Full wwPDB EM Validation Report ⓘ

Mar 18, 2023 – 02:56 PM EDT

PDB ID	:	8E2K
EMDB ID	:	EMD-27841
Title	:	Cryo-EM structure of BIRC6/HtrA2-S306A
Authors	:	Hunkeler, M.; Fischer, E.S.
Deposited on	:	2022-08-15
Resolution	:	3.21 Å(reported)

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

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

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

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

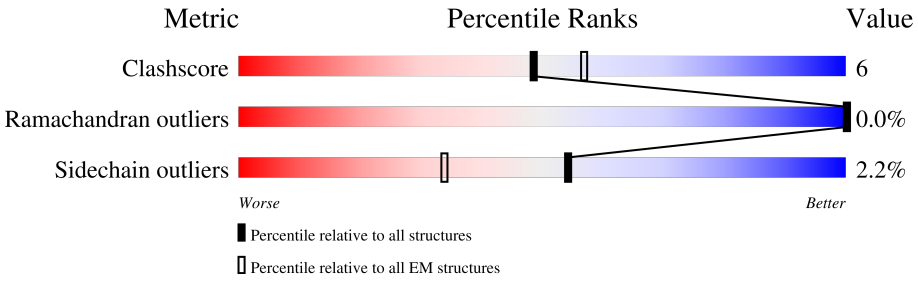
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 3.21 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4898	17% 46% 9% 44%
1	B	4898	15% 47% 9% 44%
2	X	332	28% 74% 13% • 12%
2	Y	332	26% 51% 6% 43%
2	Z	332	26% 52% 5% 43%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 96785 atoms, of which 48882 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 Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	2745	Total	C	H	N	O	S	21	0
			43316	13710	21895	3643	3918	150		
1	B	2745	Total	C	H	N	O	S	21	0
			43316	13710	21895	3643	3918	150		

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	expression tag	UNP Q9NR09
A	-39	GLY	-	expression tag	UNP Q9NR09
A	-38	ASP	-	expression tag	UNP Q9NR09
A	-37	TYR	-	expression tag	UNP Q9NR09
A	-36	LYS	-	expression tag	UNP Q9NR09
A	-35	ASP	-	expression tag	UNP Q9NR09
A	-34	HIS	-	expression tag	UNP Q9NR09
A	-33	ASP	-	expression tag	UNP Q9NR09
A	-32	GLY	-	expression tag	UNP Q9NR09
A	-31	ASP	-	expression tag	UNP Q9NR09
A	-30	TYR	-	expression tag	UNP Q9NR09
A	-29	LYS	-	expression tag	UNP Q9NR09
A	-28	ASP	-	expression tag	UNP Q9NR09
A	-27	HIS	-	expression tag	UNP Q9NR09
A	-26	ASP	-	expression tag	UNP Q9NR09
A	-25	ILE	-	expression tag	UNP Q9NR09
A	-24	ASP	-	expression tag	UNP Q9NR09
A	-23	TYR	-	expression tag	UNP Q9NR09
A	-22	LYS	-	expression tag	UNP Q9NR09
A	-21	ASP	-	expression tag	UNP Q9NR09
A	-20	ASP	-	expression tag	UNP Q9NR09
A	-19	ASP	-	expression tag	UNP Q9NR09
A	-18	ASP	-	expression tag	UNP Q9NR09
A	-17	LYS	-	expression tag	UNP Q9NR09
A	-16	GLY	-	expression tag	UNP Q9NR09
A	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	GLY	-	expression tag	UNP Q9NR09
A	-13	SER	-	expression tag	UNP Q9NR09
A	-12	GLY	-	expression tag	UNP Q9NR09
A	-11	GLY	-	expression tag	UNP Q9NR09
A	-10	LEU	-	expression tag	UNP Q9NR09
A	-9	GLU	-	expression tag	UNP Q9NR09
A	-8	VAL	-	expression tag	UNP Q9NR09
A	-7	LEU	-	expression tag	UNP Q9NR09
A	-6	PHE	-	expression tag	UNP Q9NR09
A	-5	GLN	-	expression tag	UNP Q9NR09
A	-4	GLY	-	expression tag	UNP Q9NR09
A	-3	PRO	-	expression tag	UNP Q9NR09
A	-2	SER	-	expression tag	UNP Q9NR09
A	-1	ARG	-	expression tag	UNP Q9NR09
A	0	THR	-	expression tag	UNP Q9NR09
A	1332	VAL	LEU	conflict	UNP Q9NR09
B	-40	MET	-	expression tag	UNP Q9NR09
B	-39	GLY	-	expression tag	UNP Q9NR09
B	-38	ASP	-	expression tag	UNP Q9NR09
B	-37	TYR	-	expression tag	UNP Q9NR09
B	-36	LYS	-	expression tag	UNP Q9NR09
B	-35	ASP	-	expression tag	UNP Q9NR09
B	-34	HIS	-	expression tag	UNP Q9NR09
B	-33	ASP	-	expression tag	UNP Q9NR09
B	-32	GLY	-	expression tag	UNP Q9NR09
B	-31	ASP	-	expression tag	UNP Q9NR09
B	-30	TYR	-	expression tag	UNP Q9NR09
B	-29	LYS	-	expression tag	UNP Q9NR09
B	-28	ASP	-	expression tag	UNP Q9NR09
B	-27	HIS	-	expression tag	UNP Q9NR09
B	-26	ASP	-	expression tag	UNP Q9NR09
B	-25	ILE	-	expression tag	UNP Q9NR09
B	-24	ASP	-	expression tag	UNP Q9NR09
B	-23	TYR	-	expression tag	UNP Q9NR09
B	-22	LYS	-	expression tag	UNP Q9NR09
B	-21	ASP	-	expression tag	UNP Q9NR09
B	-20	ASP	-	expression tag	UNP Q9NR09
B	-19	ASP	-	expression tag	UNP Q9NR09
B	-18	ASP	-	expression tag	UNP Q9NR09
B	-17	LYS	-	expression tag	UNP Q9NR09
B	-16	GLY	-	expression tag	UNP Q9NR09
B	-15	GLY	-	expression tag	UNP Q9NR09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	GLY	-	expression tag	UNP Q9NR09
B	-13	SER	-	expression tag	UNP Q9NR09
B	-12	GLY	-	expression tag	UNP Q9NR09
B	-11	GLY	-	expression tag	UNP Q9NR09
B	-10	LEU	-	expression tag	UNP Q9NR09
B	-9	GLU	-	expression tag	UNP Q9NR09
B	-8	VAL	-	expression tag	UNP Q9NR09
B	-7	LEU	-	expression tag	UNP Q9NR09
B	-6	PHE	-	expression tag	UNP Q9NR09
B	-5	GLN	-	expression tag	UNP Q9NR09
B	-4	GLY	-	expression tag	UNP Q9NR09
B	-3	PRO	-	expression tag	UNP Q9NR09
B	-2	SER	-	expression tag	UNP Q9NR09
B	-1	ARG	-	expression tag	UNP Q9NR09
B	0	THR	-	expression tag	UNP Q9NR09
B	1332	VAL	LEU	conflict	UNP Q9NR09

- Molecule 2 is a protein called Serine protease HTRA2, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	X	292	Total	C	H	N	O	S	0	0
			4473	1405	2248	397	418	5		
2	Y	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		
2	Z	189	Total	C	H	N	O	S	0	0
			2840	897	1422	247	272	2		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	133	MET	-	initiating methionine	UNP O43464
X	306	ALA	SER	conflict	UNP O43464
X	459	HIS	-	expression tag	UNP O43464
X	460	HIS	-	expression tag	UNP O43464
X	461	HIS	-	expression tag	UNP O43464
X	462	HIS	-	expression tag	UNP O43464
X	463	HIS	-	expression tag	UNP O43464
X	464	HIS	-	expression tag	UNP O43464
Y	133	MET	-	initiating methionine	UNP O43464
Y	306	ALA	SER	conflict	UNP O43464
Y	459	HIS	-	expression tag	UNP O43464
Y	460	HIS	-	expression tag	UNP O43464

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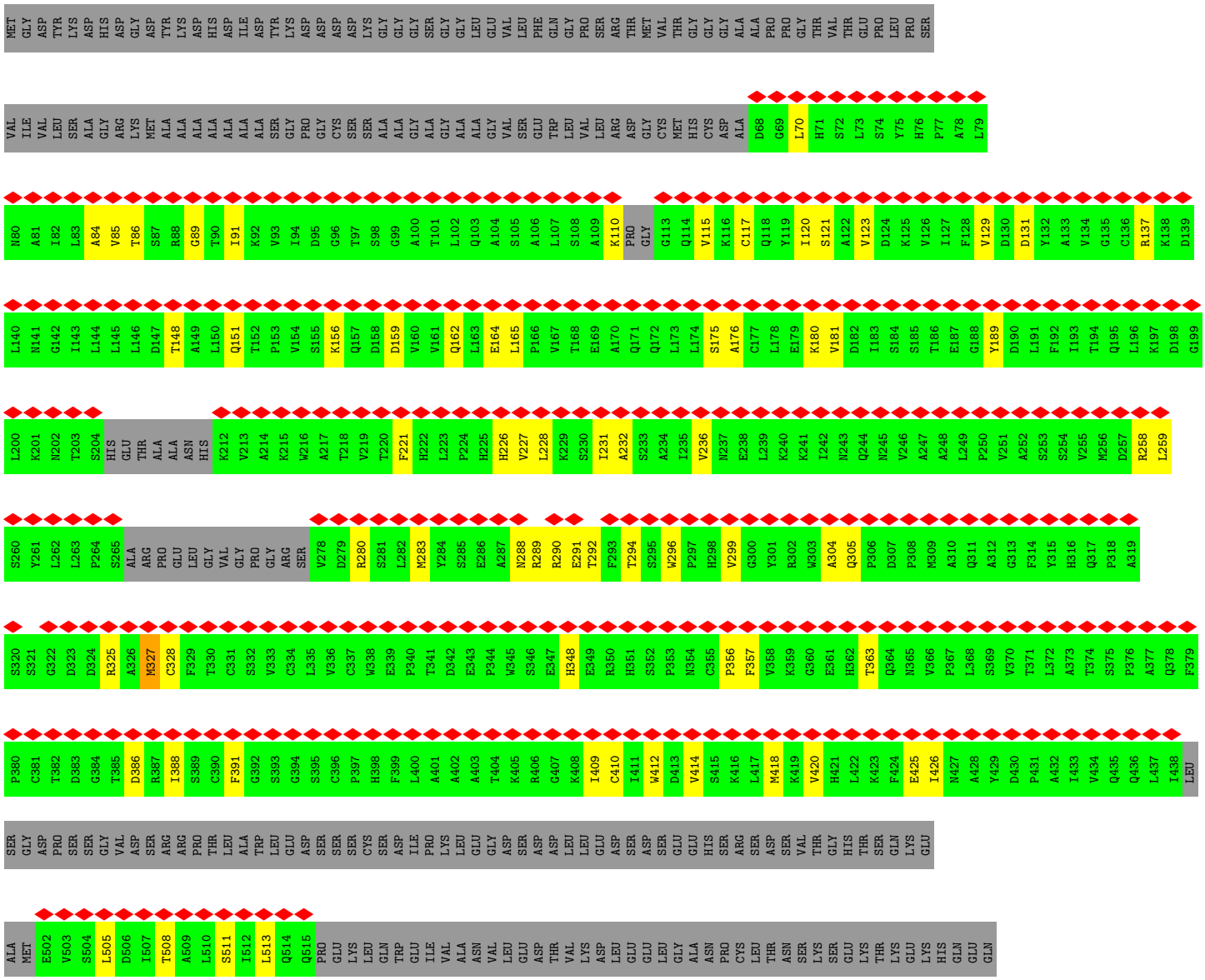
Chain	Residue	Modelled	Actual	Comment	Reference
Y	461	HIS	-	expression tag	UNP O43464
Y	462	HIS	-	expression tag	UNP O43464
Y	463	HIS	-	expression tag	UNP O43464
Y	464	HIS	-	expression tag	UNP O43464
Z	133	MET	-	initiating methionine	UNP O43464
Z	306	ALA	SER	conflict	UNP O43464
Z	459	HIS	-	expression tag	UNP O43464
Z	460	HIS	-	expression tag	UNP O43464
Z	461	HIS	-	expression tag	UNP O43464
Z	462	HIS	-	expression tag	UNP O43464
Z	463	HIS	-	expression tag	UNP O43464
Z	464	HIS	-	expression tag	UNP O43464

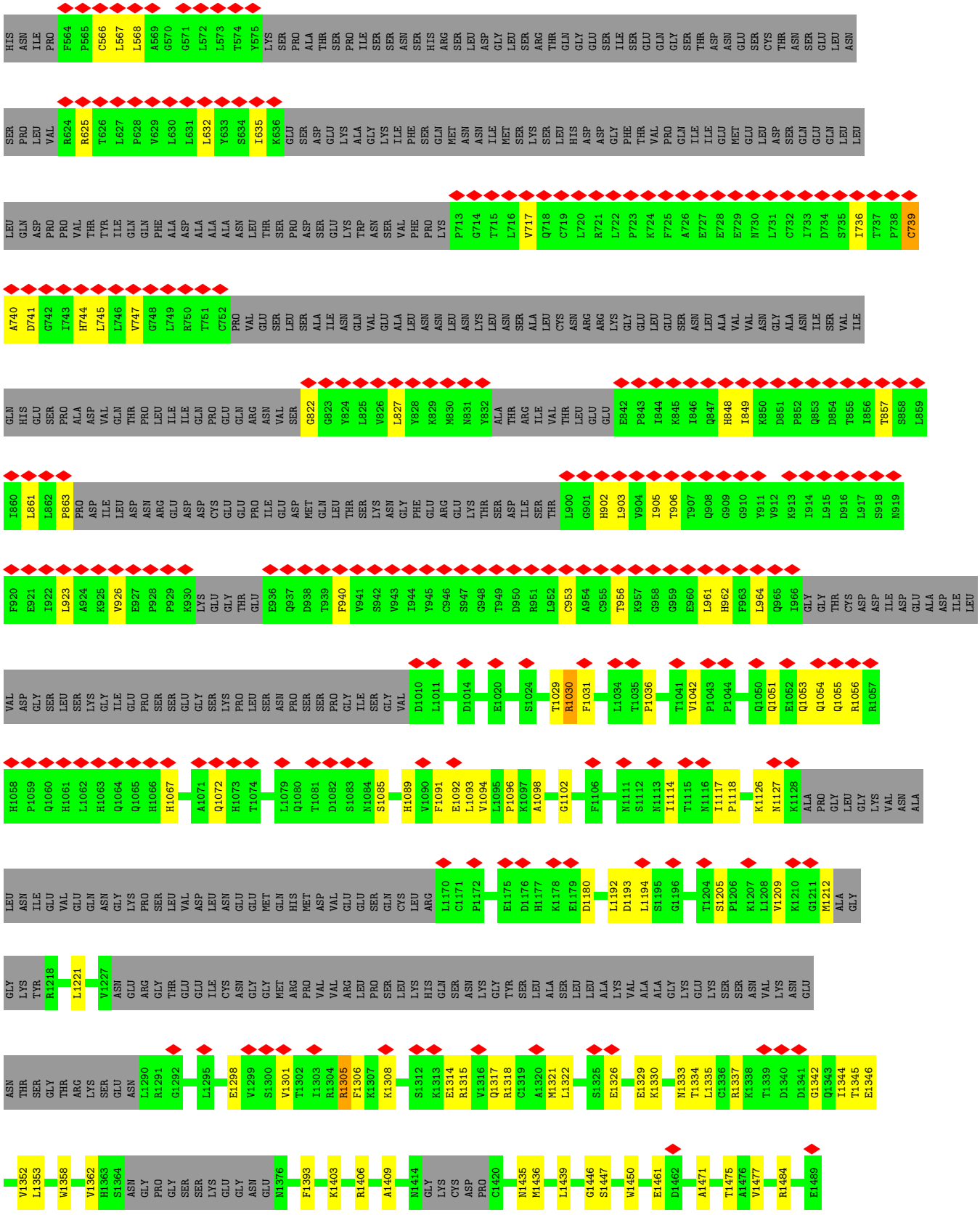
3 Residue-property plots (i)

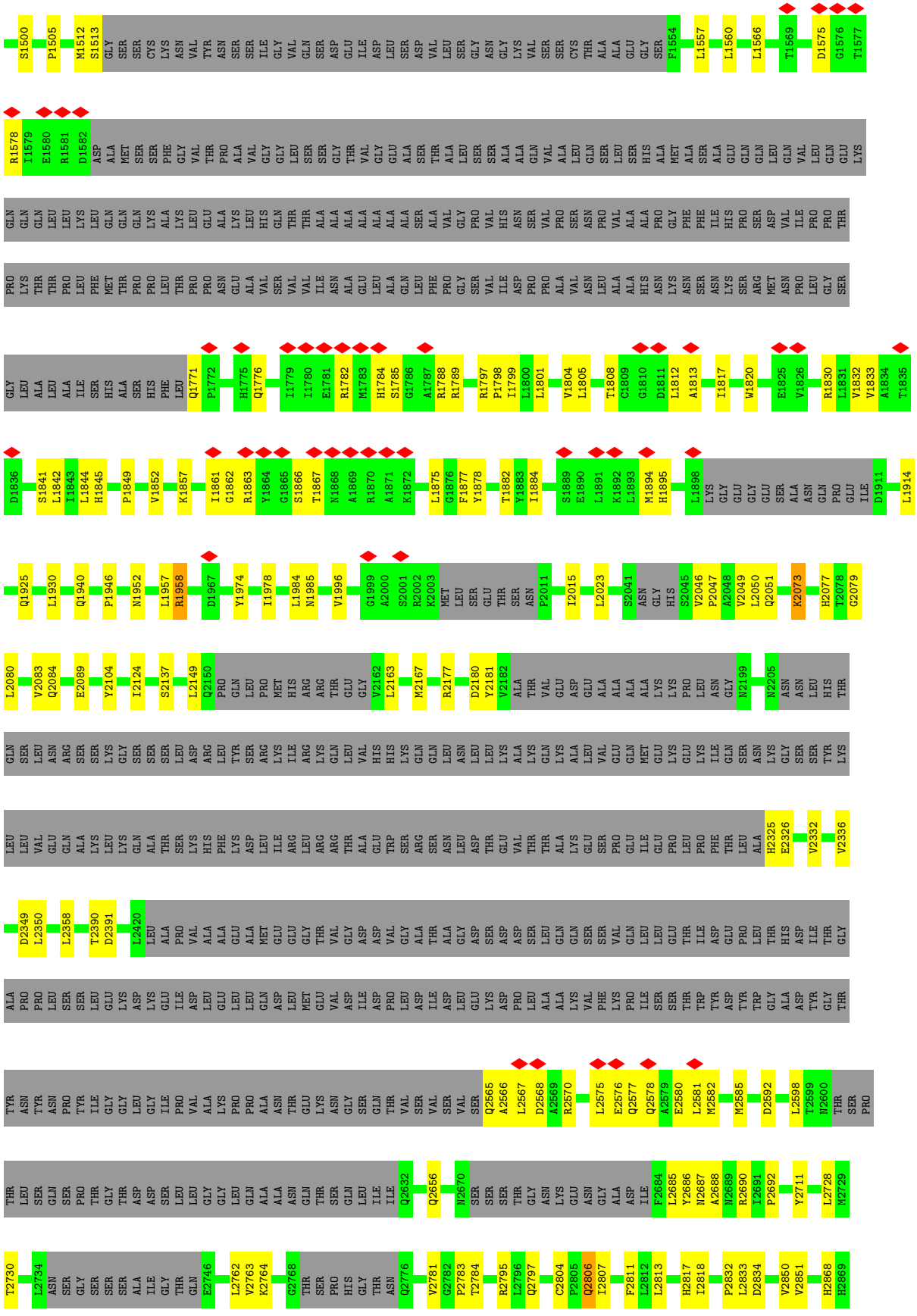
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

