Full wwPDB EM Validation Report ⓘ

Jul 27, 2025 – 11:25 PM EDT

PDB ID	:	9NWE / pdb_00009nwe
EMDB ID	:	EMD-49876
Title	:	E3 ligase UBR4-KCMF1-calmodulin complex
Authors	:	Yang, Z.; Rape, M.P.
Deposited on	:	2025-03-22
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

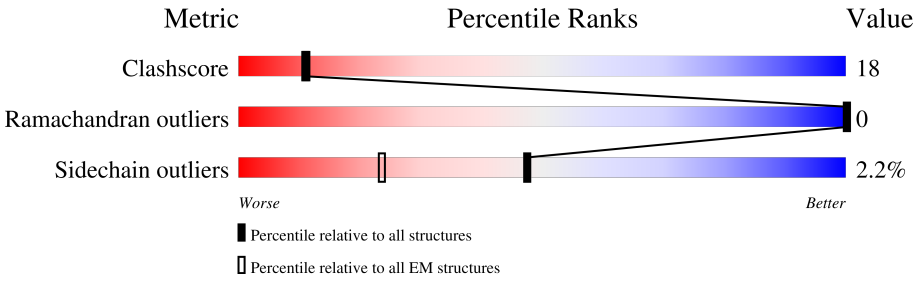
EMDB validation analysis	:	0.0.1.dev126
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	5205	8% 23% 8% 68%
1	B	5205	8% 23% 9% 68%
2	C	149	17% 45% 46% 6%
2	D	149	15% 31% 55% 10%
3	E	381	7% 6% 88%
3	F	381	7% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	A	5203	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29288 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 E3 ubiquitin-protein ligase UBR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1660	Total	C	N	O	S	0	0
			13132	8325	2255	2465	87		
1	B	1660	Total	C	N	O	S	0	0
			13134	8325	2255	2467	87		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q5T4S7
A	-20	ASP	-	expression tag	UNP Q5T4S7
A	-19	TYR	-	expression tag	UNP Q5T4S7
A	-18	LYS	-	expression tag	UNP Q5T4S7
A	-17	ASP	-	expression tag	UNP Q5T4S7
A	-16	HIS	-	expression tag	UNP Q5T4S7
A	-15	ASP	-	expression tag	UNP Q5T4S7
A	-14	GLY	-	expression tag	UNP Q5T4S7
A	-13	ASP	-	expression tag	UNP Q5T4S7
A	-12	TYR	-	expression tag	UNP Q5T4S7
A	-11	LYS	-	expression tag	UNP Q5T4S7
A	-10	ASP	-	expression tag	UNP Q5T4S7
A	-9	HIS	-	expression tag	UNP Q5T4S7
A	-8	ASP	-	expression tag	UNP Q5T4S7
A	-7	ILE	-	expression tag	UNP Q5T4S7
A	-6	ASP	-	expression tag	UNP Q5T4S7
A	-5	TYR	-	expression tag	UNP Q5T4S7
A	-4	LYS	-	expression tag	UNP Q5T4S7
A	-3	ASP	-	expression tag	UNP Q5T4S7
A	-2	ASP	-	expression tag	UNP Q5T4S7
A	-1	ASP	-	expression tag	UNP Q5T4S7
A	0	ASP	-	expression tag	UNP Q5T4S7
A	1	LYS	-	expression tag	UNP Q5T4S7
B	-21	MET	-	initiating methionine	UNP Q5T4S7
B	-20	ASP	-	expression tag	UNP Q5T4S7
B	-19	TYR	-	expression tag	UNP Q5T4S7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	LYS	-	expression tag	UNP Q5T4S7
B	-17	ASP	-	expression tag	UNP Q5T4S7
B	-16	HIS	-	expression tag	UNP Q5T4S7
B	-15	ASP	-	expression tag	UNP Q5T4S7
B	-14	GLY	-	expression tag	UNP Q5T4S7
B	-13	ASP	-	expression tag	UNP Q5T4S7
B	-12	TYR	-	expression tag	UNP Q5T4S7
B	-11	LYS	-	expression tag	UNP Q5T4S7
B	-10	ASP	-	expression tag	UNP Q5T4S7
B	-9	HIS	-	expression tag	UNP Q5T4S7
B	-8	ASP	-	expression tag	UNP Q5T4S7
B	-7	ILE	-	expression tag	UNP Q5T4S7
B	-6	ASP	-	expression tag	UNP Q5T4S7
B	-5	TYR	-	expression tag	UNP Q5T4S7
B	-4	LYS	-	expression tag	UNP Q5T4S7
B	-3	ASP	-	expression tag	UNP Q5T4S7
B	-2	ASP	-	expression tag	UNP Q5T4S7
B	-1	ASP	-	expression tag	UNP Q5T4S7
B	0	ASP	-	expression tag	UNP Q5T4S7
B	1	LYS	-	expression tag	UNP Q5T4S7

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	144	Total	C	N	O	S	0	0
			1134	696	182	247	9		
2	D	143	Total	C	N	O	S	0	0
			1127	692	181	245	9		

- Molecule 3 is a protein called E3 ubiquitin-protein ligase KCMF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	46	Total	C	N	O	S	0	0
			380	231	68	79	2		
3	F	45	Total	C	N	O	S	0	0
			371	226	67	76	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	3	Total	Zn	0
			3	3	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
4	B	3	Total Zn 3 3	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

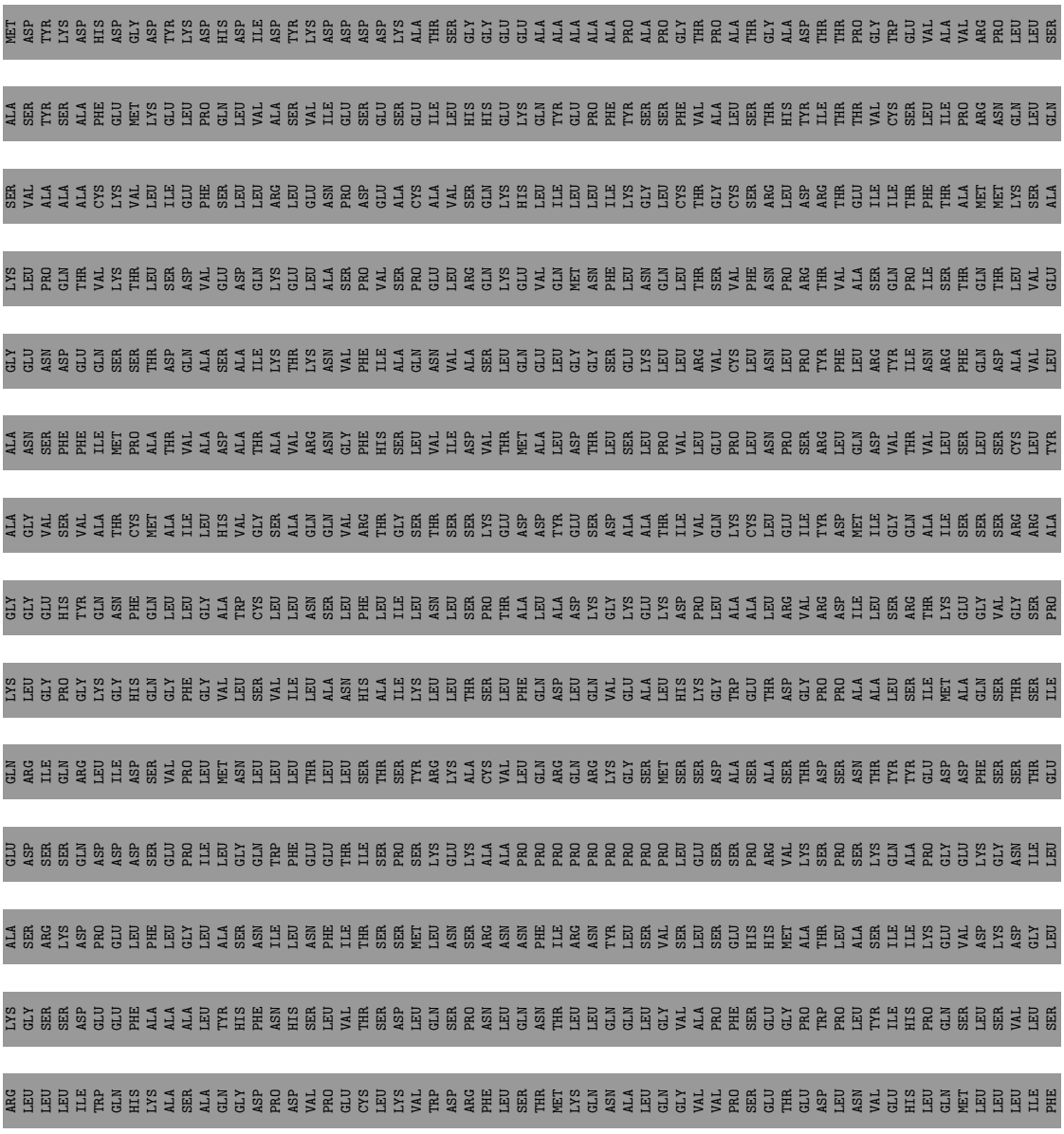
Mol	Chain	Residues	Atoms	AltConf
5	C	2	Total Ca 2 2	0
5	D	2	Total Ca 2 2	0

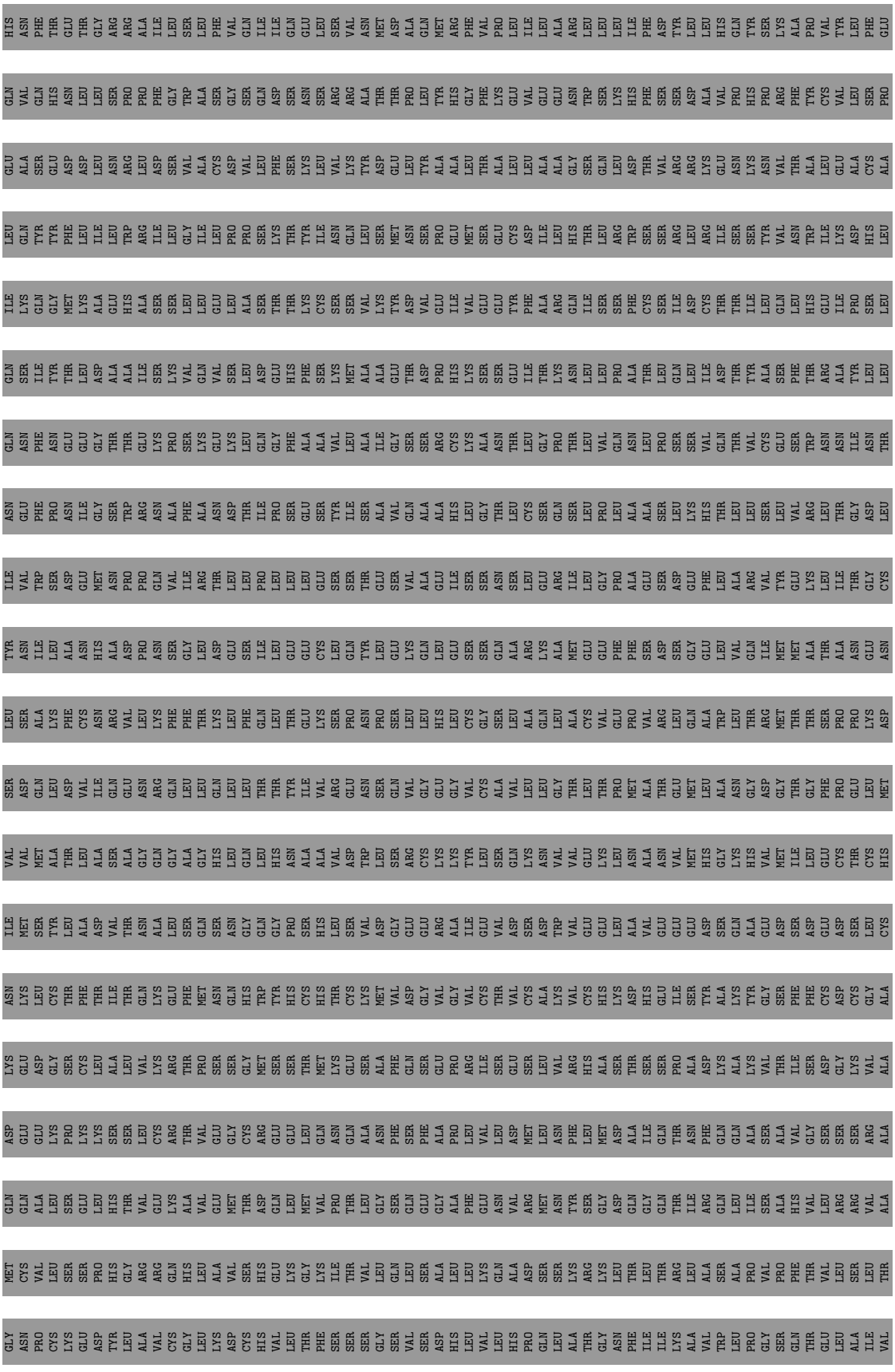
3 Residue-property plots (i)

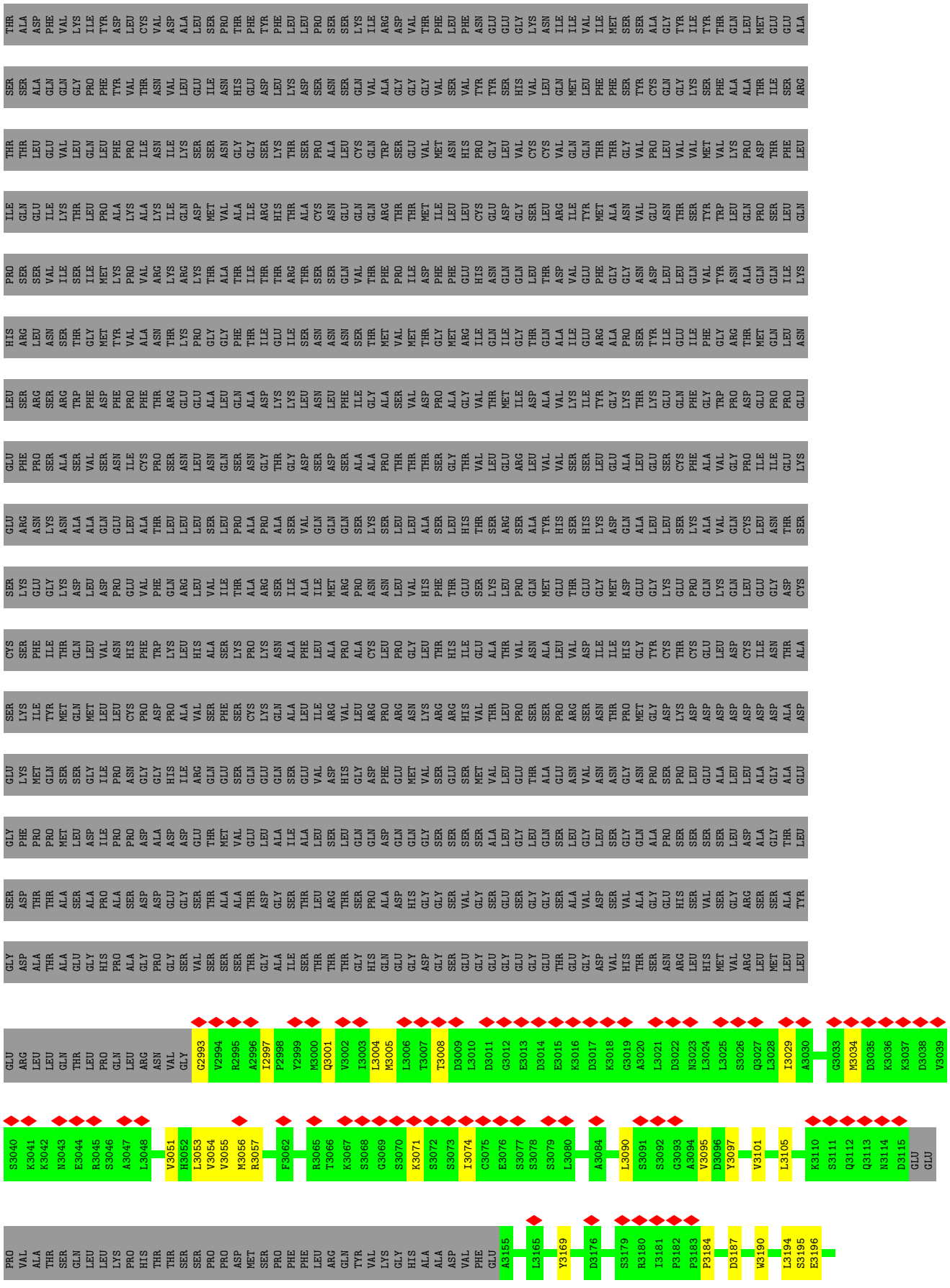
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

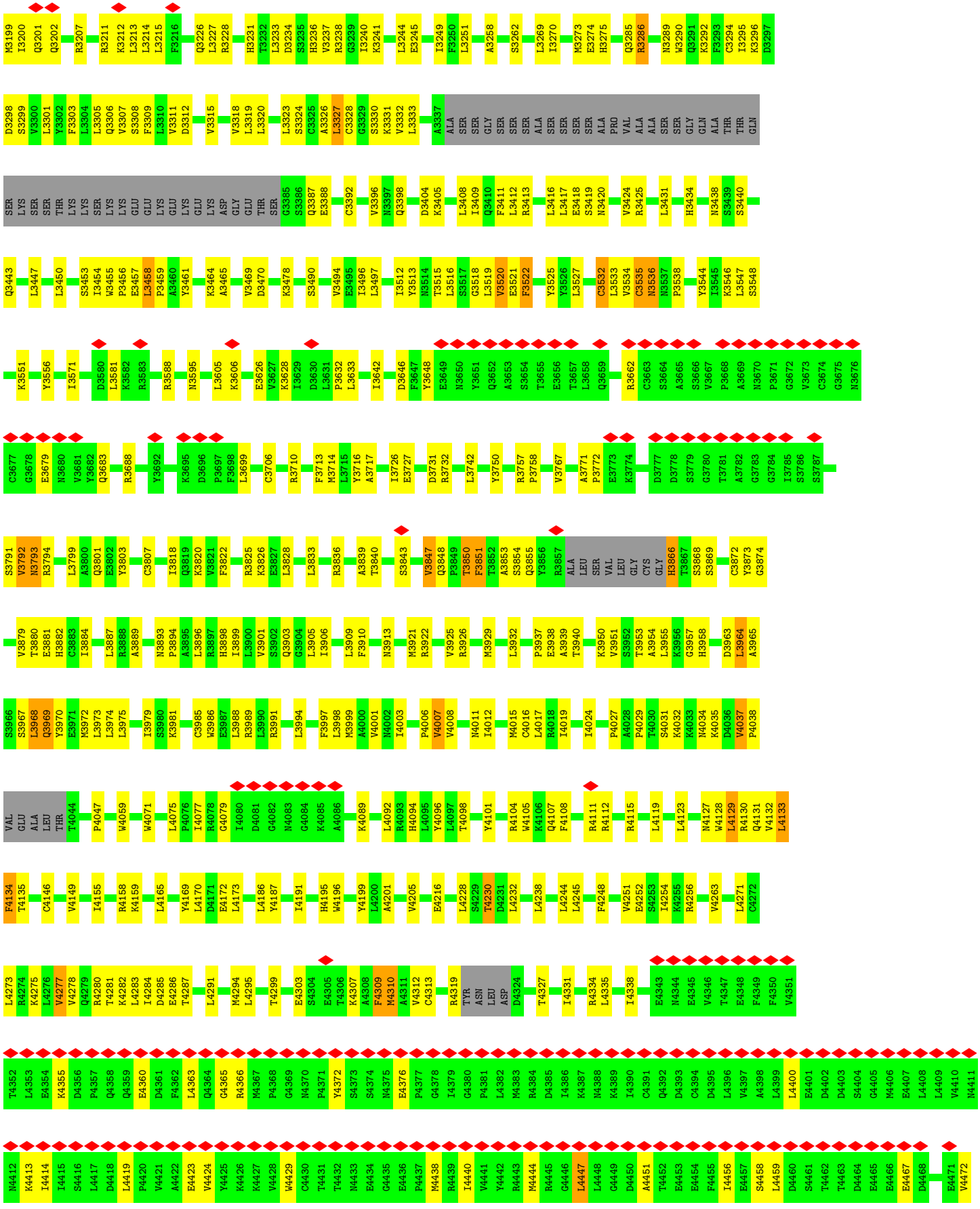
- Molecule 1: E3 ubiquitin-protein ligase UBR4

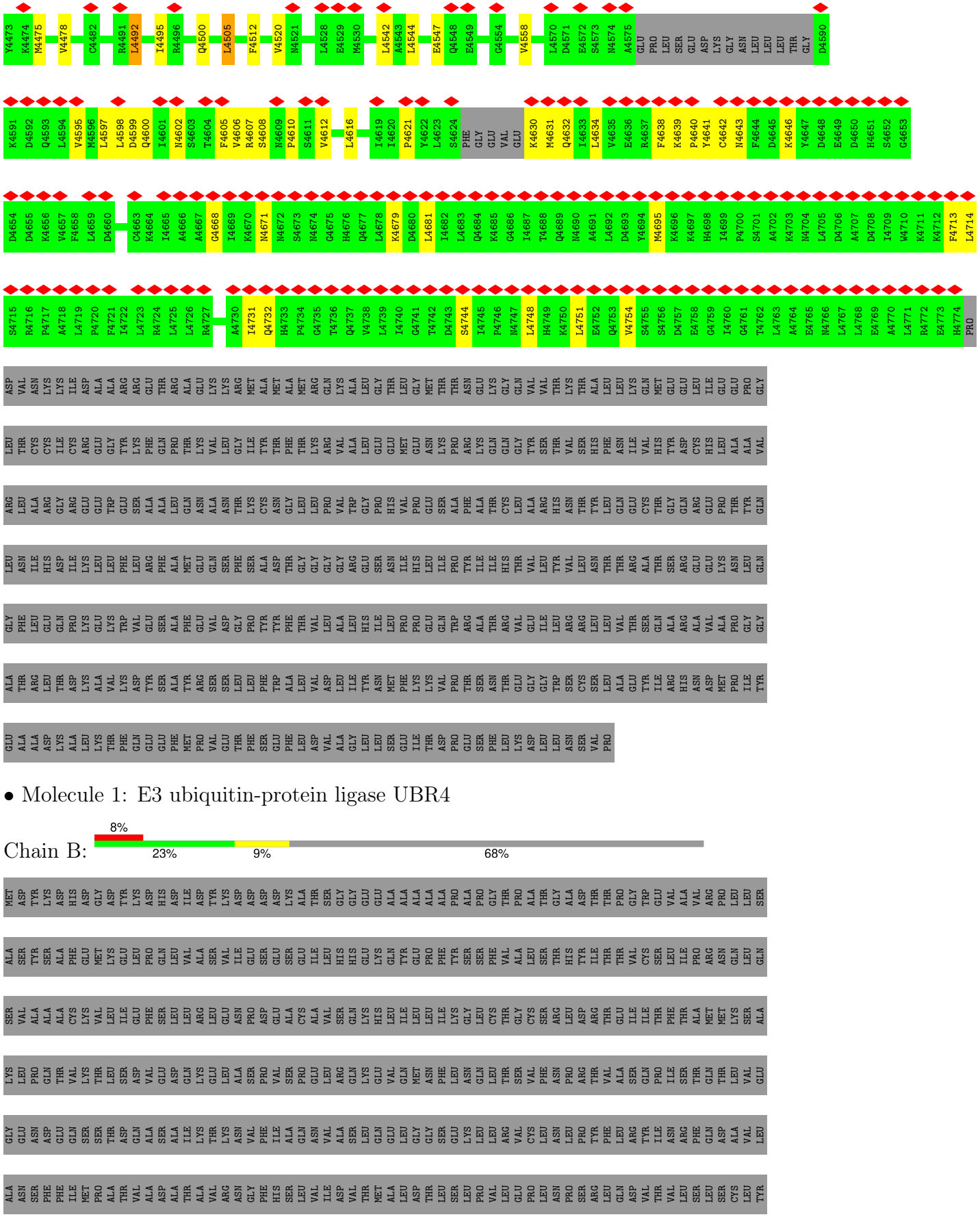
Chain A:




HIS ASN PHE THR GLU THR GLY ARG ARG ALA ILE LEU SER LEU PHE VAL GLN ILE ILE GLN GLU LEU SER VAL ASN MET ASP ALA GLN MET ARG PHE VAL PRO LEU ILE LEU ALA ARG LEU LEU LEU ILE PHE ASP TYR LEU LEU HIS GLN TYR SER LYS ALA PRO VAL TYR LEU PHE GLU
GLN VAL GLN HIS ASN LEU LEU SER PRO PRO PHE GLY TRP ALA SER GLY SER GLN ASP SER ASN SER ARG ARG ALA THR THR PRO LEU TYR HIS GLY PHE LYS GLU VAL GLU GLU ASN TRP SER LYS HIS PHE SER SER ASP ALA VAL PRO HIS PRO ARG PHE TYR CYS VAL LEU SER PRO
GLU ALA SER GLU ASP ASP LEU ASN ARG LEU ASP SER VAL ALA CYS ASP VAL LEU PHE SER LYS LEU VAL LYS TYR ASP GLU LEU TYR ALA ALA LEU THR PRO LEU TYR ALA CYS ALA ASP LEU ASN ARG ALA THR THR PRO LEU TYR HIS GLY PHE LYS GLU VAL GLU GLU ASN TRP SER LYS HIS PHE SER SER ARG LEU ARG ARG LYS GLU ASN LYS ASN VAL THR ALA LEU GLU VAL PRO ARG PHE TYR CYS VAL LEU SER PRO
LEU GLN TYR TYR PHE LEU ILE LEU TRP ARG ILE LEU LEU GLY ILE LEU PRO PRO SER LYS THR TYR ILE ASN GLN LEU SER MET ASN SER PRO GLU MET SER GLU CYS ASP ILE LEU ARG TRP SER SER ARG LEU ARG ILE SER SER TYR VAL ASN TRP ILE LYS ASP HIS LEU
ILE LYS GLN GLY MET LYS ALA GLU HIS ALA ILE SER SER LEU LEU GLU LEU ALA SER THR THR LYS CYS SER VAL LYS TYR ASP VAL GLU ILE VAL GLU GLU TYR PHE ALA ARG GLN ILE SER LEU LEU PRO ALA THR LEU ASP CYS THR ILE LEU GLN LEU ASP THR THR ILE LEU GLN LEU HIS GLU ILE PRO SER LEU
GLN SER ILE TYR THR LEU ASP ALA ALA ILE ASP PRO HIS LYS LYS SER SER GLU ILE THR LYS ASN LEU LEU PRO ALA THR LEU GLN LEU ILE ASP THR TYR ALA SER PHE THR ARG ALA TYR LEU LEU
GLN ASN PHE ASN GLU GLU GLY THR THR GLU LYS GLU LYS LEU ALA ILE GLY SER SER ARG CYS SER VAL ASN GLN VAL LEU PRO SER SER VAL GLN THR THR VAL CYS GLU SER TRP ASN ASN LEU PRO SER LEU LYS HIS THR LEU GLN THR VAL CYS SER ILE ASP CYS THR LEU ASP THR LEU ILE LEU ARG LEU THR GLY ASP LEU
ASN GLU PHE PRO ASN ILE GLY TRP ARG ASN ALA PHE ALA ASP THR ILE PRO SER GLU SER TYR ILE SER ALA VAL GLN ALA ALA HIS LEU LEU GLY THR LEU CYS SER GLN SER LEU SER LEU LYS HIS THR LEU LEU LEU ARG LEU THR GLY ASP LEU
ILE VAL TRP SER ASP GLU MET ASN PRO PRO GLN VAL ILE ARG THR LEU LEU LEU GLU SER SER THR GLU SER VAL ALA GLU ILE SER SER ASN SER LEU CYS SER GLN SER LEU PRO LEU ALA ALA SER LEU LYS HIS THR LEU LEU SER LEU VAL ARG LEU THR GLY CYS
TYR ASN ILE LEU ALA ASN HIS ALA ASP PRO ASN SER GLY LEU GLN LEU GLU SER SER GLN ALA ARG LYS ALA MET GLU GLU PHE PHE SER ASP SER GLY GLU LEU VAL GLN ILE MET MET ALA THR ALA ASN GLU ASN
LEU SER ALA LYS PHE CYS ASN ARG VAL LEU LYS PHE PHE THR LYS LEU PHE GLN LEU THR GLU LYS SER PRO ASN PRO SER LEU LEU HIS LEU CYS GLY SER LEU ALA GLN LEU LEU ALA CYS VAL GLU PRO VAL ARG LEU GLN ALA TRP LEU LEU THR ARG MET THR THR SER PRO PRO LYS ASP
SER ASP GLN LEU ASP VAL ILE GLN GLU ASN ARG GLN LEU LEU LEU GLN LEU LEU THR THR TYR ILE VAL ARG GLU ASN SER GLN VAL CYS GLY GLU GLY VAL CYS ALA VAL LEU LEU GLY THR LEU THR PRO MET ALA THR ARG GLU LEU GLU LEU
VAL VAL MET ALA THR LEU SER TYR LEU SER ARG CYS LYS LYS TYR LEU SER ASP TRP LEU SER VAL ASP GLY GLU GLU ARG ALA ALA ASP TRP ALA ASP VAL THR GLU LYS LEU ASN ALA ASN VAL MET HIS GLY LYS HIS VAL MET ILE LEU GLU GLU CYS THR CYS HIS
ILE MET SER TYR LEU ALA ASP VAL THR ASN ALA LEU SER GLN GLN GLY GLN GLY PRO SER HIS LEU SER VAL ASP GLY GLU GLU ARG ALA ILE GLU VAL ASP SER ASP TRP VAL GLU GLU LEU ALA VAL GLU GLU GLU ASP SER GLN GLY ALA ASP GLU ASP SER ASP
ASN LYS LEU CYS THR PHE THR ILE THR GLN LYS GLU PHE MET ASN GLN HIS TRP TYR HIS CYS HIS THR CYS LYS MET VAL ASP GLY VAL GLY VAL CYS THR VAL CYS HIS LYS ASP HIS GLU ILE SER PHE PHE CYS ASP CYS GLY ALA
LYS GLU ASP GLY SER CYS LEU VAL LYS ARG THR PRO SER SER GLY MET SER SER THR MET LYS GLU SER ALA PHE GLN SER GLU PRO ARG ILE SER GLU SER LEU VAL ARG HIS ALA SER THR SER SER PRO ALA ASP LYS ALA LYS VAL THR ILE SER ASP LYS VAL ALA
ASP GLU GLU LYS PRO LYS LYS SER LEU CYS ARG GLU GLU LEU GLN ASN GLN ALA ASN PHE SER PHE ALA PRO LEU VAL LEU ASP MET LEU ASN PHE LEU MET ASP ALA ILE GLN THR ASN PHE GLN GLN LEU ALA SER ALA ALA VAL GLY SER SER ARG ALA
GLN GLN ALA LEU SER GLU HIS THR VAL GLU LYS ALA PHE GLU ASN VAL ARG MET ASN TYR SER GLY ASP GLN GLY GLN THR ILE ARG GLN LEU ILE SER ALA HIS VAL LEU ARG ARG VAL ALA
MET CYS VAL LEU SER SER HIS GLY HIS LEU LEU LYS GLN ALA ASP SER SER LYS ARG LYS LEU THR LEU LEU ARG LEU ALA ALA SER LEU THR
GLY ASN PRO CYS LYS GLU ASP TYR LEU ALA VAL SER SER GLY SER VAL ASP HIS LEU VAL LEU HIS PRO GLN LEU ALA THR GLY ASN PHE ILE ILE LYS ALA VAL TRP LEU PRO GLY SER GLN THR GLU LEU ALA ILE VAL

