Full wwPDB EM Validation Report ⓘ

May 5, 2022 – 04:12 pm BST

PDB ID	:	7QPG
EMDB ID	:	EMD-14120
Title	:	Human RZZ kinetochore corona complex.
Authors	:	Raisch, T.; Ciossani, G.; d'Amico, E.; Cmetowski, V.; Carmignani, S.; Maffini, S.; Merino, F.; Wohlgemuth, S.; Vetter, I.R.; Raunser, S.; Musacchio, A.
Deposited on	:	2022-01-04
Resolution	:	3.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

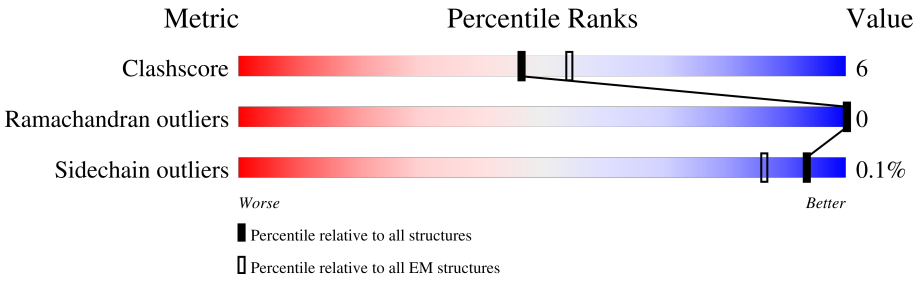
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.90 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	B	591	21% 80% 20%
1	C	591	18% 80% 20%
2	R	2464	15% 75% 15% 10%
2	S	2464	15% 74% 15% 10%
3	W	779	17% 84% 16%
3	X	779	17% 84% 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 57164 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 Protein zwilch homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	591	Total 4737	C 3031	N 791	O 898	S 17	0	0
1	C	591	Total 4737	C 3031	N 791	O 898	S 17	0	0

- Molecule 2 is a protein called Kinetochore-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	2208	Total 17614	C 11298	N 2909	O 3312	S 95	0	0
2	S	2208	Total 17614	C 11298	N 2909	O 3312	S 95	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-254	MET	-	initiating methionine	UNP A0A366VY15
R	-253	ALA	-	expression tag	UNP A0A366VY15
R	-252	HIS	-	expression tag	UNP A0A366VY15
R	-251	HIS	-	expression tag	UNP A0A366VY15
R	-250	HIS	-	expression tag	UNP A0A366VY15
R	-249	HIS	-	expression tag	UNP A0A366VY15
R	-248	HIS	-	expression tag	UNP A0A366VY15
R	-247	HIS	-	expression tag	UNP A0A366VY15
R	-246	SER	-	expression tag	UNP A0A366VY15
R	-245	SER	-	expression tag	UNP A0A366VY15
R	-244	GLY	-	expression tag	UNP A0A366VY15
R	-8	LEU	-	linker	UNP A0A366VY15
R	-7	GLU	-	linker	UNP A0A366VY15
R	-6	VAL	-	linker	UNP A0A366VY15
R	-5	LEU	-	linker	UNP A0A366VY15
R	-4	PHE	-	linker	UNP A0A366VY15
R	-3	GLN	-	linker	UNP A0A366VY15

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-2	GLY	-	linker	UNP A0A366VY15
R	-1	PRO	-	linker	UNP A0A366VY15
R	0	GLY	-	linker	UNP A0A366VY15
R	1	SER	-	linker	UNP A0A366VY15
S	-254	MET	-	initiating methionine	UNP A0A366VY15
S	-253	ALA	-	expression tag	UNP A0A366VY15
S	-252	HIS	-	expression tag	UNP A0A366VY15
S	-251	HIS	-	expression tag	UNP A0A366VY15
S	-250	HIS	-	expression tag	UNP A0A366VY15
S	-249	HIS	-	expression tag	UNP A0A366VY15
S	-248	HIS	-	expression tag	UNP A0A366VY15
S	-247	HIS	-	expression tag	UNP A0A366VY15
S	-246	SER	-	expression tag	UNP A0A366VY15
S	-245	SER	-	expression tag	UNP A0A366VY15
S	-244	GLY	-	expression tag	UNP A0A366VY15
S	-8	LEU	-	linker	UNP A0A366VY15
S	-7	GLU	-	linker	UNP A0A366VY15
S	-6	VAL	-	linker	UNP A0A366VY15
S	-5	LEU	-	linker	UNP A0A366VY15
S	-4	PHE	-	linker	UNP A0A366VY15
S	-3	GLN	-	linker	UNP A0A366VY15
S	-2	GLY	-	linker	UNP A0A366VY15
S	-1	PRO	-	linker	UNP A0A366VY15
S	0	GLY	-	linker	UNP A0A366VY15
S	1	SER	-	linker	UNP A0A366VY15

- Molecule 3 is a protein called Centromere/kinetochore protein zw10 homolog.

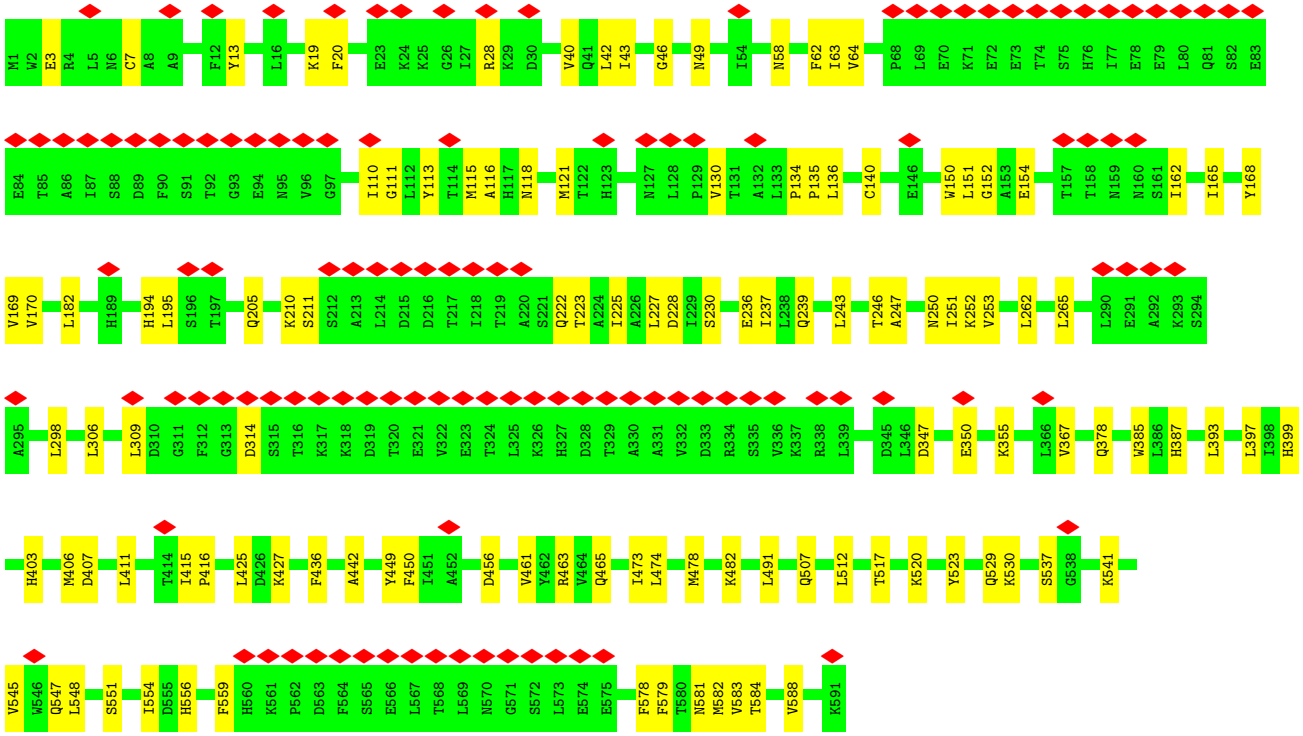
Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	779	Total	C	N	O	S	0	0
			6231	3952	1053	1189	37		
3	X	779	Total	C	N	O	S	0	0
			6231	3952	1053	1189	37		

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.

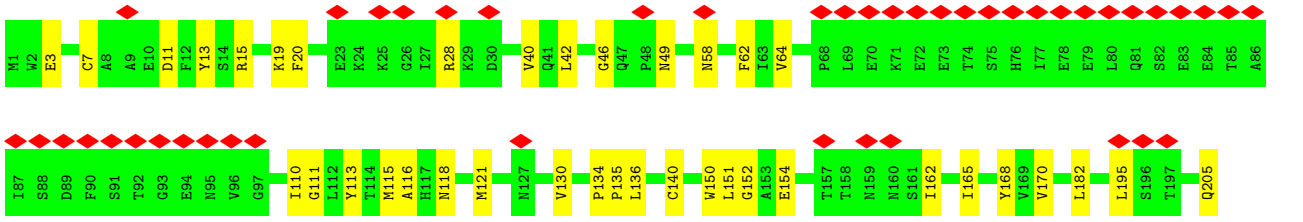
• Molecule 1: Protein zwilch homolog

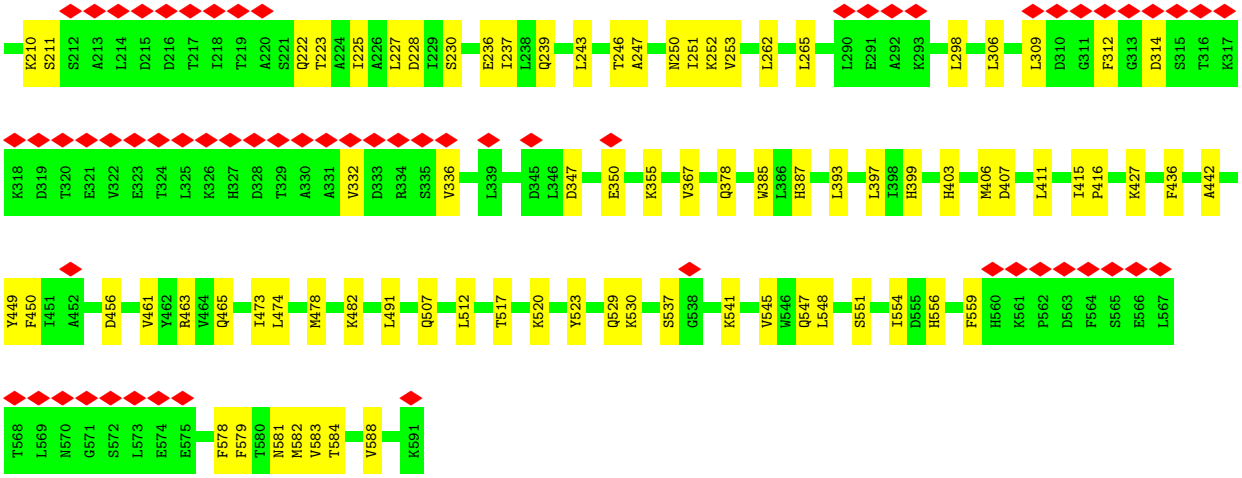
Chain B:



• Molecule 1: Protein zwilch homolog

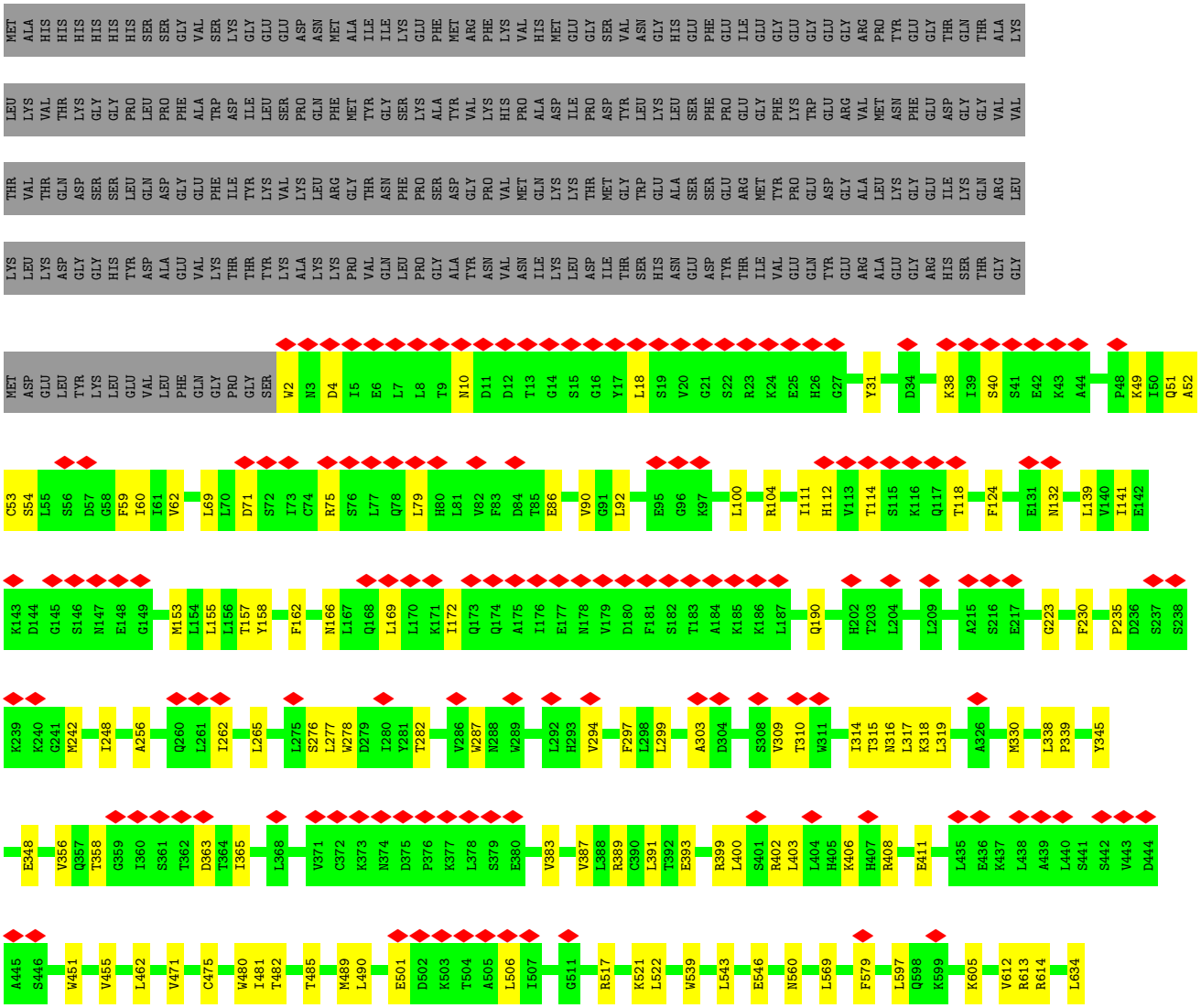
Chain C:

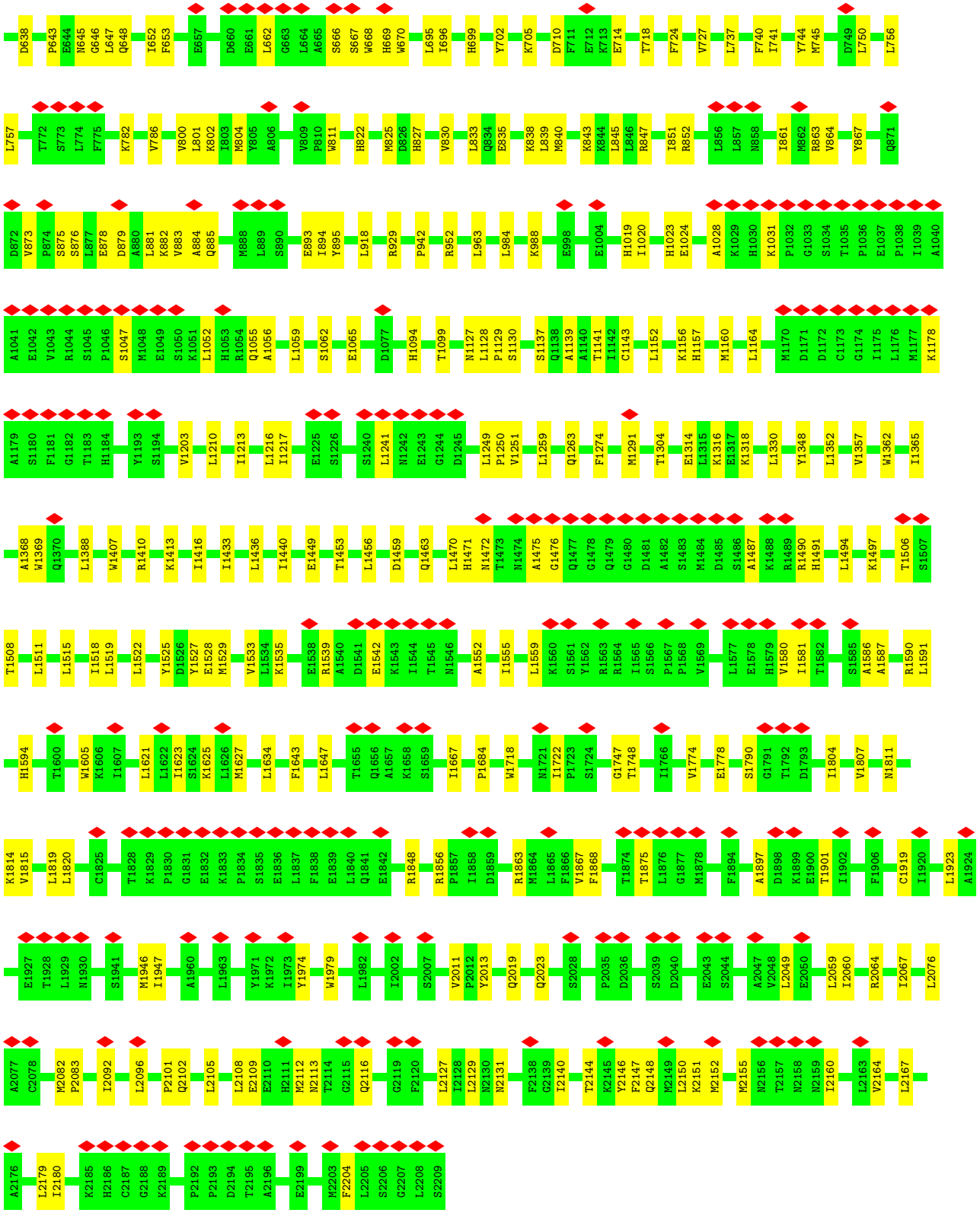




• Molecule 2: Kinetochore-associated protein 1

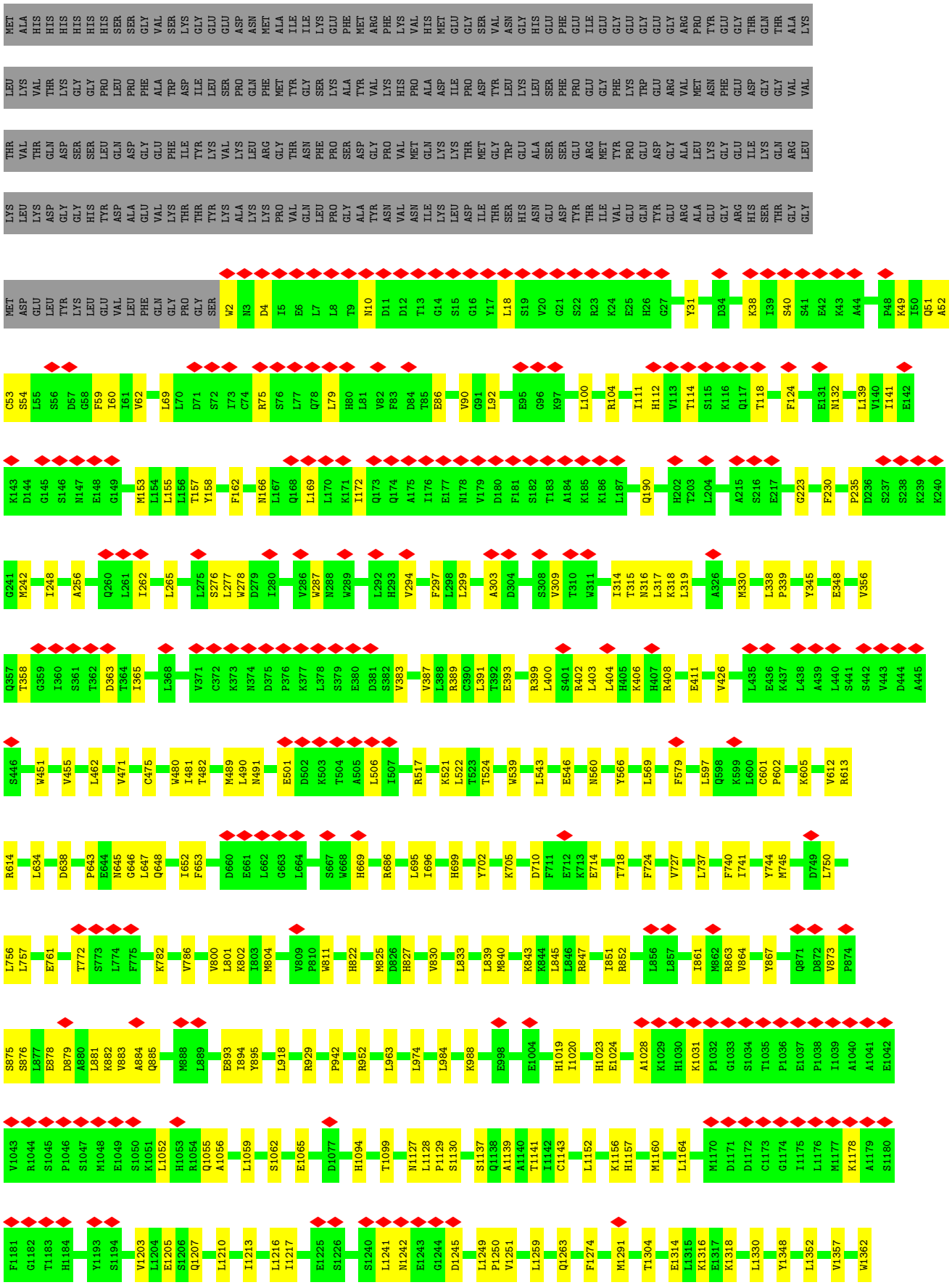
Chain R:

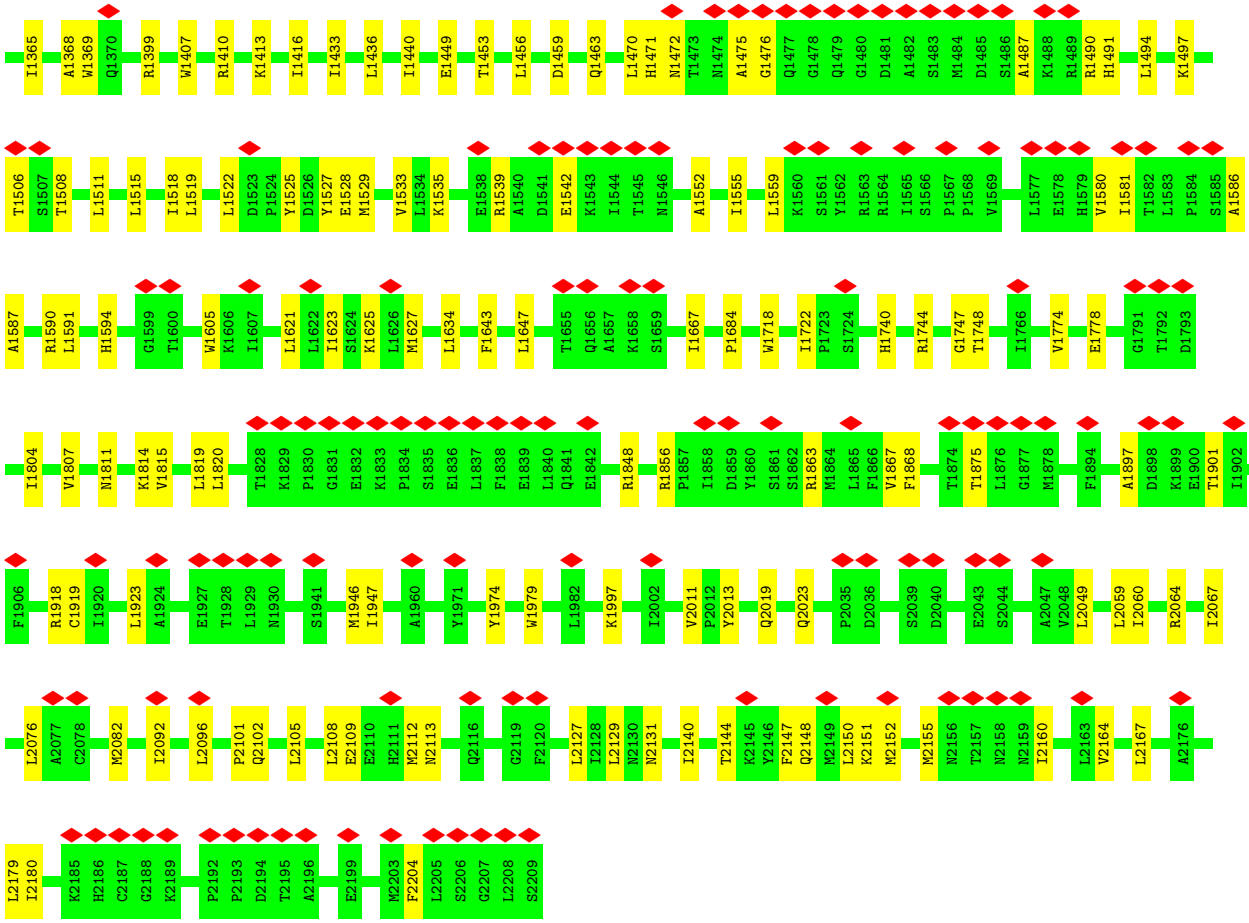




• Molecule 2: Kinetochore-associated protein 1

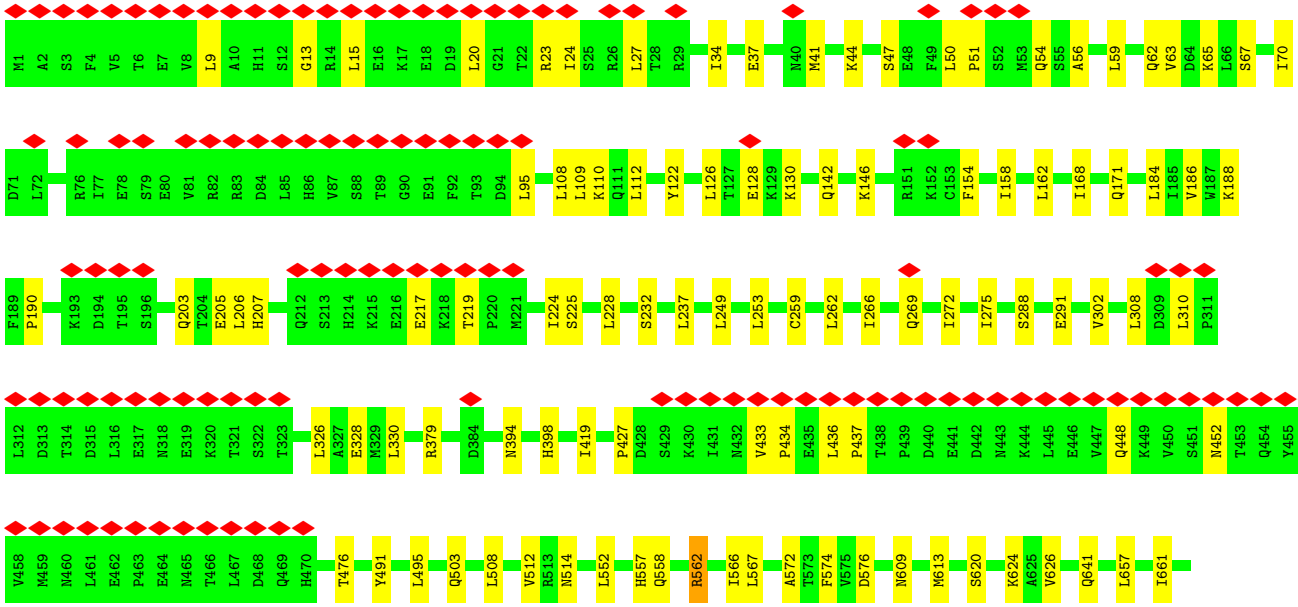
Chain S:

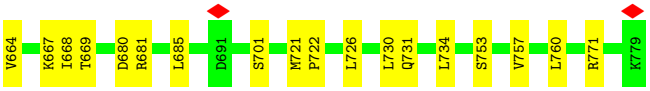

MET ALA HIS HIS HIS HIS HIS SER SER GLY VAL SER LYS GLY GLU GLU ASP ASN MET ALA ILE ILE LYS GLU PHE MET ARG PHE LYS VAL HIS MET GLU GLY SER VAL ASN GLY HIS GLU PHE GLU ILE GLU GLY GLU GLY GLU GLY ARG PRO TYR GLU GLY THR GLN THR ALA LYS
LEU LYS VAL THR LYS GLY GLY PRO LEU PRO PHE ALA TRP ASP ILE LEU SER PRO GLN PHE MET TYR LYS VAL LYS LEU ARG GLY THR ASN PHE PRO SER ASP GLY PRO VAL MET GLN ILE LYS LYS THR MET GLY TRP GLU LEU LYS LEU SER PHE PRO GLU GLY GLY PHE LYS TRP GLU GLY VAL MET ASN PHE GLU ASP LEU GLY VAL VAL
THR VAL THR GLN ASP SER SER LEU GLN ASP GLY GLU PHE ILE TYR LYS VAL LYS LEU ARG GLY THR ASN PHE PRO SER ASP GLY PRO VAL MET GLN LYS LYS THR MET GLY TRP GLU ALA SER SER SER GLU ARG MET TYR PRO GLU ASP GLY ALA LEU LYS GLY GLU ILE LYS GLN ARG LEU
LYS LEU LYS ASP GLY GLY HIS TYR ASP ALA GLU VAL LYS THR THR TYR LYS ALA LYS LYS PRO VAL GLN LEU PRO GLY ALA TYR ASN VAL ASN ILE LYS LEU ASP ILE THR SER HIS ASN GLU ASP TYR THR ILE VAL GLU GLN TYR GLU ARG ALA GLU GLY ARG HIS SER THR GLY GLY
MET ASP GLU LEU TYR LYS LEU GLU VAL LEU PHE GLN GLY PRO GLY SER W2 N3 D4 I5 E6 L7 L8 T9 N10 D11 D12 T13 G14 S15 G16 Y17 L18 S19 V20 G21 S22 R23 K24 E25 H26 G27 Y31 D34 K38 I39 S40 S41 E42 K43 A44 P48 K49 I50 Q51 A52
C53 S54 L55 S56 D57 G58 F59 I60 I61 V62 L69 L70 D71 S72 I73 C74 R75 S76 L77 Q78 L79 H80 L81 V82 F83 D84 T85 E86 V90 G91 L92 E95 G96 K97 L100 R104 I111 H112 V113 T114 S115 K116 Q117 T118 F124 E131 N132 L139 V140 I141 E142
K143 D144 G145 S146 N147 E148 G149 M153 L154 L155 L156 T157 Y158 F162 N166 L167 Q168 L169 L170 K171 I172 Q173 Q174 A175 I176 E177 N178 V179 D180 F181 S182 T183 A184 K185 K186 L187 Q190 H202 T203 L204 A215 S216 E217 G223 F230 P235 D236 S237 S238 K239 K240
G241 M242 I248 A256 Q260 L261 I262 L265 L275 S276 L277 W278 D279 I280 V286 W287 N288 W289 L292 H293 V294 F297 L298 L299 A303 D304 S308 V309 T310 W311 I314 T315 N316 L317 K318 L319 A326 M330 L338 P339 Y345 E348 V356
Q357 T358 G359 I360 S361 T362 D363 T364 I365 L368 V371 C372 K373 N374 D375 P376 K377 L378 S379 E380 D381 S382 V383 V387 L388 R389 C390 L391 T392 E393 R399 L400 S401 R402 L403 L404 H405 K406 H407 R408 E411 V426 L435 E436 K437 L438 A439 L440 S441 S442 V443 D444 A445
S446 W451 V455 L462 V471 C475 W480 I481 T482 M489 L490 N491 E501 D502 K503 T504 A505 L506 I507 R517 K521 L522 T523 T524 W539 L543 E546 N560 Y566 L569 F579 L597 Q598 K599 L600 C601 P602 K605 V612 R613
R614 L634 D638 P643 E644 N645 G646 L647 Q648 I652 F653 D660 E661 L662 G663 L664 S667 W668 H669 R686 L695 I696 H699 Y702 K705 D710 F711 E712 K713 E714 T718 F724 V727 L737 F740 I741 Y744 M745 D749 L750
L756 L757 E761 T772 S773 L774 F775 K782 V786 V800 L801 K802 I803 M804 V809 P810 W811 H822 M825 D826 H827 V830 L833 L839 M840 K843 K844 L845 L846 R847 I851 R852 L856 L857 I861 M862 R863 V864 Y867 Q871 D872 V873 P874
S875 S876 L877 E878 D879 A880 L881 K882 V883 A884 Q885 M888 L889 E893 I894 Y895 L918 R929 P942 R952 L963 L974 L984 K988 E998 E1004 H1019 I1020 H1023 E1024 A1028 K1029 H1030 K1031 P1032 G1033 S1034 T1035 P1036 E1037 P1038 I1039 A1040 A1041 E1042
V1043 R1044 S1045 P1046 S1047 M1048 E1049 S1050 K1051 L1052 H1053 R1054 Q1055 A1056 L1059 S1062 E1065 D1077 H1094 T1099 N1127 L1128 P1129 S1130 S1137 Q1138 A1139 A1140 T1141 I1142 C1143 L1152 K1156 H1157 M1160 L1164 M1170 D1171 D1172 C1173 G1174 I1175 L1176 M1177 K1178 A1179 S1180
F1181 G1182 T1183 H1184 Y1193 S1194 V1203 L1204 E1205 S1206 Q1207 L1210 I1213 L1216 I1217 E1225 S1226 S1240 L1241 N1242 E1243 G1244 D1245 L1249 P1250 V1251 L1259 Q1263 F1274 M1291 T1304 E1314 L1315 K1316 E1317 K1318 L1330 Y1348 L1352 V1357 W1362



• Molecule 3: Centromere/kinetochore protein zw10 homolog

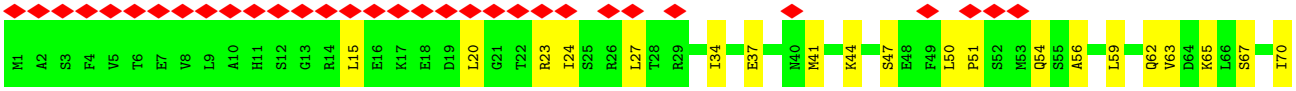
Chain W:

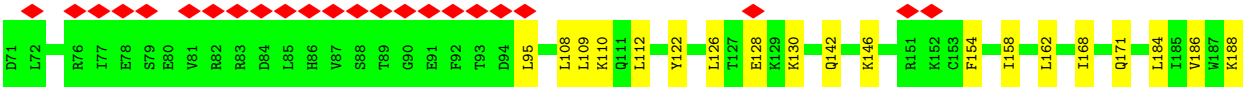


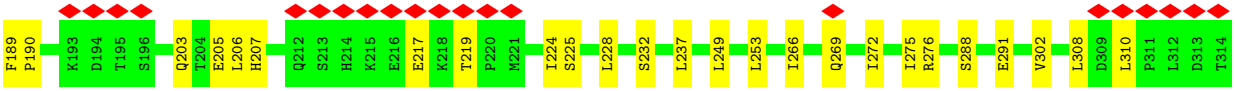


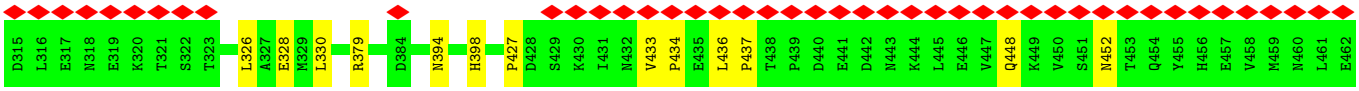
• Molecule 3: Centromere/kinetochore protein zw10 homolog

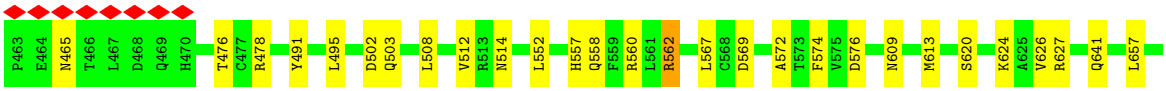
Chain X:

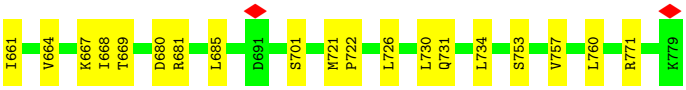












4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191979	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	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	3.677	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.051	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	540.0, 540.0, 540.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.8, 1.8, 1.8	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	B	0.24	0/4840	0.39	0/6563
1	C	0.24	0/4840	0.39	0/6563
2	R	0.23	0/17950	0.40	0/24302
2	S	0.23	0/17950	0.40	0/24302
3	W	0.24	0/6340	0.39	0/8565
3	X	0.24	0/6340	0.39	0/8565
All	All	0.24	0/58260	0.40	0/78860