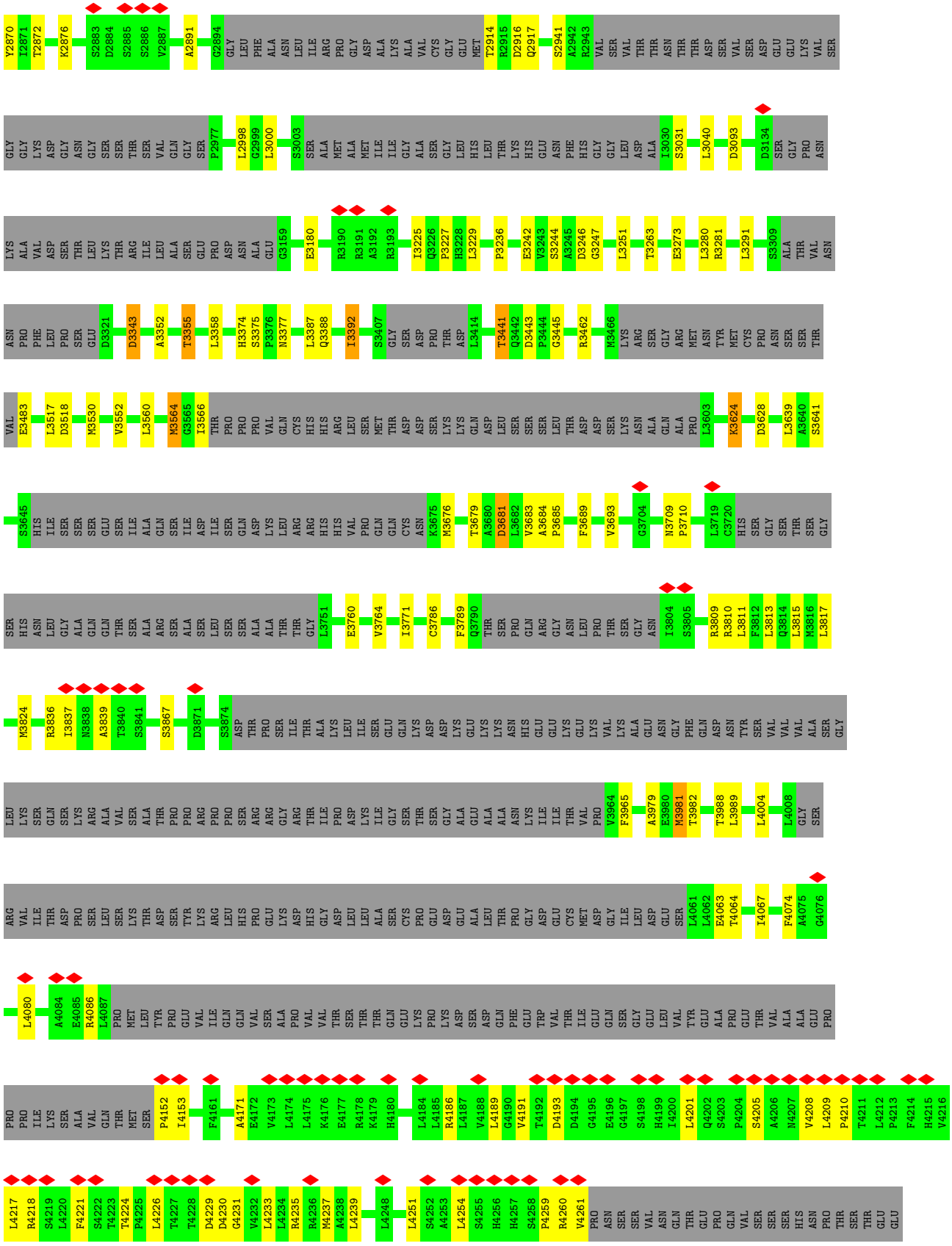
- Molecule 1: Baculoviral IAP repeat-containing protein 6

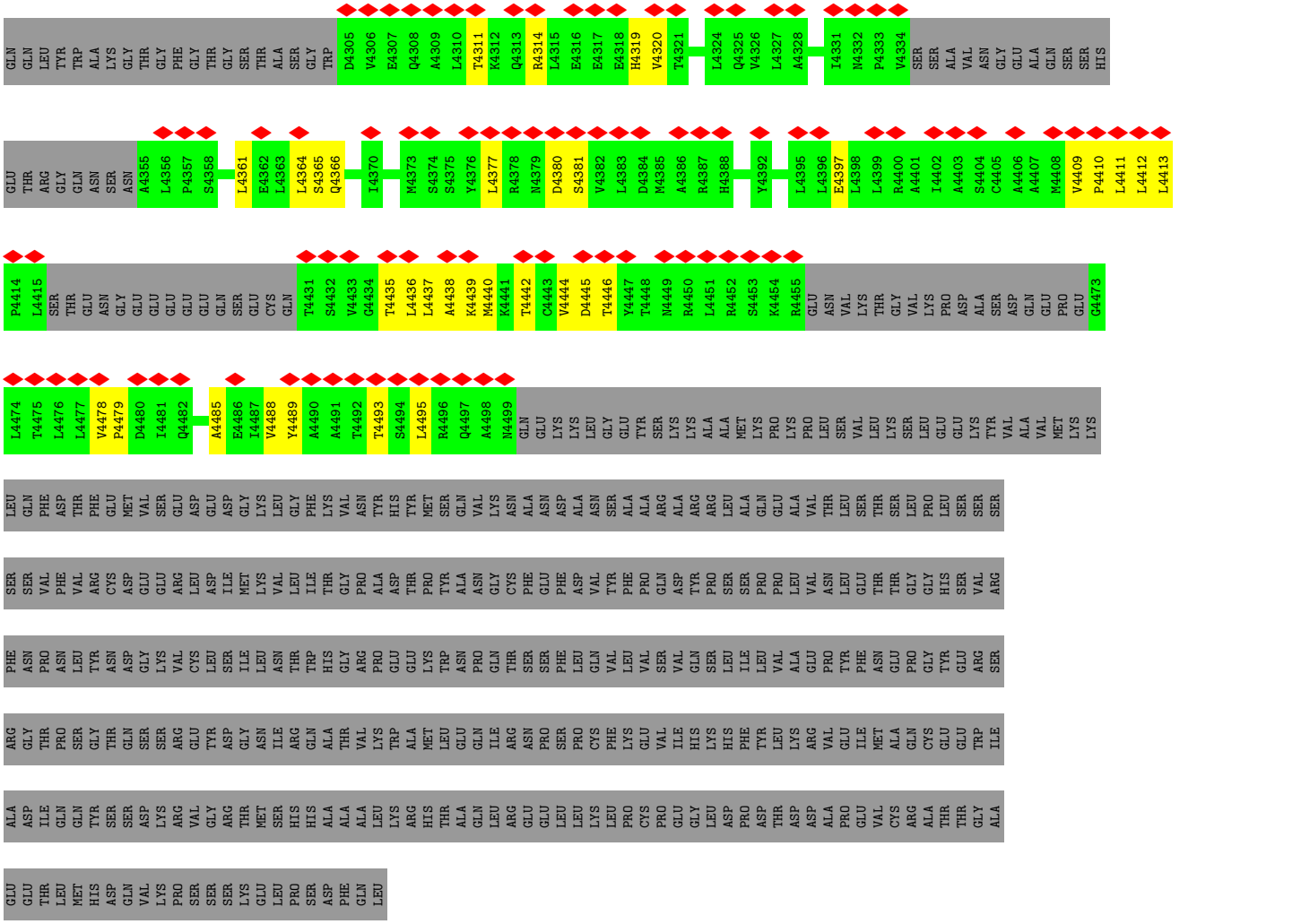
Chain A:





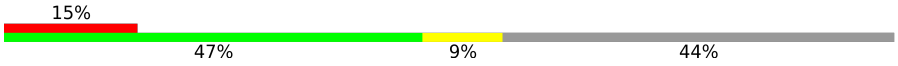


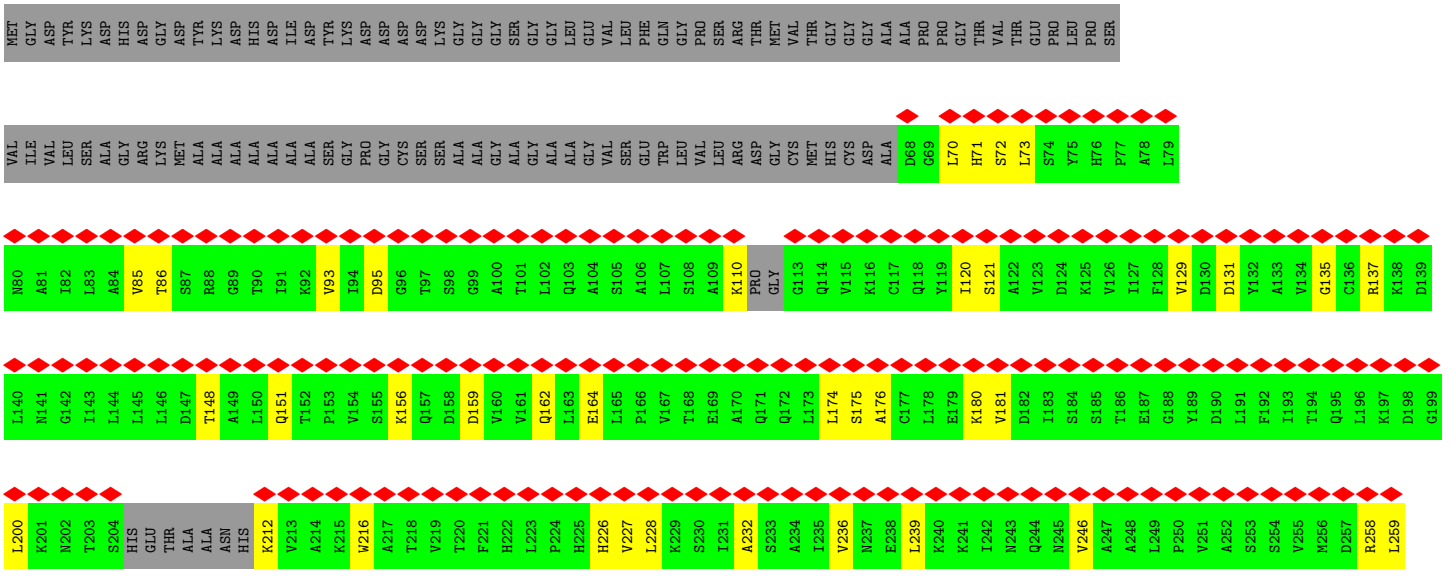


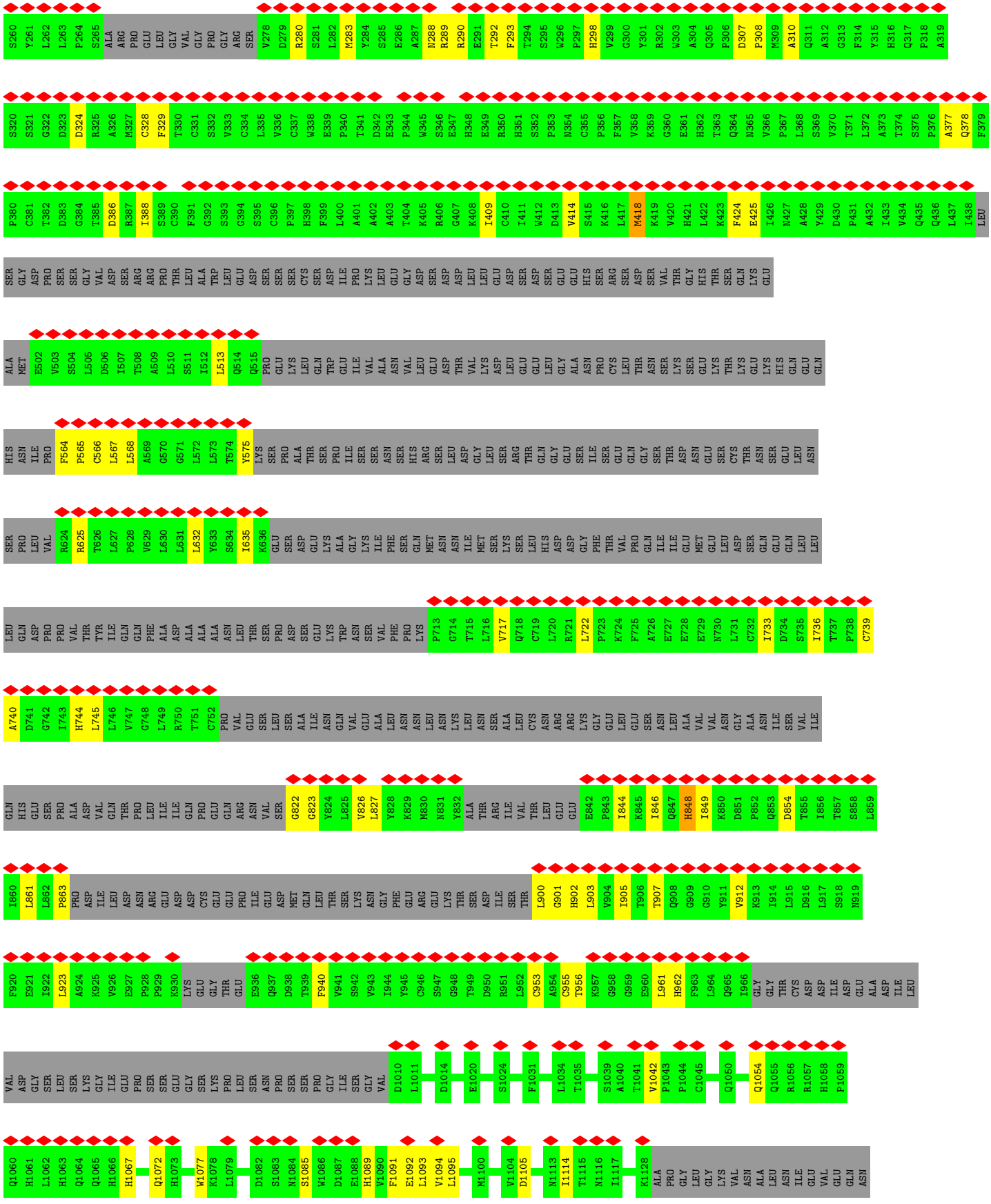


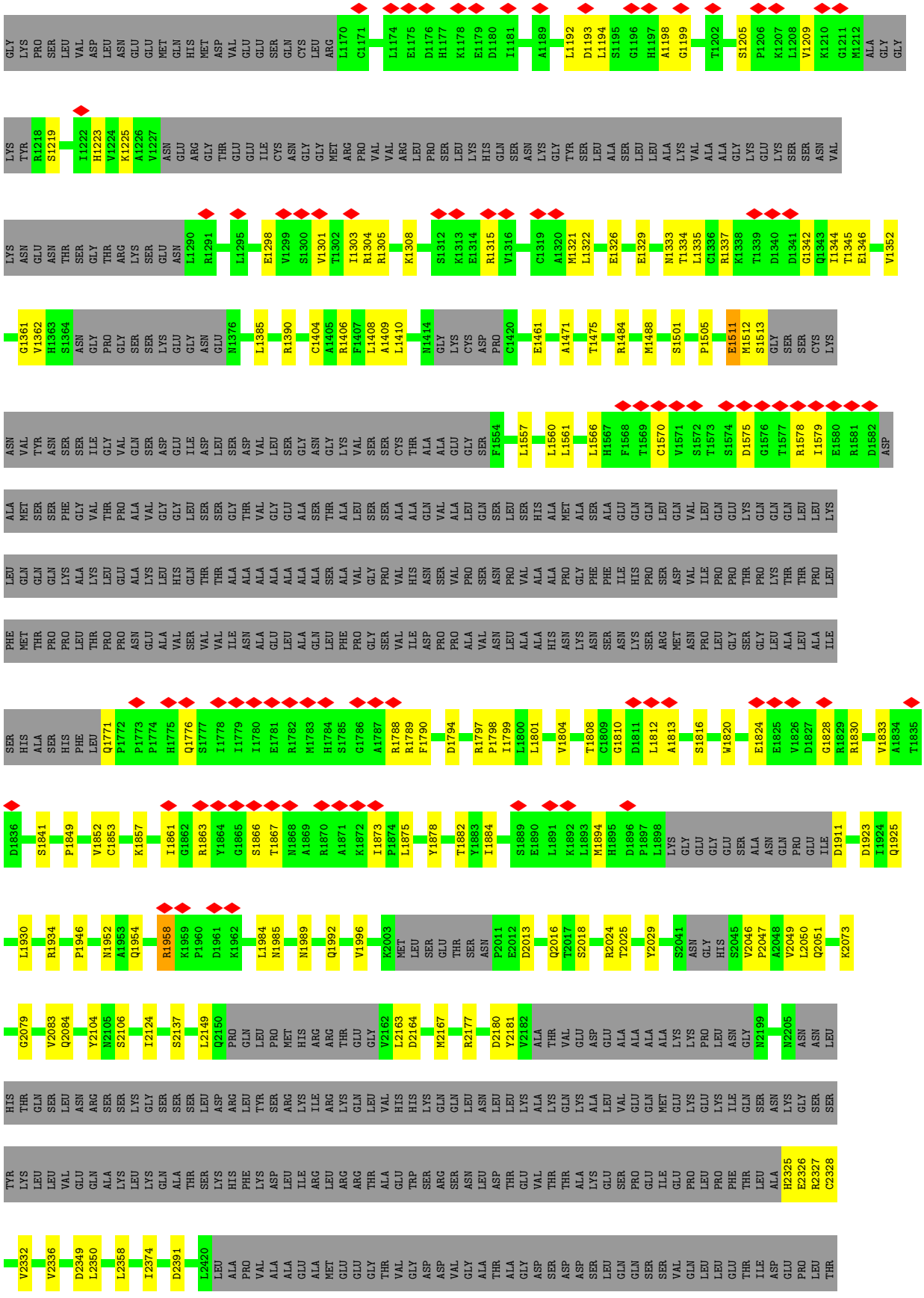
• Molecule 1: Baculoviral IAP repeat-containing protein 6