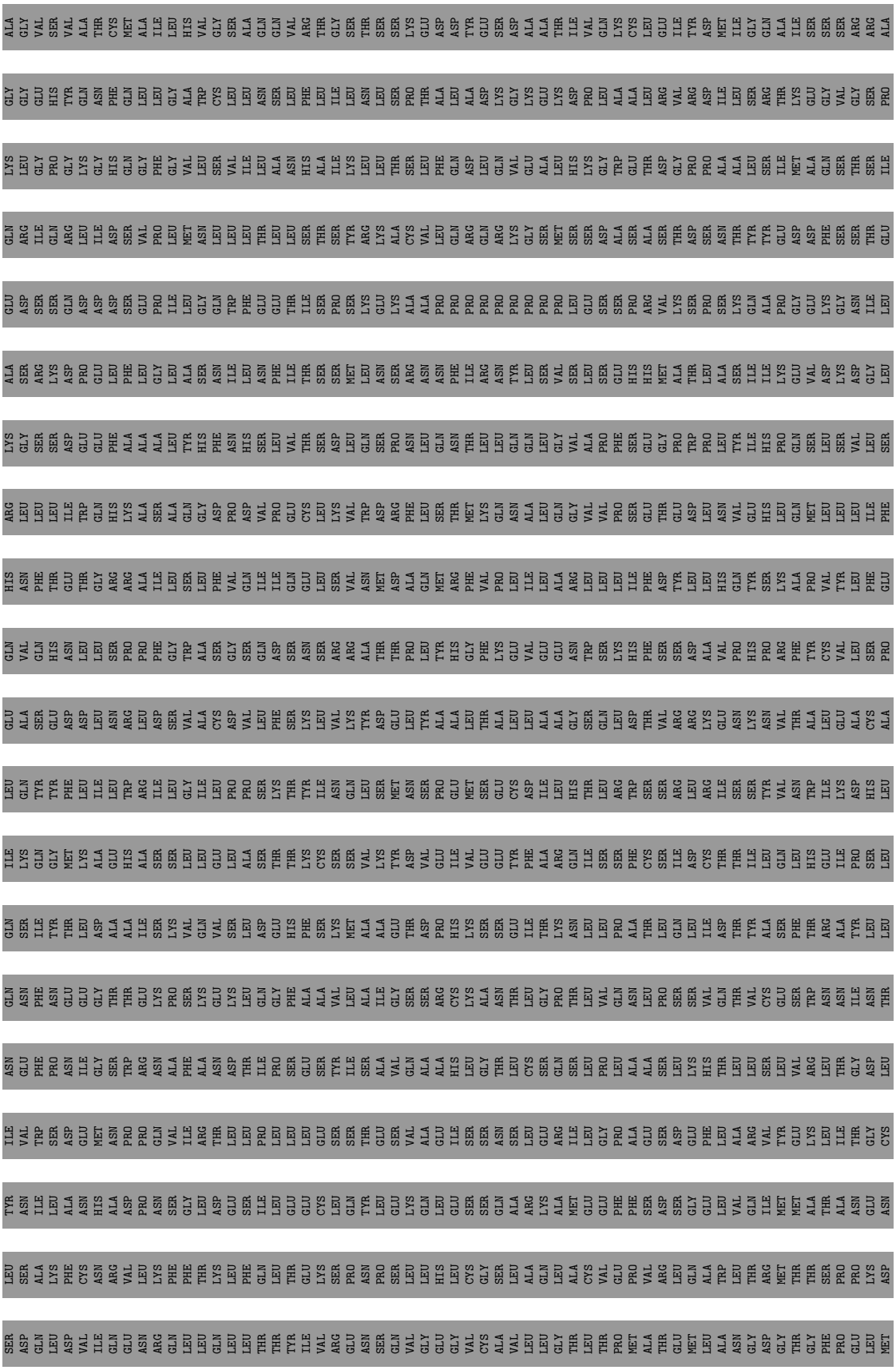

THR ALA ASP PHE VAL LYS ILE TYR ASP LEU CYS VAL ASP ALA LEU SER PRO THR PHE TYR PHE LEU LEU PRO SER SER LYS ILE ARG ASP VAL THR PHE LEU PHE ASN GLU GLU GLY LYS ASN ILE ILE VAL ILE MET SER SER ALA GLY TYR ILE TYR THR GLN LEU GLU ASN GLY GLY GLY LYS SER PHE ALA ALA THR ILE SER ARG
SER SER ALA GLN GLN GLY PRO PHE TYR VAL THR ASN VAL LEU GLU ILE ASN ASP LEU LYS ASP SER ASN HIS GLU ASP LEU LYS THR SER PRO ASN SER GLN VAL ALA GLY GLY GLY VAL SER VAL TYR TYR SER HIS VAL LEU GLN MET LEU PHE PHE SER TYR CYS GLN GLY LYS SER PHE ALA ALA THR ILE SER
THR THR LEU GLU VAL LEU GLN LEU PHE PRO ILE ASN ILE LYS SER SER ASN GLY GLY SER LYS THR SER PRO ALA LEU CYS GLN TRP SER GLU VAL MET ASN HIS PRO GLY LEU VAL CYS CYS VAL GLN GLN THR THR GLY VAL PRO LEU VAL VAL MET VAL LYS PRO ASP THR PHE LEU
ILE GLN GLU ILE LYS THR LEU PRO ALA LYS ALA LYS ILE GLN ASP MET VAL ALA ILE ARG HIS THR ALA CYS ASN GLU GLN GLN GLN ARG THR THR MET ILE LEU LEU CYS GLU ASP GLY SER LEU ARG ILE TYR MET ALA ASN VAL GLU ASN THR SER TYR TRP LEU GLN LEU SER ALA GLN
PRO SER SER VAL ILE SER ILE MET LYS PRO VAL ARG LYS ARG LYS THR ALA ALA THR ILE THR THR ARG THR SER SER GLN VAL THR PHE PRO ILE ASP PHE PHE GLU HIS ASN GLN GLN LEU THR ASP VAL GLU PHE GLY GLY ASN ASP LEU LEU GLN VAL TYR ASN ALA GLN PHE ILE LYS
HIS ARG LEU ASN SER THR GLY MET TYR VAL ALA ASN THR LYS PRO GLY GLY PHE THR ILE GLU ILE ILE GLU ILE SER SER ASN ASN SER THR MET VAL MET THR GLY MET ARG ILE GLN ILE GLY THR GLN ALA ILE GLU ARG ALA PRO SER TYR ILE GLU LEU GLN ILE PHE PHE GLY ARG THR MET GLN LEU LEU ASN
LEU SER ARG SER ARG TRP PHE ASP PHE PRO PHE THR ARG GLU GLU ALA LEU GLN ALA ASP LYS LYS LEU ASN LEU PHE ILE GLY ALA ALA SER VAL ASP PRO THR THR THR SER GLY THR VAL THR MET ILE ASP ALA ALA VAL LYS ILE TYR GLY LYS THR LYS GLU GLN PHE GLY TRP PRO ASP GLU PRO PRO GLU
GLU PHE PRO SER ALA SER VAL SER ASN ILE CYS PRO SER ASN GLN SER ASN GLY THR GLY ASP SER ASP SER ALA ALA PRO THR THR THR SER GLY THR VAL LEU GLU SER ASP ALA ALA LEU GLU SER CYS PHE ALA VAL GLY PRO ILE ILE GLU GLU LYS
GLU ARG ASN LYS ASN ALA ALA GLN GLU LEU ALA THR LEU LEU LEU SER LEU LEU PRO ALA ALA SER VAL GLN GLN GLN SER LYS SER LEU LEU LEU ALA SER LEU HIS THR SER ARG SER ALA TYR HIS SER HIS LYS ASP GLN ALA LEU LEU SER LYS ALA VAL GLN CYS LEU ASN THR SER
SER LYS GLU GLY LYS ASP LEU ASP PRO GLU VAL PHE GLN ARG ARG LEU VAL ILE THR ALA ARG SER ILE ALA ILE MET ARG PRO ASN ASN LEU VAL HIS PHE THR GLU SER LYS LEU PRO GLN MET GLU THR GLU GLY MET ASP GLU GLY LYS GLU PRO GLN LYS GLN LEU GLU GLY ASP CYS
CYS SER PHE ILE THR GLN LEU VAL ASN HIS PHE TRP LYS LEU HIS ALA SER LYS PRO LYS ASN ALA PHE LEU ALA PRO ALA CYS LEU PRO GLY LEU THR HIS ILE GLU SER ALA THR VAL ASN ALA LEU VAL ASP ILE ILE HIS GLY TYR CYS THR CYS GLU LEU ASP CYS ILE ASN THR ALA
SER LYS ILE TYR MET GLN MET LEU LEU CYS PRO ASP PRO ALA ILE SER PHE SER CYS LYS GLN LEU ALA SER ILE LEU ARG VAL LEU ARG PRO ARG ASN LYS ARG ARG HIS VAL THR LEU LEU PRO SER SER PRO ARG SER ASN THR PRO MET GLY ASP LYS ASP ASP ASP ASP ASP ASP ASP ASP
GLU LYS MET GLN SER SER GLY ILE PRO ASN GLY GLY HIS ILE ARG GLN GLU SER GLN GLU GLN SER GLU VAL ASP HIS GLY ASP PHE GLU MET VAL SER GLU SER SER MET VAL LEU GLU THR ALA GLU ASN VAL ASN ASN GLY ASN PRO SER PRO LEU GLU GLU ALA LEU LEU LEU ALA ALA GLY ALA ASP
GLY PHE PRO PRO MET LEU ASP ILE PRO PRO ASP ALA ASP GLU THR MET VAL GLU LEU ALA ILE ALA LEU SER LEU GLN GLN GLN GLY SER SER SER ALA LEU GLY LEU GLN SER LEU GLY LEU SER SER GLY GLN ALA PRO SER SER SER SER LEU ASP ASP THR LEU
SER ASP THR THR ALA SER ASP ASP GLU GLY SER THR LEU ARG THR SER PRO ALA ASP HIS GLY GLY SER GLU GLY SER GLU SER GLY GLY SER ALA VAL ASP SER VAL ALA GLY GLU HIS SER VAL SER GLY ASP ALA ALA ALA ASP ASP ALA ASP ALA TYR
GLY ASP ALA THR ALA GLU GLY SER VAL SER SER THR GLY HIS GLN GLU GLY ASP GLY SER GLU GLY GLU GLY GLU GLY GLU THR GLU GLY ASP VAL HIS THR SER ARG LEU HIS MET VAL ARG LEU MET LEU LEU
GLU ARG LEU LEU GLN THR GLN LEU ARG ASN VAL G2993 V2994 R2995 A2996 I2997 P2998 Y2999 M3000 Q3001 V3002 I3003 L3004 M3005 L3006 T3007 T3008 D3009 L3010 D3011 G3012 E3013 D3014 E3015 K3016 D3017 K3018 G3019 A3020 L3021 D3022 N3023 L3024 L3025 S3026 Q3027 L3028 I3029 A3030 G3033 M3034 D3035 K3036 K3037 D3038 V3039
S3040 K3041 K3042 N3043 E3044 R3045 S3046 A3047 L3048 V3051 H3052 L3053 V3054 V3055 M3056 R3057 F3062 R3065 T3066 K3067 S3068 G3069 S3070 K3071 S3072 S3073 I3074 C3075 E3076 S3077 S3078 S3079 L3080 A3084 L3090 S3091 S3092 G3093 A3094 V3095 D3096 Y3097 V3101 L3105 K3110 S3111 Q3112 Q3113 N3114 D3115 GLU GLU
PRO VAL ALA THR SER GLN LEU LEU LYS PRO HIS THR THR SER PRO PRO ASP MET SER PRO PHE PHE LEU ARG GLN TYR VAL LYS GLY HIS ALA ALA ASP VAL PHE GLU A3155 L3165 Y3169 D3176 S3179 R3180 I3181 P3182 P3183 P3184 D3187 W3190 L3194 S3195 E3196

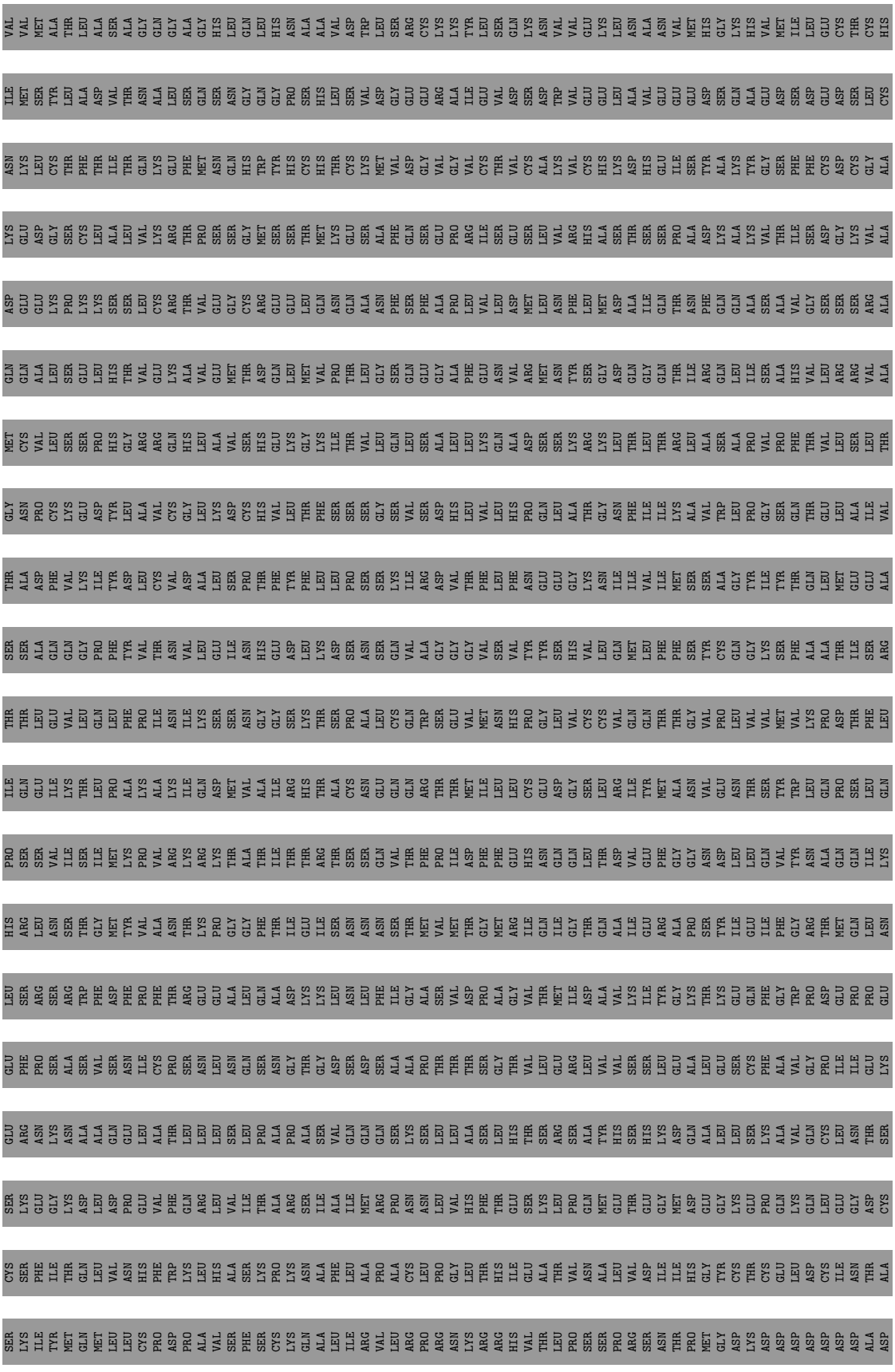


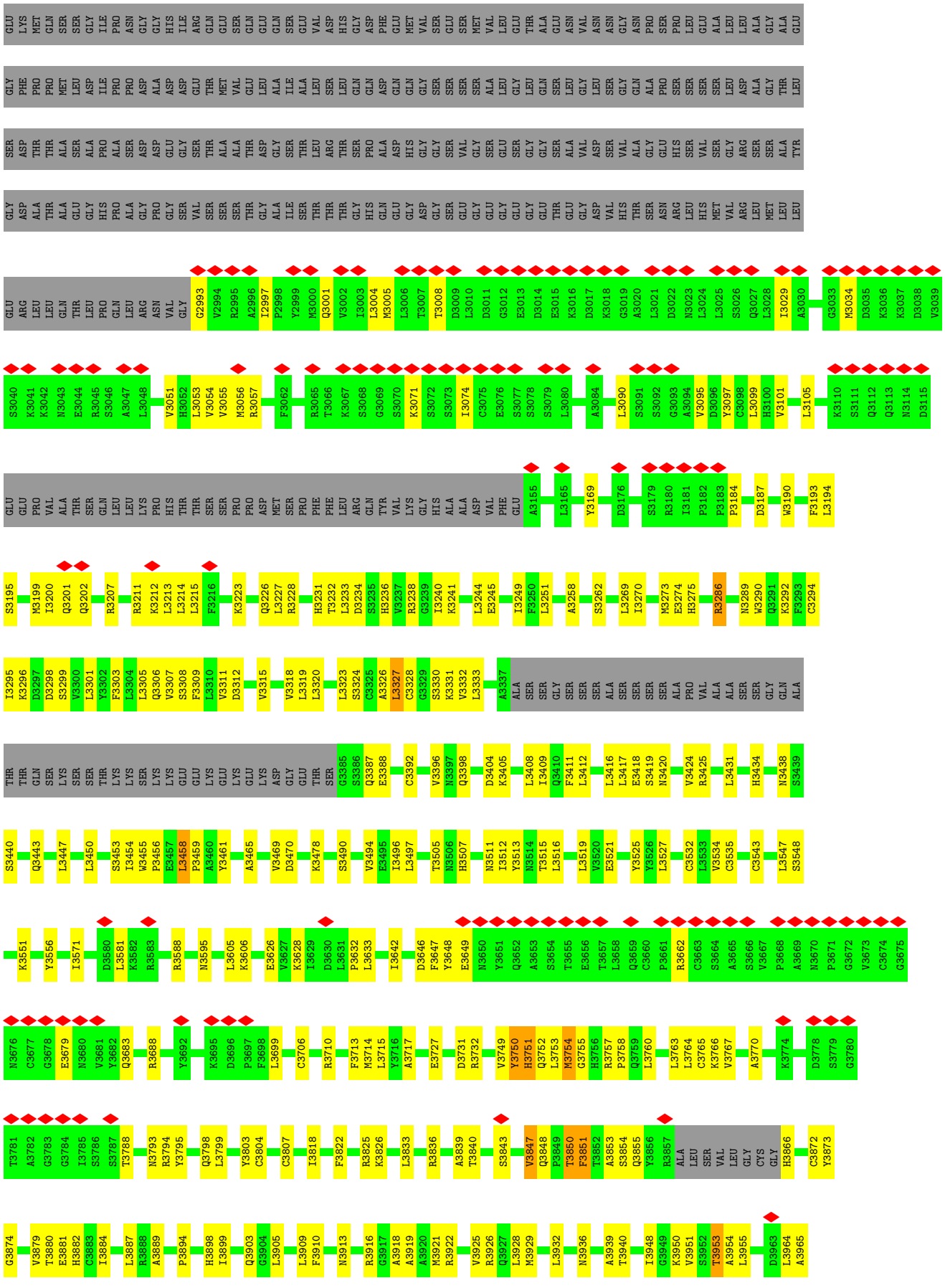


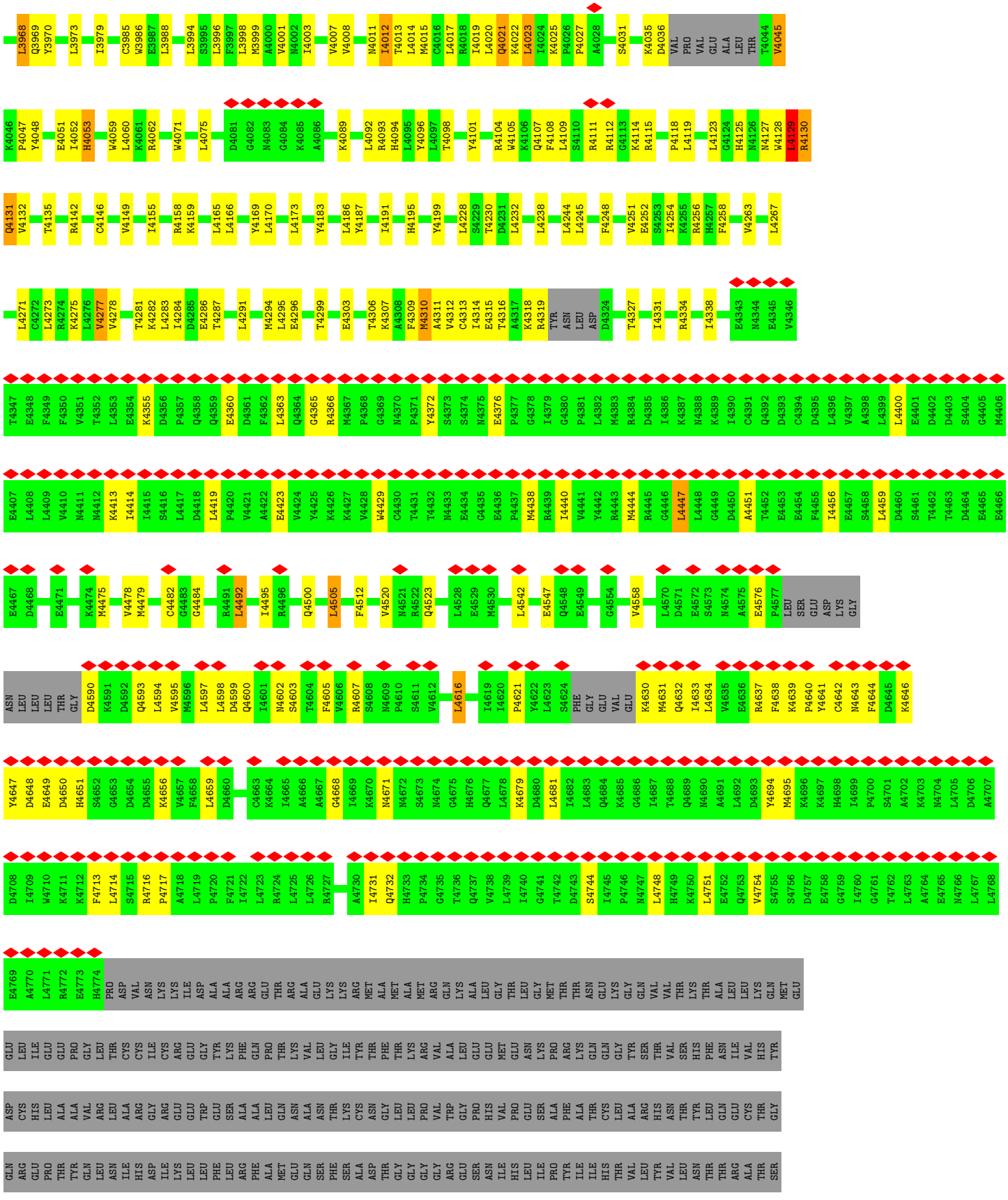
• Molecule 1: E3 ubiquitin-protein ligase UBR4

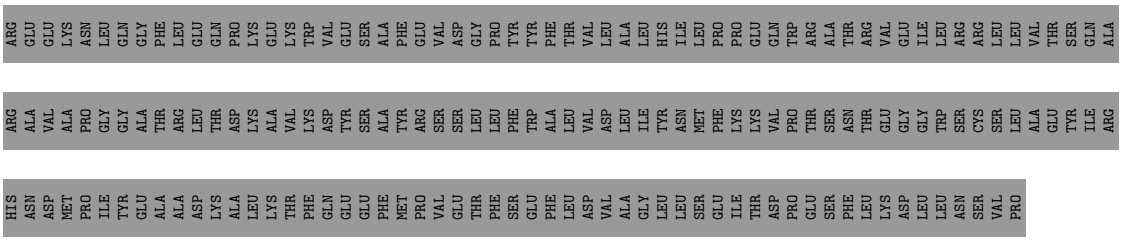
Chain B:


ALA GLY VAL SER VAL ALA THR CYS MET ALA ILE LEU HIS VAL GLY SER ALA GLN GLN VAL ARG THR GLY SER GLU ASP ASP TYR GLU SER ASP ALA ALA THR ILE VAL GLN LYS CYS LEU GLU ILE TYR ASP MET ILE GLY GLN ALA ILE SER SER ARG
GLY GLY GLU HIS TYR GLN ASN PHE GLN LEU LEU GLY ALA TRP CYS LEU LEU ASN SER LEU PHE LEU ILE LEU ASN GLU SER PRO THR ALA LEU ALA ASP LYS GLY LYS GLU GLY VAL GLY SER PRO
LYS LEU GLY PRO GLY LYS GLY HIS GLN GLY PHE GLY VAL LEU SER VAL ILE LEU ALA ASN HIS ALA ILE LYS LEU LEU THR SER LEU PHE GLN ASP LEU GLN VAL GLU ALA LEU LYS ASP PRO GLY TRP GLU THR ASP GLY PRO PRO ALA ALA LEU SER ILE MET ALA GLN SER THR SER ILE
GLN ARG ILE GLN ARG LEU ILE ASP SER VAL PRO LEU MET ASN LEU LEU LEU THR LEU LEU SER THR SER SER TYR ARG LYS ALA CYS VAL LEU GLN ARG ARG LYS GLY SER MET SER SER ASP ALA SER ALA SER THR ASP SER ASN ALA ASP PHE SER SER THR GLU
GLU ASP SER SER GLN ASP ASP SER GLU PRO PRO ILE LEU GLY GLN TRP PHE GLU GLU THR ILE SER PRO SER LYS GLU LYS ALA ALA PRO PRO PRO PRO PRO PRO LEU GLU SER SER SER PRO ARG VAL LYS SER PRO SER LYS GLN LYS ALA PRO GLY GLU LYS GLY ASN ILE LEU
ALA SER ARG LYS ASP PRO GLU LEU PHE ILE LEU ASN PHE ILE THR SER SER MET LEU ASN ASN SER ARG ASN ASN ASN PHE ILE ARG ASN TYR LEU SER VAL SER LEU SER SER GLU HIS HIS MET ALA THR LEU ALA SER ILE ILE LYS GLU VAL ASP GLY LEU
LYS GLY SER SER ASP GLU GLU PHE ALA ALA LEU TYR HIS PHE ASN HIS SER LEU VAL THR SER ASP LEU GLN SER ASN THR LEU LEU GLN GLN LEU GLY VAL ALA PRO PHE SER GLU GLY PRO TRP PRO LEU TYR ILE HIS PRO GLN SER LEU SER VAL LEU SER
ARG LEU LEU LEU ILE TRP GLN HIS LYS ALA SER ALA GLN GLY ASP PRO ASP VAL PRO GLU CYS LEU LYS VAL TRP ASP ARG PHE LEU SER THR MET LYS GLN ASN ALA LEU GLN GLY VAL VAL PRO SER GLU THR GLU ASP LEU ASN VAL GLU HIS LEU ASP ILE PHE
HIS ASN PHE THR GLU THR GLY ARG ARG ALA ILE LEU SER LEU PHE VAL GLN ILE ILE GLN GLU LEU SER VAL ASN MET ASP ALA GLN MET ARG PHE VAL PRO LEU ILE LEU ALA ARG LEU GLN LEU ILE PHE ASP TYR LEU LEU HIS GLN TYR SER LYS ALA PRO VAL TYR LEU PHE GLU
GLN VAL GLN HIS ASN LEU LEU SER PRO PRO PHE GLY TRP ALA SER GLY SER GLN ASP SER ASN SER ARG ARG ALA THR THR PRO LEU TYR HIS GLY PHE LYS GLU VAL GLU GLU ASN TRP SER LYS HIS PHE SER SER ASP ALA VAL PRO HIS PRO ARG PHE TYR CYS VAL LEU SER PRO
GLU ALA SER GLU ASP ASP LEU ASN ARG LEU ASP SER VAL PHE SER LYS LEU VAL LYS TYR ASP GLU LEU TYR ALA ALA LEU THR ALA LEU LEU ALA ALA GLY SER GLN LEU ASP THR VAL ARG ARG LYS GLU VAL ASN VAL THR ALA LEU GLU LEU ASP
LEU GLN TYR TYR PHE LEU ILE ILE LEU TRP ARG ILE LEU LEU GLY ILE LEU PRO PRO SER LYS THR THR TYR ILE ASN GLN LEU SER MET ASN SER PRO GLU MET SER GLU CYS ASP ILE LEU HIS THR LEU ARG TRP SER SER SER ARG LEU ARG ILE SER ASN VAL THR GLU ASP ILE LYS
ILE LYS GLN GLY MET LYS ALA GLU HIS ALA ILE SER SER VAL LYS TYR ASP VAL GLU ILE VAL GLU GLU TYR PHE ALA ARG GLN ILE SER SER PHE CYS SER ILE ASP CYS THR THR THR ILE GLU LEU GLN ILE GLN LEU HIS GLU ILE PRO SER LEU
GLN SER ILE TYR THR LEU ASP ALA ALA ILE SER LYS VAL GLN VAL SER LEU LYS MET ALA ALA GLU THR ASP PRO HIS LYS SER SER GLU ILE THR LYS ASN LEU LEU PRO ALA THR LEU GLN LEU ILE ASP THR TYR THR ILE ALA SER PHE THR ARG ALA TYR LEU LEU
GLN ASN PHE ASN GLU GLU GLY THR THR GLU LYS PRO SER LYS LEU GLY PHE ALA ALA VAL LEU ALA ILE GLY SER SER ARG CYS LYS ALA ASN THR LEU GLY PRO THR LEU VAL GLN ASN LEU PRO SER SER VAL GLN THR THR ASN ASN ASN ILE ASN THR
ASN GLU PHE PRO ASN ILE GLY SER TRP PHE PRO SER GLU VAL SER TYR ILE SER ALA VAL GLN ALA ALA HIS LEU LEU GLY THR LEU CYS SER GLN SER LEU PRO LEU ALA ALA SER LEU SER LEU LYS HIS THR LEU LEU THR ILE GLY ASP LEU
ILE VAL TRP SER ASP GLU MET ASN PRO PRO GLN VAL LEU SER SER THR GLU SER VAL ALA GLU ILE SER SER GLN ASN SER ARG ILE LEU GLY PRO ALA GLU SER ASP GLU PHE LEU ALA ARG VAL TYR GLU LYS LEU LEU ILE THR GLY CYS
TYR ASN ILE LEU ALA ASN HIS ALA ASP PRO ASN SER GLY LEU GLN LEU GLU SER SER GLN ALA ARG LYS ALA MET GLU GLU PHE PHE SER ASP SER GLY GLU LEU VAL GLN ILE MET MET ALA THR ALA ASN GLY GLU
LEU SER ALA LYS PHE CYS LEU SER LEU LEU HIS LEU CYS GLY SER LEU ALA CYS VAL GLU PRO VAL ARG LEU GLN ALA TRP THR LEU ARG MET THR THR SER PRO PRO LYS ASP
SER ASP GLN LEU ASP VAL ARG GLN LEU GLU GLY VAL CYS ALA VAL LEU LEU GLY THR LEU THR PRO MET ALA THR GLU MET LEU ALA ASN GLY ASP GLY THR GLY PHE PRO GLU LEU MET


VAL VAL MET ALA THR LEU ALA SER ALA GLY GLN GLY ALA GLY HIS LEU GLN LEU HIS ASN ALA ALA VAL ASP TRP LEU SER ARG CYS LYS LYS TYR LEU SER GLN LYS ASN VAL VAL GLU LYS LEU ASN ALA ASN VAL MET HIS GLY LYS HIS VAL MET ILE LEU GLU CYS THR CYS HIS
ILE MET SER TYR LEU ALA ASP VAL THR ASN ALA LEU SER GLN SER ASN GLY GLN GLY PRO SER HIS LEU SER VAL ASP GLY GLU GLU ARG ALA ILE GLU VAL ASP SER ASP TRP VAL GLU GLU LEU ALA VAL ASP GLY GLU GLU ASP SER ASP GLU GLY GLN ALA GLU ASP SER ASP GLU ASP SER LEU CYS
ASN LYS LEU CYS THR PHE THR ILE THR GLN LYS GLU PHE MET ASN GLN HIS TRP TYR HIS CYS HIS THR CYS LYS MET VAL ASP GLY VAL GLY VAL CYS THR VAL CYS ALA LYS VAL CYS HIS LYS ASP HIS GLU ILE SER TYR ALA LYS TYR GLY PHE PHE CYS ASP CYS GLY ALA
LYS GLU ASP GLY SER CYS LEU ALA LEU VAL LYS ARG THR PRO SER SER GLY MET SER SER THR MET LYS GLU SER ALA LEU VAL LYS ARG THR SER GLN SER GLU SER GLU PRO ARG ILE SER GLU SER LEU VAL ARG HIS ALA SER THR SER SER PRO ALA ASP LYS ALA LYS VAL THR ILE SER ASP GLU ASP GLY LYS VAL ALA
ASP GLU GLU LYS PRO LYS LYS SER LEU CYS ARG THR VAL GLU GLY CYS ARG GLU GLU LEU GLN ASN GLN ALA ASN PHE SER PHE ALA PRO LEU VAL LEU ASP MET LEU ASN PHE LEU MET ASP ALA ILE GLN THR ASN PHE GLN GLN ALA SER ALA ALA VAL GLY SER ARG ALA
GLN GLN ALA LEU SER GLU LEU HIS THR VAL GLU LYS ALA VAL GLU MET THR ASP GLN LEU MET VAL PRO THR LEU GLY SER GLN GLU GLY ALA PHE GLU ASN VAL ARG MET ASN TYR SER GLY ASP GLN GLY GLY THR ILE ARG GLN LEU GLN ALA SER GLN THR GLU LEU ILE SER ALA HIS VAL LEU ARG ARG VAL VAL ALA
MET CYS VAL LEU SER SER PRO HIS GLY ARG ARG GLN HIS LEU ALA VAL SER HIS GLU LYS GLY LYS ILE THR VAL LEU GLN LEU LEU LYS GLN ALA ASP SER SER LYS ARG LYS LEU THR LEU THR ARG LEU ALA SER LEU THR VAL LEU SER LEU THR
GLY ASN PRO CYS LYS GLU ASP TYR LEU ALA VAL CYS GLY LEU ALA SER SER SER GLY SER VAL SER ASP HIS LEU VAL LEU THR PHE SER SER GLY LEU GLN LEU ALA THR GLY ASN PHE ILE ILE LYS ALA VAL TRP LEU PRO GLY PHE SER GLN THR GLU LEU ALA ILE VAL
THR ALA ASP PHE VAL LYS ILE TYR ASP LEU CYS VAL ASP ALA LEU SER PRO THR PHE TYR PHE LEU LEU PRO SER SER LYS ILE ARG ASP VAL THR PHE LEU PHE ASN GLU GLU GLY LYS ASN ILE ILE VAL ILE MET SER SER ALA GLY TYR ILE TYR THR GLN LEU GLU GLU ALA
SER SER ALA GLN GLN GLY PRO PHE TYR VAL THR ASN VAL LEU GLU ILE ASN HIS GLU ASP LEU ASP SER ASN SER GLN SER GLN VAL ALA ALA GLY GLY GLY VAL GLY GLY LYS SER PHE ALA ALA THR ILE SER ARG
THR THR LEU GLU VAL LEU GLN LEU PHE PRO ILE ASN ILE LYS SER SER ASN GLY GLY SER LYS THR SER PRO ALA LEU CYS GLN TRP SER GLU VAL MET ASN HIS PRO GLY LEU VAL CYS CYS VAL GLN GLN THR THR GLY VAL PRO LEU LEU VAL VAL MET VAL LYS PRO ASP THR PHE LEU
ILE GLN GLU ILE LYS THR LEU PRO ALA LYS ALA ALA LYS ILE GLN ASP MET VAL ALA ILE ARG HIS THR ALA CYS ASN GLU GLN GLN ARG THR MET MET ILE LEU LEU CYS GLU ASP GLY SER LEU ARG ILE TYR MET ALA ASN VAL GLU ASN THR LEU VAL LEU GLU LEU ARG
PRO SER SER VAL ILE SER ILE MET LYS PRO VAL ALA ARG LYS ARG LYS THR ALA THR ILE THR THR ARG THR SER SER GLN VAL THR PHE PRO ILE ASP PHE PHE GLU HIS ASN GLN GLN LEU THR ASP VAL GLU ASN ASP LEU LEU VAL GLN VAL TYR ASN ALA GLN PRO SER LEU ILE
HIS ARG LEU ASN SER THR GLY MET TYR VAL ALA ASN THR LYS PRO GLY GLY PHE THR ILE GLU ILE SER ASN ASN SER THR MET VAL MET THR ASP GLY MET ARG ILE GLN ILE GLY THR GLN ALA ILE GLU ARG ALA PRO SER TYR ILE GLU ILE PHE GLY ARG THR MET GLN LEU ASN
LEU SER ARG SER ARG TRP PHE PRO PHE THR ARG GLU GLU ALA LEU GLN ALA ASP LYS LYS LEU ASN LEU PHE ILE GLY ALA SER VAL ASP PRO ALA GLY VAL THR MET ILE ASP ALA GLY TYR LYS ILE TYR GLY LYS THR LYS GLU GLN PHE GLY TRP PRO ASP GLU PRO GLU
GLU PHE PRO SER ALA SER VAL SER ASN ILE CYS PRO SER ASN LEU ASN GLN SER ASP SER ASN GLY THR GLY ASP SER ALA ALA PRO THR THR THR VAL ILE LEU VAL ARG LEU ASP VAL VAL VAL SER SER LEU GLU ALA LEU GLU SER CYS PHE ALA VAL GLY PRO ILE ILE GLU LYS
GLU ARG ASN LYS ASN ALA GLN LEU LEU LEU SER LEU PRO ALA ALA THR LEU LEU ALA SER VAL GLN GLN GLU SER LYS SER LEU LEU ALA ALA PRO ALA SER ARG SER ALA TYR HIS SER HIS LYS ASP GLN ALA LEU GLU SER LYS ALA ALA VAL GLN CYS LEU ASN THR SER
SER LYS GLU GLY LYS ASP PRO GLU VAL PHE GLN ARG LEU ILE THR ALA ARG SER ILE ALA ILE MET ARG PRO ASN ASN LEU VAL HIS PHE THR GLU SER LYS LEU PRO GLN MET GLU THR GLU GLY GLN GLN LYS GLN LEU ILE ASP CYS
CYS SER PHE ILE THR GLN LEU VAL ASN HIS PHE TRP LYS LEU HIS ALA SER LYS PRO LYS ASN ALA PHE LEU ALA PRO ALA CYS LEU PRO GLY LEU THR HIS ILE GLU ALA THR VAL ASN ALA LEU VAL ASP ILE ILE HIS GLY TYR CYS THR CYS GLU LEU ASP CYS ILE ASN THR ALA
SER LYS ILE TYR MET GLN MET LEU LEU CYS PRO ASP PRO ALA VAL SER PHE SER CYS LYS GLN ALA LEU ILE ARG VAL LEU ARG PRO ARG ASN LYS ARG ARG HIS VAL THR LEU PRO SER SER PRO ARG SER ASN THR PRO MET GLY ASP LYS ASP ASP ASP ASP ASP ASP ASP ASP

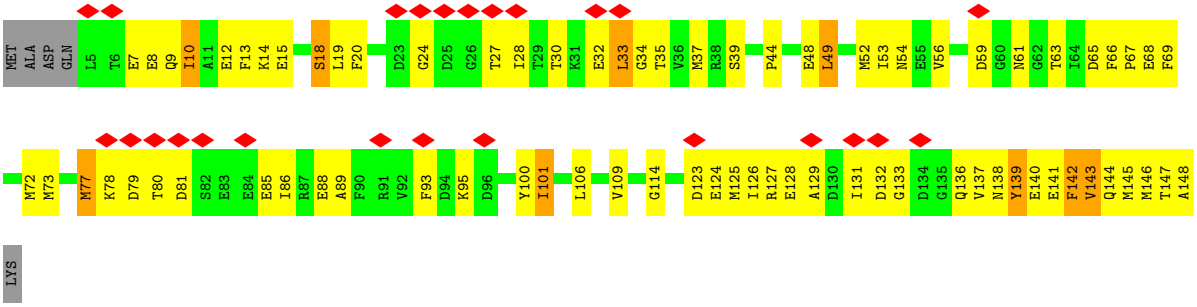

GLU LYS MET GLN SER SER GLY ILE PRO ASN GLY GLY HIS ILE ARG GLN GLU SER GLN GLU GLN SER GLU VAL ASP HIS GLY ASP PHE GLU MET VAL SER GLU SER MET VAL LEU LEU ALA GLU ASN VAL ASN ASN GLY ASN PRO SER PRO LEU GLU ALA LEU LEU ALA GLY ALA GLU
GLY PHE PRO PRO MET LEU ASP ILE PRO PRO ASP ASP ALA ASP GLU THR MET VAL GLU ALA ILE SER THR LEU ALA LEU SER LEU GLN GLN GLN GLY SER LEU GLY LEU SER GLN GLN ALA PRO SER SER SER SER SER LEU ASP ALA LEU THR
SER ASP THR THR ALA SER ALA PRO ALA SER ASP ASP GLU GLY SER THR ALA ALA THR ASP GLY ALA ILE SER THR LEU ARG THR SER PRO ALA ASP HIS GLY GLY SER VAL GLY SER GLU GLY GLY SER ALA VAL ASP SER VAL ALA GLY GLU HIS SER VAL SER GLY ARG SER SER THR LEU
GLY ASP ALA THR ALA GLU GLY HIS PRO ALA GLY PRO GLY SER VAL SER SER SER THR GLY THR THR GLY HIS GLN GLU GLY ASP GLY SER GLU GLY GLU GLY GLU GLY GLU THR GLU GLY ASP VAL HIS THR SER ASN ARG LEU HIS MET VAL ARG LEU MET LEU LEU
GLU ARG LEU LEU GLN THR LEU PRO GLN LEU ARG ASN VAL GLY G2993 V2994 R2995 A2996 I2997 P2998 Y2999 M3000 Q3001 V3002 I3003 L3004 M3005 L3006 T3007 T3008 D3009 L3010 D3011 D3011 G3012 E3013 D3014 E3015 K3016 D3017 K3018 G3019 A3020 L3021 D3022 N3023 L3024 L3025 S3026 Q3027 L3028 I3029 A3030 G3033 M3034 D3035 K3036 K3037 D3038 V3039
S3040 K3041 K3042 N3043 E3044 R3045 S3046 A3047 L3048 V3051 H3052 L3053 V3054 V3055 M3056 R3057 F3082 R3065 T3066 K3067 S3068 G3069 S3070 K3071 S3072 S3073 I3074 C3076 E3076 S3077 S3078 S3079 L3080 A3084 L3090 S3091 S3092 G3093 A3094 V3095 D3096 Y3097 C3098 L3099 H3100 V3101 L3105 K3110 S3111 Q3112 Q3113 N3114 D3115
GLU GLU PRO VAL ALA THR SER GLN LEU LEU LYS PRO HIS THR THR SER SER PRO PRO ASP MET SER PRO PHE PHE LEU ARG GLN TYR VAL LYS GLY HIS ALA ALA ASP VAL PHE GLU A3155 L3165 Y3169 D3176 S3179 R3180 I3181 P3182 P3183 P3184 D3187 W3190 F3193 L3194
S3195 M3199 I3200 Q3201 Q3202 R3207 R3211 K3212 L3213 L3214 L3215 F3216 K3223 Q3226 L3227 R3228 H3231 T3232 L3233 D3234 S3235 H3236 V3237 R3238 G3239 I3240 K3241 L3244 E3245 I3249 F3250 L3251 A3258 S3262 L3269 I3270 M3273 E3274 H3275 R3286 N3289 W3290 Q3291 K3292 F3293 C3294
I3295 K3296 D3297 D3298 S3299 V3300 L3301 Y3302 F3303 L3304 L3305 Q3306 V3307 S3308 F3309 L3310 V3311 D3312 V3315 V3318 L3319 L3320 L3323 S3324 C3325 A3326 L3327 C3328 G3329 S3330 K3331 V3332 L3333 A3337 ALA SER SER GLY SER SER SER ALA SER SER SER SER ALA PRO VAL ALA ALA ALA SER SER GLY GLN ALA
THR THR GLN SER LYS SER SER THR LYS LYS SER LYS LYS GLU GLU LYS GLU LYS GLU LYS ASP GLY GLU THR SER G3385 S3386 Q3387 E3388 C3392 V3396 N3397 Q3398 D3404 K3405 L3408 I3409 Q3410 F3411 L3412 L3416 L3417 E3418 S3419 N3420 V3424 R3425 L3431 H3434 N3438 S3439
S3440 Q3443 L3447 L3450 S3453 I3454 W3455 P3456 E3457 L3458 P3459 A3460 Y3461 A3465 V3469 D3470 K3478 S3490 V3494 E3495 I3496 L3497 T3505 N3506 H3507 N3511 I3512 Y3513 N3514 T3515 L3516 L3519 V3520 E3521 Y3525 Y3526 L3527 C3532 L3533 V3534 C3535 C3543 L3547 S3548
K3551 Y3556 I3571 D3580 L3581 K3582 R3583 R3588 N3595 L3605 K3606 E3626 V3627 K3628 I3629 D3630 L3631 P3632 L3633 I3642 D3646 F3647 Y3648 E3649 N3650 Y3651 Q3652 A3653 S3654 T3655 E3656 T3657 L3658 Q3659 C3660 P3661 R3662 C3663 S3664 A3665 S3666 V3667 P3668 A3669 N3670 P3671 G3672 V3673 C3674 G3675
N3676 C3677 G3678 E3679 N3680 V3681 Y3682 Q3683 R3688 Y3692 K3695 D3696 P3697 F3698 L3699 C3706 R3710 F3713 M3714 L3715 Y3716 A3717 E3727 D3731 R3732 V3749 Y3750 H3751 Q3752 L3753 M3754 G3755 H3756 R3757 P3758 Q3759 L3760 L3763 L3764 C3765 K3766 V3767 A3770 K3774 D3778 S3779 G3780
T3781 A3782 G3783 G3784 I3785 S3786 S3787 T3788 N3793 R3794 Y3795 Q3798 L3799 Y3803 C3804 C3807 I3818 F3822 R3825 K3826 L3833 R3836 A3839 T3840 S3843 V3847 Q3848 P3849 T3850 F3851 T3852 A3853 S3854 Q3855 Y3856 R3857 ALA LEU SER VAL LEU GLY CYS GLY H3866 C3872 Y3873
G3874 V3879 T3880 E3881 H3882 C3883 I3884 L3887 R3888 A3889 P3894 H3898 I3899 Q3903 G3904 L3905 L3909 F3910 N3913 R3916 G3917 A3918 A3919 A3920 M3921 R3922 V3925 R3926 Q3927 L3928 M3929 L3932 N3936 A3939 T3940 I3948 G3949 K3950 V3951 S3952 T3953 A3954 L3955 D3963 L3964 A3965


L3968 Q3969 Y3970 L3973 I3979 C3985 W3986 E3987 L3988 L3994 S3995 L3996 F3997 L3998 M3999 A4000 V4001 M4002 I4003 V4007 V4008 N4011 I4012 T4013 L4014 M4015 C4016 L4017 R4018 I4019 L4020 Q4021 K4022 L4023 I4024 K4025 P4026 P4027 A4028 S4031 K4035 D4036 VAL PRO VAL GLU ALA LEU THR T4044 V4045
K4046 P4047 Y4048 E4051 I4052 H4053 W4059 L4060 K4061 R4062 W4071 L4075 D4081 G4082 N4083 G4084 K4085 A4086 K4089 L4092 R4093 H4094 L4095 Y4096 L4097 T4098 Y4101 R4104 W4105 K4106 Q4107 F4108 L4109 S4110 R4111 R4112 G4113 K4114 R4115 P4118 L4119 L4123 G4124 H4125 N4126 N4127 W4128 L4129 R4130
Q4131 V4132 T4135 R4142 C4146 V4149 I4155 R4158 K4159 L4165 L4166 Y4169 L4170 L4173 Y4183 L4186 Y4187 I4191 H4195 Y4199 L4228 S4229 T4230 D4231 L4232 L4238 L4244 L4245 F4248 V4251 E4252 S4253 I4254 K4255 R4256 H4257 F4258 V4263 L4267
L4271 C4272 L4273 R4274 K4275 L4276 V4277 V4278 T4281 K4282 L4283 I4284 D4285 E4286 T4287 L4291 M4294 L4295 E4296 T4299 E4303 T4306 K4307 A4308 F4309 M4310 A4311 V4312 C4313 I4314 E4315 T4316 A4317 K4318 R4319 TYR ASN LEU ASP D4324 T4327 I4331 R4334 I4338 E4343 N4344 E4345 V4346
T4347 E4348 F4349 F4350 V4351 T4352 L4353 E4354 K4355 D4356 P4357 Q4358 Q4359 E4360 D4361 F4362 L4363 Q4364 G4365 R4366 M4367 P4368 G4369 N4370 P4371 Y4372 S4373 S4374 N4375 E4376 P4377 G4378 I4379 G4380 P4381 L4382 M4383 R4384 D4385 I4386 K4387 N4388 K4389 I4390 C4391 Q4392 D4393 C4394 D4395 L4396 V4397 A4398 L4399 L4400 E4401 D4402 D4403 S4404 G4405 M4406
E4407 L4408 L4409 V4410 N4411 N4412 K4413 I4414 I4415 S4416 L4417 D4418 L4419 P4420 V4421 A4422 E4423 V4424 Y4425 K4426 K4427 V4428 W4429 C4430 T4431 T4432 N4433 E4434 G4435 E4436 P4437 M4438 R4439 I4440 V4441 Y4442 R4443 M4444 R4445 G4446 L4447 L4448 G4449 D4450 A4451 T4452 E4453 E4454 F4455 I4456 E4457 S4458 L4459 D4460 S4461 T4462 T4463 D4464 E4465 E4466
E4467 D4468 E4471 K4474 M4475 V4478 M4479 C4482 G4483 G4484 R4491 L4492 I4495 R4496 Q4500 L4505 F4512 V4520 N4521 R4522 Q4523 L4528 E4529 M4530 L4542 E4547 Q4548 E4549 G4554 V4558 L4570 D4571 E4572 S4573 N4574 A4575 E4576 P4577 LEU SER GLU ASP LYS GLY
ASN LEU LEU LEU THR GLY D4590 K4591 D4592 Q4593 L4594 V4595 M4596 L4597 L4598 D4599 Q4600 I4601 N4602 S4603 T4604 F4605 V4606 R4607 S4608 N4609 P4610 S4611 V4612 L4616 I4619 I4620 P4621 Y4622 L4623 S4624 PHE GLY GLU VAL GLU K4630 M4631 Q4632 I4633 L4634 V4635 E4636 R4637 F4638 K4639 P4640 Y4641 C4642 N4643 F4644 D4645 K4646
Y4647 D4648 E4649 D4650 H4651 S4652 G4653 D4654 D4655 K4656 V4657 F4658 L4659 D4660 C4663 K4664 I4665 A4666 A4667 G4668 I4669 K4670 N4671 N4672 S4673 N4674 G4675 H4676 Q4677 L4678 K4679 D4680 L4681 I4682 L4683 Q4684 K4685 G4686 I4687 T4688 Q4689 M4690 A4691 L4692 D4693 Y4694 M4695 K4696 K4697 H4698 I4699 P4700 S4701 A4702 K4703 N4704 L4705 D4706 A4707
D4708 I4709 W4710 K4711 K4712 F4713 L4714 S4715 R4716 P4717 A4718 L4719 P4720 F4721 I4722 L4723 R4724 I4725 L4726 R4727 A4730 I4731 Q4732 H4733 P4734 G4735 T4736 Q4737 V4738 L4739 I4740 G4741 T4742 D4743 S4744 I4745 P4746 N4747 L4748 H4749 K4750 L4751 E4752 Q4753 V4754 S4755 S4756 D4757 E4758 G4759 I4760 G4761 T4762 L4763 A4764 E4765 N4766 L4767 L4768
E4769 A4770 L4771 R4772 E4773 H4774 PRO ASP VAL ASN LYS LYS ILE ASP ALA ARG ARG GLU THR ARG ALA GLU LYS LYS ARG MET ALA MET ALA ARG GLN LYS ALA LEU GLY THR LEU GLY MET THR THR ASN GLU LYS GLY GLN VAL VAL THR LYS THR ALA LEU LEU LEU LYS GLN MET GLU
GLU LEU ILE GLU GLU PRO GLY LEU THR CYS CYS ILE CYS ARG GLU GLY TYR LYS PHE GLN PRO THR LYS VAL LEU GLY ILE TYR THR PHE THR LYS ARG VAL ALA LEU GLU GLU MET GLU ASN LYS PRO ARG LYS GLN GLN GLY GLY TYR SER THR VAL SER HIS PHE ASN LEU GLN GLU ILE VAL HIS TYR
ASP CYS HIS LEU ALA ALA VAL ARG LEU ALA ARG GLY ARG GLU GLU TRP GLU SER ALA ALA LEU GLN ASN ALA ASN THR LYS CYS ASN GLY LEU LEU LEU PRO VAL TRP GLY PRO HIS VAL PRO GLU SER ALA PHE ALA THR CYS LEU ALA ARG HIS ASN THR TYR LEU GLN GLU CYS THR GLY
GLN ARG GLU PRO THR TYR GLN LEU ASN ILE HIS ASP ILE LYS LEU LEU PHE LEU ARG PHE ALA MET GLU GLN SER PHE SER ALA ASP THR GLY GLY GLY GLY ARG GLU SER ASN ILE HIS LEU LEU ILE PRO TYR ILE ILE HIS THR VAL LEU TYR VAL THR LEU ASN THR THR ARG GLU ALA THR GLY



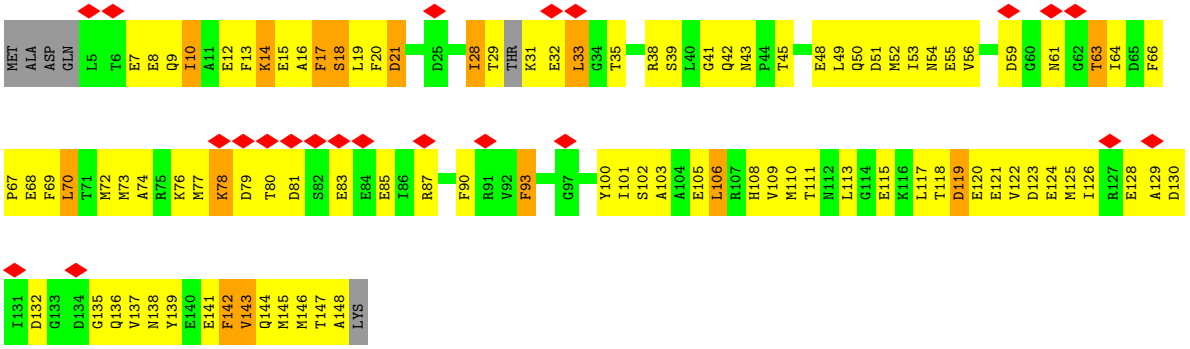
• Molecule 2: Calmodulin-1

Chain C:



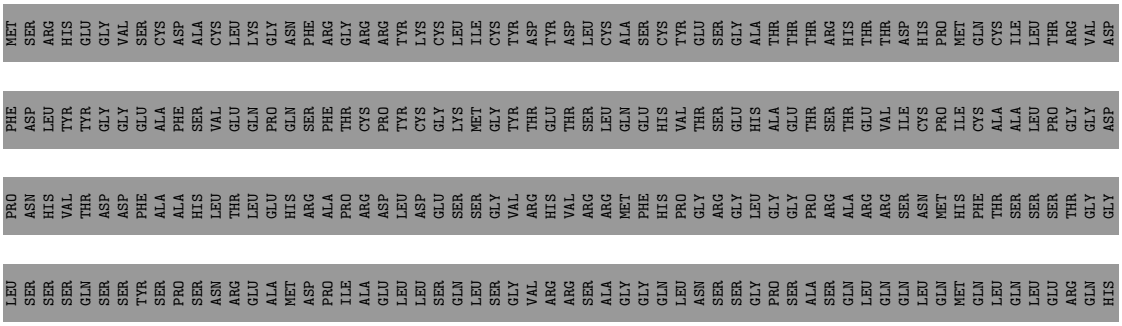
• Molecule 2: Calmodulin-1

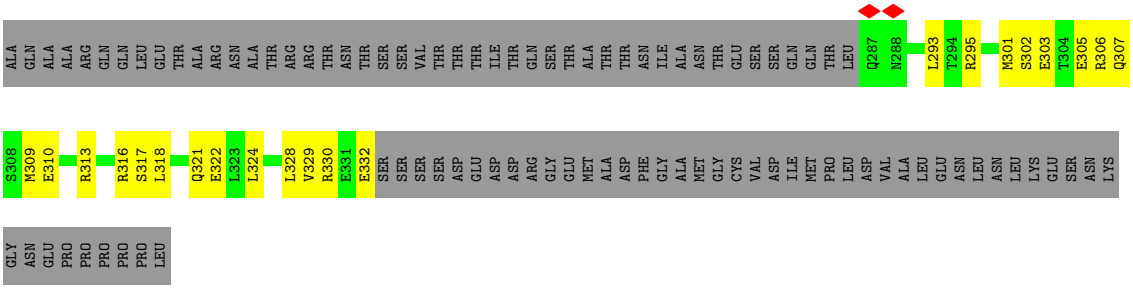
Chain D:



• Molecule 3: E3 ubiquitin-protein ligase KCMF1

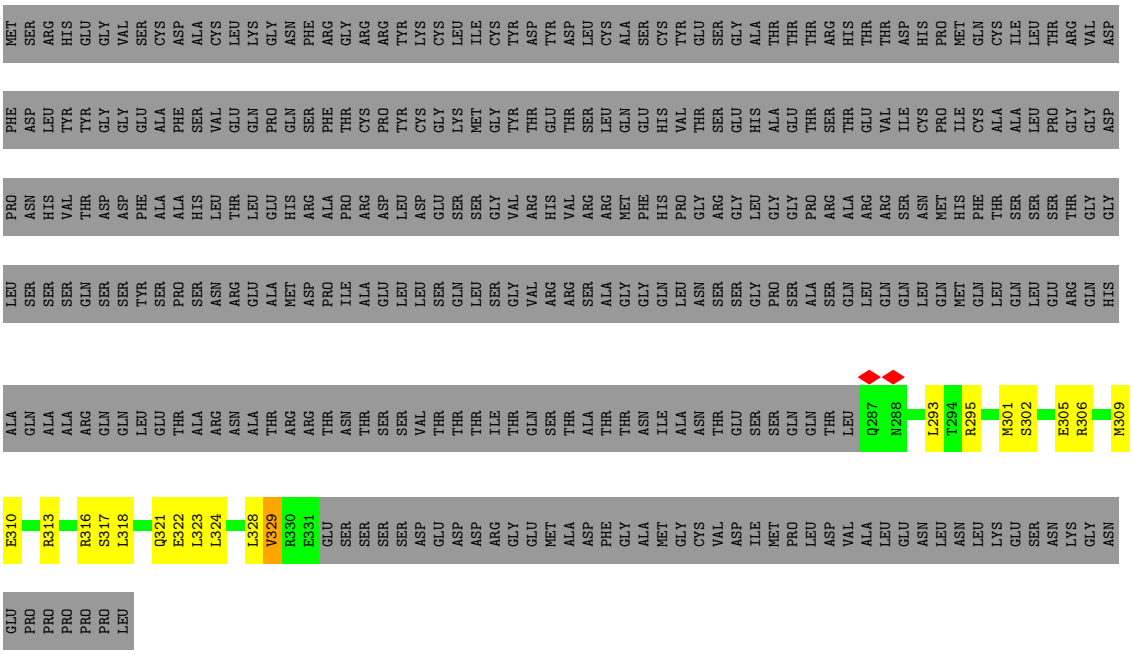
Chain E:





• Molecule 3: E3 ubiquitin-protein ligase KCMF1

Chain F: 7% 88%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87263	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.493	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.146	Depositor
Map size (Å)	419.19998, 419.19998, 419.19998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	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: CA, 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	A	0.61	1/13355 (0.0%)	0.90	24/18055 (0.1%)
1	B	0.64	6/13357 (0.0%)	0.91	24/18057 (0.1%)
2	C	1.06	2/1146 (0.2%)	1.31	5/1539 (0.3%)
2	D	1.14	2/1138 (0.2%)	1.34	8/1526 (0.5%)
3	E	0.36	0/382	0.68	0/511
3	F	0.35	0/373	0.77	1/499 (0.2%)
All	All	0.66	11/29751 (0.0%)	0.94	62/40187 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4013	THR	C-O	-6.08	1.17	1.24
1	B	4023	LEU	C-O	-6.06	1.17	1.24
1	A	3968	LEU	C-O	-5.96	1.16	1.24
2	D	14	LYS	CA-C	-5.91	1.45	1.52
2	C	14	LYS	CA-C	-5.89	1.45	1.52
2	D	18	SER	N-CA	-5.53	1.39	1.46
1	B	4020	LEU	C-O	-5.34	1.17	1.24
1	B	4131	GLN	C-O	-5.33	1.18	1.24
2	C	18	SER	N-CA	-5.32	1.40	1.46
1	B	4014	LEU	C-O	-5.28	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4021	GLN	C-O	-5.13	1.18	1.24

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	3792	VAL	CA-C-N	-17.13	96.38	120.71
1	A	3792	VAL	C-N-CA	-17.13	96.38	120.71
1	A	3792	VAL	O-C-N	13.47	136.41	122.54
1	A	3969	GLN	CB-CA-C	-12.40	91.86	110.96
2	C	86	ILE	N-CA-C	-11.11	97.20	111.09
2	D	106	LEU	N-CA-C	-9.97	100.49	111.36
1	A	3969	GLN	CA-C-N	-9.22	107.92	120.28
1	A	3969	GLN	C-N-CA	-9.22	107.92	120.28
1	A	3331	LYS	N-CA-C	-9.13	101.28	111.14
1	B	3331	LYS	N-CA-C	-8.96	101.46	111.14
2	C	139	TYR	N-CA-C	-8.93	101.44	111.71
1	B	4021	GLN	N-CA-C	-8.63	101.83	111.07
1	A	3973	LEU	N-CA-C	-7.65	102.92	111.71
1	A	3851	PHE	N-CA-C	-7.60	102.99	111.28
1	A	4134	PHE	CB-CA-C	7.51	122.86	110.17
1	B	3851	PHE	N-CA-C	-7.50	103.11	111.28
1	A	4133	LEU	CA-C-N	-7.41	111.01	122.49
1	A	4133	LEU	C-N-CA	-7.41	111.01	122.49
2	D	142	PHE	N-CA-C	-6.99	103.74	111.36
2	D	119	ASP	N-CA-C	-6.87	104.76	113.01
2	C	142	PHE	N-CA-C	-6.83	103.83	111.28
1	B	3750	TYR	CB-CA-C	-6.78	99.15	110.68
1	B	4023	LEU	CA-C-O	-6.76	113.66	120.90
1	B	4129	LEU	N-CA-C	-6.52	104.17	111.28
2	C	143	VAL	CB-CA-C	-6.16	104.08	111.97
1	B	4021	GLN	CA-C-O	-6.16	114.35	120.82
2	D	143	VAL	CB-CA-C	-6.06	104.21	111.97
1	A	3296	LYS	N-CA-C	-5.97	105.48	112.89
1	A	3535	CYS	CB-CA-C	-5.94	98.60	110.42
1	B	4131	GLN	CA-C-N	-5.87	113.56	120.72
1	B	4131	GLN	C-N-CA	-5.87	113.56	120.72
1	B	3296	LYS	N-CA-C	-5.78	105.72	112.89
2	D	110	MET	N-CA-C	-5.67	105.10	111.28
1	B	4130	ARG	N-CA-C	-5.66	104.80	110.97
1	A	3968	LEU	N-CA-C	-5.63	105.02	112.34
1	A	3970	TYR	CA-C-N	-5.59	112.23	120.28
1	A	3970	TYR	C-N-CA	-5.59	112.23	120.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	10	ILE	N-CA-C	-5.56	104.25	112.04
2	C	10	ILE	N-CA-C	-5.55	104.28	112.04
1	A	4744	SER	CA-C-N	5.41	124.66	120.33
1	A	4744	SER	C-N-CA	5.41	124.66	120.33
1	A	3327	LEU	CA-C-O	-5.38	115.16	120.70
1	A	3716	TYR	N-CA-C	-5.38	103.87	110.65
3	F	329	VAL	O-C-N	5.36	128.31	122.63
1	B	4052	ILE	CA-C-N	-5.31	114.74	122.86
1	B	4052	ILE	C-N-CA	-5.31	114.74	122.86
1	B	4012	ILE	CA-C-O	-5.25	115.94	121.41
2	D	74	ALA	N-CA-C	-5.24	105.46	111.07
1	B	3751	HIS	CB-CA-C	5.24	120.73	110.67
1	B	3327	LEU	CA-C-O	-5.21	115.34	120.70
1	B	4014	LEU	N-CA-C	-5.19	105.62	111.28
1	B	4744	SER	CA-C-N	5.18	124.47	120.33
1	B	4744	SER	C-N-CA	5.18	124.47	120.33
1	B	4023	LEU	CA-C-N	5.16	127.52	120.46
1	B	4023	LEU	C-N-CA	5.16	127.52	120.46
1	B	4021	GLN	N-CA-CB	5.12	117.44	110.01
1	B	3854	SER	CA-C-N	-5.05	114.20	122.79
1	B	3854	SER	C-N-CA	-5.05	114.20	122.79
1	A	3866	HIS	CA-CB-CG	5.02	118.82	113.80
2	D	17	PHE	N-CA-C	-5.02	105.81	111.28
1	A	3854	SER	CA-C-N	-5.01	114.27	122.79
1	A	3854	SER	C-N-CA	-5.01	114.27	122.79

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3286	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	B	4112	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	13132	0	13358	477	0
1	B	13134	0	13352	460	0
2	C	1134	0	1063	91	0
2	D	1127	0	1055	112	0
3	E	380	0	376	30	0
3	F	371	0	370	17	0
4	A	3	0	0	3	0
4	B	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
All	All	29288	0	29574	1056	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 18.