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	B	4737	0	4766	76	0
1	C	4737	0	4766	74	0
2	R	17614	0	17942	235	0
2	S	17614	0	17942	235	0
3	W	6231	0	6339	78	0
3	X	6231	0	6339	82	0
All	All	57164	0	58094	749	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 (749) 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:B:223:THR:HA	1:B:252:LYS:O	1.73	0.89
1:C:223:THR:HA	1:C:252:LYS:O	1.73	0.89
2:R:277:LEU:HB3	2:R:287:TRP:HB3	1.70	0.73
2:S:277:LEU:HB3	2:S:287:TRP:HB3	1.70	0.73
3:W:613:MET:O	3:W:681:ARG:NH1	2.22	0.72
3:X:613:MET:O	3:X:681:ARG:NH1	2.22	0.72
2:R:1868:PHE:HE1	2:R:1875:THR:H	1.37	0.71
1:C:545:VAL:HB	1:C:583:VAL:HB	1.71	0.71
3:W:288:SER:OG	3:W:291:GLU:OE1	2.09	0.71
3:W:436:LEU:HB3	3:W:562:ARG:HH12	1.56	0.70
2:S:1868:PHE:HE1	2:S:1875:THR:H	1.37	0.70
2:S:1407:TRP:HE1	2:S:1453:THR:HG21	1.57	0.70
1:B:545:VAL:HB	1:B:583:VAL:HB	1.71	0.69
2:R:60:ILE:HD11	2:R:92:LEU:HG	1.74	0.69
2:R:54:SER:HB3	2:R:358:THR:HG22	1.74	0.69
2:S:60:ILE:HD11	2:S:92:LEU:HG	1.74	0.69
3:X:288:SER:OG	3:X:291:GLU:OE1	2.09	0.69
2:S:54:SER:HB3	2:S:358:THR:HG22	1.74	0.69
3:X:436:LEU:HB3	3:X:562:ARG:HH12	1.56	0.69
2:R:1407:TRP:HE1	2:R:1453:THR:HG21	1.57	0.69
3:X:232:SER:HA	3:X:237:LEU:HD22	1.76	0.68
2:R:884:ALA:HB3	2:R:894:ILE:HD11	1.76	0.68
2:S:1552:ALA:HA	2:S:1555:ILE:HD12	1.76	0.68
2:R:1552:ALA:HA	2:R:1555:ILE:HD12	1.76	0.67
2:S:884:ALA:HB3	2:S:894:ILE:HD11	1.76	0.67
3:W:232:SER:HA	3:W:237:LEU:HD22	1.76	0.67
3:X:558:GLN:O	3:X:562:ARG:NH2	2.27	0.67
3:W:206:LEU:HD23	3:W:275:ILE:HD12	1.76	0.67
3:W:558:GLN:O	3:W:562:ARG:NH2	2.27	0.67
3:W:59:LEU:HD23	3:W:62:GLN:HE21	1.60	0.66
2:R:666:SER:O	2:S:1918:ARG:NH2	2.27	0.65
2:R:2083:PRO:O	2:S:491:ASN:ND2	2.17	0.65
3:X:206:LEU:HD23	3:X:275:ILE:HD12	1.76	0.65
1:C:140:CYS:O	1:C:556:HIS:HE1	1.78	0.65
1:B:140:CYS:O	1:B:556:HIS:HE1	1.78	0.64
2:R:1527:TYR:OH	2:R:1591:LEU:O	2.15	0.64
3:X:59:LEU:HD23	3:X:62:GLN:HE21	1.60	0.64
2:S:881:LEU:HA	2:S:894:ILE:HD13	1.79	0.64
2:S:963:LEU:HD13	2:S:984:LEU:HA	1.80	0.64
1:B:530:LYS:HB2	1:B:547:GLN:HE21	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:605:LYS:HB2	2:S:652:ILE:HD11	1.79	0.64
1:C:225:ILE:HG12	1:C:251:ILE:HG23	1.80	0.64
2:R:605:LYS:HB2	2:R:652:ILE:HD11	1.79	0.64
2:S:18:LEU:HD12	2:S:38:LYS:HD2	1.78	0.63
1:C:530:LYS:HB2	1:C:547:GLN:HE21	1.63	0.63
2:R:18:LEU:HD12	2:R:38:LYS:HD2	1.78	0.63
2:S:1127:ASN:HB3	2:S:1130:SER:HB3	1.81	0.63
2:R:963:LEU:HD13	2:R:984:LEU:HA	1.80	0.63
1:B:347:ASP:HA	1:B:385:TRP:HD1	1.64	0.63
2:R:881:LEU:HA	2:R:894:ILE:HD13	1.79	0.63
2:S:303:ALA:HA	2:S:406:LYS:HE2	1.81	0.63
2:R:455:VAL:HG22	2:R:480:TRP:HZ3	1.64	0.63
2:R:2060:ILE:HG13	2:R:2082:MET:HE1	1.81	0.63
2:S:1527:TYR:OH	2:S:1591:LEU:O	2.15	0.63
2:R:363:ASP:HB3	2:R:399:ARG:HH22	1.64	0.63
2:R:1440:ILE:O	2:R:1497:LYS:NZ	2.32	0.62
3:W:184:LEU:HD13	3:W:224:ILE:HG12	1.81	0.62
2:S:1440:ILE:O	2:S:1497:LYS:NZ	2.32	0.62
2:R:1127:ASN:HB3	2:R:1130:SER:HB3	1.80	0.62
2:R:303:ALA:HA	2:R:406:LYS:HE2	1.80	0.62
2:S:455:VAL:HG22	2:S:480:TRP:HZ3	1.64	0.62
1:C:347:ASP:HA	1:C:385:TRP:HD1	1.64	0.62
3:X:184:LEU:HD13	3:X:224:ILE:HG12	1.81	0.62
1:B:225:ILE:HG12	1:B:251:ILE:HG23	1.80	0.62
2:R:2148:GLN:O	2:R:2151:LYS:HB2	2.00	0.62
2:S:2148:GLN:O	2:S:2151:LYS:HB2	2.00	0.62
1:B:211:SER:HB3	1:B:223:THR:HB	1.83	0.61
1:B:306:LEU:HD23	1:B:309:LEU:HD12	1.82	0.61
2:S:1330:LEU:HD13	2:S:1348:TYR:HE1	1.65	0.61
1:C:436:PHE:HB3	1:C:442:ALA:HB3	1.83	0.61
3:W:37:GLU:HB3	3:W:41:MET:HE1	1.82	0.61
1:B:140:CYS:O	1:B:556:HIS:CE1	2.53	0.61
2:S:2060:ILE:HG13	2:S:2082:MET:HE1	1.83	0.61
1:C:140:CYS:O	1:C:556:HIS:CE1	2.53	0.61
2:S:265:LEU:HD22	2:S:277:LEU:HD11	1.83	0.61
2:S:363:ASP:HB3	2:S:399:ARG:HH22	1.64	0.61
2:R:265:LEU:HD22	2:R:277:LEU:HD11	1.83	0.60
2:S:873:VAL:HB	2:S:876:SER:HB3	1.83	0.60
3:W:108:LEU:HB3	3:W:154:PHE:HZ	1.66	0.60
1:B:194:HIS:CG	2:R:310:THR:HB	2.36	0.60
1:C:309:LEU:HD23	1:C:314:ASP:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:37:GLU:HB3	3:X:41:MET:HE1	1.83	0.60
1:C:211:SER:HB3	1:C:223:THR:HB	1.83	0.60
2:S:1684:PRO:HG2	2:S:1718:TRP:HD1	1.66	0.60
1:C:195:LEU:HD13	1:C:537:SER:HB3	1.84	0.60
2:R:1684:PRO:HG2	2:R:1718:TRP:HD1	1.66	0.60
1:B:169:VAL:HG11	2:R:282:THR:HG21	1.82	0.60
1:B:436:PHE:HB3	1:B:442:ALA:HB3	1.83	0.60
1:C:306:LEU:HD23	1:C:309:LEU:HD12	1.82	0.60
2:R:1330:LEU:HD13	2:R:1348:TYR:HE1	1.65	0.60
3:X:108:LEU:HB3	3:X:154:PHE:HZ	1.66	0.60
3:X:626:VAL:HG21	3:X:685:LEU:HD12	1.84	0.60
1:B:195:LEU:HD13	1:B:537:SER:HB3	1.84	0.59
1:B:309:LEU:HD23	1:B:314:ASP:HA	1.83	0.59
3:W:626:VAL:HG21	3:W:685:LEU:HD12	1.84	0.59
3:X:436:LEU:HD22	3:X:562:ARG:HH22	1.68	0.59
2:S:2102:GLN:HG3	2:S:2144:THR:HG21	1.84	0.59
1:B:243:LEU:HD13	1:B:517:THR:HG22	1.85	0.59
2:R:873:VAL:HB	2:R:876:SER:HB3	1.82	0.59
2:R:481:ILE:HG13	2:R:482:THR:HG23	1.84	0.59
2:R:1491:HIS:NE2	2:R:1528:GLU:HG3	2.18	0.59
3:W:436:LEU:HD22	3:W:562:ARG:HH22	1.68	0.59
2:R:276:SER:HG	2:R:278:TRP:HE1	1.49	0.59
2:R:86:GLU:OE1	2:R:104:ARG:NH2	2.36	0.58
1:B:450:PHE:HA	1:B:463:ARG:HD3	1.85	0.58
1:C:450:PHE:HA	1:C:463:ARG:HD3	1.85	0.58
2:S:481:ILE:HG13	2:S:482:THR:HG23	1.84	0.58
3:W:41:MET:HG3	3:W:44:LYS:HD2	1.85	0.58
3:X:448:GLN:O	3:X:452:ASN:ND2	2.37	0.58
1:B:130:VAL:HG23	1:B:162:ILE:HD12	1.86	0.58
1:C:130:VAL:HG23	1:C:162:ILE:HD12	1.86	0.57
2:S:223:GLY:HA3	2:S:256:ALA:HB3	1.86	0.57
2:R:223:GLY:HA3	2:R:256:ALA:HB3	1.86	0.57
2:R:365:ILE:HB	2:R:391:LEU:HB2	1.86	0.57
2:S:724:PHE:HZ	2:S:737:LEU:HD13	1.69	0.57
2:S:1491:HIS:NE2	2:S:1528:GLU:HG3	2.18	0.57
1:B:559:PHE:HB2	1:B:579:PHE:HE1	1.70	0.57
2:R:1216:LEU:HD11	2:R:1251:VAL:HG13	1.86	0.57
2:R:2102:GLN:HG3	2:R:2144:THR:HG21	1.84	0.57
2:S:1774:VAL:HG22	2:S:1819:LEU:HD21	1.86	0.57
3:X:41:MET:HG3	3:X:44:LYS:HD2	1.85	0.57