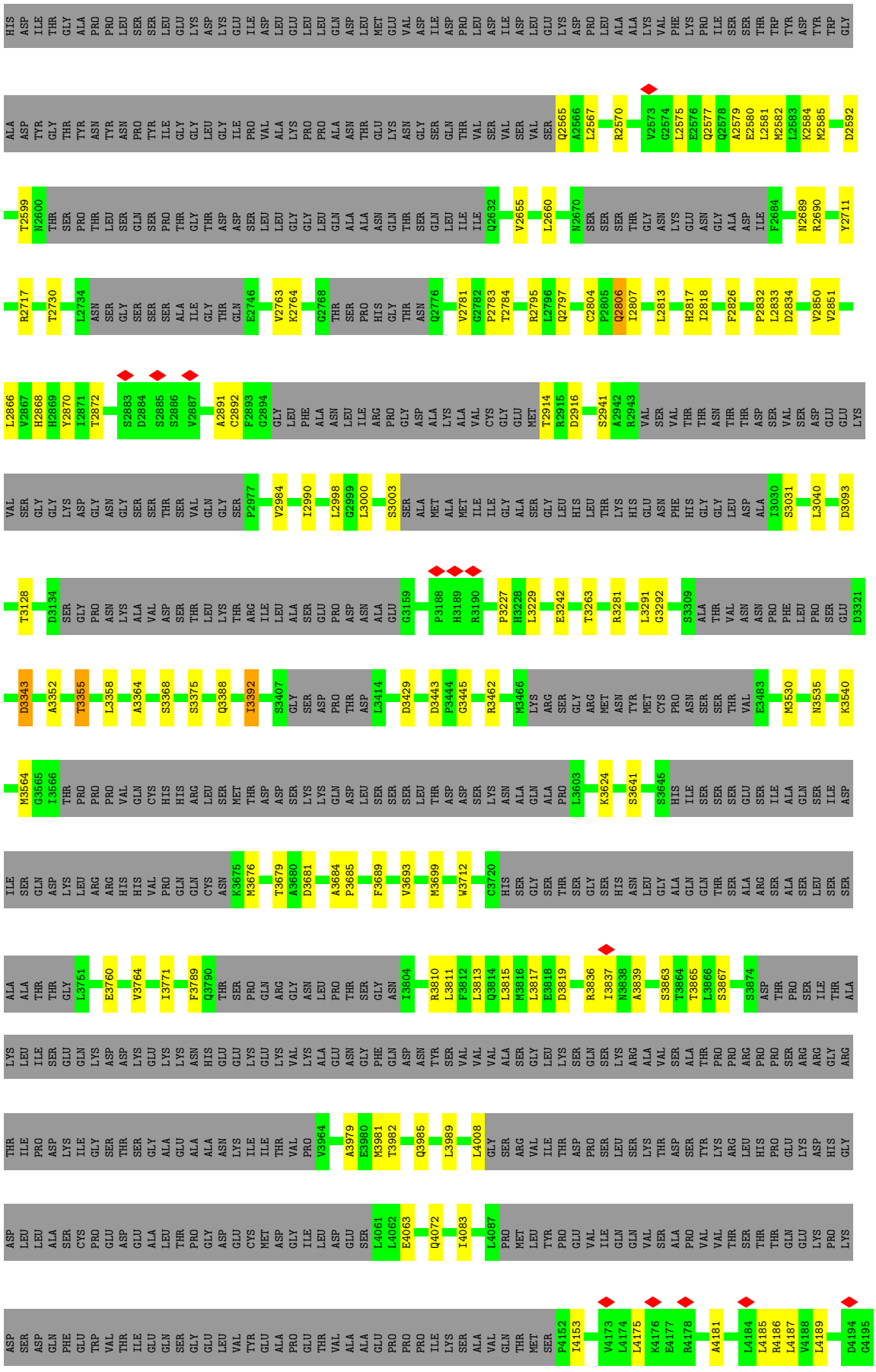
Chain B:

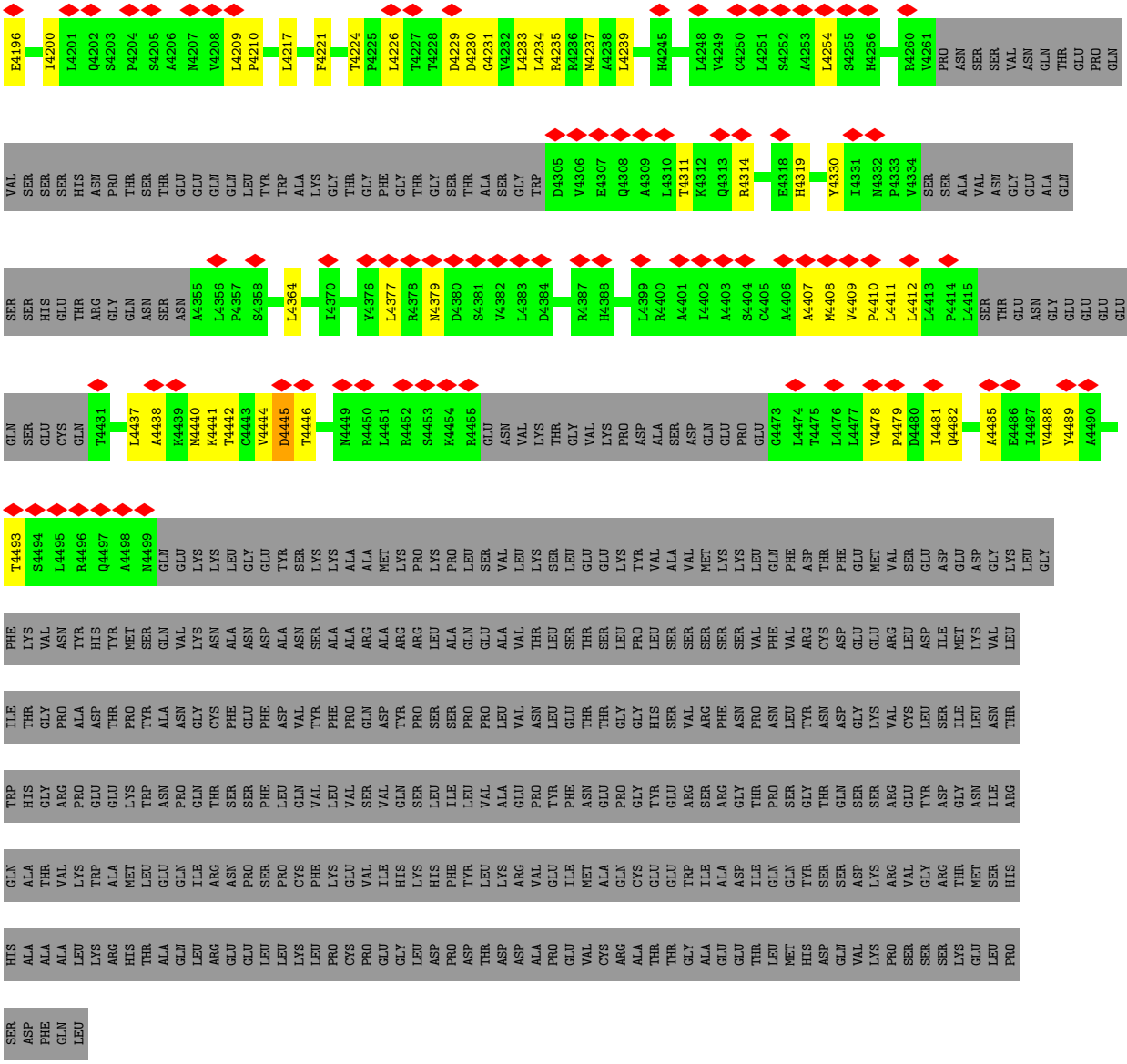





S260 Y261 L262 L263 P264 S265 ALA ARG PRO GLU LEU GLY VAL GLY PRO GLY ARG SER V278 D279 R280 S281 L282 M283 Y284 S285 E286 A287 N288 R289 R290 E291 T292 F293 T294 S295 W296 P297 H298 V299 G300 Y301 R302 W303 A304 Q305 P306 D307 P308 M309 A310 Q311 A312 G313 F314 Y315 H316 Q317 P318 A319
S320 S321 G322 D323 D324 R325 A326 M327 C328 F329 T330 C331 S332 V333 C334 L335 V336 C337 W338 E339 P340 T341 D342 E343 P344 W345 S346 E347 H348 E349 R350 H351 S352 P353 N354 C355 P356 F357 V358 K359 G360 E361 H362 T363 Q364 N365 V366 P367 L368 S369 V370 T371 L372 A373 T374 S375 P376 A377 Q378 F379
P380 C381 T382 D383 G384 T385 D386 R387 I388 S389 C390 F391 G392 S393 G394 S395 C396 P397 H398 F399 L400 A401 A402 A403 T404 K405 R406 G407 K408 I409 C410 I411 W412 D413 V414 S415 K416 L417 M418 K419 V420 H421 L422 K423 F424 E425 I426 N427 A428 Y429 D430 P431 A432 I433 V434 Q435 Q436 L437 I438 LEU
SER GLY ASP PRO SER SER GLY VAL ASP SER ARG ARG PRO THR LEU ALA TRP LEU GLU ASP SER SER SER CYS SER ASP ILE PRO LYS LEU GLU GLY ASP SER ASP ASP LEU LEU GLU ASP SER ASP SER GLU GLU HIS SER ARG SER ASP SER VAL THR GLY HIS THR SER GLN LYS GLU
ALA MET E502 V503 S504 L505 D506 I507 T508 A509 L510 S511 I512 L513 Q514 Q515 PRO GLU LYS LEU GLN TRP GLU ILE VAL ALA ASN VAL LEU GLU ASP THR VAL LYS ASP LEU GLU GLU LEU GLY ALA ASN PRO CYS LEU THR ASN SER LYS SER GLU LYS THR LYS GLU LYS HIS GLN GLU GLN
HIS ASN ILE PRO F564 P565 C566 L567 L568 A569 G570 G571 L572 L573 T574 Y575 LYS SER PRO ALA THR SER PRO ILE SER SER ASN SER HIS ARG SER LEU ASP GLY LEU SER ARG THR GLN GLY GLU SER ILE SER GLU GLN GLY SER THR ASP ASN GLU SER CYS THR ASN SER GLU LEU ASN
SER PRO LEU VAL R624 R625 T626 L627 P628 V629 L630 L631 L632 Y633 S634 I635 K636 GLU SER ASP GLU LYS ALA GLY LYS ILE PHE SER GLN MET ASN ASN ILE MET SER LYS SER LEU HIS ASP ASP GLY PHE THR VAL PRO GLN ILE ILE GLU MET GLU LEU ASP SER GLN GLU GLN LEU LEU
LEU GLN ASP PRO PRO PRO VAL THR TYR ILE GLN GLN PHE ALA ASP ALA ALA ALA ASN LEU THR SER PRO ASP SER GLU LYS TRP ASN SER SER VAL PHE PRO LYS P713 G714 T715 L716 V717 Q718 C719 L720 R721 L722 P723 K724 F725 A726 E727 E728 E729 N730 L731 C732 I733 D734 S735 I736 T737 P738 C739
A740 D741 G742 I743 H744 L745 L746 V747 G748 L749 R750 T751 C752 PRO VAL GLU SER LEU SER ALA ILE ASN GLN VAL GLU ALA LEU ASN ASN LEU ASN LYS LEU ASN SER ALA LEU CYS ASN ARG ARG LYS GLY GLU LEU GLU SER ASN LEU ALA VAL VAL ASN GLY ALA ASN ILE SER VAL ILE
GLN HIS GLU SER PRO ALA ASP VAL GLN THR PRO LEU ILE ILE GLN PRO GLU GLN ARG ASN VAL SER G822 G823 Y824 L825 V826 L827 Y828 K829 M830 N831 Y832 ALA THR ARG ILE VAL THR LEU GLU GLU E842 P843 I844 K845 I846 Q847 H848 I849 K850 D851 P852 Q853 D854 T855 I856 T857 S858 L859
I860 L861 L862 P863 PRO ASP ILE LEU ASP ASN ARG GLU ASP ASP CYS GLU GLU PRO ILE GLU ASP MET GLN LEU THR SER LYS ASN GLY PHE GLU ARG GLU LYS THR SER ASP ILE SER THR L900 G901 H902 L903 V904 I905 T906 T907 Q908 G909 G910 Y911 V912 K913 I914 L915 D916 L917 S918 N919
F920 E921 I922 L923 A924 K925 V926 E927 P928 P929 K930 LYS GLU GLY THR GLU E936 Q937 D938 T939 F940 V941 S942 V943 I944 Y945 C946 S947 G948 T949 D950 R951 L952 C953 A954 C955 T956 K957 G958 G959 E960 L961 H962 F963 L964 Q965 I966 GLY GLY THR CYS ASP ILE ASP GLU ALA ASP ILE LEU
VAL ASP GLY SER LEU SER LYS GLY ILE GLU PRO SER SER GLU GLY SER LYS PRO LEU SER ASN PRO SER SER PRO GLY ILE SER GLY VAL D1010 L1011 D1014 E1020 S1024 F1031 L1034 T1035 S1039 A1040 T1041 V1042 P1043 P1044 C1045 Q1050 Q1054 Q1055 R1056 R1057 H1058 P1059
Q1060 H1061 L1062 H1063 Q1064 Q1065 H1066 H1067 Q1072 H1073 W1077 K1078 L1079 D1082 S1083 N1084 S1085 W1086 D1087 E1088 H1089 V1090 F1091 E1092 L1093 V1094 L1095 M1100 V1104 D1105 N1113 I1114 T1115 N1116 I1117 K1128 ALA PRO GLY LEU GLY LYS VAL ASN ALA LEU ASN ILE GLU VAL GLU GLN ASN

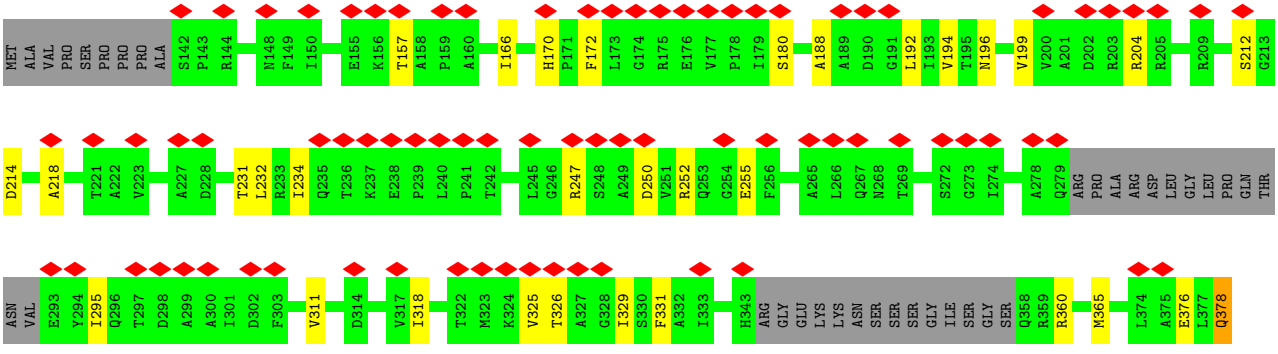


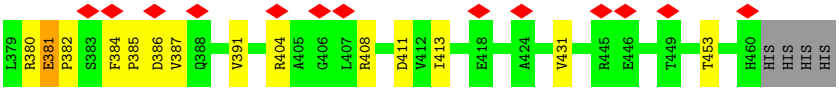

HIS ASP ILE THR GLY ALA PRO PRO LEU SER SER LEU GLU LYS ASP LYS GLU ILE ASP LEU GLU LEU LEU GLN ASP LEU MET GLU VAL ASP ILE ASP PRO LEU ASP ILE ASP LEU GLU LYS ASP PRO LEU ALA ALA LYS VAL PHE LYS PRO ILE SER SER THR TRP TYR ASP TRP TYR
ALA ASP TYR GLY THR TYR ASN TYR ASN PRO TYR ILE GLY GLY LEU GLY ILE PRO VAL ALA LYS PRO PRO ALA ASN THR GLU LYS ASN GLY SER GLN THR VAL SER VAL SER Q2565 A2566 L2567 R2570 V2573 G2574 L2575 E2576 Q2577 Q2578 A2579 E2580 L2581 M2582 L2583 K2584 M2585 D2592
T2599 N2600 THR SER PRO THR LEU SER GLN SER PRO THR GLY THR ASP ASP SER LEU LEU GLY GLY LEU GLN ALA ALA ASN GLN THR SER GLN LEU ILE ILE Q2632 V2655 L2660 N2670 SER SER SER THR GLY ASN LYS GLU ASN GLY ALA ASP ILE F2684 N2689 R2690 Y2711
R2717 T2730 L2734 ASN SER GLY SER SER SER ALA ILE GLY THR GLN E2746 V2763 K2764 G2768 THR SER PRO HIS GLY THR ASN Q2776 V2781 G2782 P2783 T2784 R2795 L2796 Q2797 C2804 P2805 Q2806 I2807 L2813 H2817 I2818 F2826 P2832 L2833 D2834 V2850 V2851
L2866 V2867 H2868 H2869 V2870 I2871 T2872 S2883 D2884 S2885 S2886 V2887 A2891 C2892 F2893 G2894 GLY LEU PHE ALA ASN LEU ILE ARG PRO GLY ASP ALA LYS ALA VAL CYS GLY GLU MET T2914 R2915 D2916 S2941 A2942 R2943 VAL SER VAL THR THR THR ASN THR THR ASP SER VAL SER ASP GLU GLU LYS
VAL SER GLY GLY LYS ASP GLY ASN GLY SER SER THR SER VAL GLN GLY SER P2977 V2984 I2990 L2998 G2999 L3000 S3003 SER ALA MET ALA MET ILE ILE GLY ALA SER GLY LEU HIS LEU THR LYS HIS GLU ASN PHE HIS GLY GLY LEU ASP ALA I3030 S3031 L3040 D3093
T3128 D3134 SER GLY PRO ASN LYS ALA VAL ASP SER THR LEU LYS THR ARG ILE LEU ALA SER GLU PRO ASP ASN ALA GLU G3159 P3188 H3189 R3190 P3227 H3228 L3229 E3242 T3263 R3281 L3291 G3292 S3309 ALA THR VAL ASN ASN PRO PHE LEU PRO SER GLU D3321
D3343 A3352 T3355 L3358 A3364 S3368 S3375 Q3388 I3392 S3407 GLY SER ASP PRO THR ASP L3414 D3429 D3443 P3444 G3445 R3462 M3466 LYS ARG SER GLY ARG MET ASN TYR MET CYS PRO ASN SER SER THR VAL E3483 M3530 N3535 K3540
M3564 G3565 I3566 THR PRO PRO PRO VAL GLN CYS HIS HIS ARG LEU SER MET THR ASP ASP SER LYS LYS GLN ASP LEU SER SER SER LEU THR ASP GLU GLN ALA PRO L3603 K3624 S3641 S3645 HIS ILE SER SER SER SER GLU GLU SER ILE ALA GLN SER ILE ASP
ILE SER GLN ASP LYS LEU ARG ARG HIS HIS VAL PRO GLN GLN CYS ASN K3675 M3676 T3679 A3680 D3681 A3684 P3685 F3689 V3693 M3699 W3712 C3720 HIS SER GLY SER THR SER GLY SER HIS ASN LEU GLY ALA GLN GLN THR SER ALA ARG SER ALA SER LEU SER SER
ALA ALA THR THR GLY L3751 E3760 V3764 I3771 F3789 Q3790 THR SER PRO GLN ARG GLY ASN LEU PRO THR SER GLY ASN I3804 R3810 L3811 F3812 L3813 Q3814 L3815 M3816 L3817 E3818 D3819 R3836 I3837 N3838 A3839 S3863 T3864 T3865 L3866 S3867 S3874 ASP THR PRO SER ILE THR ALA
LYS LEU ILE SER GLU GLN LYS ASP LYS GLU LYS LYS LYS ASN HIS GLU GLU LYS LYS GLU LYS VAL LYS ALA GLU ASN GLY PHE GLN ASP ASN TYR SER VAL VAL ALA SER GLY LEU LYS SER GLN SER LYS ARG ALA VAL SER ALA THR PRO PRO PRO ARG PRO PRO SER ARG ARG GLY ARG
THR ILE PRO ASP LYS ILE GLY SER THR SER GLY ALA GLU ALA ASN LYS ILE ILE THR VAL PRO V3964 A3979 E3980 M3981 T3982 Q3985 L3989 L4008 GLY SER ARG VAL ILE THR ASP PRO SER LEU SER LYS THR ASP SER TYR LYS ARG LEU HIS PRO GLU LYS ASP HIS GLY
ASP LEU LEU ALA SER CYS PRO GLU ALA LEU THR PRO GLY ASP ILE LEU ASP GLU SER L4061 L4062 E4063 Q4072 I4083 L4087 PRO MET LEU TYR PRO GLU VAL ILE GLN GLN VAL SER ALA PRO VAL VAL THR SER THR THR GLN GLU LYS PRO LYS
ASP SER ASP GLN PHE GLU TRP VAL THR ILE GLU GLU GLN SER GLY GLU LEU VAL TYR GLU ALA PRO GLU THR VAL ALA ALA GLU PRO PRO PRO ILE LYS SER ALA VAL GLN THR MET SER P4152 I4153 V4173 L4174 L4175 K4176 E4177 R4178 A4181 L4184 L4185 R4186 L4187 V4188 L4189 D4194 G4195



• Molecule 2: Serine protease HTRA2, mitochondrial

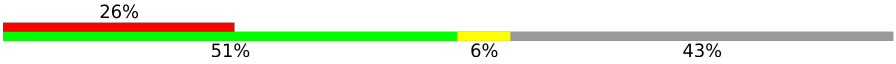
Chain X:

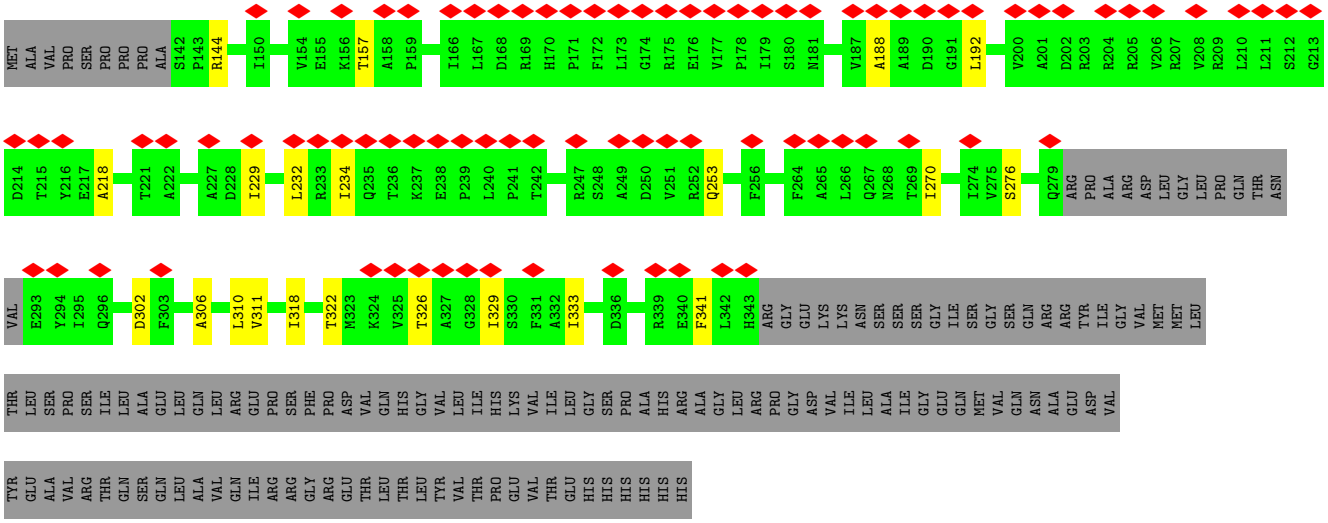




• Molecule 2: Serine protease HTRA2, mitochondrial

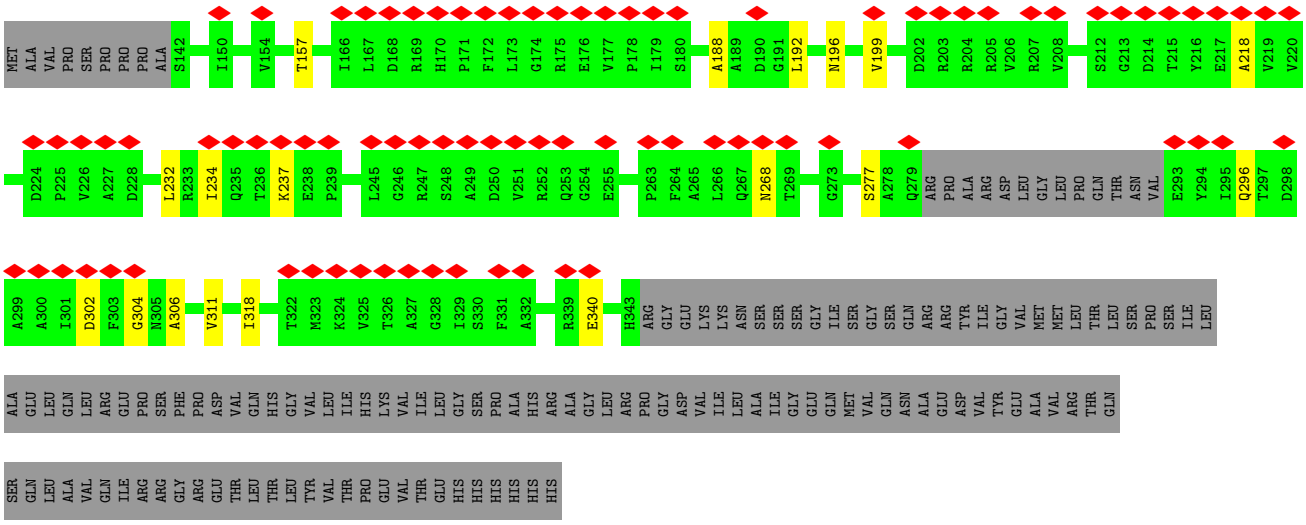
Chain Y:





• Molecule 2: Serine protease HTRA2, mitochondrial

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73712	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.659	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.384	Depositor
Minimum map value	-0.530	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.215	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/21893	0.49	0/29721
1	B	0.28	0/21893	0.50	0/29721
2	X	0.28	0/2263	0.56	0/3082
2	Y	0.27	0/1442	0.56	0/1967
2	Z	0.27	0/1442	0.56	0/1967
All	All	0.28	0/48933	0.50	0/66458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	21421	21895	21819	301	0
1	B	21421	21895	21819	268	0
2	X	2225	2248	2250	28	0
2	Y	1418	1422	1424	13	0
2	Z	1418	1422	1424	12	0
All	All	47903	48882	48736	603	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 6.