All (1056) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4032:LYS:CE	3:E:307:GLN:HG3	1.25	1.55
1:A:4307:LYS:CG	1:A:4475:MET:HE1	1.45	1.44
1:A:4307:LYS:HG3	1:A:4475:MET:CE	1.47	1.42
1:A:4032:LYS:CE	3:E:307:GLN:CG	2.11	1.28
1:B:4098:THR:OG1	2:D:113:LEU:HD21	1.18	1.26
1:A:4032:LYS:HE3	3:E:307:GLN:CG	1.66	1.25
1:A:4307:LYS:CG	1:A:4475:MET:CE	2.09	1.24
1:B:3270:ILE:CD1	1:B:3632:PRO:HG2	1.66	1.24
1:A:3270:ILE:CD1	1:A:3632:PRO:HG2	1.66	1.23
1:B:4307:LYS:CG	1:B:4475:MET:HE1	1.67	1.22
1:A:3270:ILE:HD13	1:A:3632:PRO:HG2	1.25	1.14
1:A:4309:PHE:HE1	1:A:4338:ILE:CD1	1.59	1.14
1:B:3328:CYS:SG	1:B:3333:LEU:HD11	1.90	1.12
1:B:4314:ILE:HD11	1:B:4479:MET:SD	1.88	1.11
1:A:3328:CYS:SG	1:A:3333:LEU:HD11	1.89	1.10
1:A:4271:LEU:HD11	1:A:4331:ILE:HD11	1.29	1.10
1:A:4310:MET:SD	1:A:4338:ILE:HG21	1.89	1.10
1:A:4032:LYS:HE2	3:E:307:GLN:HG3	1.13	1.10
1:B:3270:ILE:HD13	1:B:3632:PRO:HG2	1.25	1.09
1:B:4271:LEU:HD11	1:B:4331:ILE:HD11	1.28	1.07
1:A:4309:PHE:HE1	1:A:4338:ILE:HD11	1.19	1.05
2:C:106:LEU:HD22	2:C:126:ILE:HD11	1.38	1.04
1:A:3269:LEU:HB3	1:A:3633:LEU:CD1	1.89	1.03
1:B:4098:THR:OG1	2:D:113:LEU:CD2	2.05	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3791:SER:O	1:B:3521:GLU:N	1.89	1.03
1:B:4307:LYS:HG3	1:B:4475:MET:HE1	1.09	1.03
1:A:4309:PHE:CE1	1:A:4338:ILE:HD11	1.93	1.03
1:A:3532:CYS:HB3	1:A:3869:SER:H	1.25	1.02
1:B:3269:LEU:HB3	1:B:3633:LEU:CD1	1.89	1.02
2:D:103:ALA:HB2	2:D:126:ILE:HG13	1.41	1.01
1:A:3839:ALA:HB1	1:B:4500:GLN:NE2	1.74	1.00
1:A:4500:GLN:NE2	1:B:3839:ALA:HB1	1.78	0.97
1:A:3793:ASN:HA	1:B:3521:GLU:HG3	1.45	0.97
1:B:4309:PHE:CE1	1:B:4338:ILE:HD11	2.00	0.97
2:D:50:GLN:O	2:D:53:ILE:HG22	1.65	0.97
1:B:4648:ASP:HA	1:B:4717:PRO:HD2	1.46	0.96
1:B:4671:ASN:HB2	1:B:4732:GLN:OE1	1.66	0.96
1:A:4671:ASN:HB2	1:A:4732:GLN:OE1	1.66	0.95
1:B:4271:LEU:CD1	1:B:4331:ILE:HD11	1.98	0.94
1:A:4032:LYS:HE2	3:E:307:GLN:CG	1.81	0.94
1:A:3532:CYS:HB3	1:A:3869:SER:N	1.84	0.93
1:A:4309:PHE:CE1	1:A:4338:ILE:CD1	2.50	0.93
2:D:101:ILE:HB	2:D:137:VAL:HB	1.47	0.93
1:A:4271:LEU:CD1	1:A:4331:ILE:HD11	1.98	0.92
1:A:4032:LYS:HE3	3:E:307:GLN:HG3	0.93	0.92
2:C:24:GLY:HA3	2:C:28:ILE:HD12	1.52	0.91
1:A:3328:CYS:SG	1:A:3333:LEU:CD1	2.58	0.90
1:B:3328:CYS:SG	1:B:3333:LEU:CD1	2.58	0.90
1:A:4307:LYS:CG	1:A:4475:MET:HE3	2.02	0.90
2:C:138:ASN:HB3	2:C:140:GLU:HG2	1.53	0.90
1:A:3532:CYS:HG	4:A:5203:ZN:ZN	0.86	0.89
1:A:4307:LYS:CG	1:A:4478:VAL:HG21	2.02	0.89
1:A:3794:ARG:N	1:B:3521:GLU:OE2	2.04	0.89
1:B:3270:ILE:CD1	1:B:3632:PRO:CG	2.51	0.88
1:A:3535:CYS:SG	4:A:5203:ZN:ZN	1.62	0.88
1:A:3270:ILE:CD1	1:A:3632:PRO:CG	2.50	0.87
1:B:4307:LYS:CG	1:B:4475:MET:CE	2.52	0.87
1:A:4307:LYS:HG2	1:A:4478:VAL:HG21	1.58	0.86
2:C:69:PHE:CZ	2:C:73:MET:SD	2.67	0.86
2:C:106:LEU:CD2	2:C:126:ILE:HD11	2.05	0.86
1:B:4296:GLU:HG2	1:B:4334:ARG:HH22	1.40	0.86
1:B:3419:SER:O	1:B:3420:ASN:CG	2.19	0.85
1:B:3327:LEU:O	1:B:3392:CYS:SG	2.34	0.85
1:B:4309:PHE:HE1	1:B:4338:ILE:HD11	1.36	0.85
1:A:3419:SER:O	1:A:3420:ASN:CG	2.19	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3327:LEU:O	1:A:3392:CYS:SG	2.35	0.85
2:C:106:LEU:HD22	2:C:126:ILE:CD1	2.07	0.85
2:C:80:THR:O	2:C:81:ASP:OD1	1.94	0.85
1:B:4444:MET:HE3	1:B:4447:LEU:HD13	1.58	0.84
1:A:4275:LYS:NZ	1:A:4327:THR:HG21	1.93	0.84
1:A:4307:LYS:HG2	1:A:4475:MET:HE3	1.57	0.84
1:A:4444:MET:HE3	1:A:4447:LEU:HD13	1.58	0.84
2:D:106:LEU:HD22	2:D:126:ILE:CD1	2.09	0.83
1:A:3269:LEU:HB3	1:A:3633:LEU:HD11	1.61	0.83
1:A:3419:SER:O	1:A:3420:ASN:OD1	1.96	0.82
1:A:4714:LEU:HD11	1:A:4754:VAL:HG11	1.59	0.82
1:A:4232:LEU:HD13	1:B:3750:TYR:HB2	1.61	0.82
1:B:3419:SER:O	1:B:3420:ASN:OD1	1.96	0.82
1:B:4714:LEU:HD11	1:B:4754:VAL:HG11	1.59	0.82
1:B:3979:ILE:HG21	1:B:4019:ILE:HG23	1.62	0.82
1:B:4275:LYS:NZ	1:B:4327:THR:HG21	1.94	0.82
1:B:4307:LYS:HG2	1:B:4475:MET:HE1	1.60	0.81
1:A:3839:ALA:HB1	1:B:4500:GLN:HE21	1.41	0.81
1:B:3269:LEU:HB3	1:B:3633:LEU:HD11	1.61	0.81
1:B:3516:LEU:HD22	1:B:3799:LEU:HD21	1.63	0.81
1:A:4500:GLN:HE21	1:B:3839:ALA:HB1	1.46	0.81
1:A:3997:PHE:HB2	1:A:4016:CYS:HB3	1.63	0.80
1:B:3270:ILE:HD13	1:B:3632:PRO:CG	2.11	0.80
2:C:49:LEU:C	2:C:49:LEU:HD13	2.06	0.80
1:B:4313:CYS:HB3	1:B:4331:ILE:HG23	1.64	0.79
1:A:3516:LEU:HD22	1:A:3799:LEU:HD21	1.63	0.79
1:A:4632:GLN:HA	1:A:4681:LEU:HD21	1.62	0.79
1:B:3330:SER:HA	1:B:3333:LEU:HB2	1.64	0.79
1:A:4307:LYS:HD2	1:A:4478:VAL:CG2	2.12	0.79
1:A:3793:ASN:ND2	1:B:3519:LEU:O	2.12	0.79
1:B:3588:ARG:HD2	1:B:3646:ASP:OD2	1.83	0.79
2:D:106:LEU:CD2	2:D:126:ILE:HD11	2.12	0.79
1:A:3532:CYS:CB	1:A:3869:SER:H	1.96	0.78
1:A:3330:SER:HA	1:A:3333:LEU:HB2	1.64	0.78
1:A:3532:CYS:SG	4:A:5203:ZN:ZN	1.72	0.78
1:A:3588:ARG:HD2	1:A:3646:ASP:OD2	1.82	0.78
1:A:4029:PRO:O	1:A:4034:ASN:OD1	2.01	0.78
2:D:106:LEU:HD22	2:D:126:ILE:HD11	1.66	0.78
2:D:101:ILE:HD11	2:D:142:PHE:HD1	1.48	0.77
1:B:3315:VAL:HG22	1:B:3633:LEU:HD21	1.66	0.77
1:B:4027:PRO:HB2	3:F:313:ARG:HH21	1.49	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3968:LEU:CD1	1:A:4012:ILE:HD11	2.14	0.77
2:D:137:VAL:HG13	2:D:141:GLU:HB2	1.67	0.77
2:D:50:GLN:O	2:D:53:ILE:CG2	2.32	0.77
1:B:4307:LYS:HG2	1:B:4475:MET:CE	2.14	0.76
1:A:3315:VAL:HG22	1:A:3633:LEU:HD21	1.67	0.76
1:A:3793:ASN:HD22	1:B:3519:LEU:C	1.93	0.76
1:B:4108:PHE:CD1	2:D:148:ALA:HB3	2.21	0.76
1:B:4105:TRP:CZ3	2:D:106:LEU:HD11	2.21	0.76
1:A:4108:PHE:CD1	2:C:148:ALA:HB3	2.21	0.76
1:A:3951:VAL:HG13	1:A:4012:ILE:HD13	1.67	0.75
1:B:4296:GLU:HG2	1:B:4334:ARG:NH2	2.01	0.75
2:C:140:GLU:HG3	2:C:141:GLU:HG3	1.68	0.75
1:A:3054:VAL:HA	1:A:3057:ARG:HD2	1.68	0.75
1:A:3532:CYS:HB2	1:A:3868:SER:HA	1.68	0.75
1:A:3955:LEU:HD21	1:A:4012:ILE:HD12	1.67	0.75
1:A:3270:ILE:HD13	1:A:3632:PRO:CG	2.10	0.74
1:A:3240:ILE:HD11	1:A:3275:HIS:HB2	1.70	0.74
1:A:4105:TRP:CD1	2:C:145:MET:HG3	2.22	0.74
1:B:3054:VAL:HA	1:B:3057:ARG:HD2	1.68	0.74
1:A:3965:ALA:HA	1:A:4011:ASN:HD21	1.53	0.74
1:A:4307:LYS:CD	1:A:4475:MET:HE1	2.16	0.74
1:A:4310:MET:HG3	1:A:4335:LEU:HD23	1.70	0.74
1:A:3459:PRO:HA	1:A:3879:VAL:HG21	1.69	0.74
1:B:3459:PRO:HA	1:B:3879:VAL:HG21	1.69	0.74
1:A:3954:ALA:HB3	1:A:3968:LEU:HD11	1.70	0.73
1:B:4105:TRP:CD1	2:D:145:MET:HG3	2.22	0.73
1:B:4127:ASN:HD21	1:B:4165:LEU:HD21	1.53	0.73
2:C:139:TYR:O	2:C:143:VAL:HG23	1.88	0.73
2:C:140:GLU:HG3	2:C:141:GLU:N	2.04	0.73
1:B:3240:ILE:HD11	1:B:3275:HIS:HB2	1.70	0.73
2:C:69:PHE:CE1	2:C:73:MET:SD	2.82	0.72
1:B:4105:TRP:HZ2	2:D:129:ALA:HB2	1.55	0.72
1:A:4310:MET:CG	1:A:4335:LEU:HD23	2.19	0.72
2:C:24:GLY:CA	2:C:28:ILE:HD12	2.20	0.71
1:A:3793:ASN:HA	1:B:3521:GLU:CG	2.21	0.71
1:B:3547:LEU:HD13	1:B:3715:LEU:HD11	1.73	0.71
1:A:3968:LEU:HD12	1:A:4012:ILE:HD11	1.72	0.71
1:A:3791:SER:HB3	1:B:3521:GLU:O	1.91	0.71
2:D:147:THR:O	2:D:148:ALA:C	2.34	0.71
1:A:3518:GLY:HA2	1:B:3770:ALA:HB1	1.73	0.70
1:A:3791:SER:HB3	1:B:3804:CYS:SG	2.31	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3270:ILE:HD12	1:B:3632:PRO:HG2	1.72	0.70
2:C:147:THR:O	2:C:148:ALA:C	2.34	0.70
1:B:4598:LEU:HD12	1:B:4634:LEU:HD22	1.73	0.70
1:A:4011:ASN:O	1:A:4015:MET:HG2	1.90	0.70
2:C:137:VAL:HG13	2:C:141:GLU:HB2	1.73	0.69
2:D:118:THR:O	2:D:122:VAL:HG23	1.90	0.69
1:A:4492:LEU:HD12	1:A:4512:PHE:HE2	1.57	0.69
1:A:3836:ARG:O	1:A:3840:THR:OG1	2.11	0.69
1:B:4492:LEU:HD12	1:B:4512:PHE:HE2	1.57	0.69
1:B:3556:TYR:O	1:B:3606:LYS:HE3	1.93	0.68
1:A:4105:TRP:HZ2	2:C:129:ALA:HB2	1.58	0.68
1:A:3270:ILE:HD12	1:A:3632:PRO:HG2	1.72	0.68
1:B:3836:ARG:O	1:B:3840:THR:OG1	2.11	0.68
1:B:4238:LEU:HG	1:B:4287:THR:HG21	1.74	0.68
1:B:4314:ILE:HG21	1:B:4484:GLY:HA2	1.74	0.68
1:A:4232:LEU:HD12	1:B:3750:TYR:CG	2.29	0.68
1:A:4238:LEU:HG	1:A:4287:THR:HG21	1.74	0.68
1:B:4123:LEU:HD13	1:B:4165:LEU:HD22	1.75	0.68
2:C:140:GLU:HG3	2:C:141:GLU:H	1.59	0.68
1:A:3556:TYR:O	1:A:3606:LYS:HE3	1.93	0.68
1:B:4314:ILE:HD12	1:B:4482:CYS:SG	2.34	0.68
1:A:4037:VAL:HG13	1:A:4038:PRO:HD3	1.76	0.67
1:B:3244:LEU:HB3	1:B:3249:ILE:HB	1.75	0.67
1:B:4643:ASN:HB3	1:B:4646:LYS:HB3	1.77	0.67
2:C:24:GLY:HA3	2:C:28:ILE:CD1	2.24	0.67
1:A:3258:ALA:HB3	1:A:3847:VAL:HG22	1.75	0.67
1:B:3258:ALA:HB3	1:B:3847:VAL:HG22	1.75	0.67
1:A:4232:LEU:HD12	1:B:3750:TYR:CD2	2.30	0.67
1:A:4307:LYS:CD	1:A:4475:MET:CE	2.71	0.67
1:A:3244:LEU:HB3	1:A:3249:ILE:HB	1.76	0.66
1:A:3839:ALA:CB	1:B:4500:GLN:NE2	2.55	0.66
1:A:4094:HIS:O	1:A:4098:THR:HG23	1.96	0.66
1:B:4094:HIS:O	1:B:4098:THR:HG23	1.95	0.66
1:A:4089:LYS:HA	1:A:4092:LEU:HD12	1.77	0.66
1:B:4314:ILE:CD1	1:B:4479:MET:SD	2.77	0.66
1:A:3190:TRP:H	1:A:3190:TRP:CD1	2.12	0.66
1:A:3940:THR:HG21	1:A:3985:CYS:HB3	1.76	0.66
1:B:3241:LYS:O	1:B:3245:GLU:HG2	1.95	0.66
1:B:4309:PHE:CD1	1:B:4338:ILE:HD11	2.30	0.66
1:A:3241:LYS:O	1:A:3245:GLU:HG2	1.95	0.66
1:B:3527:LEU:HD21	1:B:3757:ARG:HD3	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3270:ILE:HD12	1:A:3632:PRO:CG	2.26	0.65
1:A:3826:LYS:N	1:B:4228:LEU:CD1	2.55	0.65
1:B:3190:TRP:CD1	1:B:3190:TRP:H	2.12	0.65
1:B:3290:TRP:NE1	1:B:3326:ALA:HB2	2.12	0.65
1:B:3408:LEU:HD12	1:B:3411:PHE:HE2	1.61	0.65
1:A:4495:ILE:HG21	1:A:4505:LEU:HD12	1.78	0.65
1:A:4600:GLN:HB3	1:A:4606:VAL:HG21	1.79	0.65
1:A:3290:TRP:NE1	1:A:3326:ALA:HB2	2.11	0.65
1:A:3408:LEU:HD12	1:A:3411:PHE:HE2	1.62	0.65
1:B:3497:LEU:HD11	1:B:3913:ASN:HD21	1.62	0.65
1:B:4307:LYS:HG2	1:B:4478:VAL:HG21	1.78	0.65
1:A:3447:LEU:HA	1:A:3450:LEU:HD12	1.79	0.64
1:B:3994:LEU:HD23	1:B:4060:LEU:HD21	1.78	0.64
1:B:3270:ILE:HD12	1:B:3632:PRO:CG	2.26	0.64
2:C:137:VAL:HA	2:C:141:GLU:OE1	1.98	0.64
1:A:4228:LEU:CD1	1:B:3826:LYS:N	2.54	0.64
1:B:4495:ILE:HG21	1:B:4505:LEU:HD12	1.78	0.64
1:B:3803:TYR:HA	1:B:3807:CYS:HB2	1.80	0.64
1:A:3211:ARG:HH21	1:A:3228:ARG:HH22	1.45	0.64
1:A:3818:ILE:HD12	1:B:4230:THR:CG2	2.28	0.64
2:C:140:GLU:CG	2:C:141:GLU:H	2.10	0.64
1:A:3791:SER:CB	1:B:3804:CYS:SG	2.86	0.63
1:A:3792:VAL:O	1:A:3793:ASN:C	2.35	0.63
1:A:4309:PHE:HE1	1:A:4338:ILE:HD13	1.58	0.63
1:B:3447:LEU:HA	1:B:3450:LEU:HD12	1.80	0.63
1:B:4258:PHE:HE1	2:D:19:LEU:HD21	1.63	0.63
1:A:3803:TYR:HA	1:A:3807:CYS:HB2	1.80	0.63
1:A:4310:MET:CG	1:A:4335:LEU:CD2	2.77	0.63
1:A:4307:LYS:CD	1:A:4478:VAL:CG2	2.77	0.63
1:A:4500:GLN:NE2	1:B:3839:ALA:O	2.32	0.63
1:B:3211:ARG:HH21	1:B:3228:ARG:HH22	1.44	0.63
1:A:3464:LYS:HE3	1:A:3534:VAL:HG13	1.81	0.63
1:A:3497:LEU:HD11	1:A:3913:ASN:HD21	1.62	0.63
1:A:3905:LEU:HD23	1:A:3932:LEU:HD11	1.81	0.63
1:A:4307:LYS:HD2	1:A:4478:VAL:HG22	1.81	0.63
2:C:140:GLU:CG	2:C:141:GLU:N	2.62	0.62
2:C:143:VAL:O	2:C:144:GLN:C	2.42	0.62
2:D:21:ASP:HA	2:D:28:ILE:HA	1.80	0.62
2:D:106:LEU:CD2	2:D:126:ILE:CD1	2.74	0.62
2:D:143:VAL:O	2:D:144:GLN:C	2.41	0.62
2:D:122:VAL:O	2:D:126:ILE:HG12	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3273:MET:HE1	1:A:3318:VAL:HG21	1.82	0.62
1:A:4228:LEU:HB3	1:B:3822:PHE:CD1	2.35	0.62
1:A:4232:LEU:CD1	1:B:3750:TYR:CG	2.82	0.62
1:B:4295:LEU:HD11	1:B:4309:PHE:HE2	1.64	0.62
1:B:3273:MET:HE1	1:B:3318:VAL:HG21	1.81	0.62
1:B:3850:THR:HG22	1:B:3853:ALA:HB3	1.82	0.62
2:D:29:THR:HG23	2:D:31:LYS:HB2	1.81	0.62
1:A:4230:THR:CG2	1:B:3818:ILE:HD12	2.28	0.62
1:A:3791:SER:O	1:B:3521:GLU:CA	2.47	0.61
1:A:3825:ARG:NH1	1:B:4278:VAL:O	2.33	0.61
1:A:3822:PHE:CD1	1:B:4228:LEU:HB3	2.36	0.61
1:A:3850:THR:HG22	1:A:3853:ALA:HB3	1.82	0.61
1:A:3965:ALA:O	1:A:3969:GLN:HB2	1.99	0.61
1:A:4032:LYS:HE3	3:E:307:GLN:CB	2.29	0.61
1:B:4313:CYS:HB3	1:B:4331:ILE:CG2	2.29	0.61
1:A:3794:ARG:HB3	1:B:3521:GLU:OE2	2.00	0.61
1:A:4500:GLN:NE2	1:B:3839:ALA:CB	2.58	0.61
2:C:33:LEU:CD2	2:C:72:MET:HE1	2.30	0.61
1:A:3332:VAL:HG21	1:A:3434:HIS:NE2	2.15	0.61
1:A:4032:LYS:HB3	1:A:4035:LYS:HD2	1.83	0.61
2:C:49:LEU:C	2:C:49:LEU:CD1	2.74	0.61
1:B:3332:VAL:HG21	1:B:3434:HIS:NE2	2.15	0.60
2:C:33:LEU:HD21	2:C:72:MET:HE1	1.83	0.60
1:B:4022:LYS:O	1:B:4023:LEU:C	2.42	0.60
2:C:10:ILE:HG13	2:C:66:PHE:HZ	1.67	0.60
1:A:4278:VAL:O	1:B:3825:ARG:NH1	2.33	0.60
2:D:50:GLN:C	2:D:53:ILE:HG22	2.26	0.60
1:A:3201:GLN:HA	1:A:3207:ARG:HH21	1.68	0.59
1:A:4130:ARG:HA	1:A:4133:LEU:HB2	1.84	0.59
1:A:4134:PHE:O	1:A:4135:THR:C	2.44	0.59
3:F:302:SER:O	3:F:306:ARG:N	2.34	0.59
1:A:4029:PRO:HB2	1:A:4034:ASN:HA	1.85	0.59
1:B:3894:PRO:O	1:B:3898:HIS:ND1	2.35	0.59
2:C:100:TYR:HB3	2:C:136:GLN:HB3	1.85	0.59
1:A:3240:ILE:HD11	1:A:3275:HIS:CB	2.33	0.59
1:A:3270:ILE:O	1:A:3274:GLU:HG2	2.03	0.59
1:A:3792:VAL:C	1:B:3521:GLU:HG3	2.27	0.59
1:A:4429:TRP:CE2	1:A:4438:MET:HA	2.38	0.59
1:B:4096:TYR:CE1	2:D:48:GLU:HG2	2.38	0.59
1:A:3901:VAL:HG11	1:A:3939:ALA:HB2	1.84	0.59
1:B:4429:TRP:CE2	1:B:4438:MET:HA	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3270:ILE:O	1:B:3274:GLU:HG2	2.03	0.58
2:C:141:GLU:O	2:C:144:GLN:HB3	2.02	0.58
1:A:4643:ASN:HB3	1:A:4646:LYS:HB3	1.85	0.58
2:C:93:PHE:HB3	2:C:101:ILE:HD12	1.85	0.58
1:A:4277:VAL:HG21	1:B:3732:ARG:HH22	1.68	0.58
1:B:3240:ILE:HD11	1:B:3275:HIS:CB	2.33	0.58
1:B:3683:GLN:OE1	1:B:3688:ARG:HD2	2.03	0.58
2:D:106:LEU:HD22	2:D:126:ILE:HD13	1.83	0.58
1:B:3299:SER:O	1:B:3303:PHE:HB3	2.04	0.58
1:B:4105:TRP:HZ3	2:D:106:LEU:HD11	1.67	0.58
1:B:4109:LEU:HD12	1:B:4114:LYS:HB2	1.85	0.58
1:B:4714:LEU:CD1	1:B:4754:VAL:HG11	2.32	0.58
2:D:111:THR:HA	2:D:115:GLU:O	2.04	0.58
1:A:3001:GLN:O	1:A:3005:MET:HG2	2.04	0.58
1:A:3683:GLN:OE1	1:A:3688:ARG:HD2	2.03	0.58
1:A:3469:VAL:HG21	1:A:3882:HIS:HB3	1.86	0.58
1:A:3792:VAL:CG1	1:A:3793:ASN:N	2.66	0.58
1:A:3965:ALA:HA	1:A:4011:ASN:ND2	2.18	0.58
1:A:4271:LEU:HD11	1:A:4331:ILE:CD1	2.19	0.58
2:D:78:LYS:HB3	2:D:80:THR:HG23	1.84	0.58
2:D:106:LEU:HD23	2:D:126:ILE:HD11	1.86	0.58
1:A:4101:TYR:CD2	2:C:89:ALA:HB2	2.39	0.58
1:A:4307:LYS:HG3	1:A:4475:MET:HE1	0.64	0.58
1:A:3732:ARG:HH22	1:B:4277:VAL:HG21	1.68	0.58
1:A:4032:LYS:HE3	3:E:307:GLN:CA	2.34	0.58
1:B:4295:LEU:O	1:B:4299:THR:HG23	2.03	0.58
2:C:49:LEU:HD11	2:C:53:ILE:HD12	1.85	0.58
1:A:3327:LEU:HD12	1:A:3431:LEU:HD11	1.85	0.58
1:B:3679:GLU:CD	1:B:3683:GLN:HE22	2.11	0.58
1:B:3754:MET:O	1:B:3758:PRO:HD3	2.04	0.58
2:D:20:PHE:HB3	2:D:32:GLU:HB3	1.86	0.58
1:A:3839:ALA:O	1:B:4500:GLN:NE2	2.36	0.58
1:A:4307:LYS:HD3	1:A:4475:MET:SD	2.43	0.58
1:A:3679:GLU:CD	1:A:3683:GLN:HE22	2.11	0.57
1:B:4263:VAL:HG12	1:B:4312:VAL:HG11	1.85	0.57
1:A:3792:VAL:HG12	1:A:3793:ASN:N	2.19	0.57
1:A:3299:SER:O	1:A:3303:PHE:HB3	2.04	0.57
1:A:3894:PRO:O	1:A:3898:HIS:ND1	2.35	0.57
1:B:4314:ILE:CD1	1:B:4482:CYS:SG	2.92	0.57
1:B:4355:LYS:HE3	1:B:4365:GLY:O	2.04	0.57
1:B:3034:MET:SD	1:B:3034:MET:N	2.77	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3298:ASP:OD1	1:B:3298:ASP:N	2.38	0.57
1:A:3979:ILE:HG12	1:A:3989:ARG:HB3	1.86	0.57
1:B:3327:LEU:HD12	1:B:3431:LEU:HD11	1.85	0.57
1:A:3964:LEU:HD23	1:A:4011:ASN:HD22	1.70	0.57
1:A:4307:LYS:CB	1:A:4478:VAL:HG21	2.34	0.57
1:B:3469:VAL:HG21	1:B:3882:HIS:HB3	1.86	0.57
1:B:4492:LEU:HD12	1:B:4512:PHE:CE2	2.40	0.57
2:D:101:ILE:HD11	2:D:142:PHE:CD1	2.34	0.57
1:A:3324:SER:O	1:A:3328:CYS:SG	2.62	0.57
1:B:3001:GLN:O	1:B:3005:MET:HG2	2.04	0.57
1:B:3964:LEU:HD23	1:B:4011:ASN:HD22	1.70	0.57
1:B:4314:ILE:HD13	1:B:4484:GLY:HA3	1.86	0.57
1:A:3290:TRP:HE1	1:A:3326:ALA:HB2	1.70	0.57
1:A:4714:LEU:CD1	1:A:4754:VAL:HG11	2.32	0.57
1:A:4355:LYS:HE3	1:A:4365:GLY:O	2.04	0.56
1:B:4419:LEU:HD13	1:B:4459:LEU:HG	1.87	0.56
2:D:59:ASP:HB2	2:D:63:THR:HG21	1.87	0.56
1:A:4492:LEU:HD12	1:A:4512:PHE:CE2	2.40	0.56
1:A:3972:MET:HE2	1:A:4015:MET:HB2	1.86	0.56
1:A:4313:CYS:HB3	1:A:4331:ILE:HG23	1.87	0.56
1:B:4602:ASN:HA	1:B:4607:ARG:HH21	1.71	0.56
1:A:4232:LEU:HD13	1:B:3750:TYR:CB	2.33	0.56
3:E:302:SER:O	3:E:306:ARG:N	2.34	0.56
1:A:4713:PHE:HE1	1:A:4751:LEU:HD21	1.71	0.56
1:B:3324:SER:O	1:B:3328:CYS:SG	2.62	0.56
1:B:4271:LEU:HD11	1:B:4331:ILE:CD1	2.18	0.56
1:A:4423:GLU:HB3	1:A:4459:LEU:HD13	1.88	0.56
2:C:124:GLU:O	2:C:128:GLU:HG2	2.06	0.56
1:A:3187:ASP:OD1	1:A:3190:TRP:NE1	2.39	0.56
1:B:3290:TRP:HE1	1:B:3326:ALA:HB2	1.70	0.56
1:A:4024:ILE:HD11	3:E:324:LEU:HD12	1.88	0.56
1:A:4130:ARG:HB2	1:A:4169:TYR:CE1	2.41	0.56
1:B:3662:ARG:NH2	1:B:3679:GLU:OE2	2.39	0.56
1:B:4307:LYS:HE3	1:B:4475:MET:SD	2.45	0.56
1:B:4105:TRP:CZ3	2:D:106:LEU:CD1	2.87	0.56
1:A:4602:ASN:HA	1:A:4607:ARG:HH21	1.71	0.55
3:E:301:MET:O	3:E:306:ARG:NH1	2.39	0.55
1:B:3409:ILE:HG12	1:B:3450:LEU:HD22	1.88	0.55
1:B:4129:LEU:HD21	1:B:4149:VAL:HG22	1.86	0.55
1:B:4105:TRP:HZ3	2:D:106:LEU:CD1	2.18	0.55
1:B:4131:GLN:O	1:B:4135:THR:HG23	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4258:PHE:CE1	2:D:19:LEU:HD21	2.40	0.55
1:B:4713:PHE:HE1	1:B:4751:LEU:HD21	1.71	0.55
3:F:301:MET:O	3:F:306:ARG:NH1	2.39	0.55
1:A:4105:TRP:CD2	2:C:145:MET:HE2	2.42	0.55
1:B:3201:GLN:HA	1:B:3207:ARG:HH21	1.72	0.55
1:B:4594:LEU:O	1:B:4598:LEU:HG	2.06	0.55
2:D:137:VAL:CG1	2:D:141:GLU:HB2	2.35	0.55
1:A:3662:ARG:NH2	1:A:3679:GLU:OE2	2.39	0.55
1:A:3833:LEU:HD12	1:A:3836:ARG:NH2	2.22	0.55
1:B:3833:LEU:HD12	1:B:3836:ARG:NH2	2.22	0.55
1:A:3292:LYS:O	1:A:3295:ILE:HG22	2.07	0.55
1:B:4045:VAL:HG21	1:B:4075:LEU:HB2	1.89	0.55
1:A:3409:ILE:HG12	1:A:3450:LEU:HD22	1.88	0.55
1:B:4423:GLU:HB3	1:B:4459:LEU:HD13	1.88	0.55
2:D:137:VAL:HG13	2:D:141:GLU:CB	2.36	0.55
1:A:4595:VAL:HG21	1:A:4630:LYS:HA	1.88	0.55
1:B:3292:LYS:O	1:B:3295:ILE:HG22	2.07	0.55
1:B:4105:TRP:CD2	2:D:145:MET:HE2	2.42	0.55
1:A:3954:ALA:CB	1:A:3968:LEU:HD21	2.37	0.54
1:B:3955:LEU:HD21	1:B:4012:ILE:HD12	1.89	0.54
1:B:4017:LEU:HD11	1:B:4132:VAL:HG11	1.88	0.54
2:D:28:ILE:HD12	2:D:33:LEU:HA	1.88	0.54
1:B:3187:ASP:OD1	1:B:3190:TRP:NE1	2.39	0.54
1:A:3521:GLU:HG3	1:B:3793:ASN:HA	1.89	0.54
1:A:4295:LEU:O	1:A:4299:THR:HG23	2.07	0.54
1:A:3298:ASP:N	1:A:3298:ASP:OD1	2.38	0.54
1:A:4263:VAL:HG12	1:A:4312:VAL:HG11	1.89	0.54
1:B:4129:LEU:HD23	1:B:4165:LEU:HD23	1.90	0.54
1:B:4355:LYS:CE	1:B:4365:GLY:O	2.56	0.54
1:A:3757:ARG:HB3	1:A:3758:PRO:HD3	1.88	0.54
1:B:4107:GLN:O	1:B:4111:ARG:HG2	2.07	0.54
1:B:4647:TYR:HD1	1:B:4717:PRO:HB2	1.72	0.54
1:A:3034:MET:SD	1:A:3034:MET:N	2.77	0.54
1:A:4105:TRP:CZ2	2:C:129:ALA:HB2	2.42	0.54
1:A:4107:GLN:O	1:A:4111:ARG:HG2	2.07	0.54
1:B:3706:CYS:O	1:B:3710:ARG:NH1	2.41	0.54
1:B:4595:VAL:HG21	1:B:4630:LYS:HB3	1.90	0.54
1:B:3881:GLU:HG2	1:B:3921:MET:HG3	1.88	0.54
1:B:4642:CYS:HA	1:B:4659:LEU:HD13	1.90	0.54
1:A:3706:CYS:O	1:A:3710:ARG:NH1	2.41	0.54
1:A:4032:LYS:HE3	3:E:307:GLN:HA	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4355:LYS:CE	1:A:4365:GLY:O	2.56	0.54
1:A:3881:GLU:HG2	1:A:3921:MET:HG3	1.89	0.53
1:A:4123:LEU:HD13	1:A:4165:LEU:HD22	1.90	0.53
1:B:4309:PHE:CD1	1:B:4338:ILE:CD1	2.91	0.53
2:C:33:LEU:CD1	2:C:72:MET:HE1	2.38	0.53
1:A:3513:TYR:CZ	1:A:3525:TYR:HB3	2.44	0.53
1:A:3818:ILE:HD12	1:B:4230:THR:HG21	1.90	0.53
1:A:4307:LYS:CG	1:A:4478:VAL:CG2	2.84	0.53
1:A:4309:PHE:CE1	1:A:4338:ILE:HD13	2.38	0.53
1:B:4314:ILE:HG22	1:B:4318:LYS:HE3	1.91	0.53
2:D:109:VAL:O	2:D:113:LEU:HG	2.07	0.53
1:B:4423:GLU:CB	1:B:4459:LEU:HD13	2.38	0.53
2:D:117:LEU:HB3	2:D:121:GLU:HB2	1.91	0.53
1:A:3512:ILE:O	1:A:3516:LEU:HG	2.08	0.53
1:A:4228:LEU:HB3	1:B:3822:PHE:CE1	2.42	0.53
1:A:4230:THR:HG21	1:B:3818:ILE:HD12	1.90	0.53
1:A:3793:ASN:CA	1:B:3521:GLU:HG3	2.30	0.53
1:A:3822:PHE:CE1	1:B:4228:LEU:HB3	2.44	0.53
1:B:3512:ILE:O	1:B:3516:LEU:HG	2.08	0.53
1:B:4547:GLU:HG2	1:B:4605:PHE:CE2	2.44	0.53
2:C:59:ASP:HB3	2:C:63:THR:HB	1.89	0.53
1:A:3547:LEU:O	1:A:3551:LYS:HG3	2.09	0.53
1:A:4307:LYS:HB3	1:A:4478:VAL:HG21	1.91	0.53
1:B:4129:LEU:HB3	1:B:4169:TYR:HE2	1.74	0.53
1:B:4314:ILE:CG2	1:B:4484:GLY:HA2	2.39	0.53
1:A:4245:LEU:HD23	1:A:4294:MET:HE1	1.90	0.53
1:B:3408:LEU:HD12	1:B:3411:PHE:CE2	2.44	0.53
1:B:3404:ASP:N	1:B:3404:ASP:OD1	2.41	0.53
1:B:3419:SER:HB3	1:B:3425:ARG:HG3	1.91	0.53
1:B:3751:HIS:O	1:B:3755:GLY:N	2.42	0.53
2:C:30:THR:HB	2:C:53:ILE:HG12	1.90	0.53
1:A:4105:TRP:CE2	2:C:145:MET:HE2	2.44	0.52
1:B:4306:THR:HG22	1:B:4338:ILE:CG2	2.40	0.52
2:D:138:ASN:CG	2:D:139:TYR:H	2.17	0.52
1:A:4096:TYR:CE1	2:C:48:GLU:HG2	2.44	0.52
1:B:3547:LEU:O	1:B:3551:LYS:HG3	2.09	0.52
1:A:4032:LYS:CE	3:E:307:GLN:HG2	2.28	0.52
1:B:3199:MET:HE1	1:B:3232:THR:HA	1.90	0.52
1:B:3763:LEU:O	1:B:3767:VAL:HG23	2.10	0.52
1:B:4245:LEU:HD23	1:B:4294:MET:HE1	1.90	0.52
1:A:3535:CYS:SG	1:A:3872:CYS:SG	3.07	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3513:TYR:CZ	1:B:3525:TYR:HB3	2.44	0.52
1:B:4017:LEU:CD1	1:B:4132:VAL:HG11	2.40	0.52
1:B:4195:HIS:CD2	2:D:35:THR:HG21	2.45	0.52
2:C:78:LYS:HB2	2:C:80:THR:HG23	1.90	0.52
2:D:105:GLU:HA	2:D:108:HIS:HB2	1.91	0.52
1:B:3309:PHE:HE1	1:B:3411:PHE:HB3	1.74	0.52
1:B:4309:PHE:CE1	1:B:4338:ILE:CD1	2.85	0.52
1:A:3324:SER:OG	1:A:3333:LEU:HD11	2.10	0.52
1:A:3771:ALA:HB1	1:B:3919:ALA:HB2	1.91	0.52
1:B:3749:VAL:O	1:B:3750:TYR:C	2.52	0.52
2:C:49:LEU:HD13	2:C:49:LEU:O	2.09	0.52
3:F:324:LEU:O	3:F:328:LEU:HG	2.10	0.52
1:A:3727:GLU:H	1:A:3731:ASP:HB2	1.75	0.52
1:A:4195:HIS:CD2	2:C:35:THR:HG21	2.44	0.52
1:A:4310:MET:HG2	1:A:4335:LEU:CD2	2.40	0.52
1:B:3324:SER:OG	1:B:3333:LEU:HD11	2.10	0.52
1:B:4048:TYR:HD1	1:B:4048:TYR:H	1.58	0.52
1:B:4647:TYR:OH	1:B:4656:LYS:HA	2.09	0.52
2:D:145:MET:SD	2:D:146:MET:N	2.83	0.52
1:A:3309:PHE:HE1	1:A:3411:PHE:HB3	1.74	0.52
1:B:4306:THR:HG22	1:B:4338:ILE:HG23	1.92	0.52
2:D:117:LEU:O	2:D:118:THR:C	2.53	0.52
1:A:3419:SER:HB3	1:A:3425:ARG:HG3	1.92	0.51
1:B:3936:ASN:HB3	1:B:3939:ALA:HB3	1.93	0.51
1:B:4105:TRP:CE2	2:D:145:MET:HE2	2.44	0.51
1:B:4155:ILE:HB	1:B:4158:ARG:HD2	1.92	0.51
1:A:3522:PHE:H	1:A:3522:PHE:HD1	1.57	0.51
1:A:4423:GLU:CB	1:A:4459:LEU:HD13	2.39	0.51
1:B:3097:TYR:O	1:B:3101:VAL:HG12	2.10	0.51
1:B:3850:THR:CG2	1:B:3853:ALA:HB3	2.39	0.51
1:B:3965:ALA:HA	1:B:4011:ASN:ND2	2.24	0.51
2:C:49:LEU:HD11	2:C:53:ILE:CD1	2.40	0.51
1:A:3200:ILE:HG22	1:A:3202:GLN:H	1.75	0.51
1:A:4128:TRP:HA	1:A:4131:GLN:HG2	1.93	0.51
2:C:33:LEU:HD11	2:C:72:MET:HE1	1.91	0.51
2:C:145:MET:SD	2:C:146:MET:N	2.83	0.51
2:D:18:SER:O	2:D:21:ASP:N	2.41	0.51
1:A:3850:THR:CG2	1:A:3853:ALA:HB3	2.40	0.51
1:B:3405:LYS:HB2	1:B:3450:LEU:HD21	1.93	0.51
1:B:3458:LEU:HD11	1:B:3465:ALA:HB1	1.93	0.51
1:B:4282:LYS:O	1:B:4286:GLU:HG2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3097:TYR:O	1:A:3101:VAL:HG12	2.10	0.51
1:A:3968:LEU:N	1:A:3968:LEU:HD23	2.25	0.51
1:A:3998:LEU:O	1:A:4001:VAL:HG12	2.10	0.51
1:B:3200:ILE:HG22	1:B:3202:GLN:H	1.76	0.51
1:B:4129:LEU:HB3	1:B:4169:TYR:CE2	2.46	0.51
2:D:10:ILE:HA	2:D:13:PHE:CD2	2.46	0.51
1:B:3095:VAL:HG12	1:B:3190:TRP:CZ3	2.46	0.51
1:B:3226:GLN:HA	1:B:3289:ASN:ND2	2.26	0.51
2:C:106:LEU:CD2	2:C:126:ILE:CD1	2.80	0.51
1:A:3053:LEU:HA	1:A:3056:MET:HE2	1.93	0.51
1:A:3536:ASN:O	1:A:3538:PRO:HD3	2.11	0.51
1:A:4130:ARG:HB2	1:A:4169:TYR:CZ	2.46	0.51
1:B:3440:SER:OG	1:B:3443:GLN:OE1	2.20	0.51
1:B:3519:LEU:HD13	1:B:3767:VAL:HG11	1.93	0.51
1:B:4643:ASN:O	1:B:4647:TYR:HB2	2.10	0.51
1:B:3053:LEU:HA	1:B:3056:MET:HE2	1.93	0.51
1:B:3954:ALA:HB3	1:B:3968:LEU:HD11	1.93	0.51
1:A:3818:ILE:HD12	1:B:4230:THR:HG23	1.92	0.51
1:A:4230:THR:HG23	1:B:3818:ILE:HD12	1.92	0.51
2:C:10:ILE:HA	2:C:13:PHE:CD2	2.46	0.51
2:D:100:TYR:CD1	2:D:136:GLN:HB2	2.46	0.50
3:E:324:LEU:O	3:E:328:LEU:HG	2.10	0.50
1:A:3405:LYS:HB2	1:A:3450:LEU:HD21	1.93	0.50
1:A:4155:ILE:HB	1:A:4158:ARG:HD2	1.92	0.50
1:B:3273:MET:HE3	1:B:3273:MET:O	2.11	0.50
1:B:4035:LYS:O	1:B:4036:ASP:C	2.54	0.50
1:B:4599:ASP:HA	1:B:4602:ASN:HD22	1.76	0.50
1:A:3307:VAL:O	1:A:3311:VAL:HG13	2.12	0.50
1:A:3458:LEU:HD11	1:A:3465:ALA:HB1	1.92	0.50
1:A:4282:LYS:O	1:A:4286:GLU:HG2	2.11	0.50
1:B:3307:VAL:O	1:B:3311:VAL:HG13	2.12	0.50
2:D:118:THR:OG1	2:D:120:GLU:HB2	2.12	0.50
1:A:4077:ILE:HG13	1:A:4079:GLY:H	1.76	0.50
1:B:4306:THR:CG2	1:B:4338:ILE:HG23	2.42	0.50
2:C:7:GLU:HA	2:C:10:ILE:HG22	1.93	0.50
1:A:3095:VAL:HG12	1:A:3190:TRP:CZ3	2.46	0.50
1:A:3212:LYS:HA	1:A:3215:LEU:HG	1.94	0.50
1:A:4108:PHE:O	1:A:4112:ARG:HG3	2.12	0.50
1:A:4307:LYS:CD	1:A:4478:VAL:HG21	2.40	0.50
1:A:4438:MET:HE3	1:A:4440:ILE:HD11	1.94	0.50
1:A:4492:LEU:CD1	1:A:4512:PHE:CE2	2.95	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4089:LYS:HA	1:B:4092:LEU:HD12	1.92	0.50
1:B:4307:LYS:HA	1:B:4310:MET:HE2	1.93	0.50
1:B:4492:LEU:CD1	1:B:4512:PHE:CE2	2.95	0.50
2:D:14:LYS:HD3	2:D:66:PHE:CD2	2.46	0.50
1:B:4310:MET:HE1	1:B:4478:VAL:HG21	1.94	0.49
2:C:44:PRO:HB2	2:C:48:GLU:HB2	1.94	0.49
2:D:87:ARG:HG3	2:D:139:TYR:HE1	1.77	0.49
1:A:3273:MET:HE3	1:A:3273:MET:O	2.11	0.49
1:A:3404:ASP:OD1	1:A:3404:ASP:N	2.41	0.49
1:A:3968:LEU:HD13	1:A:4012:ILE:HD11	1.92	0.49
1:B:3588:ARG:HG3	1:B:3648:TYR:CZ	2.47	0.49
1:A:4310:MET:HE1	1:A:4475:MET:HE3	1.94	0.49
1:B:4505:LEU:HD22	1:B:4558:VAL:HG11	1.93	0.49
2:C:65:ASP:H	2:C:68:GLU:HB3	1.78	0.49
3:E:309:MET:O	3:E:313:ARG:HG2	2.12	0.49
1:A:3726:ILE:HD12	1:A:3828:LEU:HA	1.94	0.49
1:A:4275:LYS:HZ2	1:A:4327:THR:HG21	1.72	0.49
1:A:4355:LYS:NZ	1:A:4363:LEU:O	2.40	0.49
1:B:3940:THR:HG21	1:B:3985:CYS:HB3	1.93	0.49
1:B:4523:GLN:NE2	1:B:4576:GLU:OE1	2.46	0.49
1:A:3408:LEU:HD12	1:A:3411:PHE:CE2	2.44	0.49
1:A:4098:THR:HA	2:C:93:PHE:CE2	2.47	0.49
1:B:4438:MET:HE3	1:B:4440:ILE:HD11	1.94	0.49
2:D:124:GLU:O	2:D:128:GLU:HG2	2.12	0.49
1:A:3324:SER:HG	1:A:3333:LEU:HD11	1.78	0.49
1:A:3548:SER:HA	1:A:3551:LYS:HE2	1.95	0.49
1:A:4001:VAL:C	1:A:4003:ILE:N	2.69	0.49
3:F:301:MET:SD	3:F:306:ARG:HG3	2.53	0.49
1:A:3262:SER:HA	1:A:3833:LEU:HD23	1.95	0.49
1:A:4310:MET:HG2	1:A:4335:LEU:HD23	1.92	0.49
1:A:4608:SER:O	1:A:4610:PRO:HD3	2.13	0.49
1:A:3412:LEU:HD22	1:A:3454:ILE:HD12	1.95	0.49
1:A:3850:THR:O	1:A:3851:PHE:C	2.56	0.49
1:A:4505:LEU:HD22	1:A:4558:VAL:HG11	1.93	0.49
1:B:3412:LEU:HD22	1:B:3454:ILE:HD12	1.95	0.49
1:A:3988:LEU:HD12	1:A:3988:LEU:H	1.77	0.48
3:E:301:MET:SD	3:E:306:ARG:HG3	2.53	0.48
1:A:4032:LYS:HE2	3:E:307:GLN:CD	2.38	0.48
1:B:3968:LEU:CD1	1:B:4012:ILE:HD11	2.43	0.48
1:B:4071:TRP:O	1:B:4075:LEU:HD12	2.13	0.48
1:A:3309:PHE:CE1	1:A:3411:PHE:HB3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3955:LEU:HD21	1:A:4012:ILE:CD1	2.41	0.48
1:B:4252:GLU:O	1:B:4256:ARG:HG3	2.13	0.48
2:D:105:GLU:O	2:D:109:VAL:HG23	2.14	0.48
2:D:145:MET:SD	2:D:146:MET:SD	3.12	0.48
1:A:3308:SER:HA	1:A:3319:LEU:HD13	1.95	0.48
1:A:4424:VAL:HA	1:A:4459:LEU:HD21	1.95	0.48
1:B:3292:LYS:HA	1:B:3295:ILE:HG22	1.96	0.48
2:C:132:ASP:OD1	2:C:133:GLY:N	2.47	0.48
2:D:103:ALA:HB2	2:D:126:ILE:CG1	2.30	0.48
1:A:4071:TRP:O	1:A:4075:LEU:HD12	2.13	0.48
1:B:4108:PHE:CE2	2:D:146:MET:O	2.66	0.48
3:F:309:MET:O	3:F:313:ARG:HG2	2.12	0.48
1:A:4252:GLU:O	1:A:4256:ARG:HG3	2.13	0.48
1:A:4310:MET:HE1	1:A:4475:MET:CE	2.44	0.48
1:B:3262:SER:HA	1:B:3833:LEU:HD23	1.95	0.48
1:B:3749:VAL:HA	1:B:3752:GLN:HG3	1.95	0.48
1:B:4021:GLN:HE21	1:B:4025:LYS:HE2	1.78	0.48
2:C:52:MET:O	2:C:56:VAL:HG22	2.13	0.48
2:D:7:GLU:HA	2:D:10:ILE:HG22	1.94	0.48
1:A:4159:LYS:HZ3	1:A:4196:TRP:CD1	2.31	0.48
1:A:3418:GLU:HG2	1:A:3461:TYR:CE1	2.49	0.48
1:A:4310:MET:HG3	1:A:4335:LEU:CD2	2.41	0.48
1:B:3169:TYR:HD1	1:B:3213:LEU:HD13	1.79	0.48
1:B:3226:GLN:OE1	1:B:3227:LEU:HD22	2.14	0.48
1:B:3309:PHE:CE1	1:B:3411:PHE:HB3	2.48	0.48
1:B:3964:LEU:HD22	1:B:4007:VAL:HG12	1.95	0.48
1:B:4053:HIS:CE1	1:B:4118:PRO:HB3	2.49	0.48
2:D:33:LEU:HD13	2:D:64:ILE:HG21	1.95	0.48
1:A:4299:THR:HG22	1:A:4309:PHE:CE2	2.49	0.48
1:B:4135:THR:O	1:B:4142:ARG:NH1	2.36	0.48
1:A:3169:TYR:HD1	1:A:3213:LEU:HD13	1.79	0.48
1:A:4108:PHE:CE2	2:C:146:MET:O	2.67	0.48
1:B:3955:LEU:HD12	1:B:3999:MET:HE3	1.96	0.48
1:B:4651:HIS:HD2	1:B:4656:LYS:HB2	1.78	0.48
2:C:100:TYR:CB	2:C:136:GLN:HB3	2.44	0.48
1:A:3071:LYS:HB3	1:A:3074:ILE:HB	1.95	0.47
1:A:4134:PHE:CD2	1:A:4172:GLU:HG2	2.49	0.47
1:B:4071:TRP:CE2	1:B:4075:LEU:HD11	2.49	0.47
1:A:3884:ILE:HD11	1:A:3913:ASN:HD22	1.79	0.47
1:A:3954:ALA:HB3	1:A:3968:LEU:HD21	1.96	0.47
1:A:4230:THR:CG2	1:B:3818:ILE:HG23	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3212:LYS:HA	1:B:3215:LEU:HG	1.95	0.47
1:B:3872:CYS:O	1:B:3873:TYR:C	2.57	0.47
1:B:3850:THR:O	1:B:3851:PHE:C	2.56	0.47
1:B:3884:ILE:HD11	1:B:3913:ASN:HD22	1.80	0.47
2:C:145:MET:SD	2:C:146:MET:SD	3.12	0.47
1:A:3533:LEU:HD12	1:A:3533:LEU:H	1.80	0.47
1:A:3588:ARG:HG3	1:A:3648:TYR:CZ	2.49	0.47
2:C:49:LEU:CD1	2:C:53:ILE:HD12	2.44	0.47
2:D:20:PHE:HE1	2:D:35:THR:CG2	2.26	0.47
1:A:3292:LYS:HA	1:A:3295:ILE:HG22	1.96	0.47
1:A:3872:CYS:O	1:A:3873:TYR:C	2.57	0.47
1:A:4071:TRP:CE2	1:A:4075:LEU:HD11	2.49	0.47
1:A:4129:LEU:HD11	1:A:4149:VAL:HG21	1.95	0.47
1:A:4695:MET:HE1	1:A:4748:LEU:HD21	1.96	0.47
1:B:3308:SER:HA	1:B:3319:LEU:HD13	1.96	0.47
1:B:3548:SER:HA	1:B:3551:LYS:HE2	1.95	0.47
1:B:4101:TYR:HB3	2:D:146:MET:SD	2.55	0.47
2:C:19:LEU:HD23	2:C:19:LEU:HA	1.77	0.47
1:A:4101:TYR:HB3	2:C:146:MET:SD	2.55	0.47
1:A:4119:LEU:HD23	3:E:329:VAL:HG21	1.96	0.47
1:A:4413:LYS:HD3	1:A:4456:ILE:HD11	1.96	0.47
1:B:3455:TRP:CZ3	1:B:3458:LEU:HD22	2.50	0.47
1:B:4275:LYS:HZ2	1:B:4327:THR:HG21	1.72	0.47
1:B:4642:CYS:SG	1:B:4643:ASN:N	2.88	0.47
1:B:4644:PHE:HB3	1:B:4694:TYR:CD2	2.49	0.47
2:C:66:PHE:HB3	2:C:67:PRO:HD3	1.97	0.47
1:A:3226:GLN:HA	1:A:3289:ASN:ND2	2.28	0.47
1:A:3456:PRO:HA	1:A:3496:ILE:HD11	1.96	0.47
1:A:4006:PRO:HG2	1:B:3507:HIS:O	2.14	0.47
1:A:4419:LEU:HD13	1:A:4459:LEU:HG	1.96	0.47
1:B:3417:LEU:HD13	1:B:3461:TYR:CD2	2.49	0.47
1:B:3515:THR:O	1:B:3519:LEU:HG	2.15	0.47
1:B:4109:LEU:HG	1:B:4115:ARG:HB2	1.97	0.47
1:B:4119:LEU:HD11	3:F:329:VAL:HG11	1.97	0.47
1:B:4311:ALA:O	1:B:4315:GLU:HG2	2.15	0.47
1:B:4413:LYS:HD3	1:B:4456:ILE:HD11	1.96	0.47
2:C:131:ILE:HD11	2:C:144:GLN:HG2	1.96	0.47
1:A:3005:MET:O	1:A:3008:THR:OG1	2.33	0.47
1:A:3571:ILE:HG12	1:A:3717:ALA:HB2	1.97	0.47
1:B:3194:LEU:HD13	1:B:3214:LEU:HD21	1.97	0.47
1:B:3324:SER:HG	1:B:3333:LEU:HD11	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3727:GLU:H	1:B:3731:ASP:HB2	1.80	0.47
1:B:3969:GLN:O	1:B:3973:LEU:HG	2.15	0.47
1:B:4307:LYS:HG2	1:B:4475:MET:HE3	1.96	0.47
2:D:102:SER:HB2	2:D:105:GLU:OE1	2.15	0.47
1:A:3298:ASP:HB3	1:A:3398:GLN:CD	2.39	0.47
1:B:3298:ASP:HB3	1:B:3398:GLN:CD	2.39	0.47
1:B:3456:PRO:HA	1:B:3496:ILE:HD11	1.96	0.47
1:A:3515:THR:O	1:A:3519:LEU:HG	2.15	0.47
1:A:3750:TYR:HB2	1:B:4232:LEU:HD13	1.22	0.47
2:C:28:ILE:HG22	2:C:32:GLU:HG2	1.96	0.47
2:D:103:ALA:CB	2:D:126:ILE:HG13	2.28	0.47
1:A:3226:GLN:OE1	1:A:3227:LEU:HD22	2.14	0.46
1:A:3417:LEU:HD13	1:A:3461:TYR:CD2	2.49	0.46
1:A:3732:ARG:NH2	1:B:4277:VAL:HG21	2.30	0.46
1:B:3004:LEU:O	1:B:3008:THR:HG23	2.16	0.46
1:B:3418:GLU:HG2	1:B:3461:TYR:CE1	2.49	0.46
1:A:3527:LEU:HD21	1:A:3757:ARG:HD3	1.98	0.46
1:B:3005:MET:O	1:B:3008:THR:OG1	2.33	0.46
2:D:119:ASP:HA	2:D:122:VAL:HG23	1.96	0.46
1:A:3090:LEU:HD11	1:A:3184:PRO:HB3	1.97	0.46
1:A:3419:SER:HB3	1:A:3425:ARG:CG	2.46	0.46
1:A:3793:ASN:ND2	1:B:3519:LEU:C	2.68	0.46
1:A:3848:GLN:C	1:A:3850:THR:H	2.24	0.46
1:B:3071:LYS:HB3	1:B:3074:ILE:HB	1.96	0.46
1:B:3301:LEU:HD23	1:B:3301:LEU:HA	1.76	0.46
1:B:3419:SER:HB3	1:B:3425:ARG:CG	2.45	0.46
1:B:3905:LEU:HD23	1:B:3932:LEU:HD11	1.96	0.46
1:A:3455:TRP:CZ3	1:A:3458:LEU:HD22	2.50	0.46
1:A:4001:VAL:C	1:A:4003:ILE:H	2.22	0.46
1:A:4101:TYR:HA	1:A:4104:ARG:HB2	1.97	0.46
1:A:4232:LEU:HD13	1:B:3750:TYR:CG	2.50	0.46
1:B:4639:LYS:HB2	1:B:4640:PRO:HD3	1.97	0.46
2:C:12:GLU:O	2:C:15:GLU:HB3	2.16	0.46
2:D:70:LEU:HA	2:D:73:MET:HG2	1.97	0.46
1:A:3887:LEU:HD13	1:A:3905:LEU:HD21	1.98	0.46
1:A:4419:LEU:HD22	1:A:4459:LEU:HD12	1.97	0.46
1:B:4634:LEU:HA	1:B:4637:ARG:HD2	1.98	0.46
1:B:4640:PRO:O	1:B:4643:ASN:ND2	2.48	0.46
2:D:42:GLN:OE1	2:D:77:MET:HG3	2.16	0.46
2:D:69:PHE:HA	2:D:72:MET:HE2	1.98	0.46
1:A:4281:THR:HG22	1:A:4283:LEU:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4640:PRO:C	1:A:4642:CYS:H	2.24	0.46
1:B:3305:LEU:HB2	1:B:3323:LEU:HD21	1.96	0.46
1:A:3301:LEU:HD23	1:A:3301:LEU:HA	1.76	0.46
1:A:3305:LEU:HB2	1:A:3323:LEU:HD21	1.96	0.46
1:A:3478:LYS:HD2	1:A:3478:LYS:HA	1.83	0.46
1:A:4195:HIS:NE2	2:C:35:THR:HG21	2.30	0.46
1:A:4631:MET:O	1:A:4634:LEU:HG	2.15	0.46
1:B:3909:LEU:HD22	1:B:3925:VAL:HG13	1.98	0.46
1:B:4310:MET:HE1	1:B:4478:VAL:CG2	2.45	0.46
1:B:4646:LYS:HE2	1:B:4651:HIS:HA	1.96	0.46
2:D:93:PHE:HB2	2:D:109:VAL:HG21	1.97	0.46
1:A:3226:GLN:HA	1:A:3289:ASN:HD22	1.81	0.46
1:A:4277:VAL:HG21	1:B:3732:ARG:NH2	2.30	0.46
1:A:4467:GLU:HB3	1:A:4472:VAL:HG21	1.98	0.46
1:B:3848:GLN:C	1:B:3850:THR:H	2.24	0.46
2:D:20:PHE:HD1	2:D:32:GLU:HB3	1.80	0.46
1:A:4310:MET:SD	1:A:4338:ILE:HD13	2.55	0.46
1:B:3190:TRP:CD1	1:B:3190:TRP:N	2.83	0.46
1:B:3910:PHE:HB2	1:B:3929:MET:HE1	1.97	0.46
1:B:4101:TYR:HA	1:B:4104:ARG:HB2	1.97	0.46
1:B:4281:THR:HG22	1:B:4283:LEU:H	1.81	0.46
1:B:4695:MET:HE1	1:B:4748:LEU:HD21	1.96	0.46
2:C:73:MET:O	2:C:77:MET:N	2.48	0.46
2:D:12:GLU:O	2:D:15:GLU:HB3	2.16	0.46
1:A:3234:ASP:O	1:A:3238:ARG:HG2	2.16	0.46
1:A:3791:SER:O	1:B:3521:GLU:HB2	2.16	0.46
1:A:3818:ILE:HG23	1:B:4230:THR:CG2	2.45	0.46
1:B:3757:ARG:HB3	1:B:3758:PRO:HD3	1.98	0.46
1:B:3840:THR:HG22	1:B:3843:SER:HB2	1.97	0.46
2:D:52:MET:CE	2:D:76:LYS:HB2	2.46	0.46
3:E:302:SER:OG	3:E:305:GLU:HB3	2.16	0.46
3:F:302:SER:OG	3:F:305:GLU:HB3	2.16	0.46
1:A:3825:ARG:HH21	1:B:4230:THR:HB	1.82	0.45
2:C:9:GLN:O	2:C:13:PHE:CG	2.70	0.45
1:A:3004:LEU:O	1:A:3008:THR:HG23	2.15	0.45
1:A:4128:TRP:HA	1:A:4131:GLN:CG	2.47	0.45
1:A:4639:LYS:HB3	1:A:4640:PRO:HD3	1.98	0.45
1:A:3909:LEU:HD22	1:A:3925:VAL:HG13	1.98	0.45
1:A:3910:PHE:HB2	1:A:3929:MET:HE1	1.97	0.45
1:B:3090:LEU:HD11	1:B:3184:PRO:HB3	1.97	0.45
1:B:3571:ILE:HG12	1:B:3717:ALA:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3714:MET:HE3	1:B:3714:MET:HB3	1.78	0.45
1:B:4047:PRO:O	1:B:4048:TYR:C	2.60	0.45
2:D:51:ASP:HA	2:D:54:ASN:HD22	1.81	0.45
1:A:3251:LEU:HD12	1:A:3303:PHE:CD2	2.52	0.45
1:A:3791:SER:C	1:B:3521:GLU:HB2	2.41	0.45
1:B:3328:CYS:O	1:B:3332:VAL:HG12	2.16	0.45
1:B:3965:ALA:HA	1:B:4011:ASN:HD21	1.81	0.45
1:B:4130:ARG:O	1:B:4131:GLN:C	2.60	0.45
1:B:4316:THR:HA	1:B:4319:ARG:HD2	1.97	0.45
2:D:121:GLU:O	2:D:125:MET:HG2	2.16	0.45
1:A:3194:LEU:HD13	1:A:3214:LEU:HD21	1.97	0.45
1:A:3195:SER:HG	1:A:3231:HIS:CE1	2.32	0.45
1:A:3328:CYS:O	1:A:3332:VAL:HG12	2.16	0.45
1:A:3626:GLU:OE1	1:A:3628:LYS:HE3	2.17	0.45
1:A:3880:THR:O	1:A:3884:ILE:HG12	2.16	0.45
1:A:4307:LYS:HD3	1:A:4475:MET:CE	2.46	0.45
1:B:3626:GLU:OE1	1:B:3628:LYS:HE3	2.17	0.45
1:B:4011:ASN:O	1:B:4015:MET:HG2	2.16	0.45
1:A:3840:THR:HG22	1:A:3843:SER:HB2	1.98	0.45
1:B:3766:LYS:HB3	1:B:3795:TYR:CD2	2.52	0.45
1:B:3887:LEU:HD13	1:B:3905:LEU:HD21	1.98	0.45
2:D:39:SER:C	2:D:41:GLY:H	2.25	0.45
1:A:3826:LYS:N	1:B:4228:LEU:HD12	2.31	0.45
1:A:4170:LEU:O	1:A:4173:LEU:HB3	2.17	0.45
1:B:4170:LEU:O	1:B:4173:LEU:HB3	2.17	0.45
2:C:138:ASN:C	2:C:140:GLU:N	2.71	0.45
2:D:120:GLU:O	2:D:123:ASP:HB2	2.17	0.45
1:A:3324:SER:OG	1:A:3328:CYS:SG	2.56	0.45
1:A:4098:THR:HB	2:C:109:VAL:HG13	1.99	0.45
1:A:4299:THR:HG21	1:A:4334:ARG:HH21	1.81	0.45
1:A:4360:GLU:CD	1:A:4366:ARG:HH21	2.24	0.45
1:A:4606:VAL:HG13	1:A:4612:VAL:HG12	1.98	0.45
1:B:3051:VAL:O	1:B:3055:VAL:HG23	2.17	0.45
1:B:4413:LYS:CD	1:B:4456:ILE:HD11	2.47	0.45
1:A:3051:VAL:O	1:A:3055:VAL:HG23	2.17	0.44
1:A:3440:SER:OG	1:A:3443:GLN:OE1	2.20	0.44
1:A:3532:CYS:CB	1:A:3868:SER:HA	2.43	0.44
1:A:4047:PRO:HA	1:A:4075:LEU:HD23	1.99	0.44
1:A:4310:MET:SD	1:A:4338:ILE:CG2	2.82	0.44
1:B:3273:MET:HG3	1:B:3633:LEU:CD2	2.48	0.44
1:B:3286:ARG:HH21	1:B:3286:ARG:HG3	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3642:ILE:HD13	1:B:3713:PHE:CE1	2.52	0.44
1:B:3880:THR:O	1:B:3884:ILE:HG12	2.16	0.44
1:B:3922:ARG:NH1	1:B:3970:TYR:OH	2.50	0.44
2:D:18:SER:O	2:D:19:LEU:C	2.60	0.44
2:D:101:ILE:N	2:D:137:VAL:O	2.46	0.44
1:A:3642:ILE:HD13	1:A:3713:PHE:CE1	2.52	0.44
1:A:3951:VAL:CG1	1:A:4012:ILE:HD13	2.44	0.44
1:B:4360:GLU:CD	1:B:4366:ARG:HH21	2.24	0.44
2:C:89:ALA:HB3	2:C:142:PHE:HE2	1.81	0.44
1:A:4101:TYR:CE2	2:C:89:ALA:HB2	2.52	0.44
1:A:4598:LEU:HD12	1:A:4634:LEU:HD22	1.99	0.44
1:B:3234:ASP:O	1:B:3238:ARG:HG2	2.16	0.44
1:B:3889:ALA:HB2	3:F:293:LEU:HD13	1.99	0.44
1:B:4093:ARG:NH2	2:D:51:ASP:OD2	2.51	0.44
2:D:9:GLN:O	2:D:13:PHE:CG	2.70	0.44
1:A:4228:LEU:HD12	1:B:3826:LYS:N	2.30	0.44
1:B:3461:TYR:O	1:B:3534:VAL:HG11	2.17	0.44
1:B:3950:LYS:O	1:B:3953:THR:HG22	2.18	0.44
2:D:56:VAL:HG13	2:D:72:MET:SD	2.57	0.44
1:A:3412:LEU:O	1:A:3416:LEU:HB2	2.18	0.44
1:A:4230:THR:HB	1:B:3825:ARG:HH21	1.82	0.44
1:A:4281:THR:HB	1:A:4284:ILE:HG12	2.00	0.44
1:B:4651:HIS:CD2	1:B:4656:LYS:HB2	2.53	0.44
2:D:13:PHE:N	2:D:13:PHE:CD1	2.83	0.44
3:E:317:SER:O	3:E:321:GLN:HG3	2.17	0.44
1:A:4017:LEU:HD11	1:A:4132:VAL:HG11	1.98	0.44
1:A:4413:LYS:CD	1:A:4456:ILE:HD11	2.47	0.44
1:B:3323:LEU:O	1:B:3327:LEU:HB2	2.18	0.44
1:B:4125:HIS:HA	1:B:4165:LEU:HD12	1.99	0.44
1:B:4295:LEU:HD11	1:B:4309:PHE:CE2	2.48	0.44
1:A:3273:MET:HG3	1:A:3633:LEU:CD2	2.48	0.44
1:A:3520:VAL:HG11	1:A:3799:LEU:HD22	2.00	0.44
1:A:3957:GLY:O	1:A:3958:HIS:C	2.61	0.44
2:D:81:ASP:O	2:D:85:GLU:N	2.51	0.44
3:F:301:MET:HE1	3:F:305:GLU:HG2	2.00	0.44
1:A:3490:SER:O	1:A:3494:VAL:HG23	2.18	0.44
1:A:4115:ARG:NH2	2:C:125:MET:SD	2.91	0.44
1:B:3251:LEU:HD12	1:B:3303:PHE:CD2	2.52	0.44
1:B:4631:MET:O	1:B:4634:LEU:HG	2.18	0.44
2:D:132:ASP:OD1	2:D:132:ASP:N	2.50	0.44
3:E:301:MET:HE1	3:E:305:GLU:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4275:LYS:HZ1	1:A:4327:THR:HG21	1.79	0.43
1:A:4278:VAL:O	1:B:3825:ARG:HD3	2.18	0.43
1:A:4621:PRO:HB3	1:A:4668:GLY:HA3	2.00	0.43
1:B:3412:LEU:O	1:B:3416:LEU:HB2	2.18	0.43
1:B:3899:ILE:O	1:B:3903:GLN:HG2	2.18	0.43
1:B:4414:ILE:HD11	1:B:4451:ALA:HB1	2.00	0.43
1:B:4671:ASN:CB	1:B:4732:GLN:OE1	2.54	0.43
2:C:85:GLU:HA	2:C:88:GLU:HB2	2.00	0.43
2:C:145:MET:O	2:C:147:THR:N	2.51	0.43
2:D:42:GLN:HE22	2:D:76:LYS:HG3	1.82	0.43
2:D:90:PHE:HB2	2:D:142:PHE:CD2	2.53	0.43
1:B:3951:VAL:HA	1:B:3968:LEU:HD21	2.00	0.43
1:B:4590:ASP:OD1	1:B:4593:GLN:HG3	2.18	0.43
1:A:3294:CYS:HB3	1:A:3301:LEU:HG	1.99	0.43
1:A:3889:ALA:HB2	3:E:293:LEU:HD13	2.00	0.43
1:A:3899:ILE:O	1:A:3903:GLN:HG2	2.19	0.43
1:A:4146:CYS:HA	1:A:4186:LEU:HD22	2.00	0.43
1:B:3490:SER:O	1:B:3494:VAL:HG23	2.18	0.43
1:B:4281:THR:HB	1:B:4284:ILE:HG12	2.00	0.43
1:B:4372:TYR:HD1	1:B:4376:GLU:OE2	2.02	0.43
1:B:4600:GLN:O	1:B:4603:SER:HB3	2.18	0.43
1:B:4643:ASN:O	1:B:4644:PHE:C	2.61	0.43
2:C:54:ASN:C	2:C:56:VAL:N	2.77	0.43
1:B:3998:LEU:O	1:B:4001:VAL:HG12	2.18	0.43
1:B:4003:ILE:HB	1:B:4008:VAL:HG11	2.00	0.43
1:B:4273:LEU:HD12	1:B:4291:LEU:HD12	2.00	0.43
1:B:4310:MET:HE2	1:B:4310:MET:HB2	1.85	0.43
1:B:4646:LYS:HG2	1:B:4650:ASP:O	2.17	0.43
2:C:27:THR:HA	2:C:61:ASN:HA	2.00	0.43
2:C:138:ASN:HB3	2:C:140:GLU:CG	2.36	0.43
2:D:10:ILE:O	2:D:13:PHE:HB2	2.19	0.43
1:A:3940:THR:HG21	1:A:3985:CYS:CB	2.46	0.43
1:A:3986:TRP:CZ2	3:E:316:ARG:HG2	2.54	0.43
1:A:4299:THR:HG21	1:A:4334:ARG:HE	1.84	0.43
1:A:4599:ASP:HA	1:A:4602:ASN:HD22	1.84	0.43
1:B:2993:GLY:O	1:B:2997:ILE:HG13	2.18	0.43
1:B:3295:ILE:HD12	1:B:3295:ILE:HA	1.91	0.43
1:B:3595:ASN:HD21	1:B:3605:LEU:HD13	1.83	0.43
1:B:4109:LEU:CD1	1:B:4114:LYS:HB2	2.47	0.43
1:B:4146:CYS:HA	1:B:4186:LEU:HD22	2.01	0.43
1:A:3207:ARG:O	1:A:3211:ARG:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3595:ASN:HD21	1:A:3605:LEU:HD13	1.83	0.43
1:A:3967:SER:C	1:A:3969:GLN:N	2.72	0.43
1:A:4007:VAL:HG22	1:B:3511:ASN:HB2	2.00	0.43
1:A:4313:CYS:HB3	1:A:4331:ILE:CG2	2.47	0.43
1:A:4414:ILE:HD11	1:A:4451:ALA:HB1	2.00	0.43
1:B:3760:LEU:HD13	1:B:3760:LEU:HA	1.90	0.43
3:F:317:SER:O	3:F:321:GLN:HG3	2.18	0.43
1:A:4372:TYR:HD1	1:A:4376:GLU:OE2	2.02	0.43
3:E:295:ARG:O	3:E:295:ARG:HG2	2.19	0.43
1:A:3974:LEU:O	1:A:3975:LEU:C	2.57	0.43
1:A:4363:LEU:HD21	1:A:4444:MET:HG3	2.01	0.43
1:B:3207:ARG:O	1:B:3211:ARG:HG3	2.18	0.43
1:B:4638:PHE:HA	1:B:4641:TYR:CD2	2.54	0.43
2:D:38:ARG:HD2	2:D:43:ASN:HA	2.00	0.43
1:A:3323:LEU:O	1:A:3327:LEU:HB2	2.19	0.43
1:A:3525:TYR:HE2	1:A:3874:GLY:HA2	1.83	0.43
1:A:3699:LEU:HD23	1:A:3706:CYS:HB2	2.01	0.43
1:B:3764:LEU:HD23	1:B:3764:LEU:HA	1.70	0.43
1:B:3855:GLN:C	1:B:3855:GLN:CD	2.87	0.43
2:C:34:GLY:HA2	2:C:37:MET:HE2	2.01	0.43
2:D:73:MET:HE3	2:D:73:MET:HB2	1.67	0.43
1:A:3544:TYR:HB3	1:A:3714:MET:CE	2.48	0.43
1:A:3727:GLU:H	1:A:3731:ASP:CB	2.31	0.43
1:A:3884:ILE:HD11	1:A:3913:ASN:ND2	2.34	0.43
1:A:4029:PRO:HB3	3:E:310:GLU:OE1	2.19	0.43
1:A:4273:LEU:HD12	1:A:4291:LEU:HD12	2.00	0.43
1:B:3294:CYS:HB3	1:B:3301:LEU:HG	1.99	0.43
1:B:3396:VAL:HG11	1:B:3438:ASN:CB	2.49	0.43
1:B:4258:PHE:HE1	2:D:19:LEU:CD2	2.31	0.43
2:D:145:MET:O	2:D:147:THR:N	2.52	0.43
1:A:2993:GLY:O	1:A:2997:ILE:HG13	2.18	0.42
1:A:3997:PHE:HB2	1:A:4016:CYS:CB	2.42	0.42
2:C:13:PHE:N	2:C:13:PHE:CD1	2.83	0.42
1:A:3967:SER:O	1:A:3968:LEU:C	2.63	0.42
1:A:4003:ILE:HB	1:A:4008:VAL:HG11	2.01	0.42
1:A:4031:SER:HB3	3:E:303:GLU:OE1	2.17	0.42
1:B:3525:TYR:HE2	1:B:3874:GLY:HA2	1.84	0.42
1:B:4621:PRO:HB3	1:B:4668:GLY:HA3	2.00	0.42
2:D:28:ILE:H	2:D:28:ILE:HG12	1.48	0.42
1:A:3525:TYR:CE2	1:A:3874:GLY:HA2	2.54	0.42
1:A:3801:GLN:HA	1:B:3788:THR:HG21	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4199:TYR:HE1	2:C:39:SER:HA	1.84	0.42
1:B:3986:TRP:CZ2	3:F:316:ARG:HG2	2.54	0.42
1:B:4597:LEU:HD22	1:B:4616:LEU:HD11	2.00	0.42
1:A:3979:ILE:HD12	1:A:4019:ILE:HG21	2.01	0.42
1:A:4159:LYS:HE2	1:A:4159:LYS:HB3	1.84	0.42
1:B:3794:ARG:O	1:B:3798:GLN:HG3	2.19	0.42
1:B:4129:LEU:O	1:B:4130:ARG:C	2.62	0.42
1:B:4632:GLN:HG2	1:B:4681:LEU:HD21	2.01	0.42
1:A:3825:ARG:HD3	1:B:4278:VAL:O	2.19	0.42
1:B:3269:LEU:HB3	1:B:3633:LEU:HD12	1.92	0.42
1:B:3647:PHE:HB2	1:B:3649:GLU:HG3	2.00	0.42
2:D:16:ALA:O	2:D:20:PHE:HD2	2.02	0.42
2:D:45:THR:OG1	2:D:48:GLU:HG3	2.19	0.42
1:A:4128:TRP:O	1:A:4129:LEU:C	2.62	0.42
1:B:3029:ILE:O	1:B:3034:MET:HE1	2.19	0.42
1:B:3525:TYR:CE2	1:B:3874:GLY:HA2	2.54	0.42
1:B:3884:ILE:HD11	1:B:3913:ASN:ND2	2.34	0.42
2:D:52:MET:O	2:D:55:GLU:HB3	2.20	0.42
1:A:3233:LEU:HD13	1:A:3290:TRP:HE3	1.85	0.42
1:A:3791:SER:O	1:B:3521:GLU:CB	2.68	0.42
1:A:3963:ASP:C	1:A:3965:ALA:N	2.77	0.42
1:B:3699:LEU:HD23	1:B:3706:CYS:HB2	2.01	0.42
1:B:3753:LEU:HD12	1:B:3753:LEU:HA	1.81	0.42
2:C:140:GLU:O	2:C:143:VAL:HB	2.18	0.42
3:F:318:LEU:O	3:F:322:GLU:HG2	2.20	0.42
1:A:3311:VAL:HG23	1:A:3312:ASP:O	2.20	0.42
1:A:3396:VAL:HG11	1:A:3438:ASN:CB	2.49	0.42
1:A:3453:SER:O	1:A:3456:PRO:HD2	2.20	0.42
1:B:3922:ARG:O	1:B:3926:ARG:HG3	2.20	0.42
1:B:4125:HIS:HA	1:B:4165:LEU:CD1	2.50	0.42
1:B:4637:ARG:O	1:B:4640:PRO:HD2	2.20	0.42
3:E:330:ARG:HE	3:E:332:GLU:HG3	1.85	0.42
1:B:3298:ASP:HB3	1:B:3398:GLN:OE1	2.20	0.42
1:B:3387:GLN:HG2	1:B:3388:GLU:N	2.35	0.42
1:A:3855:GLN:CD	1:A:3855:GLN:C	2.87	0.42
1:A:3954:ALA:CB	1:A:3968:LEU:HD11	2.47	0.42
1:A:4547:GLU:HG2	1:A:4605:PHE:CE2	2.55	0.42
1:B:3954:ALA:O	1:B:3964:LEU:HD12	2.19	0.42
1:B:4299:THR:HG21	1:B:4334:ARG:HH21	1.83	0.42
1:B:4355:LYS:NZ	1:B:4363:LEU:O	2.40	0.42
1:A:3101:VAL:O	1:A:3105:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3955:LEU:HD22	1:A:4003:ILE:HD12	2.02	0.41
1:B:4267:LEU:HD12	1:B:4267:LEU:HA	1.91	0.41
1:B:4363:LEU:HD21	1:B:4444:MET:HG3	2.00	0.41
2:C:10:ILE:O	2:C:13:PHE:HB2	2.19	0.41
2:D:130:ASP:OD2	2:D:135:GLY:N	2.48	0.41
2:D:141:GLU:O	2:D:144:GLN:HB3	2.20	0.41
1:A:3029:ILE:O	1:A:3034:MET:HE1	2.19	0.41
1:A:3522:PHE:HD2	1:A:3803:TYR:CE1	2.39	0.41
1:A:4108:PHE:HA	1:A:4111:ARG:CG	2.50	0.41
1:A:4419:LEU:HD21	1:A:4458:SER:HA	2.01	0.41
1:B:3101:VAL:O	1:B:3105:LEU:HG	2.20	0.41
1:B:3409:ILE:HD13	1:B:3454:ILE:HD11	2.01	0.41
1:B:3964:LEU:CD2	1:B:4011:ASN:HD22	2.32	0.41
2:C:18:SER:O	2:C:19:LEU:C	2.63	0.41
1:A:3269:LEU:HB3	1:A:3633:LEU:HD13	1.91	0.41
1:A:3320:LEU:HD12	1:A:3424:VAL:HG13	2.03	0.41
1:A:3991:ARG:HA	1:A:4059:TRP:CZ3	2.55	0.41
1:B:3951:VAL:HG13	1:B:4012:ILE:HD13	2.02	0.41
3:E:318:LEU:O	3:E:322:GLU:HG2	2.20	0.41
3:F:295:ARG:O	3:F:295:ARG:HG2	2.19	0.41
1:A:3332:VAL:HG11	1:A:3434:HIS:CE1	2.56	0.41
1:B:3928:LEU:O	1:B:3932:LEU:HG	2.20	0.41
1:B:4633:ILE:O	1:B:4637:ARG:HG3	2.20	0.41
2:D:121:GLU:O	2:D:122:VAL:C	2.60	0.41
2:D:139:TYR:O	2:D:143:VAL:HG23	2.21	0.41
1:B:3948:ILE:HA	1:B:3996:LEU:HD21	2.02	0.41
1:B:4128:TRP:O	1:B:4129:LEU:C	2.63	0.41
2:C:10:ILE:HG13	2:C:66:PHE:CZ	2.51	0.41
1:A:3095:VAL:HG12	1:A:3190:TRP:HZ3	1.85	0.41
1:A:3298:ASP:HB3	1:A:3398:GLN:OE1	2.20	0.41
1:A:3450:LEU:O	1:A:3454:ILE:HG13	2.21	0.41
1:A:4303:GLU:HB2	1:A:4475:MET:SD	2.61	0.41
1:A:4679:LYS:NZ	1:A:4731:ILE:O	2.54	0.41
1:B:3233:LEU:HD13	1:B:3290:TRP:HE3	1.85	0.41
1:B:3396:VAL:HG11	1:B:3438:ASN:HB3	2.03	0.41
1:B:3470:ASP:OD1	3:F:293:LEU:HG	2.20	0.41
1:B:4187:TYR:O	1:B:4191:ILE:HG12	2.21	0.41
1:B:4199:TYR:HA	2:D:20:PHE:HZ	1.85	0.41
1:B:4307:LYS:CG	1:B:4478:VAL:HG21	2.46	0.41
1:A:3190:TRP:H	1:A:3190:TRP:HD1	1.63	0.41
1:A:3306:GLN:O	1:A:3309:PHE:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3906:ILE:HD11	1:A:3939:ALA:HB1	2.02	0.41
1:A:3981:LYS:HA	1:A:3981:LYS:HD3	1.85	0.41
1:B:3320:LEU:HD23	1:B:3320:LEU:HA	1.92	0.41
1:B:3453:SER:O	1:B:3456:PRO:HD2	2.20	0.41
1:B:3505:THR:OG1	1:B:3916:ARG:NH1	2.37	0.41
1:B:4022:LYS:HE2	1:B:4022:LYS:HB3	1.79	0.41
1:B:3236:HIS:O	1:B:3240:ILE:HG12	2.21	0.41
1:B:3269:LEU:HB3	1:B:3633:LEU:HD13	1.90	0.41
1:B:3515:THR:HG21	1:B:3764:LEU:HD22	2.02	0.41
1:B:3988:LEU:H	1:B:3988:LEU:HD12	1.85	0.41
1:B:4108:PHE:HA	1:B:4111:ARG:CG	2.50	0.41
2:C:7:GLU:O	2:C:8:GLU:C	2.63	0.41
2:C:123:ASP:O	2:C:127:ARG:HG2	2.20	0.41
1:A:3190:TRP:CD1	1:A:3190:TRP:N	2.83	0.41
1:A:3236:HIS:O	1:A:3240:ILE:HG12	2.21	0.41
1:A:3470:ASP:OD1	3:E:293:LEU:HG	2.21	0.41
1:A:3556:TYR:O	1:A:3606:LYS:CE	2.67	0.41
1:A:3963:ASP:O	1:A:3964:LEU:C	2.64	0.41
1:A:4077:ILE:HG22	2:C:114:GLY:O	2.21	0.41
1:A:4216:GLU:HG2	1:A:4238:LEU:HB2	2.03	0.41
1:B:3071:LYS:HD2	1:B:3074:ILE:HB	2.03	0.41
1:B:3311:VAL:HG23	1:B:3312:ASP:O	2.20	0.41
1:B:3320:LEU:HD12	1:B:3424:VAL:HG13	2.03	0.41
1:B:3324:SER:OG	1:B:3328:CYS:SG	2.57	0.41
1:B:3443:GLN:H	1:B:3443:GLN:CD	2.29	0.41
1:B:3556:TYR:O	1:B:3606:LYS:CE	2.67	0.41
1:B:4059:TRP:CE3	3:F:323:LEU:HD21	2.56	0.41
1:B:4244:LEU:O	1:B:4248:PHE:HD1	2.03	0.41
2:D:7:GLU:O	2:D:8:GLU:C	2.64	0.41
2:D:66:PHE:HB3	2:D:67:PRO:HD3	2.02	0.41
2:D:119:ASP:HA	2:D:122:VAL:CG2	2.50	0.41
2:D:145:MET:HE3	2:D:145:MET:HB3	1.86	0.41
1:A:3409:ILE:HD13	1:A:3454:ILE:HD11	2.01	0.41
1:A:3519:LEU:HD11	1:A:3767:VAL:HG11	2.03	0.41
1:A:3937:PRO:O	1:A:3938:GLU:C	2.64	0.41
1:A:4638:PHE:HA	1:A:4641:TYR:CD2	2.56	0.41
1:B:3223:LYS:O	1:B:3227:LEU:HD23	2.21	0.41
1:B:3855:GLN:O	1:B:3855:GLN:NE2	2.54	0.41
1:B:4637:ARG:C	1:B:4640:PRO:HD2	2.46	0.41
2:C:95:LYS:HE3	2:C:109:VAL:HG23	2.03	0.41
2:D:119:ASP:OD1	2:D:119:ASP:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4129:LEU:HG	1:A:4165:LEU:HD23	2.02	0.40
1:A:4201:ALA:HA	1:A:4205:VAL:HG12	2.03	0.40
1:A:4251:VAL:HB	1:A:4254:ILE:HD12	2.02	0.40
1:A:4299:THR:HG22	1:A:4309:PHE:CZ	2.57	0.40
1:B:3053:LEU:HA	1:B:3056:MET:CE	2.50	0.40
1:B:3450:LEU:O	1:B:3454:ILE:HG13	2.21	0.40
1:B:4023:LEU:HD23	1:B:4023:LEU:HA	1.84	0.40
1:B:4679:LYS:NZ	1:B:4731:ILE:O	2.54	0.40
1:A:3742:LEU:HD13	1:A:3820:LYS:HG2	2.04	0.40
1:A:3855:GLN:O	1:A:3855:GLN:NE2	2.54	0.40
1:A:4187:TYR:O	1:A:4191:ILE:HG12	2.21	0.40
1:A:4195:HIS:NE2	2:C:35:THR:CG2	2.85	0.40
1:B:4031:SER:HB3	3:F:310:GLU:OE2	2.21	0.40
1:B:4166:LEU:O	1:B:4183:TYR:OH	2.38	0.40
1:B:4251:VAL:HB	1:B:4254:ILE:HD12	2.02	0.40
2:C:20:PHE:HE1	2:C:35:THR:CG2	2.34	0.40
2:D:29:THR:O	2:D:61:ASN:ND2	2.54	0.40
1:A:3053:LEU:HA	1:A:3056:MET:CE	2.50	0.40
1:A:3196:GLU:HA	1:A:3199:MET:HG2	2.02	0.40
1:A:3270:ILE:HD12	1:A:3632:PRO:HG3	2.03	0.40
1:A:3387:GLN:HG2	1:A:3388:GLU:N	2.35	0.40
1:A:3893:ASN:HB3	1:A:3896:LEU:HB2	2.03	0.40
1:A:3922:ARG:O	1:A:3926:ARG:HG3	2.20	0.40
1:A:3950:LYS:O	1:A:3953:THR:HG22	2.21	0.40
1:A:4027:PRO:HG2	3:E:313:ARG:HH21	1.86	0.40
1:A:4244:LEU:O	1:A:4248:PHE:HD1	2.03	0.40
1:A:4280:ARG:NH1	1:A:4285:ASP:OD2	2.52	0.40
2:D:68:GLU:O	2:D:72:MET:HG3	2.22	0.40
1:A:3289:ASN:HA	1:A:3292:LYS:NZ	2.36	0.40
1:A:3396:VAL:HG11	1:A:3438:ASN:HB3	2.03	0.40
1:A:3413:ARG:NH1	1:A:3457:GLU:OE1	2.41	0.40
1:A:3546:LYS:HG2	1:A:3714:MET:SD	2.61	0.40
1:A:4129:LEU:HD21	1:A:4149:VAL:HG22	2.03	0.40
1:B:3195:SER:HG	1:B:3231:HIS:CG	2.37	0.40
1:B:3478:LYS:HA	1:B:3478:LYS:HD2	1.83	0.40
1:B:4062:ARG:HB2	1:B:4062:ARG:NH1	2.37	0.40
1:B:4098:THR:HB	2:D:109:VAL:CG1	2.52	0.40
1:B:4159:LYS:HE2	1:B:4159:LYS:HB3	1.84	0.40
1:B:4299:THR:HG22	1:B:4309:PHE:CZ	2.56	0.40
2:D:17:PHE:HD1	2:D:69:PHE:CD2	2.40	0.40
1:A:3772:PRO:HG2	1:B:3918:ALA:HA	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4544:LEU:HD23	1:A:4605:PHE:HE1	1.87	0.40
1:B:3099:LEU:HD11	1:B:3193:PHE:CE1	2.57	0.40
1:B:3306:GLN:O	1:B:3309:PHE:HB2	2.21	0.40
1:B:3332:VAL:HG11	1:B:3434:HIS:CE1	2.56	0.40
1:B:4694:TYR:OH	1:B:4716:ARG:HD3	2.22	0.40
2:D:79:ASP:O	2:D:83:GLU:HG2	2.21	0.40
2:D:118:THR:C	2:D:120:GLU:N	2.74	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	1644/5205 (32%)	1590 (97%)	54 (3%)	0	100	100
1	B	1644/5205 (32%)	1599 (97%)	45 (3%)	0	100	100
2	C	142/149 (95%)	131 (92%)	11 (8%)	0	100	100
2	D	139/149 (93%)	127 (91%)	12 (9%)	0	100	100
3	E	44/381 (12%)	44 (100%)	0	0	100	100
3	F	43/381 (11%)	43 (100%)	0	0	100	100
All	All	3656/11470 (32%)	3534 (97%)	122 (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	A	1471/4542 (32%)	1439 (98%)	32 (2%)	47 73
1	B	1471/4542 (32%)	1443 (98%)	28 (2%)	52 76
2	C	123/127 (97%)	118 (96%)	5 (4%)	26 59
2	D	122/127 (96%)	114 (93%)	8 (7%)	14 45
3	E	45/330 (14%)	45 (100%)	0	100 100
3	F	44/330 (13%)	44 (100%)	0	100 100
All	All	3276/9998 (33%)	3203 (98%)	73 (2%)	47 73

