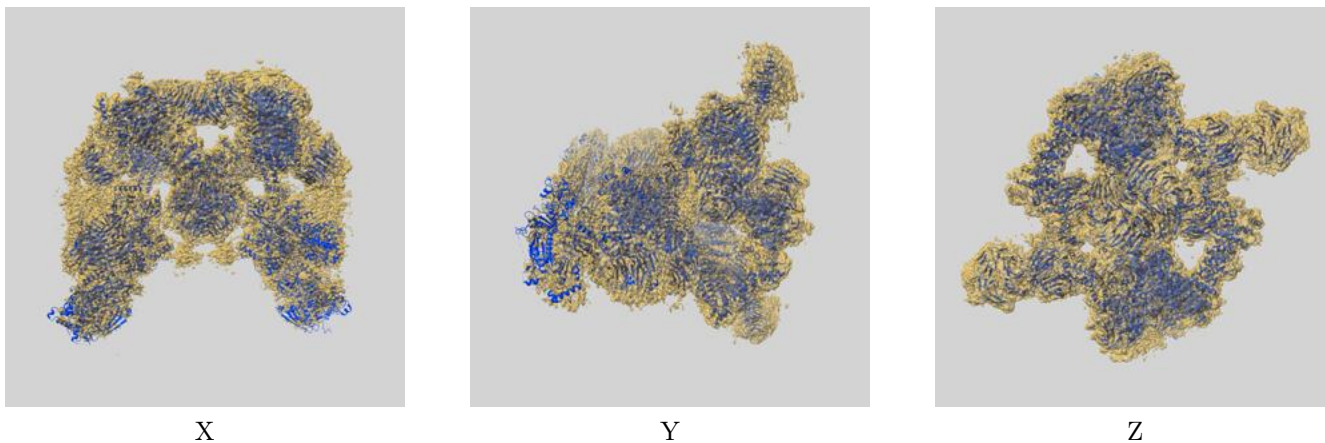
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.37	3.00
Unmasked-calculated*	3.82	7.46	3.86

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.82 differs from the reported value 2.95 by more than 10 %

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

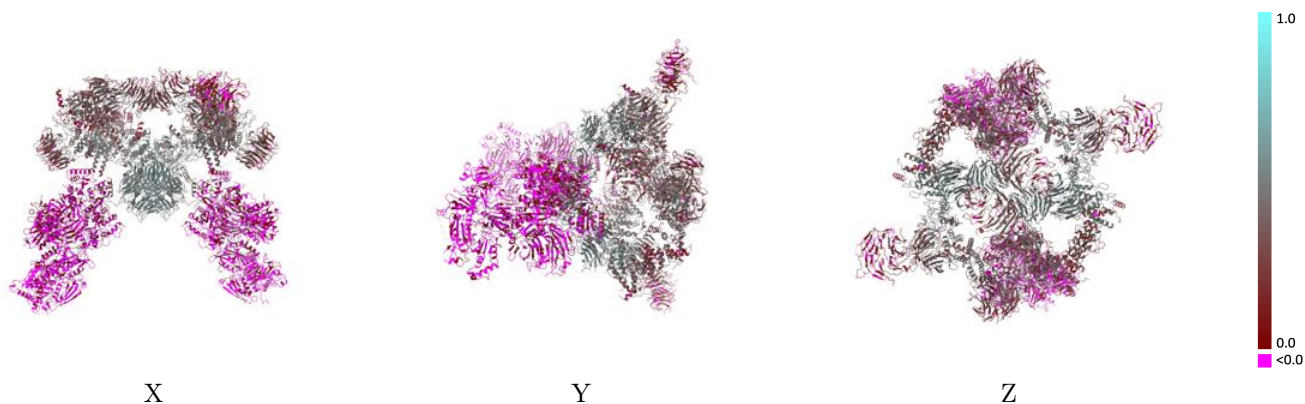
This section contains information regarding the fit between EMDB map EMD-15364 and PDB model 8ADL. Per-residue inclusion information can be found in section 3 on page 7.

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



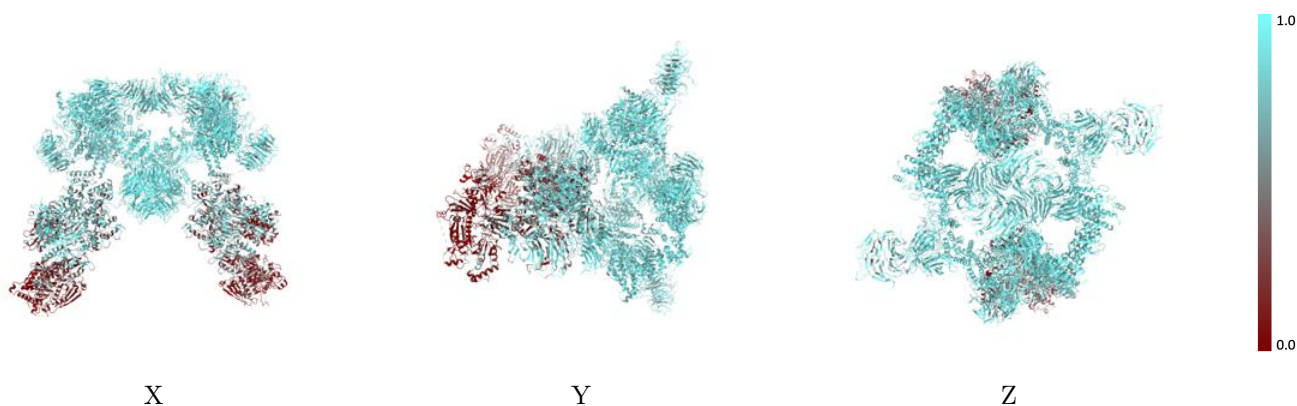
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