All (603) 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:3817:LEU:HD11	1:A:4189:LEU:HD12	1.35	1.05
1:B:1194:LEU:HD13	1:B:2565:GLN:N	1.83	0.93
1:A:3813:LEU:HD23	1:A:3817:LEU:HD12	1.52	0.92
1:A:3374:HIS:N	2:X:381:GLU:OE2	2.04	0.90
1:A:3374:HIS:ND1	2:X:381:GLU:OE1	2.05	0.89
1:A:4218:ARG:NH2	1:A:4397:GLU:OE2	2.06	0.88
1:B:822:GLY:N	1:B:849:ILE:O	2.11	0.83
1:A:164:GLU:OE1	1:A:258:ARG:NH2	2.12	0.83
1:A:1406:ARG:NH2	1:A:2580:GLU:OE1	2.12	0.82
1:B:3981:MET:O	1:B:3982:THR:OG1	1.98	0.81
1:A:2784:THR:OG1	1:B:3242:GLU:OE2	1.97	0.81
1:A:3817:LEU:O	1:A:4186:ARG:NH1	2.12	0.81
1:B:1866:SER:N	2:Z:340:GLU:OE2	2.13	0.81
1:A:3242:GLU:OE2	1:B:2784:THR:OG1	1.99	0.80
1:A:3981:MET:O	1:A:3982:THR:OG1	2.00	0.79
1:A:3809:ARG:NH2	1:B:1923:ASP:OD1	2.16	0.79
1:B:1946:PRO:O	1:B:1952:ASN:ND2	2.15	0.79
1:A:137:ARG:NH2	1:A:148:THR:O	2.17	0.78
1:B:1337:ARG:NH1	1:B:1342:GLY:O	2.18	0.77
1:B:378:GLN:NE2	1:B:418:MET:SD	2.59	0.76
1:B:1575:ASP:OD2	1:B:1789:ARG:NH2	2.20	0.75
1:B:2079:GLY:O	1:B:2083:VAL:HG23	1.86	0.75
1:B:1329:GLU:OE2	1:B:1333:ASN:ND2	2.20	0.74
1:A:2079:GLY:O	1:A:2083:VAL:HG23	1.88	0.74
1:A:4440:MET:O	1:A:4444:VAL:HG23	1.87	0.74
1:A:288:ASN:O	1:A:292:THR:HG23	1.87	0.73
2:Z:157:THR:HG21	2:Z:311:VAL:HG11	1.71	0.73
1:A:857:THR:OG1	1:A:906:THR:O	2.05	0.73
1:B:4181:ALA:O	1:B:4185:LEU:HD12	1.89	0.72
1:A:3771:ILE:HD11	1:A:3815:LEU:HD11	1.71	0.71
1:B:2891:ALA:O	1:B:3031:SER:OG	2.08	0.71
1:A:2781:VAL:HG13	1:A:2832:PRO:HB3	1.72	0.71
1:A:1799:ILE:HD12	1:A:1799:ILE:O	1.91	0.71
1:B:2781:VAL:HG13	1:B:2832:PRO:HB3	1.72	0.70
1:B:1797:ARG:NH2	1:B:1882:THR:O	2.25	0.70
1:A:1461:GLU:N	1:A:1461:GLU:OE1	2.24	0.70
1:B:1799:ILE:HD12	1:B:1799:ILE:O	1.92	0.69
1:A:131:ASP:O	1:A:388:ILE:N	2.26	0.69
1:A:226:HIS:CE1	1:A:227:VAL:HG23	2.28	0.69
1:B:3817:LEU:O	1:B:4186:ARG:NH1	2.24	0.69
1:B:1337:ARG:NH2	1:B:1344:ILE:O	2.25	0.69
1:B:1461:GLU:N	1:B:1461:GLU:OE1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3813:LEU:HD13	1:B:1930:LEU:HD11	1.76	0.68
1:B:1557:LEU:HB3	1:B:1560:LEU:HD21	1.77	0.67
1:A:1329:GLU:OE2	1:A:1333:ASN:ND2	2.28	0.67
1:B:903:LEU:HD21	1:B:905:ILE:HG23	1.76	0.67
1:A:568:LEU:CD2	1:A:736:ILE:HG21	2.25	0.67
1:B:4440:MET:O	1:B:4444:VAL:HG23	1.94	0.66
1:A:4254:LEU:HD13	1:A:4319:HIS:HB3	1.77	0.66
1:B:4230:ASP:OD1	1:B:4231:GLY:N	2.29	0.66
1:B:2149:LEU:HD21	1:B:2163:LEU:HD11	1.78	0.66
1:B:2872:THR:HG22	1:B:3000:LEU:CD1	2.25	0.66
1:A:228:LEU:HG	1:A:259:LEU:HD11	1.78	0.66
1:B:228:LEU:HG	1:B:259:LEU:HD11	1.77	0.66
1:B:3817:LEU:HD11	1:B:4189:LEU:HD12	1.77	0.66
1:A:3517:LEU:HD12	1:A:3552:VAL:HG11	1.78	0.66
1:A:1575:ASP:OD2	1:A:1789:ARG:NH2	2.28	0.65
1:A:2149:LEU:HD21	1:A:2163:LEU:HD11	1.77	0.65
1:B:1409:ALA:HB1	1:B:2582:MET:SD	2.36	0.65
1:B:2850:VAL:N	1:B:2941:SER:OG	2.30	0.65
1:B:283:MET:HE3	1:B:283:MET:HA	1.79	0.65
1:A:1054:GLN:NE2	1:A:1298:GLU:OE2	2.27	0.64
1:A:2711:TYR:O	1:A:2764:LYS:NZ	2.28	0.64
1:A:1337:ARG:NH2	1:A:1344:ILE:O	2.30	0.64
1:A:228:LEU:HD23	1:A:259:LEU:HD21	1.80	0.64
1:B:226:HIS:CE1	1:B:227:VAL:HG23	2.32	0.64
1:B:3352:ALA:O	1:B:3355:THR:HG22	1.98	0.64
1:B:568:LEU:CD2	1:B:736:ILE:HG21	2.28	0.63
1:A:414:VAL:HG22	1:A:418:MET:HE1	1.79	0.63
1:B:1808:THR:OG1	1:B:1841:SER:N	2.31	0.63
1:A:1566:LEU:HD13	1:A:1799:ILE:HD13	1.81	0.63
1:A:4412:LEU:HD13	1:A:4488:VAL:HG13	1.80	0.63
1:A:1353:LEU:HD13	1:A:1403:LYS:HB2	1.79	0.62
1:A:4489:TYR:O	1:A:4493:THR:HG23	1.99	0.62
1:B:232:ALA:O	1:B:236:VAL:HG23	1.99	0.62
1:B:3819:ASP:OD2	1:B:3863:SER:OG	2.11	0.62
1:A:2349:ASP:OD1	1:A:2350:LEU:N	2.34	0.61
1:A:3352:ALA:O	1:A:3355:THR:HG22	2.01	0.61
1:A:3374:HIS:H	2:X:381:GLU:CD	2.05	0.60
1:B:4063:GLU:OE1	1:B:4063:GLU:N	2.30	0.60
2:Z:188:ALA:HB3	2:Z:192:LEU:HB3	1.82	0.60
1:B:288:ASN:O	1:B:292:THR:HG23	2.01	0.60
1:A:1946:PRO:O	1:A:1952:ASN:ND2	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:953:CYS:SG	1:B:961:LEU:HD21	2.41	0.60
2:X:196:ASN:OD1	2:X:199:VAL:HG23	2.02	0.60
1:A:4063:GLU:OE1	1:A:4063:GLU:N	2.29	0.59
1:A:4230:ASP:OD1	1:A:4231:GLY:N	2.34	0.59
1:B:228:LEU:HD23	1:B:259:LEU:HD21	1.84	0.59
1:B:1322:LEU:HD21	1:B:1362:VAL:HG11	1.85	0.59
1:A:953:CYS:SG	1:A:961:LEU:HD21	2.42	0.59
1:A:1337:ARG:NH1	1:A:1342:GLY:O	2.36	0.59
1:B:1105:ASP:OD2	1:B:1304:ARG:NH1	2.36	0.59
1:A:232:ALA:O	1:A:236:VAL:HG23	2.03	0.59
1:B:2083:VAL:HG22	1:B:2124:ILE:HG23	1.83	0.59
1:B:1194:LEU:HD11	1:B:2567:LEU:HG	1.83	0.59
2:X:381:GLU:H	2:X:382:PRO:CD	2.16	0.59
1:B:3530:MET:HE3	1:B:3530:MET:HA	1.84	0.58
1:A:2872:THR:HG22	1:A:3000:LEU:CD1	2.32	0.58
1:B:2349:ASP:OD1	1:B:2350:LEU:N	2.36	0.58
1:A:940:PHE:CD1	1:A:956:THR:HG22	2.38	0.58
1:B:1810:GLY:O	1:B:1863:ARG:NH1	2.36	0.58
1:B:3693:VAL:HG23	1:B:3699:MET:HG2	1.85	0.58
1:B:1093:LEU:CD2	1:B:1301:VAL:HG11	2.33	0.58
1:B:280:ARG:NH2	1:B:328:CYS:O	2.37	0.57
1:A:2325:HIS:N	1:A:2326:GLU:OE1	2.38	0.57
1:A:2804:CYS:SG	1:A:2807:ILE:HG23	2.44	0.57
1:A:736:ILE:HG23	1:A:747:VAL:HG22	1.86	0.57
1:B:3229:LEU:H	1:B:3229:LEU:HD22	1.69	0.57
1:B:2325:HIS:N	1:B:2326:GLU:OE1	2.37	0.57
1:A:1042:VAL:HG12	1:A:1091:PHE:CD2	2.39	0.56
1:B:961:LEU:HD23	1:B:962:HIS:N	2.20	0.56
1:A:2891:ALA:O	1:A:3031:SER:OG	2.19	0.56
1:B:1385:LEU:HD11	1:B:1408:LEU:HD11	1.87	0.56
1:B:2804:CYS:SG	1:B:2807:ILE:HG23	2.45	0.56
1:A:3837:ILE:HG22	1:A:3839:ALA:H	1.70	0.56
1:B:1085:SER:O	1:B:1089:HIS:NE2	2.38	0.56
1:A:1808:THR:OG1	1:A:1841:SER:N	2.39	0.56
1:A:3377:ASN:OD1	2:X:381:GLU:HG2	2.05	0.56
1:A:736:ILE:CG2	1:A:745:LEU:HD11	2.35	0.56
1:A:1053:GLN:O	1:A:1056:ARG:NE	2.38	0.56
1:B:2711:TYR:O	1:B:2764:LYS:NZ	2.35	0.56
1:B:176:ALA:O	1:B:181:VAL:HG22	2.06	0.56
1:B:2013:ASP:OD1	1:B:2013:ASP:N	2.39	0.56
1:A:1813:ALA:N	1:A:1861:ILE:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4364:LEU:HB2	1:B:4411:LEU:HD11	1.87	0.56
2:X:360:ARG:NE	2:X:431:VAL:O	2.38	0.56
1:A:1322:LEU:CD2	1:A:1362:VAL:HG11	2.36	0.55
1:A:4233:LEU:HD12	1:A:4237:MET:CE	2.36	0.55
1:B:4438:ALA:O	1:B:4442:THR:HG23	2.05	0.55
1:A:1085:SER:O	1:A:1089:HIS:NE2	2.33	0.55
1:B:1093:LEU:HD21	1:B:1301:VAL:HG11	1.88	0.55
1:A:961:LEU:HD23	1:A:962:HIS:N	2.21	0.55
1:B:3771:ILE:HD11	1:B:3815:LEU:HD11	1.89	0.55
1:A:822:GLY:N	1:A:849:ILE:O	2.39	0.55
1:A:4361:LEU:O	1:A:4365:SER:N	2.40	0.55
1:B:1042:VAL:HG12	1:B:1091:PHE:CD2	2.41	0.55
1:B:4233:LEU:HD12	1:B:4237:MET:CE	2.37	0.55
1:A:2326:GLU:OE1	1:A:2326:GLU:N	2.38	0.55
1:A:3624:LYS:NZ	1:A:3628:ASP:OD2	2.36	0.55
1:A:1193:ASP:OD1	1:A:1194:LEU:N	2.38	0.54
1:A:1194:LEU:HD12	1:A:2565:GLN:N	2.23	0.54
1:B:4217:LEU:HD11	1:B:4221:PHE:CZ	2.42	0.54
1:B:4254:LEU:HD13	1:B:4319:HIS:HB3	1.89	0.54
1:A:1958:ARG:O	1:A:1958:ARG:NE	2.32	0.54
1:A:2998:LEU:HD22	1:A:3040:LEU:HD12	1.90	0.54
1:B:1193:ASP:OD1	1:B:1194:LEU:N	2.31	0.54
1:B:1054:GLN:NE2	1:B:1298:GLU:OE2	2.33	0.54
1:B:2326:GLU:OE1	1:B:2326:GLU:N	2.37	0.54
1:B:4489:TYR:O	1:B:4493:THR:HG23	2.07	0.54
1:A:1849:PRO:O	1:A:2570:ARG:NH1	2.37	0.54
1:A:3530:MET:HE3	1:A:3530:MET:HA	1.88	0.54
1:B:736:ILE:CG2	1:B:745:LEU:HD11	2.37	0.54
1:B:823:GLY:O	1:B:848:HIS:ND1	2.41	0.54
1:B:1801:LEU:HD11	1:B:1804:VAL:HG23	1.89	0.54
1:A:2850:VAL:N	1:A:2941:SER:OG	2.41	0.54
1:B:740:ALA:HB2	1:B:861:LEU:CD1	2.38	0.54
1:A:513:LEU:HD21	1:A:568:LEU:HB2	1.90	0.54
1:B:280:ARG:NH1	1:B:329:PHE:O	2.41	0.54
2:X:408:ARG:N	2:X:411:ASP:OD2	2.38	0.54
1:A:511:SER:O	1:A:568:LEU:N	2.34	0.54
1:B:298:HIS:NE2	1:B:324:ASP:OD2	2.34	0.54
1:B:3837:ILE:HG22	1:B:3839:ALA:H	1.73	0.54
1:A:903:LEU:HD21	1:A:905:ILE:HG23	1.90	0.54
1:A:2762:LEU:HD12	1:A:2811:PHE:HZ	1.72	0.54
1:A:1029:THR:OG1	1:A:1030:ARG:NH2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2868:HIS:O	1:B:2872:THR:HG23	2.08	0.53
2:X:170:HIS:O	2:X:172:PHE:N	2.38	0.53
1:B:1484:ARG:NH1	1:B:2018:SER:O	2.41	0.53
1:A:736:ILE:HG22	1:A:745:LEU:HD11	1.91	0.53
1:B:1808:THR:N	1:B:1841:SER:OG	2.39	0.53
1:A:414:VAL:HG22	1:A:418:MET:CE	2.39	0.53
1:A:1067:HIS:ND1	1:A:1072:GLN:OE1	2.39	0.53
1:A:1031:PHE:CE2	1:A:2575:LEU:HD21	2.44	0.53
1:A:89:GLY:O	1:A:115:VAL:HG21	2.09	0.53
1:A:2868:HIS:O	1:A:2872:THR:HG23	2.08	0.53
1:B:110:LYS:HD3	1:B:110:LYS:N	2.24	0.53
1:B:3679:THR:OG1	1:B:3681:ASP:OD1	2.15	0.53
1:A:740:ALA:HB2	1:A:861:LEU:CD1	2.38	0.53
1:A:1393:PHE:O	1:A:1447:SER:OG	2.24	0.53
1:A:2332:VAL:HG13	1:A:2358:LEU:HD21	1.90	0.52
1:B:567:LEU:HB2	1:B:635:ILE:HD11	1.92	0.52
1:B:722:LEU:HD11	1:B:733:ILE:HD11	1.91	0.52
1:B:1092:GLU:OE2	1:B:1094:VAL:HG23	2.08	0.52
1:A:1844:LEU:HD22	1:A:2568:ASP:HB3	1.91	0.52
1:B:826:VAL:HG12	1:B:846:ILE:CD1	2.40	0.52
1:B:4224:THR:O	1:B:4235:ARG:NH1	2.41	0.52
1:A:283:MET:HE3	1:A:283:MET:HA	1.91	0.52
1:A:1477:VAL:HG13	1:A:2023:LEU:HD22	1.89	0.52
1:A:3988:THR:OG1	1:A:4067:ILE:N	2.43	0.52
1:B:1193:ASP:HB2	1:B:1199:GLY:HA2	1.92	0.52
1:A:165:LEU:HD12	1:A:221:PHE:HE2	1.75	0.52
1:A:412:TRP:CD1	1:A:420:VAL:HG22	2.45	0.51
1:A:1042:VAL:HG12	1:A:1091:PHE:HD2	1.75	0.51
1:A:1409:ALA:HB1	1:A:2582:MET:SD	2.50	0.51
1:A:4437:LEU:HD22	1:A:4485:ALA:HB2	1.92	0.51
1:B:95:ASP:OD2	1:B:212:LYS:NZ	2.28	0.51
1:A:110:LYS:HD3	1:A:110:LYS:N	2.25	0.51
1:A:4205:SER:O	1:A:4208:VAL:HG22	2.11	0.51
1:A:1030:ARG:HD3	1:A:1895:HIS:NE2	2.26	0.51
1:A:3811:LEU:C	1:A:3811:LEU:HD23	2.31	0.51
1:A:2914:THR:HG23	1:A:2917:GLN:H	1.77	0.50
1:B:1094:VAL:HG22	1:B:1219:SER:HB2	1.92	0.50
1:B:3817:LEU:CD1	1:B:4189:LEU:HD12	2.40	0.50
1:A:926:VAL:HG21	1:A:964:LEU:HD13	1.94	0.50
1:A:2049:VAL:HG22	1:A:2050:LEU:H	1.75	0.50
1:B:1813:ALA:N	1:B:1861:ILE:O	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1335:LEU:HB2	1:B:1352:VAL:HG11	1.94	0.50
1:A:1940:GLN:HA	1:A:1940:GLN:OE1	2.12	0.50
1:A:1314:GLU:OE1	1:A:1318:ARG:NH2	2.43	0.50
2:X:188:ALA:HB3	2:X:192:LEU:HB3	1.93	0.50
1:A:1092:GLU:OE2	1:A:1094:VAL:HG23	2.12	0.49
1:B:2599:THR:HG22	1:B:2599:THR:O	2.12	0.49
1:A:566:CYS:SG	1:A:632:LEU:HD12	2.53	0.49
1:B:3811:LEU:C	1:B:3811:LEU:HD23	2.33	0.49
1:A:1322:LEU:HD21	1:A:1362:VAL:HG11	1.93	0.49
1:B:1322:LEU:CD2	1:B:1362:VAL:HG11	2.41	0.49
1:B:3789:PHE:CE2	1:B:4083:ILE:HD11	2.47	0.49
1:B:289:ARG:NH2	1:B:310:ALA:O	2.38	0.49
1:B:4364:LEU:CB	1:B:4411:LEU:HD11	2.42	0.49
2:X:325:VAL:HG21	2:X:331:PHE:CE2	2.47	0.49
1:B:1776:GLN:HB3	1:B:1875:LEU:HD12	1.95	0.49
1:B:3813:LEU:HD23	1:B:3817:LEU:HD12	1.95	0.49
1:A:129:VAL:HG11	1:A:388:ILE:HG21	1.94	0.49
1:A:1353:LEU:HD13	1:A:1403:LYS:CB	2.42	0.49
1:A:3251:LEU:HD23	1:B:2717:ARG:CG	2.43	0.49
1:B:1404:CYS:O	1:B:1408:LEU:HD23	2.12	0.49
1:B:1958:ARG:O	1:B:1958:ARG:NE	2.34	0.49
1:A:2391:ASP:N	1:A:2391:ASP:OD1	2.44	0.49
1:B:2049:VAL:HG22	1:B:2050:LEU:H	1.78	0.49
1:B:2391:ASP:OD1	1:B:2391:ASP:N	2.46	0.49
2:Z:277:SER:HB3	2:Z:296:GLN:HB3	1.95	0.49
1:A:3817:LEU:HB3	1:A:4186:ARG:HG2	1.95	0.49
1:B:1867:THR:O	1:B:1867:THR:HG22	2.13	0.49
1:A:4377:LEU:HB3	1:A:4436:LEU:HB3	1.94	0.49
1:B:1852:VAL:CG1	1:B:1884:ILE:HD13	2.43	0.49
1:A:4224:THR:O	1:A:4235:ARG:NH1	2.45	0.48
1:B:1067:HIS:ND1	1:B:1072:GLN:OE1	2.46	0.48
1:B:1406:ARG:NH2	1:B:2580:GLU:OE1	2.46	0.48
1:B:1925:GLN:HG2	1:B:1984:LEU:HD21	1.95	0.48
2:X:212:SER:OG	2:X:214:ASP:OD2	2.22	0.48
1:B:2046:VAL:N	1:B:2047:PRO:CD	2.76	0.48
1:A:176:ALA:O	1:A:181:VAL:HG22	2.14	0.48
1:A:736:ILE:HG12	1:A:747:VAL:HG13	1.94	0.48
1:A:327:MET:N	1:A:327:MET:HE2	2.28	0.48
1:B:1820:TRP:CZ3	1:B:1857:LYS:HB2	2.48	0.48
1:B:2998:LEU:HD22	1:B:3040:LEU:HD12	1.95	0.48
2:X:376:GLU:O	2:X:380:ARG:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3989:LEU:HD23	1:A:4064:THR:HG21	1.96	0.48
1:B:2763:VAL:HG21	1:B:2818:ILE:HG21	1.95	0.48
1:A:1512:MET:O	1:A:1513:SER:OG	2.20	0.48
1:B:568:LEU:HD22	1:B:736:ILE:HG21	1.95	0.48
1:A:356:PRO:HB2	1:A:363:THR:HG22	1.95	0.48
1:A:632:LEU:O	1:A:717:VAL:N	2.46	0.48
1:A:1557:LEU:HB3	1:A:1560:LEU:HD21	1.96	0.48
1:B:1824:GLU:O	1:B:1828:GLY:HA3	2.14	0.48
1:A:3281:ARG:HD2	1:B:2783:PRO:HG2	1.95	0.48
1:A:1127:ASN:ND2	1:A:1221:LEU:HD21	2.29	0.48
1:A:2180:ASP:OD1	1:A:2181:TYR:N	2.46	0.48
1:A:4364:LEU:HB2	1:A:4411:LEU:HD11	1.95	0.47
1:B:744:HIS:CD2	1:B:827:LEU:HD11	2.49	0.47
1:B:1813:ALA:HB2	1:B:1863:ARG:HA	1.95	0.47
1:B:4442:THR:O	1:B:4446:THR:HG23	2.14	0.47
1:B:1866:SER:C	2:Z:340:GLU:OE2	2.53	0.47
1:A:2763:VAL:HG21	1:A:2818:ILE:HG21	1.96	0.47
1:B:566:CYS:SG	1:B:632:LEU:HD12	2.55	0.47
1:B:1471:ALA:O	1:B:1475:THR:HG23	2.14	0.47
1:A:513:LEU:HD23	1:A:566:CYS:SG	2.54	0.47
1:A:2336:VAL:HG23	1:A:2358:LEU:HD11	1.95	0.47
1:B:3867:SER:HB3	1:B:3979:ALA:HB1	1.95	0.47
1:A:1471:ALA:O	1:A:1475:THR:HG23	2.14	0.47
1:B:1194:LEU:HD21	1:B:2581:LEU:HD23	1.96	0.47
1:B:1512:MET:O	1:B:1513:SER:OG	2.23	0.47
1:B:3867:SER:N	1:B:3979:ALA:O	2.45	0.47
1:B:4437:LEU:HD22	1:B:4485:ALA:HB2	1.95	0.47
1:A:1832:VAL:HG23	1:A:2567:LEU:O	2.15	0.47
1:A:1842:LEU:CD2	1:A:2566:ALA:HB1	2.45	0.47
1:A:3244:SER:OG	1:A:3246:ASP:OD1	2.32	0.47
1:B:1042:VAL:HG12	1:B:1091:PHE:HD2	1.78	0.47
1:B:3364:ALA:O	1:B:3368[A]:SER:OG	2.29	0.47
1:A:3639:LEU:HD11	1:A:3683:VAL:HG13	1.97	0.47
1:A:1817:ILE:HB	1:A:1832:VAL:HG12	1.96	0.47
1:A:4409:VAL:N	1:A:4410:PRO:HD2	2.30	0.47
1:B:85:VAL:HG12	1:B:86:THR:N	2.30	0.47
1:A:91:ILE:HD11	1:A:117:CYS:HB3	1.97	0.47
1:A:3709:ASN:N	1:A:3710:PRO:CD	2.78	0.47
1:A:85:VAL:HG12	1:A:86:THR:N	2.30	0.46
1:A:2083:VAL:HG22	1:A:2124:ILE:HG23	1.97	0.46
1:B:826:VAL:HG12	1:B:846:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1867:THR:OG1	2:Z:340:GLU:OE1	2.32	0.46
1:A:1117:ILE:CG2	1:A:1192:LEU:HD11	2.45	0.46
1:B:2870:TYR:OH	1:B:2916:ASP:OD1	2.24	0.46
1:A:568:LEU:HD21	1:A:736:ILE:HG21	1.98	0.46
1:A:568:LEU:HD22	1:A:736:ILE:HG21	1.97	0.46
1:A:1797:ARG:NH2	1:A:1882:THR:O	2.48	0.46
1:A:1830:ARG:HD3	1:A:1833:VAL:HG23	1.96	0.46
1:B:2336:VAL:HG23	1:B:2358:LEU:HD11	1.97	0.46
2:Y:302:ASP:O	2:Y:306:ALA:N	2.45	0.46
1:A:568:LEU:HD12	1:A:632:LEU:HD21	1.98	0.46
1:A:1209:VAL:HG13	1:A:1306:PHE:CE2	2.50	0.46
1:A:1804:VAL:HG13	1:A:1878:TYR:CD2	2.50	0.46
1:B:1361:GLY:HA3	1:B:2575:LEU:HD13	1.98	0.46
1:B:1390:ARG:HB2	1:B:1390:ARG:NH1	2.30	0.46
1:A:226:HIS:ND1	1:A:227:VAL:HG23	2.31	0.46
1:A:567:LEU:HB2	1:A:635:ILE:HD11	1.97	0.46
1:B:3535:ASN:O	1:B:3540:LYS:NZ	2.28	0.46
1:A:129:VAL:CG1	1:A:388:ILE:HG21	2.46	0.46
1:A:1117:ILE:HG21	1:A:1192:LEU:HD11	1.97	0.46
1:B:1561:LEU:HB3	1:B:1989:ASN:OD1	2.16	0.46
1:B:2025:THR:HG22	1:B:2029:TYR:CE2	2.51	0.46
1:A:1867:THR:HG22	1:A:1867:THR:O	2.14	0.46
1:A:2813:LEU:HD12	1:A:2851:VAL:HG11	1.98	0.46
1:A:3246:ASP:OD1	1:A:3247:GLY:N	2.48	0.46
1:A:4311:THR:OG1	1:A:4314:ARG:NH1	2.48	0.46
1:B:1804:VAL:HG13	1:B:1878:TYR:CD1	2.50	0.46
1:A:156:LYS:N	1:A:159:ASP:OD2	2.42	0.46
1:A:1842:LEU:HD23	1:A:2566:ALA:HB1	1.98	0.46
1:A:1957:LEU:HD21	1:B:3128:THR:HA	1.97	0.46
1:B:72:SER:O	1:B:73:LEU:HD12	2.16	0.46
1:A:2046:VAL:N	1:A:2047:PRO:CD	2.79	0.46
1:A:3813:LEU:HD22	1:A:4191:VAL:HG21	1.98	0.46
2:Y:270:ILE:HD12	2:Y:270:ILE:H	1.81	0.46
1:A:739:CYS:SG	1:A:741:ASP:N	2.87	0.45
1:B:4217:LEU:HG	1:B:4221:PHE:CE2	2.50	0.45
1:A:3227:PRO:HD2	1:A:3263:THR:O	2.16	0.45
1:A:4364:LEU:CB	1:A:4411:LEU:HD11	2.46	0.45
1:B:131:ASP:O	1:B:388:ILE:N	2.47	0.45
1:B:1484:ARG:NH2	1:B:2016:GLN:O	2.49	0.45
1:B:2104:TYR:HB2	1:B:2167:MET:HE1	1.96	0.45
1:B:4478:VAL:N	1:B:4479:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4224:THR:HG22	1:A:4231:GLY:HA2	1.97	0.45
1:B:239:LEU:HD22	1:B:246:VAL:CG1	2.46	0.45
1:B:1830:ARG:HD3	1:B:1833:VAL:HG23	1.97	0.45
1:B:2332:VAL:HG13	1:B:2358:LEU:HD21	1.98	0.45
1:B:3388:GLN:HG3	1:B:3392[B]:ILE:HD11	1.97	0.45
1:B:513:LEU:HD21	1:B:568:LEU:HB2	1.99	0.45
1:B:2177:ARG:O	1:B:2180:ASP:OD1	2.34	0.45
2:X:194:VAL:HG22	2:X:231:THR:HG22	1.98	0.45
1:B:129:VAL:HG11	1:B:388:ILE:HG21	1.99	0.45
1:B:740:ALA:HB3	1:B:901:GLY:HA3	1.98	0.45
1:B:2813:LEU:HD12	1:B:2851:VAL:HG11	1.98	0.45
1:B:4196:GLU:O	1:B:4196:GLU:HG2	2.15	0.45
1:A:291:GLU:O	1:A:294:THR:HG23	2.16	0.45
1:A:1098:ALA:HB1	1:A:1212:MET:SD	2.57	0.45
2:X:378:GLN:NE2	2:X:386:ASP:HA	2.32	0.45
1:A:740:ALA:HB1	1:A:863:PRO:HA	1.98	0.45
1:A:1436:MET:HG3	1:A:1439:LEU:HD12	1.99	0.45
1:A:1450:TRP:HZ2	1:A:1845:HIS:CE1	2.34	0.45
1:A:2080:LEU:HD12	1:A:2598:LEU:HD22	1.99	0.45
1:B:4444:VAL:HG21	1:B:4481:ILE:HD13	1.97	0.45
1:A:1930:LEU:HD11	1:B:3813:LEU:HD13	1.99	0.45
1:B:861:LEU:HD12	1:B:902:HIS:O	2.16	0.45
1:B:4377:LEU:HD22	1:B:4440:MET:HE2	1.99	0.45
1:B:4409:VAL:N	1:B:4410:PRO:HD2	2.32	0.45
1:A:3789:PHE:O	1:A:4086:ARG:NH2	2.46	0.45
1:B:2180:ASP:OD1	1:B:2181:TYR:N	2.50	0.45
1:A:357:PHE:CA	1:A:363:THR:HG21	2.47	0.45
1:A:120:ILE:HD12	1:A:120:ILE:N	2.32	0.44
1:A:1114:ILE:HD11	1:A:1118:PRO:HD3	1.98	0.44
1:B:174:LEU:HD22	1:B:200:LEU:HD12	2.00	0.44
1:B:1505:PRO:O	1:B:1985:ASN:ND2	2.38	0.44
2:X:157:THR:HG21	2:X:311:VAL:HG11	1.99	0.44
1:A:123:VAL:HG21	1:A:414:VAL:HG11	1.99	0.44
1:A:129:VAL:HG21	1:A:391:PHE:CB	2.48	0.44
1:A:226:HIS:ND1	1:A:227:VAL:N	2.65	0.44
1:A:2870:TYR:OH	1:A:2916:ASP:OD1	2.27	0.44
1:A:3225:ILE:HD11	1:A:3280:LEU:HD13	1.99	0.44
1:A:4224:THR:HG22	1:A:4231:GLY:CA	2.48	0.44
1:B:848:HIS:HD1	1:B:849:ILE:N	2.16	0.44
1:B:3227:PRO:HD2	1:B:3263:THR:O	2.18	0.44
1:B:3343:ASP:OD1	1:B:3343:ASP:N	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4235:ARG:O	1:B:4330:TYR:OH	2.31	0.44
1:B:4412:LEU:HD13	1:B:4488:VAL:HG13	1.99	0.44
1:A:1330:LYS:O	1:A:1334:THR:HG22	2.17	0.44
1:A:1335:LEU:HB2	1:A:1352:VAL:HG11	1.99	0.44
1:B:1816:SER:HB2	1:B:1833:VAL:HG22	1.99	0.44
1:B:2106:SER:OG	1:B:2164:ASP:OD1	2.35	0.44
1:B:3388:GLN:HG3	1:B:3392[A]:ILE:HD11	1.97	0.44
1:B:4407:ALA:HB3	1:B:4408:MET:HE2	1.99	0.44
1:A:2876:LYS:NZ	1:A:3273:GLU:OE2	2.50	0.44
1:A:3236:PRO:HD3	1:A:3291:LEU:HD21	2.00	0.44
2:X:391:VAL:O	2:X:413:ILE:N	2.47	0.44
1:A:3709:ASN:OD1	1:A:3709:ASN:C	2.56	0.44
1:A:4251:LEU:HD11	1:A:4320:VAL:HG13	1.99	0.44
1:B:632:LEU:O	1:B:717:VAL:N	2.50	0.44
1:A:1209:VAL:HG22	1:A:1306:PHE:CZ	2.52	0.44
1:A:1776:GLN:HB3	1:A:1875:LEU:HD12	2.00	0.44
1:A:1798:PRO:O	1:A:1884:ILE:HD11	2.18	0.44
1:A:3343:ASP:OD1	1:A:3343:ASP:N	2.49	0.44
1:A:3518:ASP:OD1	1:A:3518:ASP:N	2.48	0.44
1:A:3760:GLU:O	1:A:3764:VAL:HG23	2.17	0.44
1:A:3989:LEU:CD2	1:A:4064:THR:HG21	2.47	0.44
1:A:4495:LEU:C	1:A:4495:LEU:HD23	2.37	0.44
1:B:2180:ASP:OD1	1:B:2180:ASP:C	2.56	0.44
2:X:404:ARG:NH2	2:X:453:THR:O	2.48	0.44
1:A:1345:THR:HG22	1:A:1346:GLU:N	2.33	0.44
1:A:2834:ASP:OD1	1:A:2834:ASP:N	2.51	0.44
1:A:3251:LEU:HD23	1:B:2717:ARG:HG3	2.00	0.44
1:A:1805:LEU:O	1:A:1877:PHE:N	2.41	0.44
1:A:3443:ASP:OD1	1:A:3445:GLY:N	2.51	0.44
1:A:3679:THR:OG1	1:A:3681:ASP:OD1	2.20	0.44
1:B:151:GLN:NE2	1:B:162:GLN:O	2.48	0.44
1:A:410:CYS:SG	1:A:420:VAL:HG13	2.58	0.43
1:A:1925:GLN:HG2	1:A:1984:LEU:HD21	1.99	0.43
1:A:2051:GLN:HA	1:A:2051:GLN:OE1	2.17	0.43
1:A:4438:ALA:O	1:A:4442:THR:HG23	2.18	0.43
1:B:740:ALA:HB1	1:B:863:PRO:HA	2.00	0.43
1:B:1570:CYS:HB2	1:B:1579:ILE:HD13	2.00	0.43
1:B:4209:LEU:N	1:B:4210:PRO:HD2	2.33	0.43
2:X:318:ILE:C	2:X:318:ILE:HD12	2.39	0.43
1:A:2180:ASP:OD1	1:A:2180:ASP:C	2.56	0.43
1:A:4217:LEU:HD11	1:A:4221:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:157:THR:HG21	2:Y:311:VAL:HG11	2.00	0.43
2:Z:302:ASP:O	2:Z:306:ALA:N	2.44	0.43
1:B:740:ALA:HB2	1:B:861:LEU:HD12	2.00	0.43
1:B:3760:GLU:O	1:B:3764:VAL:HG23	2.19	0.43
1:A:2685:LEU:HD12	1:A:2686:TYR:N	2.34	0.43
1:B:1410:LEU:HG	1:B:2579:ALA:HB2	2.00	0.43
1:B:1801:LEU:HD11	1:B:1804:VAL:CG2	2.49	0.43
1:A:1091:PHE:CD1	1:A:1091:PHE:N	2.87	0.43
1:B:164:GLU:OE1	1:B:258:ARG:NH2	2.52	0.43
2:Y:188:ALA:HB3	2:Y:192:LEU:HB3	2.00	0.43
1:A:3180:GLU:OE1	1:A:3180:GLU:N	2.42	0.43
1:B:1849:PRO:HG2	1:B:2570:ARG:HE	1.84	0.43
1:A:70:LEU:HD22	1:A:84:ALA:HB1	2.01	0.43
1:A:2390:THR:HG22	1:A:2656:GLN:HG3	2.01	0.43
1:B:93:VAL:HG11	1:B:216:TRP:CZ3	2.53	0.43
1:B:120:ILE:HD12	1:B:120:ILE:N	2.33	0.43
1:A:1093:LEU:HD21	1:A:1301:VAL:HG11	2.00	0.43
1:A:1209:VAL:HG22	1:A:1306:PHE:HZ	1.84	0.43
1:A:4377:LEU:HD22	1:A:4440:MET:HE2	2.01	0.43
1:A:3387:LEU:HD22	1:A:3441:THR:HG21	2.00	0.43
1:A:3786:CYS:HG	1:A:4074:PHE:HE1	1.66	0.43
1:B:2051:GLN:OE1	1:B:2051:GLN:HA	2.19	0.43
1:B:2984:VAL:HG13	1:B:2990:ILE:HG21	2.01	0.43
2:X:381:GLU:H	2:X:382:PRO:HD2	1.84	0.43
1:A:70:LEU:HA	1:A:85:VAL:O	2.19	0.42
1:A:4478:VAL:N	1:A:4479:PRO:CD	2.82	0.42
1:B:409:ILE:HB	1:B:424:PHE:CE1	2.53	0.42
1:B:902:HIS:CD2	1:B:923:LEU:HD11	2.53	0.42
1:B:3981:MET:HG3	1:B:3985:GLN:HB2	2.01	0.42
2:X:218:ALA:HB2	2:X:234:ILE:CG2	2.49	0.42
1:A:1406:ARG:NH1	1:A:2576:GLU:HB3	2.34	0.42
1:B:827:LEU:O	1:B:844:ILE:N	2.48	0.42
1:B:1566:LEU:HD13	1:B:1799:ILE:HD13	2.00	0.42
1:B:4311:THR:OG1	1:B:4314:ARG:NH1	2.52	0.42
2:X:218:ALA:HB2	2:X:234:ILE:HG22	2.02	0.42
1:A:409:ILE:HD12	1:A:426:ILE:CD1	2.50	0.42
1:A:1914:LEU:C	1:A:1914:LEU:HD23	2.39	0.42
1:A:3684:ALA:HB3	1:A:3685:PRO:HD3	2.01	0.42
1:A:4413:LEU:CD2	1:A:4495:LEU:HD22	2.49	0.42
1:B:940:PHE:HA	1:B:956:THR:HA	2.01	0.42
1:B:1345:THR:HG22	1:B:1346:GLU:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:218:ALA:HB2	2:Z:234:ILE:CG2	2.49	0.42
1:A:1029:THR:HG22	1:A:1358:TRP:CD2	2.53	0.42
1:A:4209:LEU:N	1:A:4210:PRO:HD2	2.34	0.42
2:X:250:ASP:O	2:Y:144:ARG:NH2	2.48	0.42
1:A:296:TRP:NE1	1:A:304:ALA:O	2.53	0.42
1:A:3817:LEU:HD13	1:A:4186:ARG:HA	2.00	0.42
1:B:1223:HIS:CE1	1:B:1225:LYS:HB2	2.55	0.42
1:B:3291:LEU:HD23	1:B:3292:GLY:N	2.35	0.42
1:A:412:TRP:NE1	1:A:420:VAL:HG22	2.34	0.42
1:A:2687:ASN:OD1	1:A:2688:ALA:N	2.52	0.42
1:B:854:ASP:HA	1:B:907:THR:HB	2.01	0.42
1:B:1812:LEU:HD23	1:B:1873:ILE:HG12	2.02	0.42
1:B:2892:CYS:N	1:B:3003:SER:O	2.49	0.42
1:A:189:TYR:HA	1:A:231:ILE:HD11	2.01	0.42
1:A:1446:GLY:O	1:A:1450:TRP:CD1	2.73	0.42
1:B:73:LEU:HD13	1:B:955:CYS:SG	2.60	0.42
1:B:226:HIS:ND1	1:B:227:VAL:N	2.67	0.42
1:B:1790:PHE:CD1	1:B:1790:PHE:C	2.92	0.42
1:B:3684:ALA:HB3	1:B:3685:PRO:HD3	2.01	0.42
1:B:4221:PHE:HE1	1:B:4234:LEU:HG	1.84	0.42
2:Y:318:ILE:HD12	2:Y:318:ILE:C	2.40	0.42
1:A:426:ILE:CG2	1:A:505:LEU:HD23	2.50	0.42
1:A:902:HIS:CD2	1:A:923:LEU:HD11	2.55	0.42
1:A:1782:ARG:HB3	1:A:1784:HIS:NE2	2.34	0.42
1:A:3229:LEU:HD22	1:A:3229:LEU:H	1.85	0.42
1:A:3388:GLN:HG3	1:A:3392[B]:ILE:HD11	2.02	0.42
1:A:3965:PHE:CE2	2:X:385:PRO:HB3	2.55	0.42
1:B:137:ARG:NH2	1:B:148:THR:O	2.53	0.42
1:B:2806:GLN:NE2	1:B:2806:GLN:H	2.18	0.42
1:B:2833:LEU:HD21	1:B:2914:THR:C	2.39	0.42
1:B:3689:PHE:O	1:B:3693:VAL:HG22	2.20	0.42
2:X:326:THR:HG22	2:X:329:ILE:HB	2.02	0.42
2:Y:326:THR:HG22	2:Y:329:ILE:HB	2.02	0.42
1:A:4442:THR:O	1:A:4446:THR:HG23	2.20	0.42
1:A:2104:TYR:HB2	1:A:2167:MET:HE1	2.01	0.41
1:A:3824:MET:SD	1:A:4004:LEU:HD12	2.60	0.41
1:A:4260:ARG:HG3	1:A:4261:VAL:HG23	2.00	0.41
1:B:827:LEU:HD21	1:B:900:LEU:HD21	2.02	0.41
1:B:1334:THR:O	1:B:1344:ILE:HD13	2.20	0.41
1:B:4226:LEU:HD22	1:B:4226:LEU:N	2.35	0.41
1:A:1820:TRP:CZ3	1:A:1857:LYS:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2049:VAL:HG22	1:A:2050:LEU:N	2.35	0.41
1:B:1798:PRO:O	1:B:1884:ILE:HD11	2.20	0.41
1:B:2332:VAL:HG12	1:B:2374:ILE:HG23	2.01	0.41
1:B:2834:ASP:OD1	1:B:2834:ASP:N	2.52	0.41
1:A:2806:GLN:NE2	1:A:2806:GLN:H	2.19	0.41
1:A:3355:THR:HG23	1:A:3358:LEU:HB2	2.02	0.41
1:A:4080:LEU:HD12	1:A:4171:ALA:HB1	2.01	0.41
1:B:156:LYS:N	1:B:159:ASP:OD2	2.45	0.41
1:B:564:PHE:N	1:B:565:PRO:CD	2.83	0.41
1:B:1114:ILE:HG23	1:B:1114:ILE:O	2.20	0.41
1:A:1322:LEU:HD22	1:A:1362:VAL:HG11	2.02	0.41
2:Z:302:ASP:O	2:Z:306:ALA:HB2	2.20	0.41
1:A:4226:LEU:N	1:A:4226:LEU:HD22	2.36	0.41
1:B:70:LEU:O	1:B:71:HIS:HB3	2.20	0.41
1:B:135:GLY:HA2	1:B:377:ALA:HA	2.02	0.41
1:B:289:ARG:O	1:B:293:PHE:CD2	2.73	0.41
1:B:736:ILE:HG22	1:B:745:LEU:HD11	2.01	0.41
1:B:4441:LYS:O	1:B:4445:ASP:OD1	2.39	0.41
2:Y:322:THR:CG2	2:Y:333:ILE:HG12	2.50	0.41
1:A:3566:ILE:HD12	1:A:3566:ILE:N	2.36	0.41
1:B:912:VAL:HG13	1:B:940:PHE:HD2	1.86	0.41
1:B:940:PHE:CD1	1:B:956:THR:HG22	2.55	0.41
1:B:1042:VAL:HG11	1:B:1077:TRP:CE2	2.55	0.41
1:B:1992:GLN:O	1:B:1996:VAL:HG23	2.20	0.41
1:B:2655:VAL:HG11	1:B:2660:LEU:HD22	2.02	0.41
1:B:3712:TRP:CD1	1:B:3712:TRP:N	2.89	0.41
1:A:283:MET:O	1:A:289:ARG:NH1	2.43	0.41
1:A:1450:TRP:CZ2	1:A:1845:HIS:HE1	2.39	0.41
1:A:1500:SER:HB3	1:A:1974:TYR:OH	2.20	0.41
1:A:2177:ARG:O	1:A:2180:ASP:OD1	2.38	0.41
1:A:2868:HIS:CE1	1:A:2872:THR:HG21	2.56	0.41
1:A:4152:PRO:HA	1:A:4201:LEU:HD21	2.03	0.41
1:B:414:VAL:HA	1:B:418:MET:HA	2.02	0.41
1:B:2567:LEU:HD21	1:B:2584:LYS:HD3	2.03	0.41
1:B:4153:ILE:O	1:B:4153:ILE:HG23	2.21	0.41
1:A:1974:TYR:O	1:A:1978:ILE:HG12	2.21	0.41
1:A:2149:LEU:CD2	1:A:2163:LEU:HD11	2.48	0.41
1:A:4153:ILE:HG23	1:A:4153:ILE:O	2.21	0.41
1:B:2826:PHE:HB3	1:B:2866:LEU:HD21	2.03	0.41
1:B:3985:GLN:O	1:B:3989:LEU:HG	2.21	0.41
2:Z:196:ASN:OD1	2:Z:199:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:ARG:NH2	1:A:328:CYS:O	2.53	0.41
1:A:744:HIS:HB3	1:A:827:LEU:HD11	2.02	0.41
1:A:1102:GLY:H	1:A:1305:ARG:HA	1.85	0.41
1:A:1126:LYS:HG2	1:A:1180:ASP:O	2.21	0.41
1:A:1785:SER:HB2	1:A:1866:SER:O	2.21	0.41
1:A:1812:LEU:HA	1:A:1862:GLY:HA2	2.02	0.41
1:A:2833:LEU:HD21	1:A:2914:THR:C	2.41	0.41
1:B:307:ASP:HB3	1:B:308:PRO:HD3	2.03	0.41
1:B:1095:LEU:CD2	1:B:1303:ILE:HD13	2.51	0.41
1:B:3429:ASP:OD2	1:B:3836:ARG:NH1	2.52	0.41
1:B:3865:THR:OG1	1:B:3979:ALA:O	2.38	0.41
2:X:166:ILE:N	2:X:180:SER:O	2.40	0.41
2:X:295:ILE:O	2:X:331:PHE:HA	2.21	0.41
2:Y:229:ILE:HD12	2:Y:341:PHE:CB	2.50	0.41
2:Y:322:THR:HG21	2:Y:333:ILE:HG12	2.03	0.41
2:Z:268:ASN:HB2	2:Z:304:GLY:HA3	2.03	0.41
1:A:1863:ARG:O	1:A:1866:SER:OG	2.29	0.41
1:A:2692:PRO:HG3	1:A:2728:LEU:HB3	2.03	0.41
1:A:3689:PHE:O	1:A:3693:VAL:HG22	2.20	0.41
1:B:226:HIS:ND1	1:B:227:VAL:HG23	2.36	0.41
1:B:575:TYR:N	1:B:575:TYR:CD1	2.88	0.41
1:B:2327:ARG:HD2	1:B:2328:CYS:N	2.36	0.41
1:B:3443:ASP:OD1	1:B:3445:GLY:N	2.54	0.41
1:B:4187:LEU:HG	1:B:4200:ILE:HD13	2.03	0.41
1:A:151:GLN:NE2	1:A:162:GLN:O	2.55	0.40
1:A:299:VAL:O	1:A:305:GLN:NE2	2.54	0.40
1:A:1801:LEU:HD11	1:A:1804:VAL:HG23	2.03	0.40
1:A:4259:PRO:HB3	1:A:4366:GLN:O	2.21	0.40
1:B:1511:GLU:HA	1:B:1557:LEU:O	2.21	0.40
1:B:4008:LEU:HD23	1:B:4008:LEU:N	2.36	0.40
2:Z:318:ILE:C	2:Z:318:ILE:HD12	2.41	0.40
1:A:1114:ILE:O	1:A:1114:ILE:HG23	2.21	0.40
1:A:1317:GLN:O	1:A:1321:MET:HG3	2.21	0.40
1:A:2567:LEU:HD11	1:A:2581:LEU:HG	2.04	0.40
1:A:3560:LEU:O	1:A:3564:MET:HG3	2.22	0.40
1:A:4435:THR:O	1:A:4439:LYS:HG3	2.20	0.40
1:B:1501:SER:OG	1:B:2024:ARG:NH2	2.54	0.40
1:B:2049:VAL:HG22	1:B:2050:LEU:N	2.36	0.40
1:B:3355:THR:HG23	1:B:3358:LEU:HB2	2.02	0.40
2:Y:253:GLN:NE2	2:Y:276:SER:O	2.49	0.40
2:Y:310:LEU:HG	2:Y:318:ILE:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:THR:O	1:A:508:THR:HG22	2.21	0.40
1:A:1051:GLN:O	1:A:1055:GLN:N	2.44	0.40
1:A:1852:VAL:CG1	1:A:1884:ILE:HD13	2.52	0.40
1:A:2073:LYS:HE3	1:A:2077:HIS:CE1	2.56	0.40
1:A:4380:ASP:OD1	1:A:4380:ASP:N	2.45	0.40
1:B:1209:VAL:HG11	1:B:1322:LEU:HD11	2.03	0.40
1:B:1511:GLU:HG3	1:B:1557:LEU:O	2.22	0.40
2:X:252:ARG:N	2:X:255:GLU:OE2	2.44	0.40
2:Y:218:ALA:HB2	2:Y:234:ILE:CG2	2.51	0.40
1:A:85:VAL:CG1	1:A:86:THR:N	2.85	0.40
1:A:1036:PRO:O	1:A:1096:PRO:HG2	2.22	0.40
1:A:1321:MET:HE2	1:A:1321:MET:HB2	1.96	0.40
1:A:1484:ARG:NH2	1:A:2015:ILE:O	2.54	0.40
1:A:1505:PRO:O	1:A:1985:ASN:ND2	2.50	0.40
1:A:2783:PRO:HG2	1:B:3281:ARG:CD	2.52	0.40
1:A:4186:ARG:NE	1:A:4193:ASP:O	2.45	0.40
1:A:4217:LEU:HG	1:A:4221:PHE:CE2	2.57	0.40
1:B:1192:LEU:HA	1:B:1198:ALA:O	2.21	0.40
1:B:1321:MET:HB2	1:B:1321:MET:HE2	1.92	0.40
1:B:4235:ARG:HE	1:B:4330:TYR:HA	1.87	0.40
1:A:3388:GLN:HG3	1:A:3392[A]:ILE:HD11	2.02	0.40
1:A:3867:SER:N	1:A:3979:ALA:O	2.47	0.40
1:B:4072:GLN:HG2	1:B:4175:LEU:HD13	2.04	0.40
1:B:4445:ASP:OD1	1:B:4482:GLN:NE2	2.52	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	2668/4898 (54%)	2615 (98%)	53 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	2668/4898 (54%)	2616 (98%)	52 (2%)	0	100 100
2	X	286/332 (86%)	270 (94%)	15 (5%)	1 (0%)	41 74
2	Y	185/332 (56%)	178 (96%)	7 (4%)	0	100 100
2	Z	185/332 (56%)	178 (96%)	7 (4%)	0	100 100
All	All	5992/10792 (56%)	5857 (98%)	134 (2%)	1 (0%)	100 100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	X	381	GLU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	2440/4249 (57%)	2382 (98%)	58 (2%)	49 76
1	B	2440/4249 (57%)	2386 (98%)	54 (2%)	52 78
2	X	241/276 (87%)	234 (97%)	7 (3%)	42 72
2	Y	153/276 (55%)	152 (99%)	1 (1%)	84 93
2	Z	153/276 (55%)	151 (99%)	2 (1%)	69 86
All	All	5427/9326 (58%)	5305 (98%)	122 (2%)	54 78