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3237	VAL
1	A	3285	GLN
1	A	3286	ARG
1	A	3458	LEU
1	A	3520	VAL
1	A	3522	PHE
1	A	3532	CYS
1	A	3536	ASN
1	A	3581	LEU
1	A	3793	ASN
1	A	3847	VAL
1	A	3850	THR
1	A	3866	HIS
1	A	3964	LEU
1	A	3994	LEU
1	A	3999	MET
1	A	4007	VAL
1	A	4037	VAL
1	A	4127	ASN
1	A	4129	LEU
1	A	4230	THR
1	A	4277	VAL
1	A	4309	PHE
1	A	4310	MET
1	A	4400	LEU
1	A	4447	LEU
1	A	4492	LEU
1	A	4505	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	4520	VAL
1	A	4542	LEU
1	A	4597	LEU
1	A	4616	LEU
1	B	3286	ARG
1	B	3458	LEU
1	B	3532	CYS
1	B	3535	CYS
1	B	3543	CYS
1	B	3581	LEU
1	B	3754	MET
1	B	3765	CYS
1	B	3847	VAL
1	B	3850	THR
1	B	3866	HIS
1	B	3953	THR
1	B	3968	LEU
1	B	4045	VAL
1	B	4051	GLU
1	B	4053	HIS
1	B	4129	LEU
1	B	4277	VAL
1	B	4303	GLU
1	B	4310	MET
1	B	4400	LEU
1	B	4447	LEU
1	B	4492	LEU
1	B	4505	LEU
1	B	4520	VAL
1	B	4542	LEU
1	B	4616	LEU
1	B	4649	GLU
2	C	33	LEU
2	C	49	LEU
2	C	77	MET
2	C	79	ASP
2	C	101	ILE
2	D	21	ASP
2	D	28	ILE
2	D	33	LEU
2	D	49	LEU
2	D	63	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	70	LEU
2	D	78	LYS
2	D	93	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3170	GLN
1	A	3397	ASN
1	A	3438	ASN
1	A	3491	GLN
1	A	3591	ASN
1	A	3639	ASN
1	A	3683	GLN
1	A	3768	ASN
1	A	3855	GLN
1	A	3866	HIS
1	A	4011	ASN
1	A	4127	ASN
1	A	4161	GLN
1	A	4233	GLN
1	A	4500	GLN
1	A	4602	ASN
1	A	4643	ASN
1	B	3397	ASN
1	B	3438	ASN
1	B	3491	GLN
1	B	3591	ASN
1	B	3639	ASN
1	B	3650	ASN
1	B	3683	GLN
1	B	3768	ASN
1	B	3855	GLN
1	B	3866	HIS
1	B	3958	HIS
1	B	4002	ASN
1	B	4011	ASN
1	B	4021	GLN
1	B	4053	HIS
1	B	4500	GLN
1	B	4523	GLN
1	B	4602	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	4651	HIS
2	C	9	GLN
2	C	43	ASN
2	C	54	ASN
2	D	9	GLN
2	D	54	ASN
2	D	61	ASN
2	D	108	HIS
2	D	112	ASN
2	D	144	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 10 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.