1:C:243:LEU:HD13	1:C:517:THR:HG22	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:662:LEU:HD23	2:S:1997:LYS:HD3	1.86	0.57
2:S:86:GLU:OE1	2:S:104:ARG:NH2	2.36	0.57
3:W:67:SER:HB2	3:W:110:LYS:HZ3	1.70	0.57
2:R:724:PHE:HZ	2:R:737:LEU:HD13	1.70	0.57
3:W:142:GLN:HG2	3:W:146:LYS:HE3	1.86	0.57
1:C:210:LYS:HZ2	1:C:211:SER:H	1.53	0.57
2:S:276:SER:HG	2:S:278:TRP:HE1	1.50	0.57
3:W:448:GLN:O	3:W:452:ASN:ND2	2.37	0.57
1:C:252:LYS:HE3	1:C:507:GLN:HA	1.86	0.57
2:S:365:ILE:HB	2:S:391:LEU:HB2	1.86	0.57
2:S:727:VAL:O	2:S:782:LYS:NZ	2.38	0.56
2:R:727:VAL:O	2:R:782:LYS:NZ	2.38	0.56
1:B:40:VAL:HG22	1:B:64:VAL:HG22	1.88	0.56
1:C:559:PHE:HB2	1:C:579:PHE:HE1	1.70	0.56
3:W:217:GLU:HG3	3:W:219:THR:H	1.70	0.56
1:B:252:LYS:HE3	1:B:507:GLN:HA	1.86	0.56
2:R:2160:ILE:HG12	2:R:2164:VAL:HG23	1.86	0.56
2:R:737:LEU:HA	2:R:741:ILE:HB	1.88	0.56
2:S:2160:ILE:HG12	2:S:2164:VAL:HG23	1.86	0.56
3:X:217:GLU:HG3	3:X:219:THR:H	1.69	0.56
1:C:253:VAL:HG21	1:C:473:ILE:HA	1.88	0.56
3:X:142:GLN:HG2	3:X:146:LYS:HE3	1.86	0.56
2:S:737:LEU:HA	2:S:741:ILE:HB	1.88	0.56
2:R:1774:VAL:HG22	2:R:1819:LEU:HD21	1.86	0.55
3:W:228:LEU:HD13	3:W:326:LEU:HD21	1.88	0.55
1:C:13:TYR:HB2	1:C:116:ALA:HB1	1.88	0.55
2:R:49:LYS:NZ	2:R:132:ASN:O	2.40	0.55
1:C:40:VAL:HG22	1:C:64:VAL:HG22	1.88	0.55
1:B:253:VAL:HG21	1:B:473:ILE:HA	1.88	0.55
2:S:1216:LEU:HD11	2:S:1251:VAL:HG13	1.86	0.55
2:R:1407:TRP:HH2	2:R:1449:GLU:HG3	1.72	0.55
2:S:49:LYS:NZ	2:S:132:ASN:O	2.40	0.55
3:X:24:ILE:HG13	3:X:95:LEU:HB3	1.88	0.55
3:X:228:LEU:HD13	3:X:326:LEU:HD21	1.88	0.55
3:W:24:ILE:HG13	3:W:95:LEU:HB3	1.88	0.55
3:X:67:SER:HB2	3:X:110:LYS:HZ3	1.71	0.55
2:R:139:LEU:HD13	2:R:155:LEU:HD13	1.89	0.55
2:R:668:TRP:HE1	2:S:1918:ARG:HG3	1.72	0.55
2:R:613:ARG:NH2	2:R:653:PHE:O	2.38	0.54
1:B:13:TYR:HB2	1:B:116:ALA:HB1	1.88	0.54
1:B:227:LEU:HD11	1:B:247:ALA:HB1	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:GLU:HB3	1:C:239:GLN:HB3	1.89	0.54
2:S:1407:TRP:HH2	2:S:1449:GLU:HG3	1.72	0.54
2:R:1559:LEU:HB3	2:R:1590:ARG:HE	1.71	0.54
1:B:210:LYS:HZ2	1:B:211:SER:H	1.54	0.54
2:S:1559:LEU:HB3	2:S:1590:ARG:HE	1.71	0.54
2:S:873:VAL:HG12	2:S:875:SER:H	1.72	0.54
2:S:1820:LEU:HD11	2:S:1856:ARG:HH22	1.72	0.54
2:S:139:LEU:HD13	2:S:155:LEU:HD13	1.89	0.54
2:R:1410:ARG:HA	2:R:1413:LYS:HE2	1.89	0.54
2:R:1974:TYR:HA	2:R:1979:TRP:HE1	1.72	0.54
2:S:2101:PRO:HD2	2:S:2140:ILE:HG21	1.90	0.54
1:B:230:SER:OG	1:B:246:THR:OG1	2.26	0.54
1:C:227:LEU:HD11	1:C:247:ALA:HB1	1.88	0.54
2:S:1410:ARG:HA	2:S:1413:LYS:HE2	1.89	0.54
3:X:552:LEU:HD22	3:X:574:PHE:HB3	1.90	0.54
2:R:756:LEU:HD22	2:R:786:VAL:HG13	1.90	0.54
2:R:873:VAL:HG12	2:R:875:SER:H	1.72	0.54
2:S:4:ASP:HB3	2:S:40:SER:O	2.08	0.54
2:S:112:HIS:NE2	2:S:114:THR:OG1	2.41	0.53
2:S:501:GLU:HB3	2:S:506:LEU:HD23	1.90	0.53
3:W:552:LEU:HD22	3:W:574:PHE:HB3	1.90	0.53
2:R:112:HIS:NE2	2:R:114:THR:OG1	2.41	0.53
2:R:1820:LEU:HD11	2:R:1856:ARG:HH22	1.72	0.53
3:W:27:LEU:HD13	3:W:70:ILE:HD13	1.91	0.53
1:B:20:PHE:CZ	1:B:134:PRO:HD2	2.44	0.53
1:B:118:ASN:HB3	1:B:121:MET:HG2	1.91	0.53
1:B:236:GLU:HB3	1:B:239:GLN:HB3	1.89	0.53
2:R:501:GLU:HB3	2:R:506:LEU:HD23	1.90	0.53
2:R:811:TRP:CZ3	2:R:840:MET:HG3	2.44	0.53
2:R:1128:LEU:HB3	2:R:1129:PRO:HD3	1.91	0.53
2:S:1974:TYR:HA	2:S:1979:TRP:HE1	1.72	0.53
2:R:893:GLU:HG2	2:R:929:ARG:HH12	1.73	0.53
2:S:811:TRP:CZ3	2:S:840:MET:HG3	2.43	0.53
2:S:1128:LEU:HB3	2:S:1129:PRO:HD3	1.91	0.53
2:S:2092:ILE:HD13	2:S:2127:LEU:HD21	1.91	0.53
3:X:308:LEU:HD11	3:X:330:LEU:HD23	1.91	0.53
2:R:2049:LEU:HD13	2:S:569:LEU:HD21	1.91	0.53
2:S:827:HIS:HB3	2:S:830:VAL:HG23	1.91	0.53
1:C:20:PHE:CZ	1:C:134:PRO:HD2	2.44	0.53
2:R:2101:PRO:HD2	2:R:2140:ILE:HG21	1.90	0.53
3:X:27:LEU:HD13	3:X:70:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:SER:OG	1:C:246:THR:OG1	2.26	0.53
2:S:1152:LEU:HD21	3:X:514:ASN:HB3	1.91	0.53
2:S:1178:LYS:HE2	2:S:1203:VAL:HG13	1.91	0.52
2:S:1487:ALA:HA	2:S:1490:ARG:HE	1.74	0.52
2:R:569:LEU:HD21	2:S:2049:LEU:HD13	1.91	0.52
2:R:2105:LEU:HD23	2:R:2108:LEU:HD12	1.91	0.52
2:S:613:ARG:NH2	2:S:653:PHE:O	2.37	0.52
3:W:15:LEU:HD22	3:W:23:ARG:HH22	1.74	0.52
3:W:669:THR:HA	3:W:760:LEU:HD21	1.91	0.52
2:R:1157:HIS:HB3	2:R:1217:ILE:HD12	1.92	0.52
3:W:249:LEU:HD12	3:W:253:LEU:HB2	1.92	0.52
1:C:118:ASN:HB3	1:C:121:MET:HG2	1.91	0.52
2:S:756:LEU:HD22	2:S:786:VAL:HG13	1.90	0.52
3:X:225:SER:HB3	3:X:310:LEU:HD22	1.91	0.52
2:S:1718:TRP:CE2	2:S:1722:ILE:HD11	2.45	0.52
3:W:59:LEU:HD23	3:W:62:GLN:NE2	2.24	0.52
1:B:378:GLN:HE22	1:B:406:MET:HG2	1.74	0.52
1:B:548:LEU:HD11	1:B:578:PHE:HB3	1.92	0.52
2:R:111:ILE:HG12	2:R:118:THR:HA	1.91	0.52
2:S:893:GLU:HG2	2:S:929:ARG:HH12	1.74	0.52
3:W:225:SER:HB3	3:W:310:LEU:HD22	1.92	0.52
3:X:15:LEU:HD22	3:X:23:ARG:HH22	1.75	0.52
3:X:669:THR:HA	3:X:760:LEU:HD21	1.91	0.52
2:R:1487:ALA:HA	2:R:1490:ARG:HE	1.74	0.52
2:R:2083:PRO:HB2	2:S:491:ASN:OD1	2.09	0.52
2:S:1157:HIS:HB3	2:S:1217:ILE:HD12	1.92	0.52
2:R:1718:TRP:CE2	2:R:1722:ILE:HD11	2.45	0.52
1:C:449:TYR:O	1:C:463:ARG:NH1	2.43	0.52
2:R:4:ASP:HB3	2:R:40:SER:O	2.08	0.52
2:S:851:ILE:HD13	2:S:864:VAL:HG22	1.92	0.52
3:W:59:LEU:HA	3:W:62:GLN:HG2	1.92	0.52
3:W:308:LEU:HD11	3:W:330:LEU:HD23	1.91	0.52
1:B:449:TYR:O	1:B:463:ARG:NH1	2.43	0.52
1:C:168:TYR:OH	1:C:541:LYS:O	2.25	0.52
3:W:328:GLU:HG3	3:W:379:ARG:HG3	1.92	0.52
3:X:59:LEU:HD23	3:X:62:GLN:NE2	2.24	0.52
3:X:249:LEU:HD12	3:X:253:LEU:HB2	1.92	0.52
2:R:462:LEU:HD22	2:R:471:VAL:HG13	1.92	0.51
2:R:839:LEU:HG	2:R:843:LYS:HE3	1.92	0.51
2:R:1684:PRO:HG2	2:R:1718:TRP:CD1	2.45	0.51
1:B:170:VAL:HG22	1:B:583:VAL:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:2105:LEU:HD23	2:S:2108:LEU:HD12	1.91	0.51
2:R:522:LEU:HA	2:R:539:TRP:HH2	1.76	0.51
2:R:827:HIS:HB3	2:R:830:VAL:HG23	1.91	0.51
2:R:1062:SER:OG	2:R:1065:GLU:OE2	2.29	0.51
2:R:2092:ILE:HD13	2:R:2127:LEU:HD21	1.91	0.51