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	SER
1	A	175	SER
1	A	180	LYS
1	A	290	ARG
1	A	325	ARG
1	A	327	MET
1	A	348	HIS

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Mol	Chain	Res	Type
1	A	386	ASP
1	A	425	GLU
1	A	625	ARG
1	A	739	CYS
1	A	848	HIS
1	A	1030	ARG
1	A	1205	SER
1	A	1305	ARG
1	A	1308	LYS
1	A	1315	ARG
1	A	1326	GLU
1	A	1435	ASN
1	A	1578	ARG
1	A	1771	GLN
1	A	1788	ARG
1	A	1894	MET
1	A	1958	ARG
1	A	1996	VAL
1	A	2073	LYS
1	A	2084	GLN
1	A	2089	GLU
1	A	2137	SER
1	A	2577	GLN
1	A	2578	GLN
1	A	2585	MET
1	A	2592	ASP
1	A	2690	ARG
1	A	2795	ARG
1	A	2797	GLN
1	A	2806	GLN
1	A	3093	ASP
1	A	3343	ASP
1	A	3355	THR
1	A	3375	SER
1	A	3392[A]	ILE
1	A	3392[B]	ILE
1	A	3441	THR
1	A	3462	ARG
1	A	3483	GLU
1	A	3564	MET
1	A	3624	LYS
1	A	3641	SER

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Mol	Chain	Res	Type
1	A	3676	MET
1	A	3681	ASP
1	A	3810	ARG
1	A	3836	ARG
1	A	3981	MET
1	A	4229	ASP
1	A	4239	LEU
1	A	4381	SER
1	A	4445	ASP
1	B	121	SER
1	B	175	SER
1	B	180	LYS
1	B	290	ARG
1	B	386	ASP
1	B	418	MET
1	B	425	GLU
1	B	625	ARG
1	B	739	CYS
1	B	848	HIS
1	B	1205	SER
1	B	1305	ARG
1	B	1308	LYS
1	B	1315	ARG
1	B	1326	GLU
1	B	1488	MET
1	B	1511	GLU
1	B	1578	ARG
1	B	1771	GLN
1	B	1788	ARG
1	B	1794	ASP
1	B	1853	CYS
1	B	1894	MET
1	B	1911	ASP
1	B	1934	ARG
1	B	1954	GLN
1	B	1958	ARG
1	B	2073	LYS
1	B	2084	GLN
1	B	2137	SER
1	B	2577	GLN
1	B	2585	MET
1	B	2592	ASP

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Mol	Chain	Res	Type
1	B	2689	ASN
1	B	2690	ARG
1	B	2795	ARG
1	B	2797	GLN
1	B	2806	GLN
1	B	3093	ASP
1	B	3343	ASP
1	B	3355	THR
1	B	3375	SER
1	B	3392[A]	ILE
1	B	3392[B]	ILE
1	B	3462	ARG
1	B	3564	MET
1	B	3624	LYS
1	B	3641	SER
1	B	3676	MET
1	B	3810	ARG
1	B	4229	ASP
1	B	4239	LEU
1	B	4379	ASN
1	B	4445	ASP
2	X	204	ARG
2	X	232	LEU
2	X	247	ARG
2	X	365	MET
2	X	378	GLN
2	X	384	PHE
2	X	387	VAL
2	Y	232	LEU
2	Z	232	LEU
2	Z	237	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1840	HIS
1	A	1845	HIS
1	B	1323	GLN
1	B	1895	HIS
1	B	2565	GLN
2	X	378	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

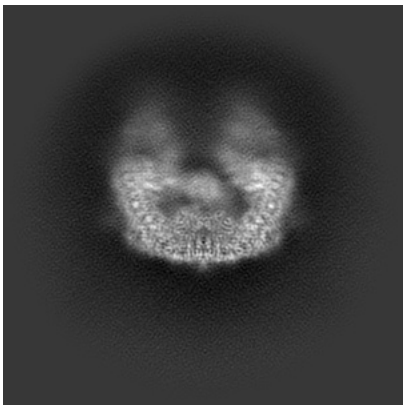
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27841. These allow visual inspection of the internal detail of the map and identification of artifacts.