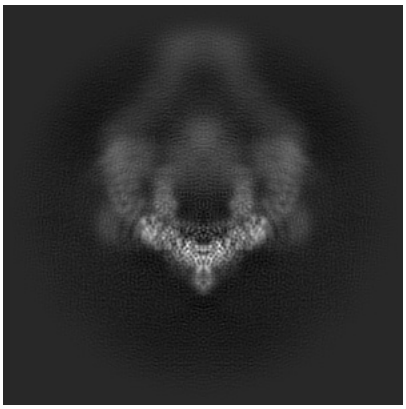
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49876. These allow visual inspection of the internal detail of the map and identification of artifacts.

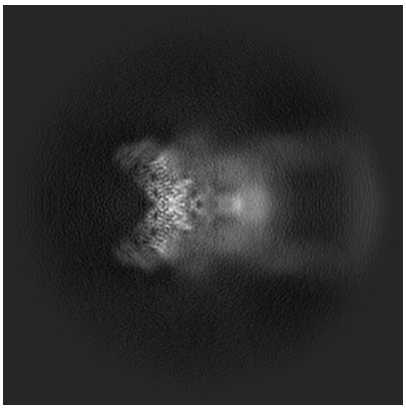
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

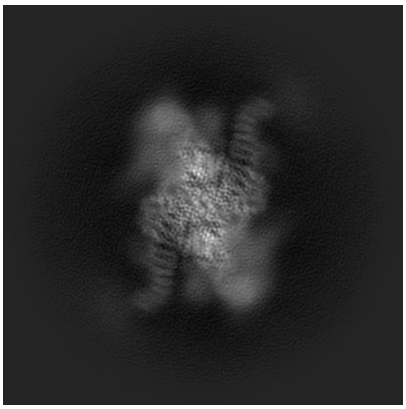
6.1.1 Primary map



X

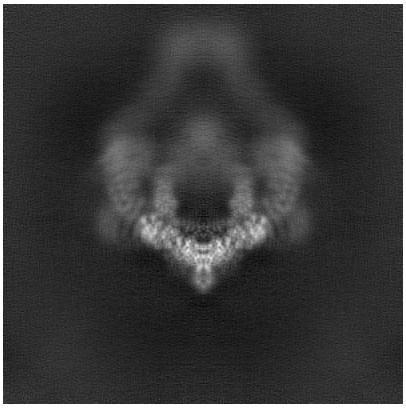


Y

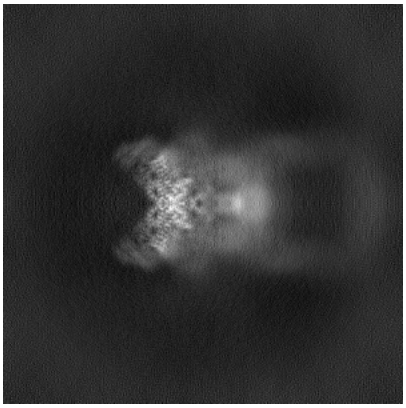


Z

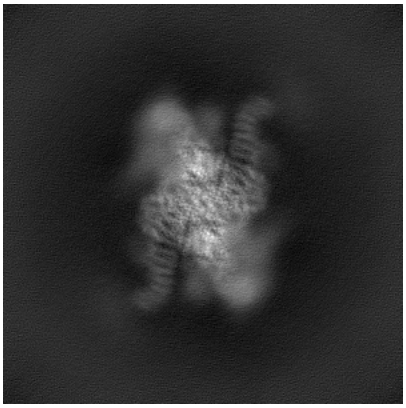
6.1.2 Raw map



X



Y

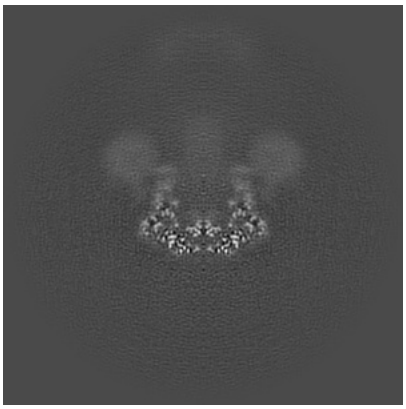


Z

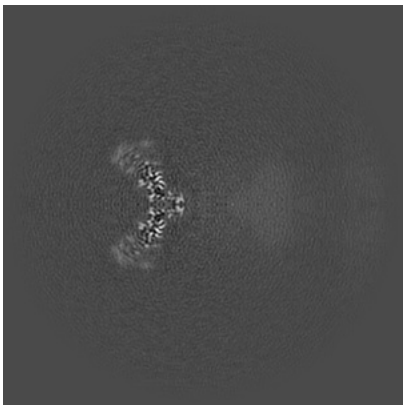
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

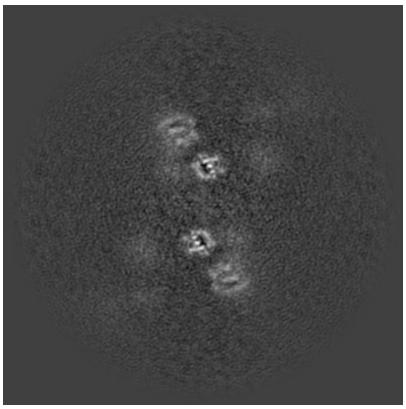
6.2.1 Primary map



X Index: 200

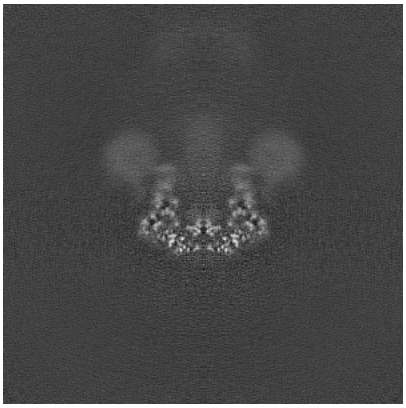


Y Index: 200

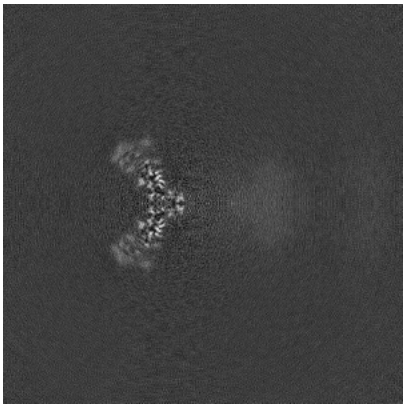


Z Index: 200

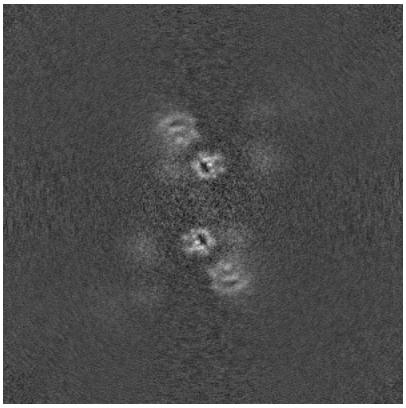
6.2.2 Raw map



X Index: 200



Y Index: 200

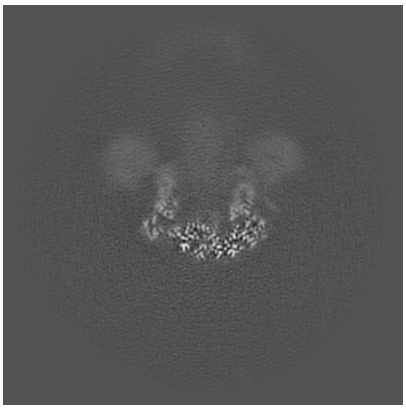


Z Index: 200

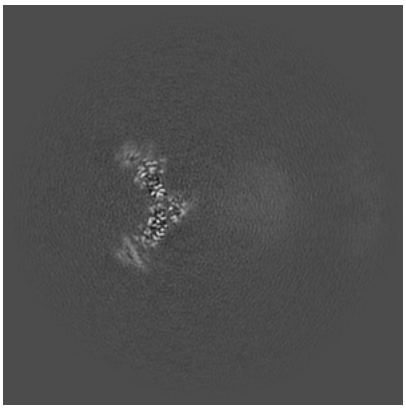
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

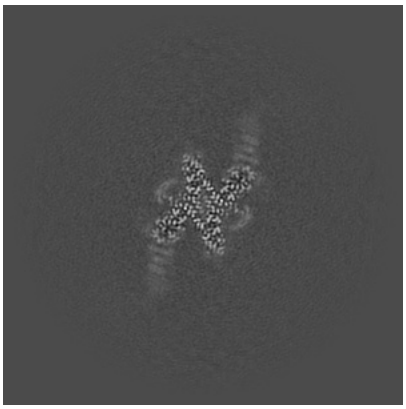
6.3.1 Primary map



X Index: 195

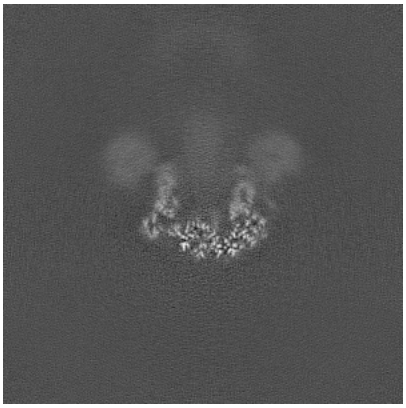


Y Index: 194

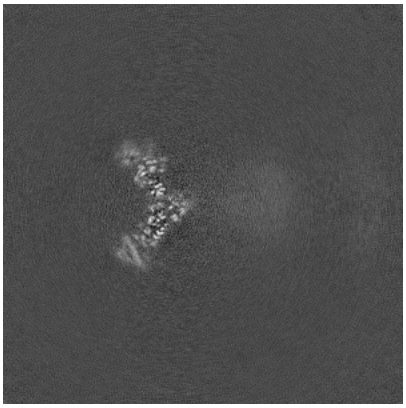


Z Index: 158

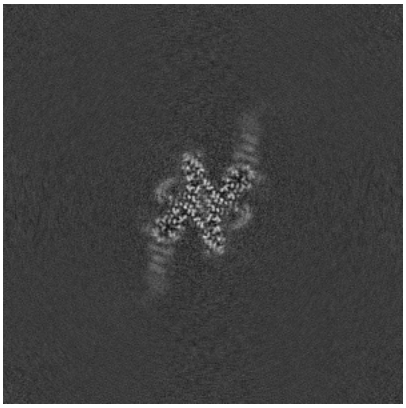
6.3.2 Raw map



X Index: 195



Y Index: 194

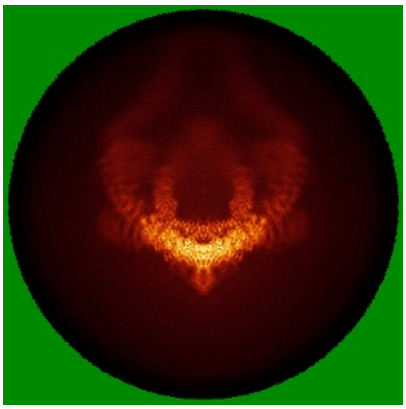


Z Index: 158

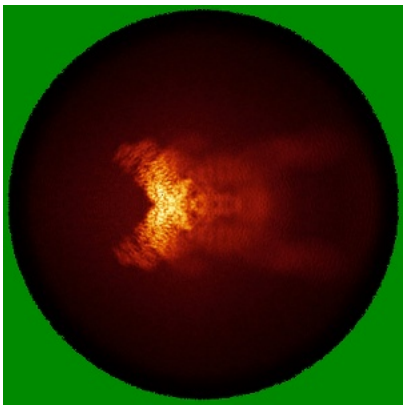
The images above show the largest variance slices of the map in three orthogonal directions.