2:S:111:ILE:HG12	2:S:118:THR:HA	1.91	0.51
2:S:462:LEU:HD22	2:S:471:VAL:HG13	1.92	0.51
2:S:839:LEU:HG	2:S:843:LYS:HE3	1.93	0.51
1:B:474:LEU:O	1:B:478:MET:HG3	2.10	0.51
1:C:378:GLN:HE22	1:C:406:MET:HG2	1.74	0.51
2:R:1178:LYS:HE2	2:R:1203:VAL:HG13	1.91	0.51
2:S:801:LEU:HD21	2:S:833:LEU:HA	1.93	0.51
2:S:1062:SER:OG	2:S:1065:GLU:OE2	2.29	0.51
1:C:548:LEU:HD11	1:C:578:PHE:HB3	1.92	0.51
2:R:666:SER:HA	2:S:1918:ARG:HE	1.76	0.51
2:R:851:ILE:HD13	2:R:864:VAL:HG22	1.92	0.51
2:R:1213:ILE:O	2:R:1217:ILE:HG12	2.11	0.51
2:S:155:LEU:HB3	2:S:162:PHE:HB2	1.93	0.51
2:S:490:LEU:HD12	2:S:522:LEU:HD12	1.93	0.51
2:S:1020:ILE:O	2:S:1024:GLU:HG3	2.11	0.51
2:S:1213:ILE:O	2:S:1217:ILE:HG12	2.11	0.51
1:C:152:GLY:HA3	1:C:168:TYR:HB2	1.93	0.50
2:R:314:ILE:HD12	2:R:339:PRO:HD3	1.92	0.50
2:R:1330:LEU:HD13	2:R:1348:TYR:CE1	2.44	0.50
2:R:1459:ASP:OD2	2:R:1506:THR:OG1	2.29	0.50
1:C:547:GLN:HB3	1:C:581:ASN:OD1	2.11	0.50
3:X:59:LEU:HA	3:X:62:GLN:HG2	1.93	0.50
1:B:165:ILE:HG22	1:B:588:VAL:HB	1.93	0.50
1:C:170:VAL:HG22	1:C:583:VAL:HG13	1.92	0.50
2:R:1020:ILE:O	2:R:1024:GLU:HG3	2.11	0.50
2:S:314:ILE:HD12	2:S:339:PRO:HD3	1.92	0.50
2:S:2019:GLN:OE1	2:S:2023:GLN:NE2	2.44	0.50
2:S:1362:TRP:O	2:S:1365:ILE:HG22	2.12	0.50
1:C:312:PHE:HE1	2:S:852:ARG:HH22	1.57	0.50
2:R:801:LEU:HD21	2:R:833:LEU:HA	1.93	0.50
2:R:2019:GLN:OE1	2:R:2023:GLN:NE2	2.44	0.50
2:S:745:MET:HG3	2:S:750:LEU:HB2	1.92	0.50
1:B:3:GLU:O	1:B:7:CYS:HB2	2.12	0.50
1:C:378:GLN:OE1	3:X:54:GLN:NE2	2.44	0.50
1:B:135:PRO:HG3	1:B:154:GLU:HG3	1.94	0.50
1:C:3:GLU:O	1:C:7:CYS:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:522:LEU:HA	2:S:539:TRP:HH2	1.75	0.50
2:S:1811:ASN:HD21	2:S:1814:LYS:HE3	1.77	0.50
2:R:745:MET:HG3	2:R:750:LEU:HB2	1.92	0.50
2:S:1946:MET:SD	2:S:1947:ILE:HG13	2.52	0.50
3:X:128:GLU:HG3	3:X:130:LYS:HD3	1.94	0.49
1:C:474:LEU:O	1:C:478:MET:HG3	2.11	0.49
1:C:582:MET:HG2	1:C:584:THR:HG23	1.94	0.49
2:R:861:ILE:HG23	2:R:883:VAL:HG12	1.94	0.49
3:X:328:GLU:HG3	3:X:379:ARG:HG3	1.92	0.49
1:B:547:GLN:HB3	1:B:581:ASN:OD1	2.11	0.49
1:C:135:PRO:HG3	1:C:154:GLU:HG3	1.94	0.49
2:R:1811:ASN:HD21	2:R:1814:LYS:HE3	1.77	0.49
1:C:165:ILE:HG22	1:C:588:VAL:HB	1.93	0.49
2:R:155:LEU:HB3	2:R:162:PHE:HB2	1.93	0.49
2:S:1684:PRO:HG2	2:S:1718:TRP:CD1	2.45	0.49
2:S:1459:ASP:OD2	2:S:1506:THR:OG1	2.29	0.49
3:X:609:ASN:OD1	3:X:667:LYS:NZ	2.39	0.49
1:B:378:GLN:NE2	1:B:406:MET:HG2	2.28	0.49
2:R:490:LEU:HD12	2:R:522:LEU:HD12	1.93	0.49
2:R:614:ARG:O	2:R:669:HIS:ND1	2.40	0.49
2:S:69:LEU:HB3	2:S:79:LEU:HB3	1.95	0.49
3:W:680:ASP:OD1	3:W:731:GLN:NE2	2.46	0.49
2:R:1362:TRP:O	2:R:1365:ILE:HG22	2.12	0.49
2:R:1491:HIS:HA	2:R:1494:LEU:HD12	1.94	0.49
2:S:387:VAL:HG11	2:S:389:ARG:HE	1.77	0.49
2:S:1330:LEU:HD13	2:S:1348:TYR:CE1	2.44	0.49
2:R:882:LYS:HA	2:R:885:GLN:HB2	1.95	0.49
3:X:50:LEU:HB3	3:X:51:PRO:HD3	1.94	0.49
1:B:152:GLY:HA3	1:B:168:TYR:HB2	1.93	0.49
1:C:49:ASN:ND2	1:C:58:ASN:O	2.46	0.49
2:S:1491:HIS:HA	2:S:1494:LEU:HD12	1.94	0.49
3:X:433:VAL:HG22	3:X:491:TYR:CD1	2.48	0.49
2:R:1152:LEU:HD21	3:W:514:ASN:HB3	1.95	0.49
3:W:433:VAL:HG22	3:W:491:TYR:CD1	2.48	0.49
1:B:42:LEU:HB2	1:B:62:PHE:CE1	2.48	0.48
1:C:520:LYS:HA	1:C:523:TYR:CE1	2.48	0.48
2:R:330:MET:SD	2:R:348:GLU:HB3	2.53	0.48
2:R:1056:ALA:HA	2:R:1059:LEU:HB2	1.95	0.48
2:R:2096:LEU:HD12	2:R:2131:ASN:HD22	1.78	0.48
1:C:378:GLN:NE2	1:C:406:MET:HG2	2.28	0.48
2:S:861:ILE:HG23	2:S:883:VAL:HG12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:50:LEU:HB3	3:W:51:PRO:HD3	1.94	0.48
3:W:394:ASN:HB3	3:W:398:HIS:CD2	2.48	0.48
2:R:318:LYS:HB2	2:R:402:ARG:HH21	1.79	0.48
2:R:1946:MET:SD	2:R:1947:ILE:HG13	2.52	0.48
2:S:984:LEU:HD11	2:S:988:LYS:HE3	1.95	0.48
3:W:186:VAL:HB	3:W:207:HIS:HB2	1.95	0.48
3:X:394:ASN:HB3	3:X:398:HIS:CD2	2.49	0.48
3:X:680:ASP:OD1	3:X:731:GLN:NE2	2.46	0.48
2:R:2116:GLN:HB3	2:S:569:LEU:HD13	1.95	0.48
2:S:1897:ALA:HB1	2:S:1901:THR:HB	1.96	0.48
2:S:2096:LEU:HD12	2:S:2131:ASN:HD22	1.78	0.48
1:B:205:GLN:HB3	1:B:530:LYS:HG2	1.96	0.48
1:C:42:LEU:HB2	1:C:62:PHE:CE1	2.48	0.48
2:R:387:VAL:HG11	2:R:389:ARG:HE	1.77	0.48
2:R:393:GLU:HB2	2:R:399:ARG:HG2	1.95	0.48
2:R:1525:TYR:CZ	2:R:1587:ALA:HA	2.49	0.48
2:R:1897:ALA:HB1	2:R:1901:THR:HB	1.96	0.48
3:X:186:VAL:HB	3:X:207:HIS:HB2	1.95	0.48
1:B:520:LYS:HA	1:B:523:TYR:CE1	2.48	0.48
2:R:1433:ILE:HD11	2:R:1456:LEU:HD13	1.95	0.48
3:X:188:LYS:HB2	3:X:205:GLU:HB2	1.94	0.48
1:C:399:HIS:O	1:C:403:HIS:ND1	2.43	0.48
2:R:984:LEU:HD11	2:R:988:LYS:HE3	1.95	0.48
2:R:1259:LEU:O	2:R:1263:GLN:HG3	2.14	0.48
2:R:2064:ARG:HA	2:R:2067:ILE:HD12	1.95	0.48
2:S:1259:LEU:O	2:S:1263:GLN:HG3	2.14	0.48
2:S:2064:ARG:HA	2:S:2067:ILE:HD12	1.95	0.48
3:X:168:ILE:O	3:X:171:GLN:HG3	2.14	0.48
2:R:69:LEU:HB3	2:R:79:LEU:HB3	1.95	0.48
2:S:393:GLU:HB2	2:S:399:ARG:HG2	1.95	0.48
3:W:419:ILE:HG21	3:X:478:ARG:HH12	1.78	0.48
1:B:49:ASN:ND2	1:B:58:ASN:O	2.46	0.48
2:R:702:TYR:CE1	2:R:744:TYR:HB2	2.49	0.48
2:S:330:MET:SD	2:S:348:GLU:HB3	2.53	0.48
2:S:882:LYS:HA	2:S:885:GLN:HB2	1.95	0.48
2:S:1471:HIS:O	2:S:1475:ALA:N	2.47	0.48
2:S:1525:TYR:CZ	2:S:1587:ALA:HA	2.49	0.48
3:W:128:GLU:HG3	3:W:130:LYS:HD3	1.94	0.48
3:W:188:LYS:HB2	3:W:205:GLU:HB2	1.94	0.48
2:S:69:LEU:HD11	2:S:92:LEU:HD11	1.96	0.47
2:S:714:GLU:OE1	2:S:718:THR:HG21	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1249:LEU:HB3	2:S:1250:PRO:HD3	1.96	0.47
2:R:166:ASN:ND2	2:R:190:GLN:O	2.47	0.47
2:R:1249:LEU:HB3	2:R:1250:PRO:HD3	1.96	0.47
2:R:1522:LEU:O	2:R:1594:HIS:NE2	2.47	0.47
2:S:647:LEU:HD22	2:S:696:ILE:HD12	1.96	0.47
2:S:1241:LEU:O	2:S:1304:THR:HG23	2.13	0.47
2:S:1470:LEU:HD11	2:S:1518:ILE:HD13	1.96	0.47
1:B:378:GLN:OE1	3:W:54:GLN:NE2	2.47	0.47
1:B:582:MET:HG2	1:B:584:THR:HG23	1.94	0.47
2:R:1028:ALA:HA	2:R:1031:LYS:HE2	1.96	0.47
2:R:1241:LEU:O	2:R:1304:THR:HG23	2.13	0.47