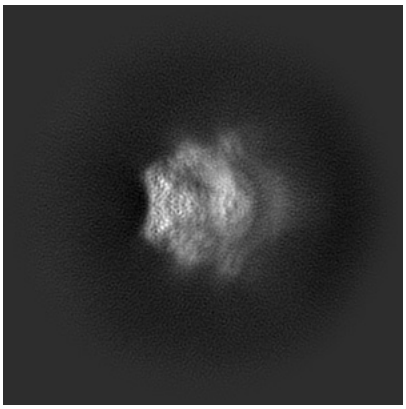
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

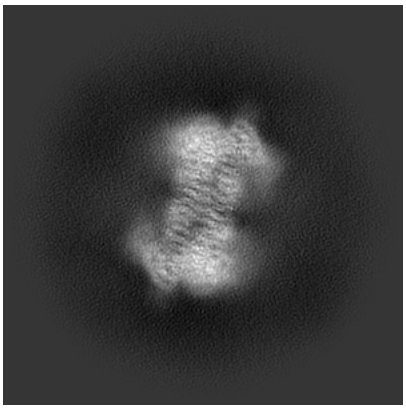
6.1.1 Primary map



X

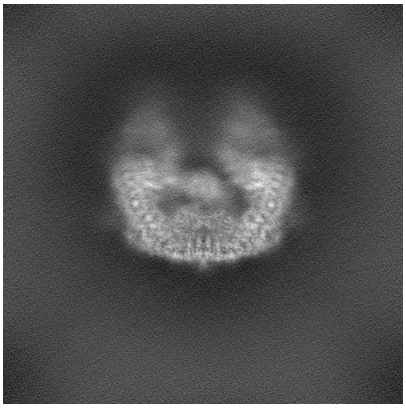


Y

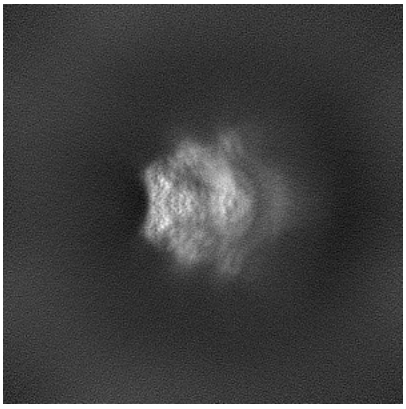


Z

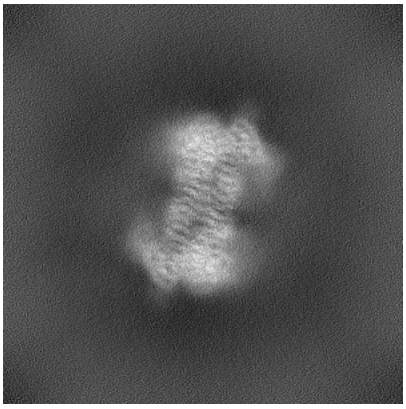
6.1.2 Raw map



X



Y

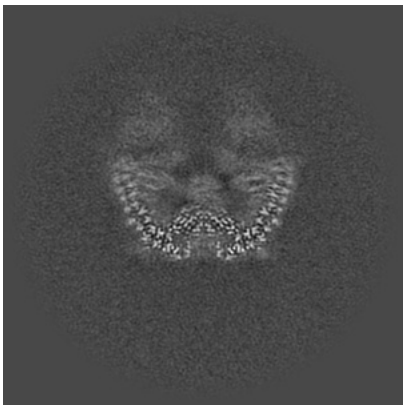


Z

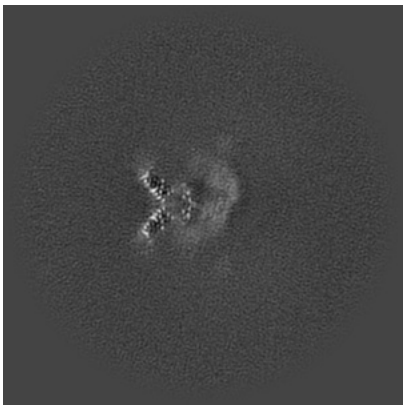
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

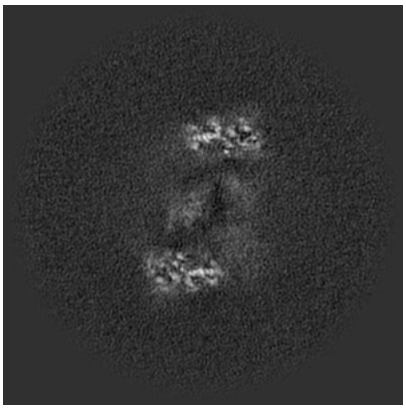
6.2.1 Primary map



X Index: 176

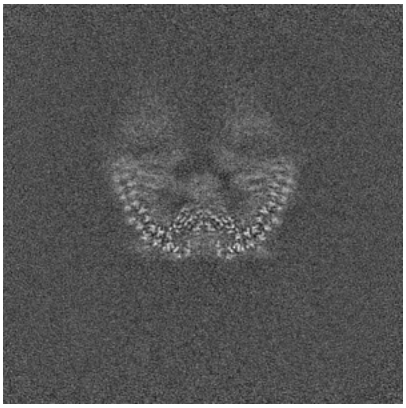


Y Index: 176

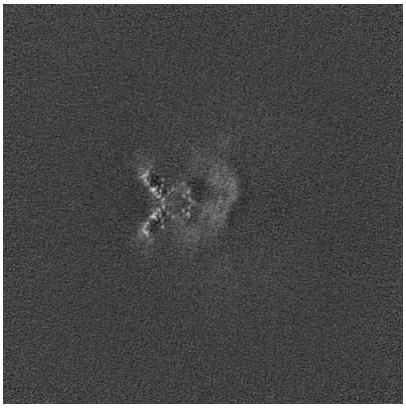


Z Index: 176

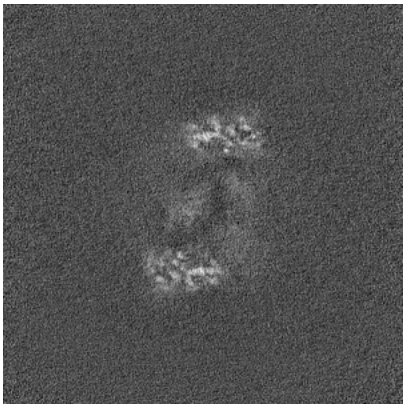
6.2.2 Raw map



X Index: 176



Y Index: 176

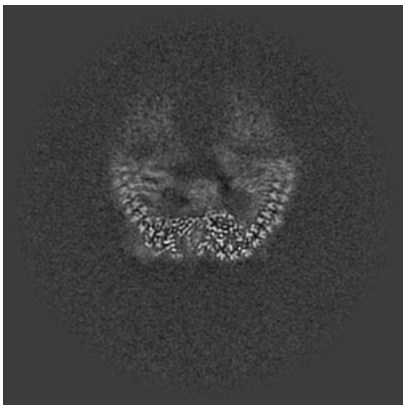


Z Index: 176

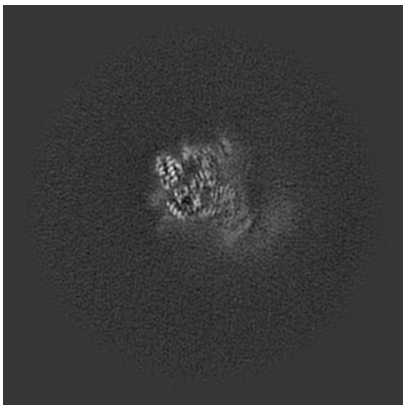
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

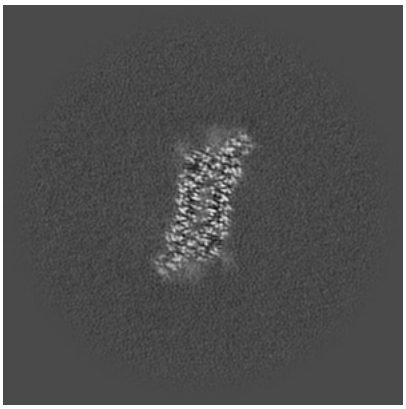
6.3.1 Primary map



X Index: 172

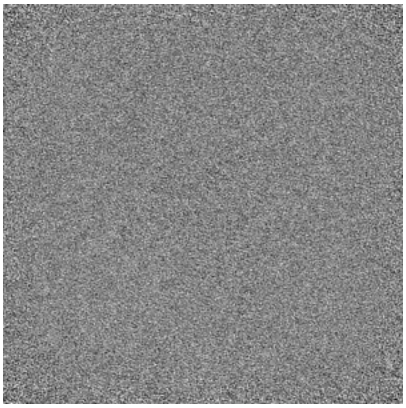


Y Index: 229

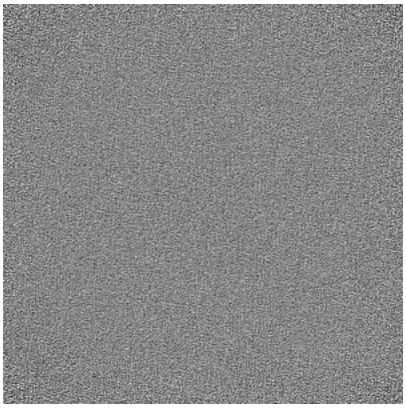


Z Index: 139

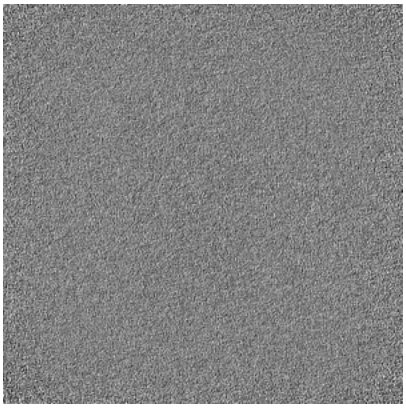
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.215. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

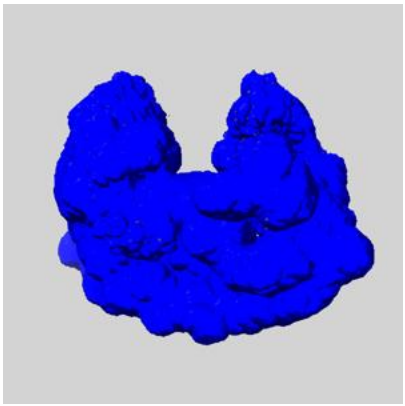
6.5 Mask visualisation (i)

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

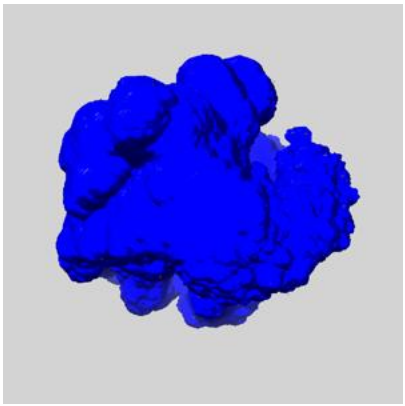
A mask typically either:

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

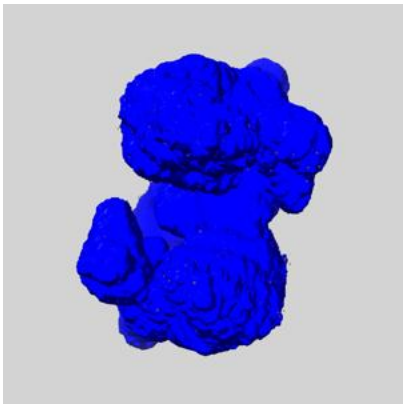
6.5.1 emd_27841_msk_1.map (i)



X

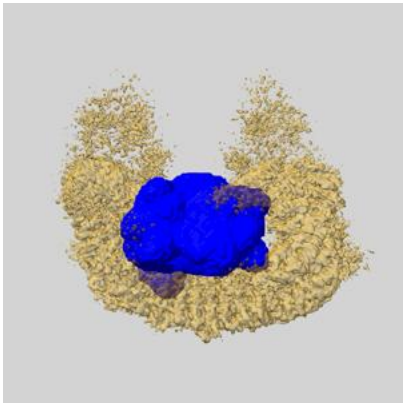


Y

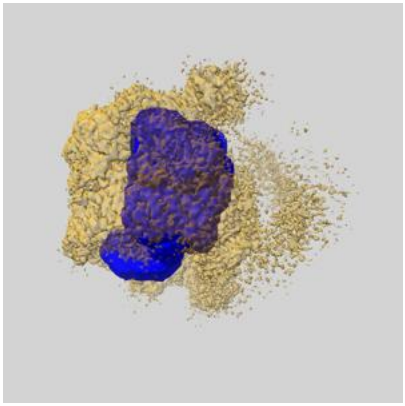


Z

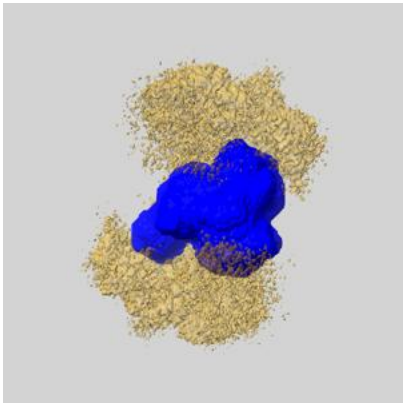
6.5.2 emd_27841_msk_2.map (i)