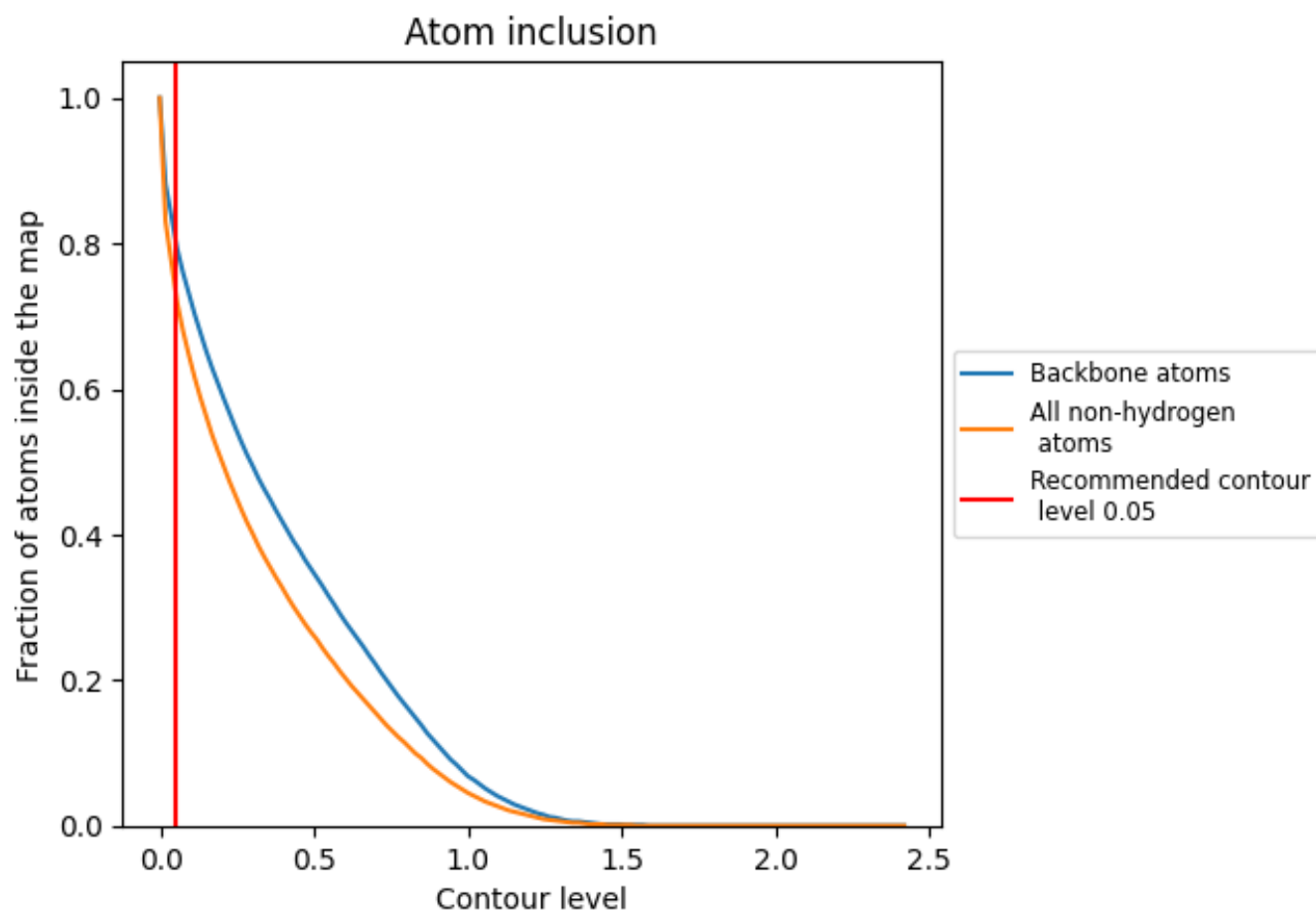
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.2180
A	 0.8510	 0.2770
B	 0.9130	 0.4550
C	 0.7580	 0.1340
D	 0.9390	 0.5170
E	 0.8970	 0.3660
F	 0.8850	 0.3740
G	 0.8790	 0.3240
H	 0.8480	 0.2860
I	 0.8560	 0.2760
J	 0.9120	 0.4540
L	 0.9430	 0.5140
M	 0.8970	 0.3670
N	 0.8780	 0.3680
O	 0.8770	 0.3210
P	 0.8510	 0.2860
Q	 0.7470	 0.1310
S	 0.5920	 0.0010
T	 0.5690	 -0.0120
U	 0.5980	 0.0380
V	 0.5940	 0.0300
W	 0.2760	 -0.0400
X	 0.2660	 -0.0380