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

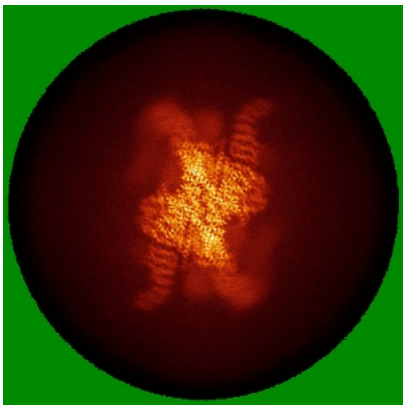
6.4.1 Primary map



X

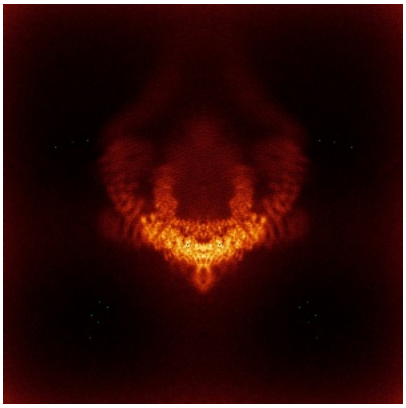


Y

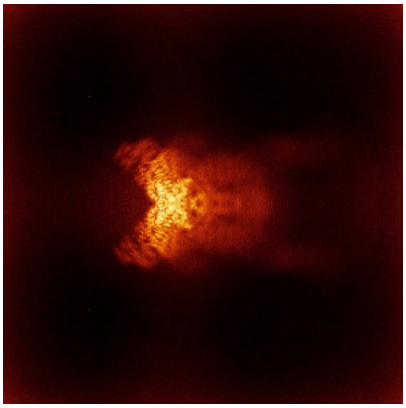


Z

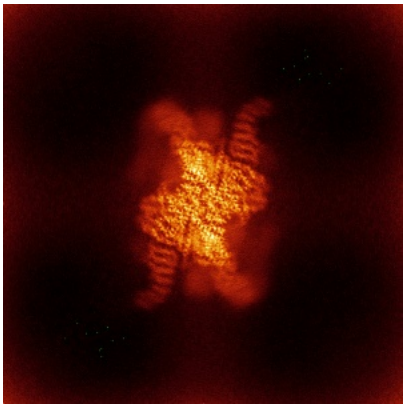
6.4.2 Raw map



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

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.146. 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

X Y Z

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

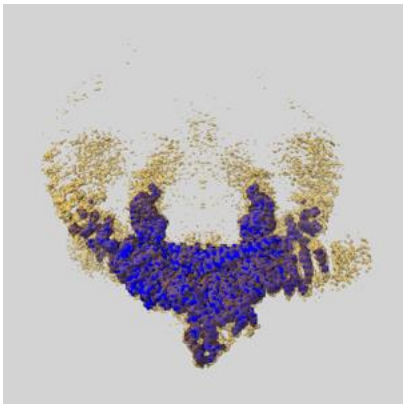
6.6 Mask visualisation

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

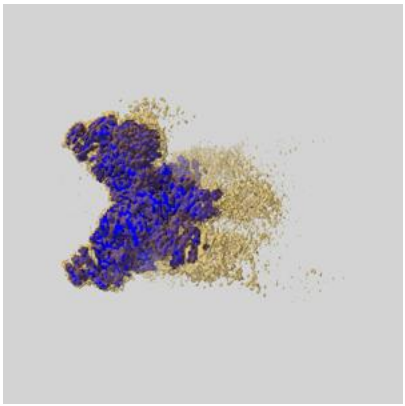
A mask typically either:

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

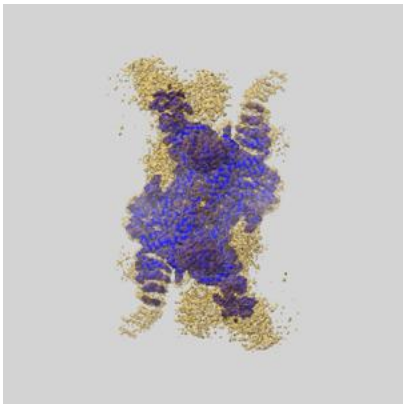
6.6.1 emd_49876_msk_1.map



X



Y

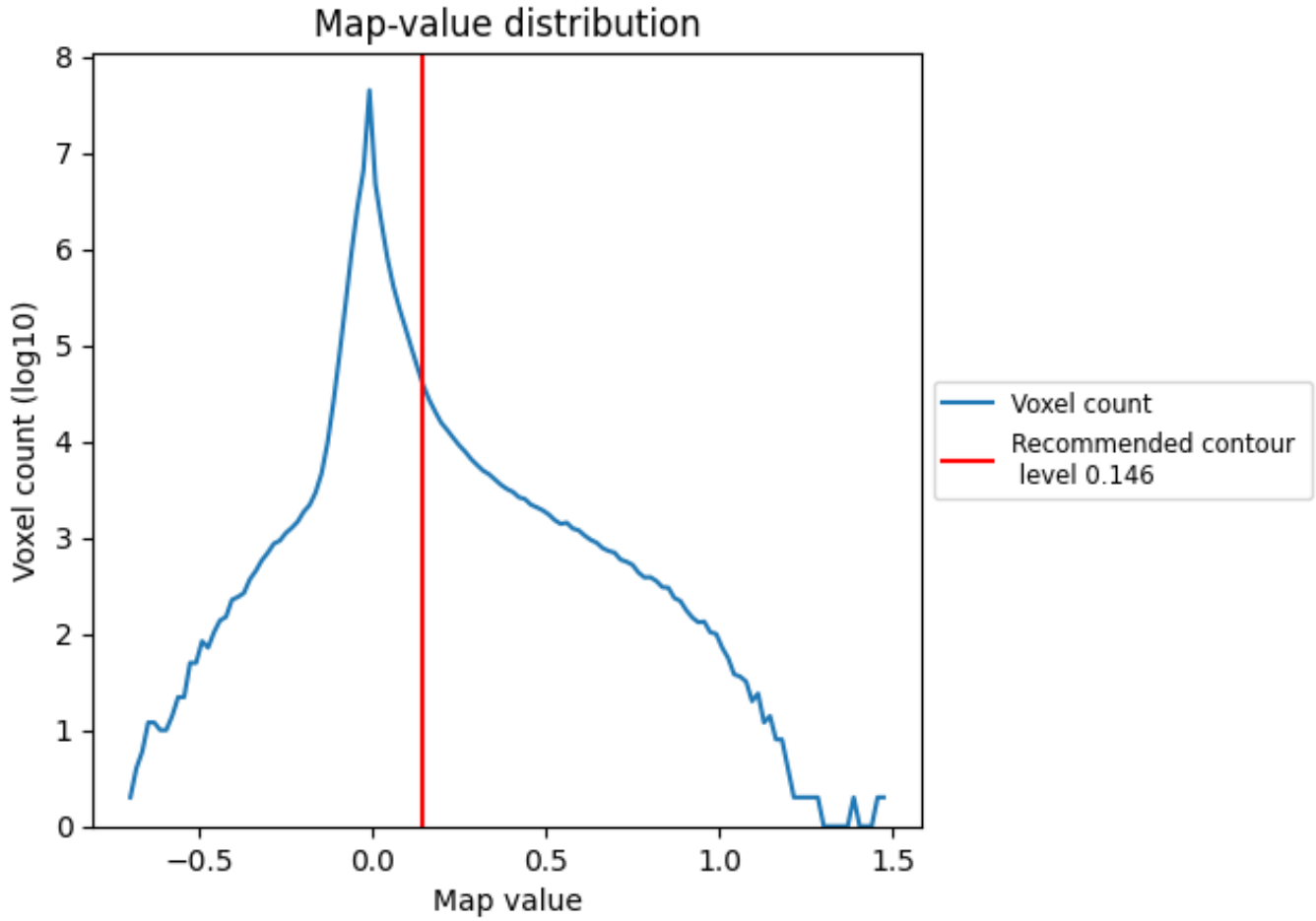


Z

7 Map analysis

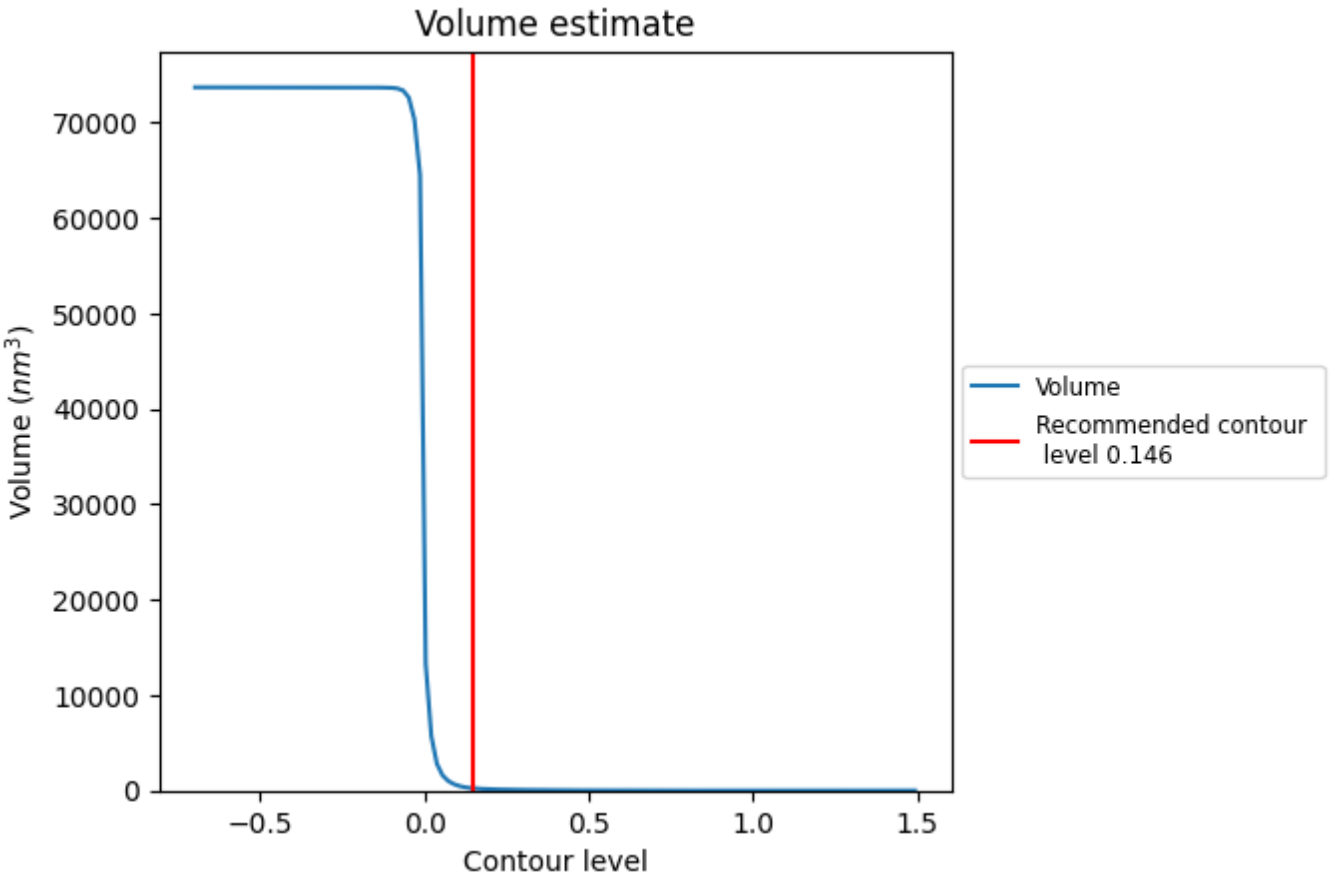
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

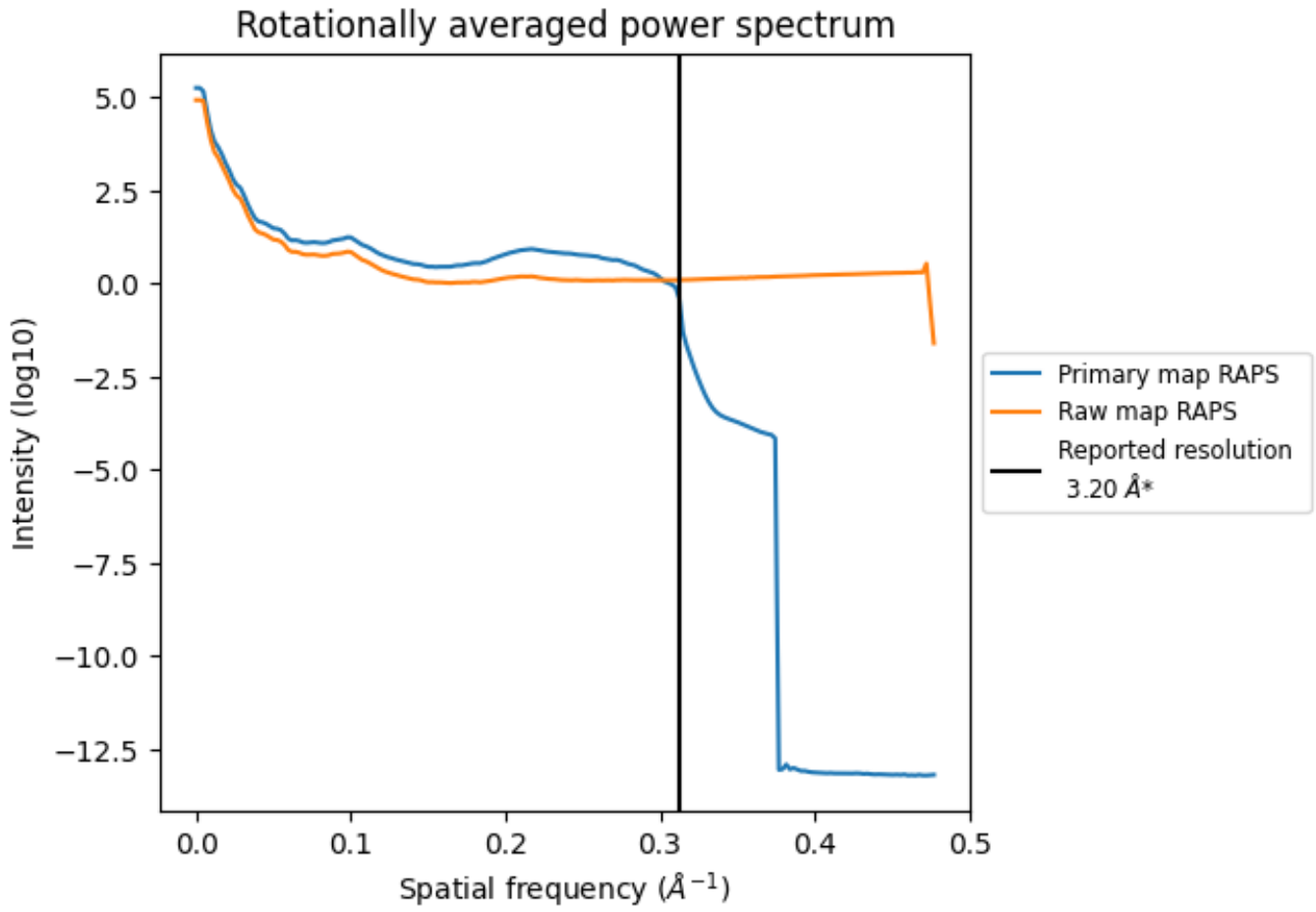
7.2 Volume estimate



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

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

7.3 Rotationally averaged power spectrum (i)

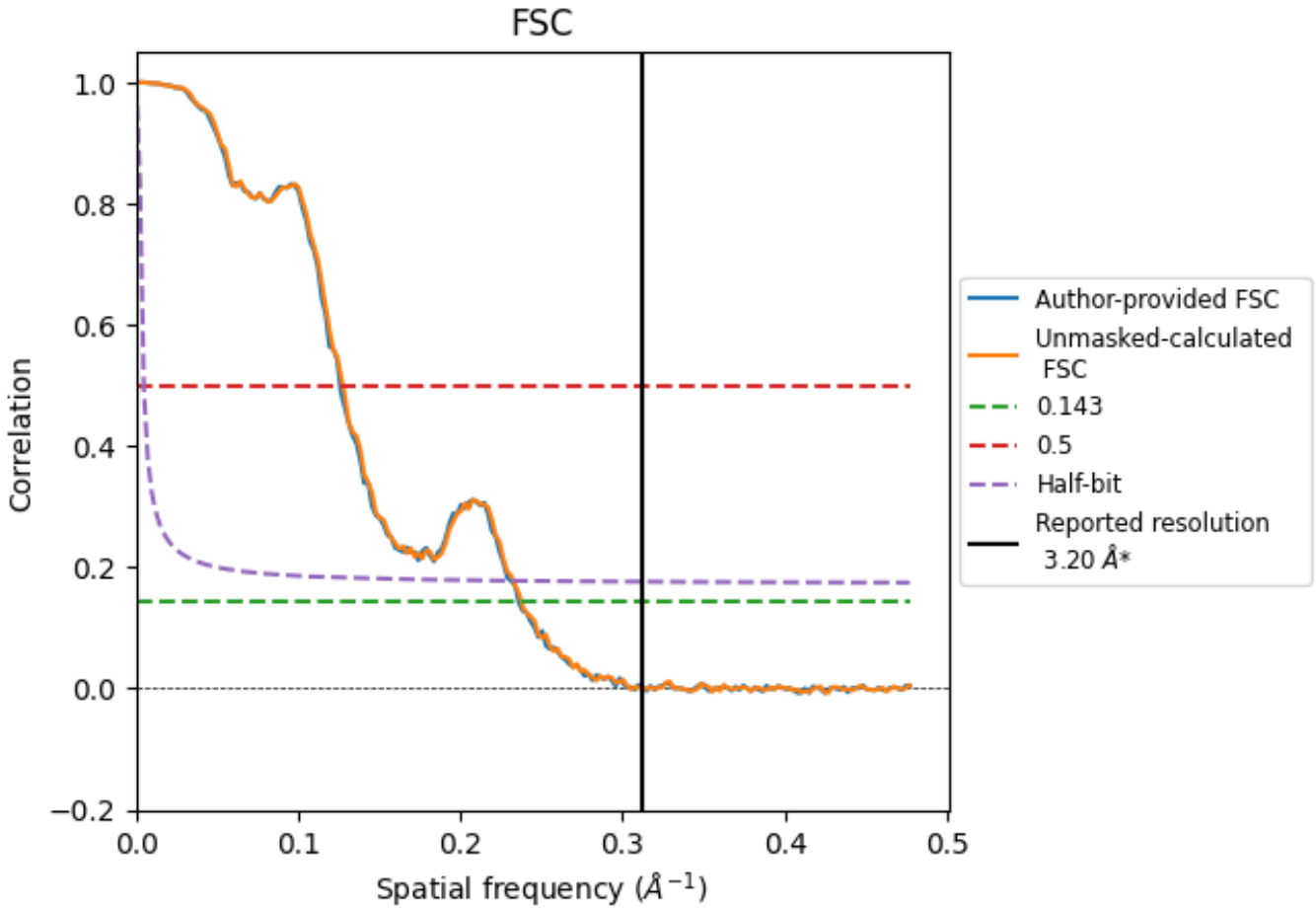


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	4.24	7.94	4.33
Unmasked-calculated*	4.21	7.84	4.30

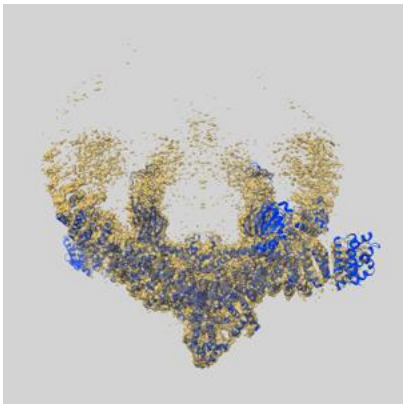
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.24 differs from the reported value 3.2 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.21 differs from the reported value 3.2 by more than 10 %

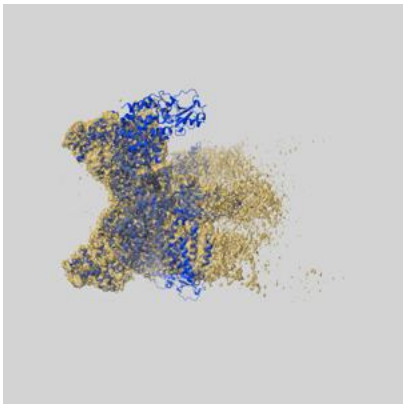
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49876 and PDB model 9NWE. Per-residue inclusion information can be found in section 3 on page 7.

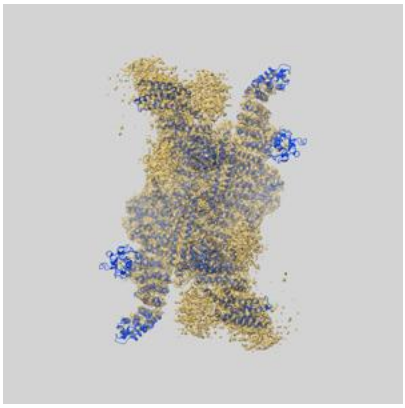
9.1 Map-model overlay



X



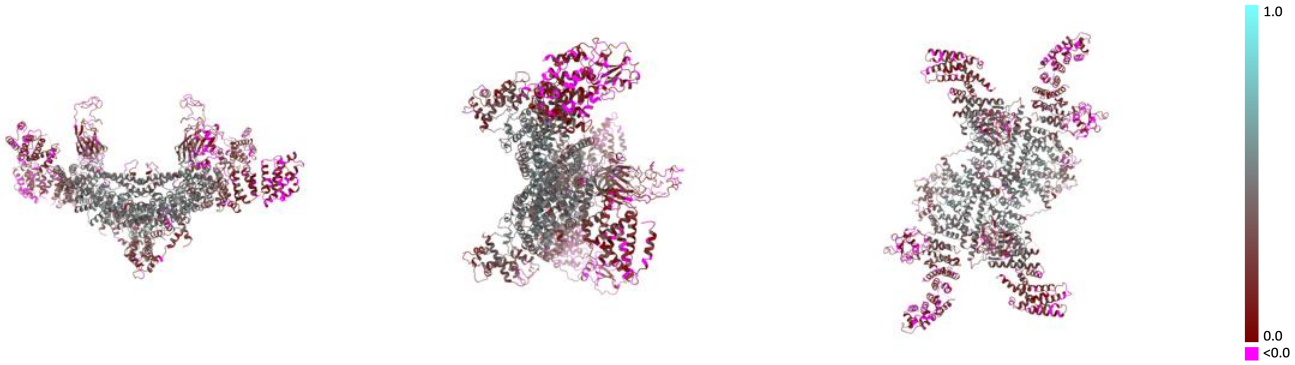
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.146 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.

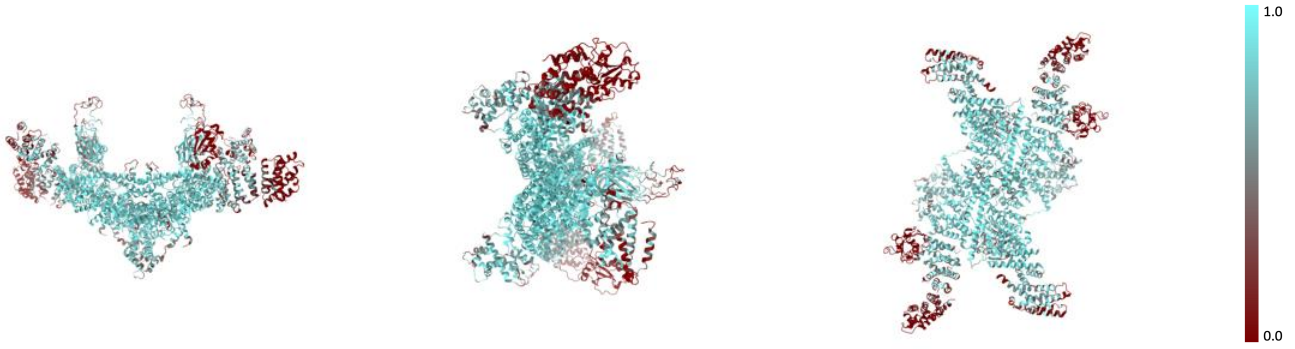
9.2 Q-score mapped to coordinate model (i)



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.

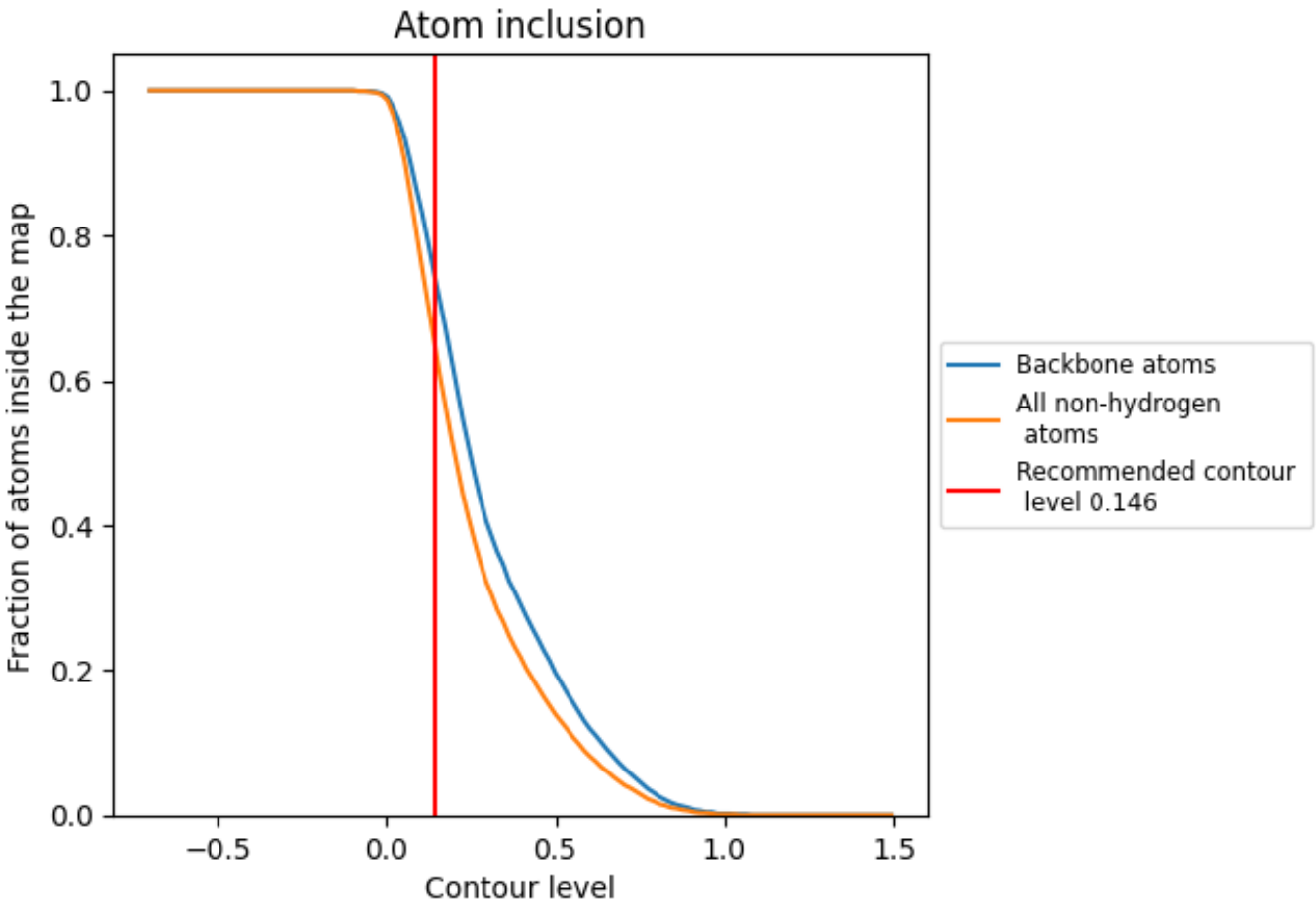
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.146).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.146) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6410	0.2850
A	0.6370	0.2880
B	0.6360	0.2870
C	0.6210	0.2260
D	0.6390	0.2360
E	0.8160	0.3900
F	0.8230	0.3850