X



Y

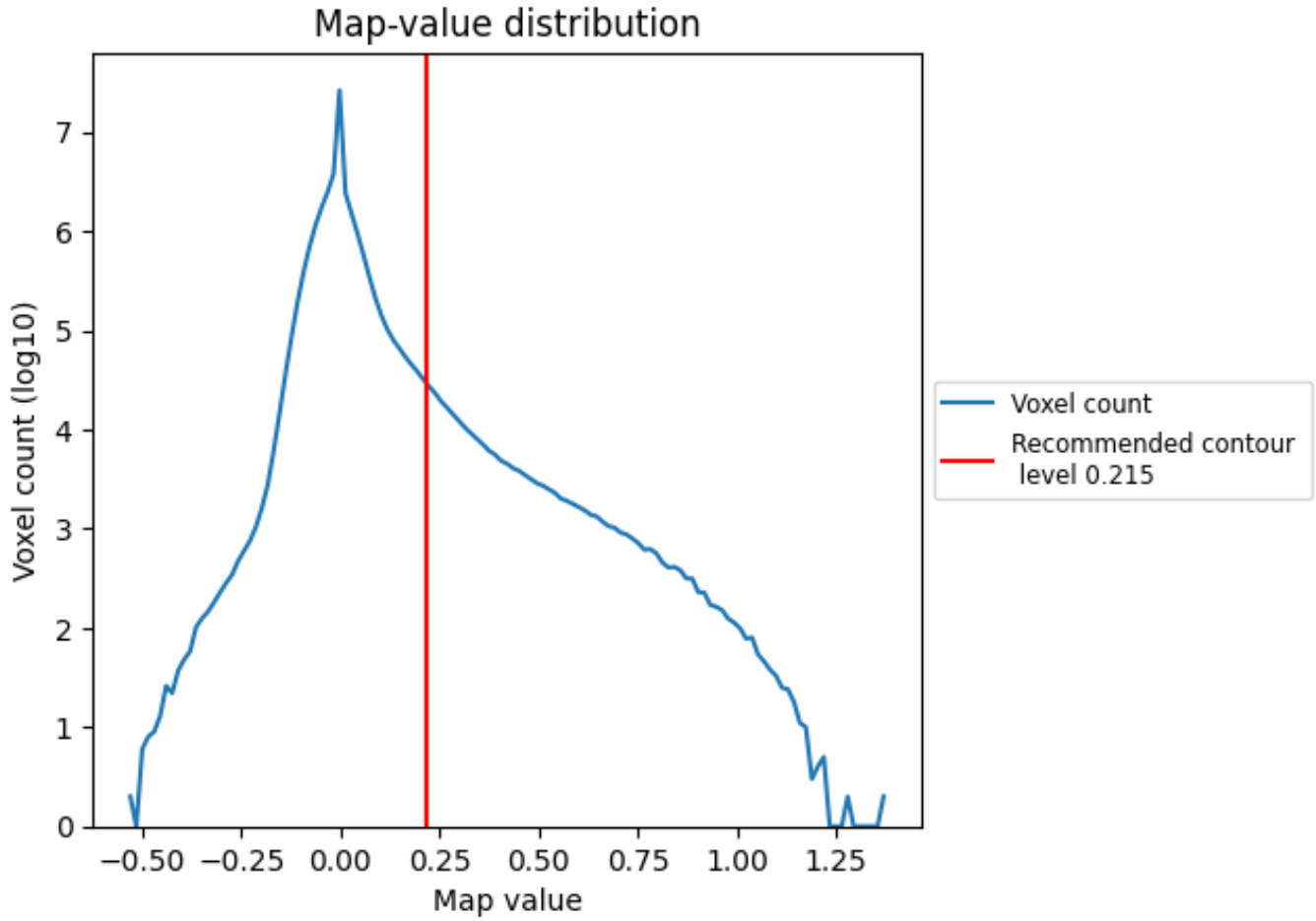


Z

7 Map analysis

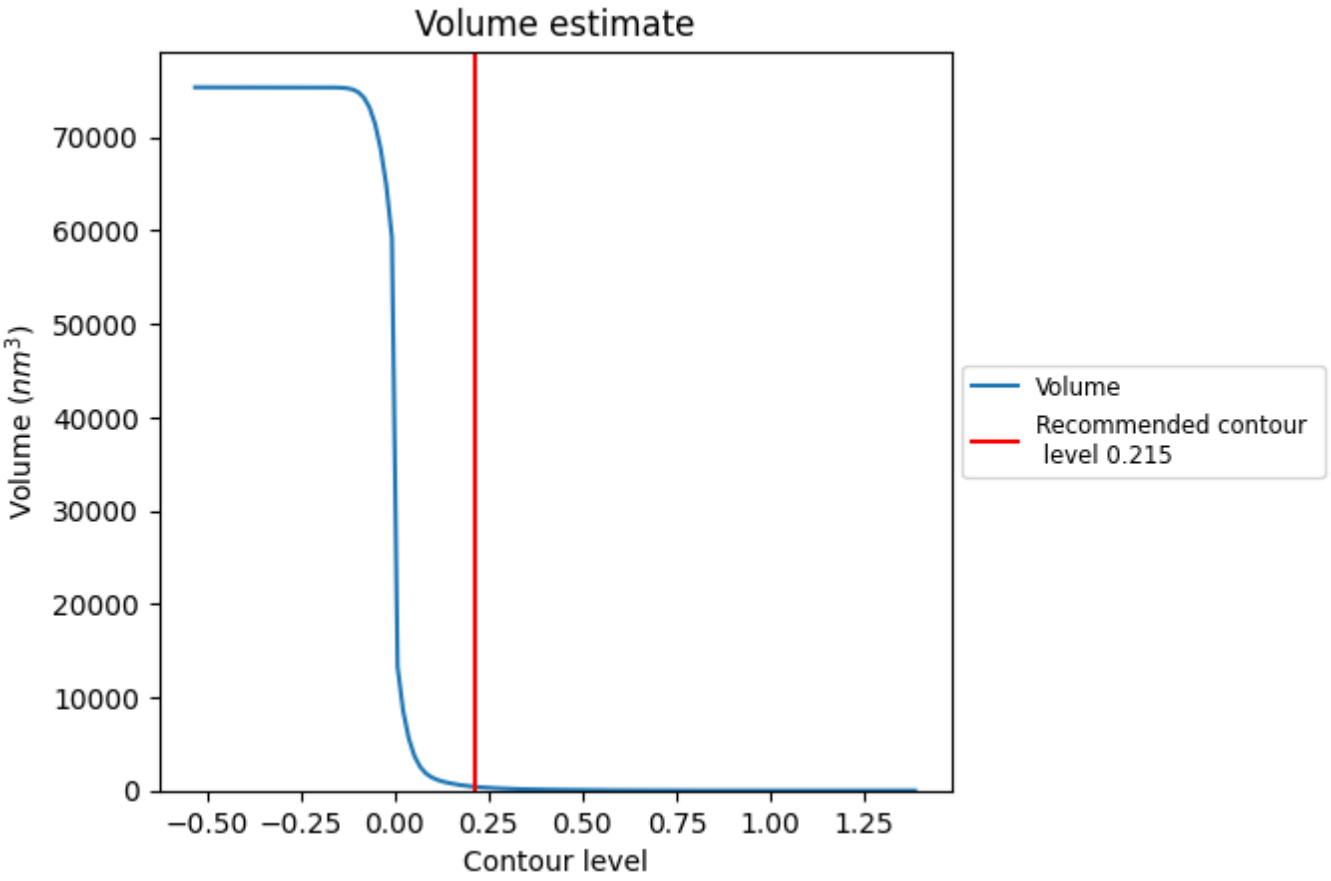
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

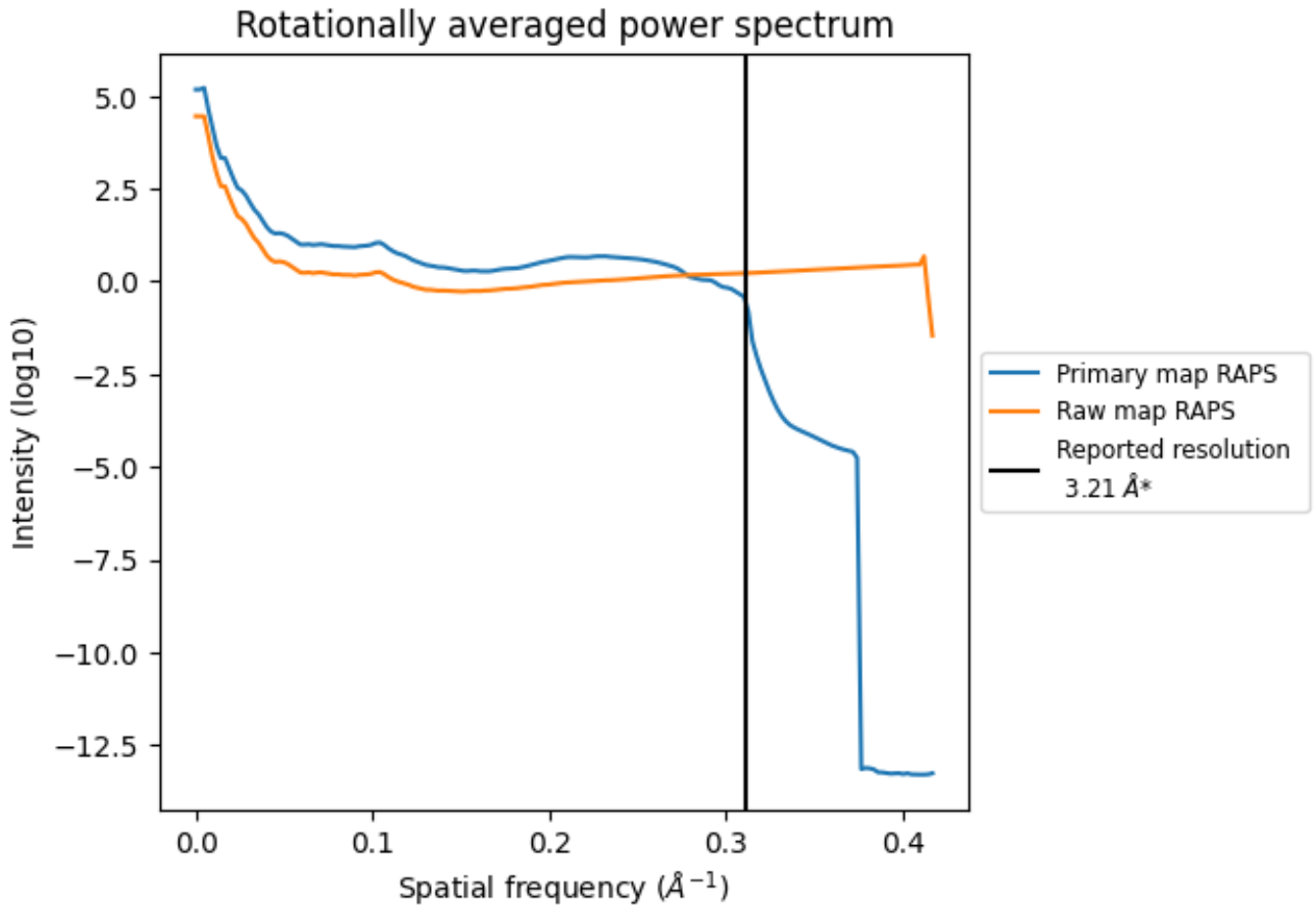
7.2 Volume estimate



The volume at the recommended contour level is 405 nm^3; this corresponds to an approximate mass of 366 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)

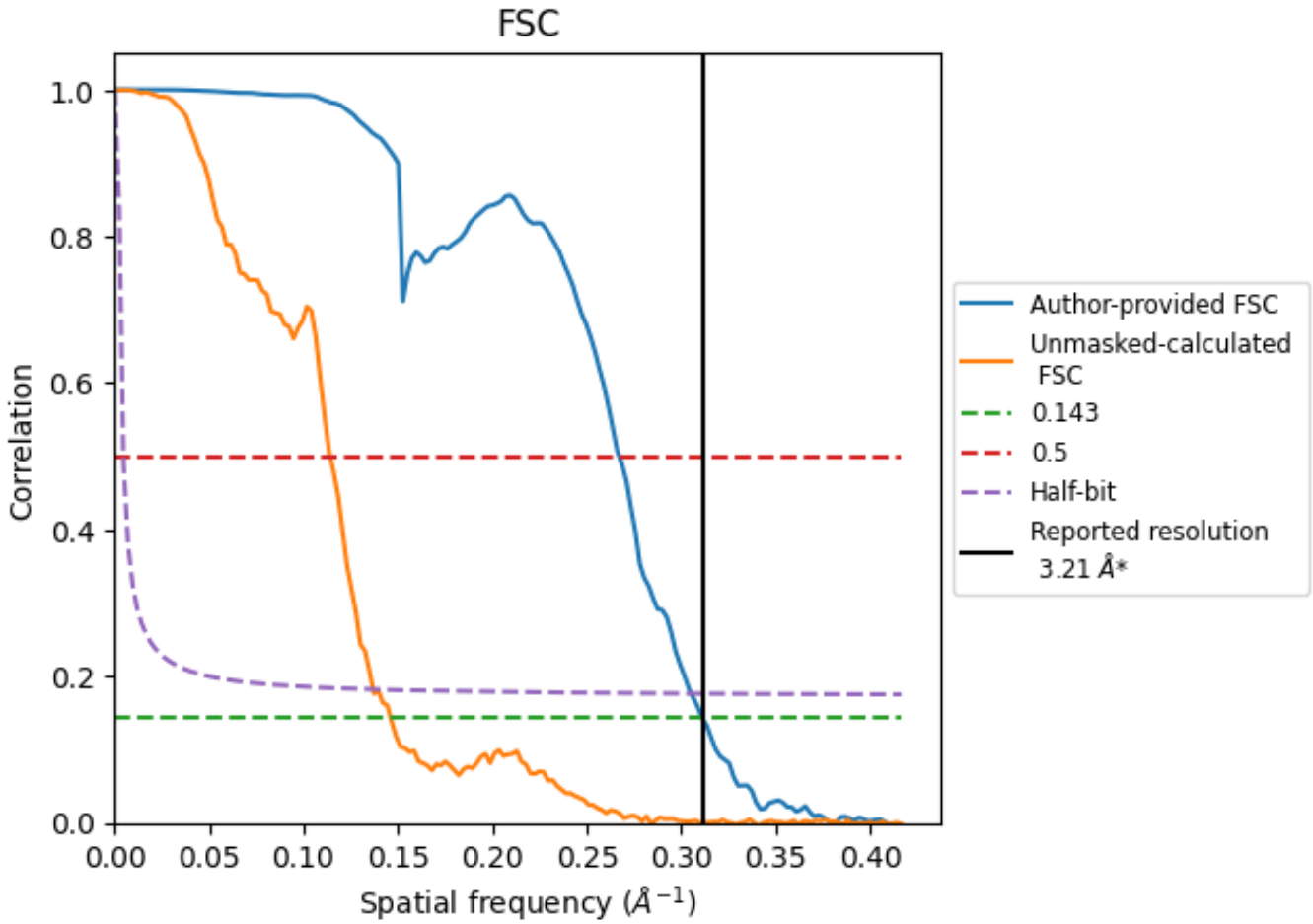


*Reported resolution corresponds to spatial frequency of 0.312 $Å^{-1}$

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)

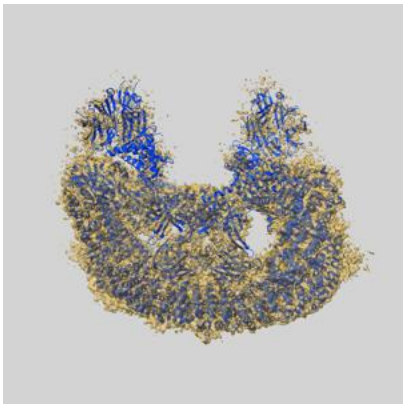
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.21	-	-
Author-provided FSC curve	3.21	3.74	3.27
Unmasked-calculated*	6.84	8.76	7.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.84 differs from the reported value 3.21 by more than 10 %

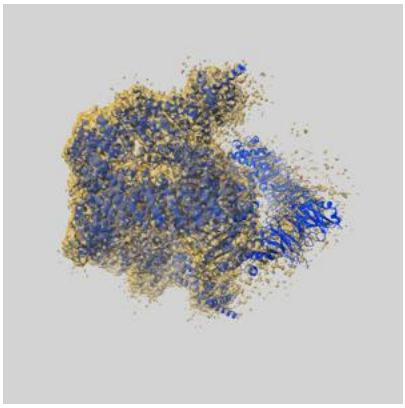
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27841 and PDB model 8E2K. Per-residue inclusion information can be found in section 3 on page 7.

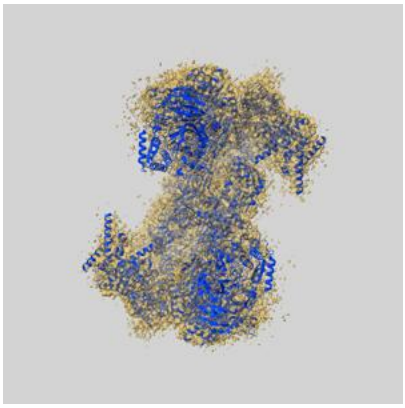
9.1 Map-model overlay



X



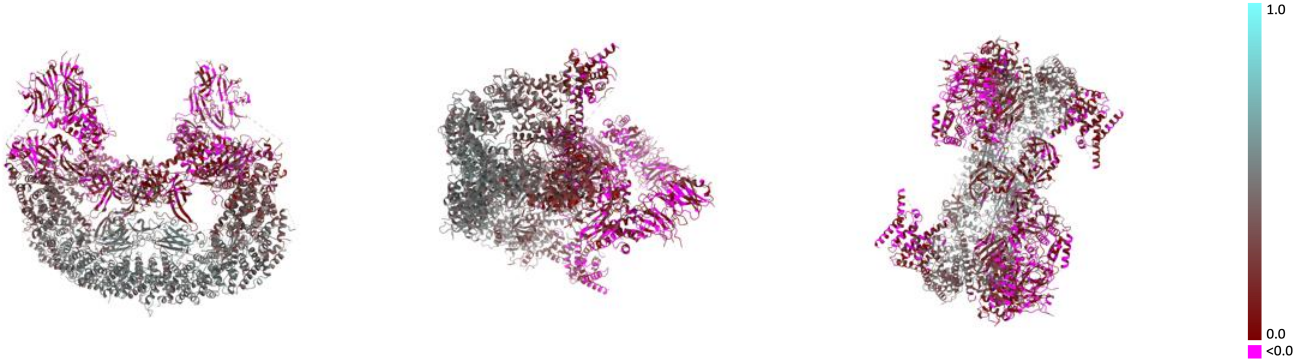
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.215 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.

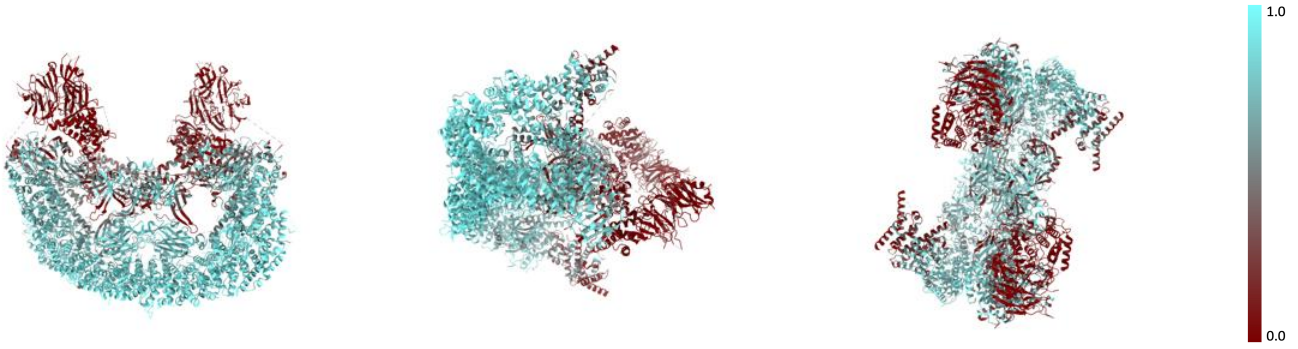
9.2 Q-score mapped to coordinate model (i)



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.

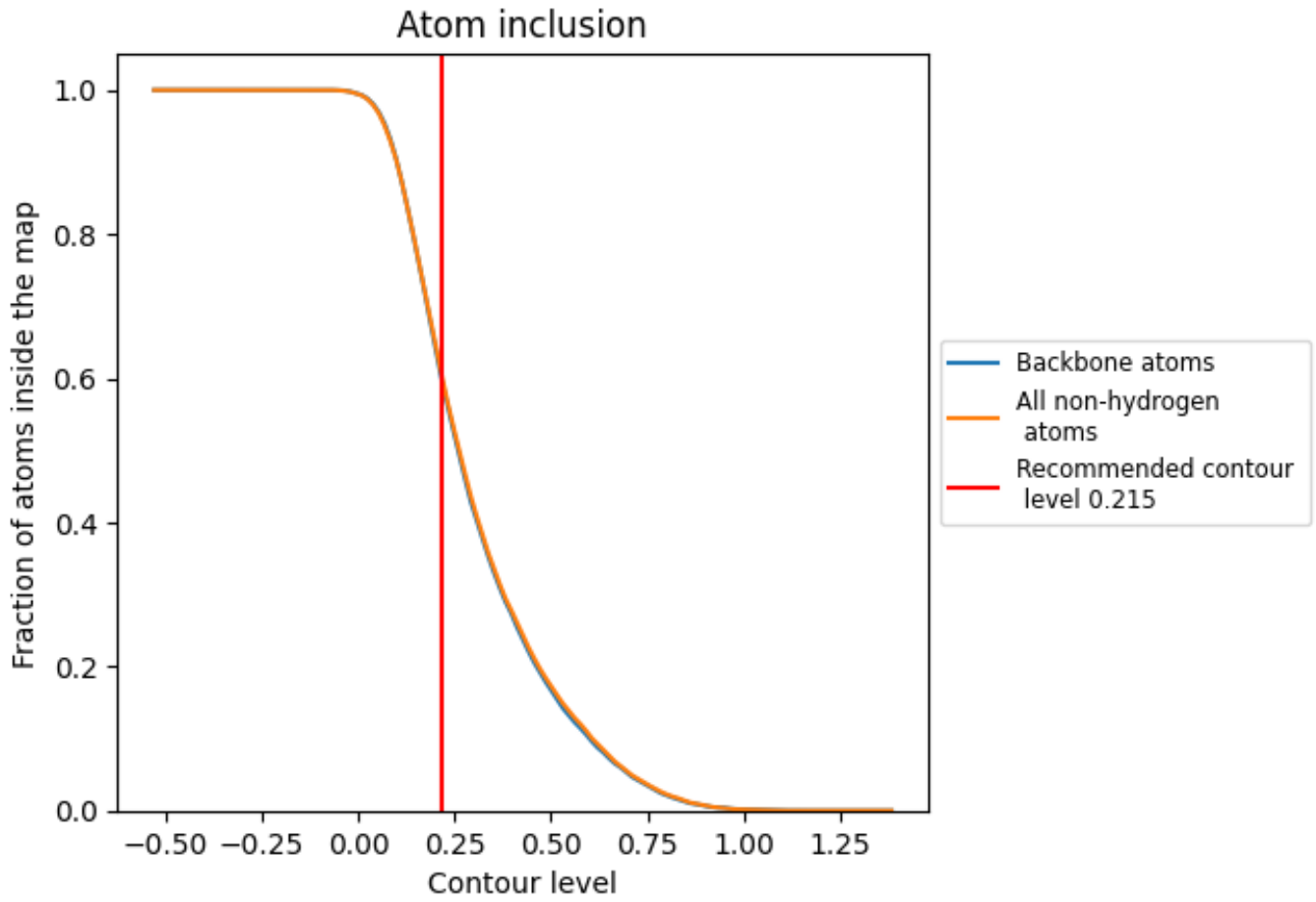
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.215).

9.4 Atom inclusion (i)



At the recommended contour level, 60% of all backbone atoms, 61% 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 (0.215) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6076	0.2770
A	0.6220	0.2830
B	0.6387	0.2890
X	0.5487	0.2640
Y	0.4590	0.1440
Z	0.4612	0.1690