2:S:702:TYR:CE1	2:S:744:TYR:HB2	2.49	0.47
3:W:62:GLN:HA	3:W:65:LYS:HG2	1.96	0.47
2:S:318:LYS:HB2	2:S:402:ARG:HH21	1.79	0.47
2:S:1056:ALA:HA	2:S:1059:LEU:HB2	1.95	0.47
3:W:609:ASN:HA	3:W:667:LYS:HD2	1.96	0.47
3:X:427:PRO:HD3	3:X:476:THR:HG22	1.97	0.47
2:R:2160:ILE:HD11	2:R:2179:LEU:HG	1.96	0.47
2:S:166:ASN:ND2	2:S:190:GLN:O	2.47	0.47
2:S:2160:ILE:HD11	2:S:2179:LEU:HG	1.96	0.47
3:W:427:PRO:HD3	3:W:476:THR:HG22	1.97	0.47
1:B:210:LYS:HZ3	1:B:222:GLN:HB3	1.79	0.47
1:B:399:HIS:O	1:B:403:HIS:ND1	2.43	0.47
2:R:1470:LEU:HD11	2:R:1518:ILE:HD13	1.96	0.47
2:S:1522:LEU:O	2:S:1594:HIS:NE2	2.47	0.47
3:X:62:GLN:HA	3:X:65:LYS:HG2	1.96	0.47
1:C:529:GLN:NE2	1:C:551:SER:OG	2.48	0.47
2:R:714:GLU:OE1	2:R:718:THR:HG21	2.14	0.47
2:R:867:TYR:HB2	3:W:47:SER:O	2.13	0.47
2:S:710:ASP:O	2:S:714:GLU:HG2	2.15	0.47
2:S:1028:ALA:HA	2:S:1031:LYS:HE2	1.96	0.47
2:S:2167:LEU:HD12	2:S:2179:LEU:HD22	1.97	0.47
3:W:168:ILE:O	3:W:171:GLN:HG3	2.14	0.47
1:C:205:GLN:HB3	1:C:530:LYS:HG2	1.96	0.47
2:R:710:ASP:O	2:R:714:GLU:HG2	2.15	0.47
2:R:2167:LEU:HD12	2:R:2179:LEU:HD22	1.97	0.47
3:W:190:PRO:HB3	3:W:203:GLN:HB2	1.97	0.47
2:R:1621:LEU:HG	2:R:1625:LYS:HE3	1.96	0.46
2:R:2109:GLU:HA	2:R:2113:ASN:HD22	1.80	0.46
2:S:294:VAL:HG11	2:S:297:PHE:HB3	1.97	0.46
2:S:1433:ILE:HD11	2:S:1456:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:2108:LEU:HA	2:R:2112:MET:HB2	1.97	0.46
2:S:86:GLU:HB2	2:S:104:ARG:HE	1.80	0.46
2:S:408:ARG:HE	2:S:411:GLU:HG3	1.81	0.46
3:W:620:SER:O	3:W:624:LYS:HG2	2.15	0.46
3:X:609:ASN:HA	3:X:667:LYS:HD2	1.96	0.46
1:B:529:GLN:NE2	1:B:551:SER:OG	2.48	0.46
2:R:169:LEU:HD23	2:R:172:ILE:HD12	1.97	0.46
2:S:1023:HIS:CG	2:S:1052:LEU:HD22	2.51	0.46
2:S:1519:LEU:HB2	2:S:1533:VAL:HG11	1.97	0.46
1:C:110:ILE:HG13	1:C:151:LEU:HB3	1.98	0.46
2:R:2011:VAL:HG12	2:R:2013:TYR:H	1.81	0.46
2:S:169:LEU:HD23	2:S:172:ILE:HD12	1.97	0.46
2:S:699:HIS:ND1	2:S:705:LYS:HG2	2.30	0.46
2:R:475:CYS:O	2:R:489:MET:HE1	2.15	0.46
2:R:647:LEU:HD22	2:R:696:ILE:HD12	1.96	0.46
2:S:1210:LEU:HA	2:S:1213:ILE:HG22	1.98	0.46
2:S:1515:LEU:HG	2:S:1533:VAL:HG13	1.97	0.46
2:S:2152:MET:O	2:S:2155:MET:HB2	2.16	0.46
3:W:41:MET:HA	3:W:44:LYS:HB2	1.98	0.46
3:X:63:VAL:HG12	3:X:110:LYS:NZ	2.31	0.46
3:X:620:SER:O	3:X:624:LYS:HG2	2.15	0.46
1:B:28:ARG:HH12	1:B:46:GLY:HA3	1.81	0.46
2:R:69:LEU:HD11	2:R:92:LEU:HD11	1.96	0.46
2:R:1210:LEU:HA	2:R:1213:ILE:HG22	1.98	0.46
2:R:1778:GLU:HA	2:R:1848:ARG:HE	1.80	0.46
2:S:1316:LYS:HE2	3:X:569:ASP:OD2	2.16	0.46
2:S:1621:LEU:HG	2:S:1625:LYS:HE3	1.96	0.46
2:S:2011:VAL:HG12	2:S:2013:TYR:H	1.81	0.46
3:W:266:ILE:HD13	3:W:302:VAL:HG21	1.98	0.46
1:B:110:ILE:HG13	1:B:151:LEU:HB3	1.98	0.46
1:C:28:ARG:HH12	1:C:46:GLY:HA3	1.81	0.46
1:C:406:MET:HG3	1:C:407:ASP:O	2.15	0.46
2:R:294:VAL:HG11	2:R:297:PHE:HB3	1.97	0.46
2:R:408:ARG:HE	2:R:411:GLU:HG3	1.81	0.46
2:R:2152:MET:O	2:R:2155:MET:HB2	2.16	0.46
2:S:1352:LEU:HB2	2:S:1357:VAL:HG22	1.98	0.46
3:W:609:ASN:OD1	3:W:667:LYS:NZ	2.39	0.46
2:R:2180:ILE:HG21	2:R:2204:PHE:HB2	1.97	0.46
2:S:2108:LEU:HA	2:S:2112:MET:HB2	1.97	0.46
2:S:2109:GLU:HA	2:S:2113:ASN:HD22	1.80	0.46
2:S:2180:ILE:HG21	2:S:2204:PHE:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:308:LEU:HD22	3:X:326:LEU:HB3	1.98	0.46
2:R:699:HIS:ND1	2:R:705:LYS:HG2	2.30	0.46
2:R:1047:SER:H	3:X:681:ARG:HH22	1.63	0.46
3:W:63:VAL:HG12	3:W:110:LYS:NZ	2.31	0.46
1:C:210:LYS:HZ3	1:C:222:GLN:HB3	1.80	0.46
2:R:309:VAL:HG13	2:R:316:ASN:HB3	1.98	0.46
2:R:757:LEU:HD21	2:R:802:LYS:HZ1	1.81	0.46
2:R:1519:LEU:HB2	2:R:1533:VAL:HG11	1.97	0.46
2:R:153:MET:CE	2:R:155:LEU:HB2	2.47	0.45
2:S:262:ILE:HG13	2:S:317:LEU:HD11	1.98	0.45
2:S:1137:SER:O	2:S:1141:THR:HG23	2.16	0.45
3:W:56:ALA:HA	3:W:59:LEU:HD12	1.98	0.45
3:X:56:ALA:HA	3:X:59:LEU:HD12	1.98	0.45
3:X:266:ILE:HD13	3:X:302:VAL:HG21	1.98	0.45
3:X:437:PRO:HB2	3:X:562:ARG:HG2	1.98	0.45
1:B:406:MET:HG3	1:B:407:ASP:O	2.15	0.45
2:R:86:GLU:HB2	2:R:104:ARG:HE	1.80	0.45
2:S:1778:GLU:HA	2:S:1848:ARG:HE	1.80	0.45
3:X:557:HIS:CE1	3:X:560:ARG:HE	2.34	0.45
2:R:1515:LEU:HG	2:R:1533:VAL:HG13	1.97	0.45
2:S:895:TYR:CZ	2:S:918:LEU:HD21	2.51	0.45
3:W:437:PRO:HB2	3:W:562:ARG:HG2	1.98	0.45
3:W:641:GLN:HE21	3:W:701:SER:HA	1.82	0.45
3:X:41:MET:HA	3:X:44:LYS:HB2	1.98	0.45
2:R:1137:SER:O	2:R:1141:THR:HG23	2.16	0.45
2:R:1919:CYS:O	2:R:1923:LEU:HG	2.17	0.45
2:S:1605:TRP:CH2	2:S:1634:LEU:HB2	2.52	0.45
3:X:190:PRO:HB3	3:X:203:GLN:HB2	1.97	0.45
1:B:168:TYR:OH	1:B:541:LYS:O	2.25	0.45
2:R:262:ILE:HG13	2:R:317:LEU:HD11	1.98	0.45
2:R:895:TYR:CZ	2:R:918:LEU:HD21	2.51	0.45
2:R:2129:LEU:HD22	2:R:2150:LEU:HD13	1.97	0.45
2:S:1919:CYS:O	2:S:1923:LEU:HG	2.17	0.45
2:R:10:ASN:OD1	2:R:75:ARG:NH2	2.50	0.45
2:R:1463:GLN:HB2	2:R:1511:LEU:HD13	1.99	0.45
2:S:153:MET:CE	2:S:155:LEU:HB2	2.47	0.45
2:S:475:CYS:O	2:S:489:MET:HE1	2.16	0.45
2:R:1605:TRP:CH2	2:R:1634:LEU:HB2	2.52	0.45
2:R:1815:VAL:O	2:R:1819:LEU:HG	2.17	0.45
2:S:10:ASN:OD1	2:S:75:ARG:NH2	2.50	0.45
2:S:51:GLN:HB3	2:S:62:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:726:LEU:O	3:X:730:LEU:HG	2.16	0.45
2:S:643:PRO:HG2	2:S:696:ILE:HG13	1.99	0.45
3:W:726:LEU:O	3:W:730:LEU:HG	2.16	0.45
2:R:521:LYS:NZ	2:R:543:LEU:O	2.50	0.45
2:R:1023:HIS:CG	2:R:1052:LEU:HD22	2.51	0.45
2:S:1291:MET:SD	3:X:502:ASP:HB2	2.57	0.45
2:R:643:PRO:HG2	2:R:696:ILE:HG13	1.99	0.45
2:R:1508:THR:OG1	2:R:1542:GLU:OE2	2.28	0.45
2:S:638:ASP:OD2	2:S:645:ASN:ND2	2.50	0.45
3:W:269:GLN:HB2	3:W:272:ILE:O	2.17	0.45
3:W:436:LEU:HB3	3:W:562:ARG:NH1	2.29	0.45
3:X:206:LEU:HB3	3:X:275:ILE:HB	1.99	0.45
2:R:1352:LEU:HB2	2:R:1357:VAL:HG22	1.98	0.44
3:W:308:LEU:HD22	3:W:326:LEU:HB3	1.98	0.44
2:R:51:GLN:HB3	2:R:62:VAL:HB	1.98	0.44
2:R:403:LEU:HD23	2:R:408:ARG:HD3	1.98	0.44
3:X:269:GLN:HB2	3:X:272:ILE:O	2.17	0.44
3:X:641:GLN:HE21	3:X:701:SER:HA	1.82	0.44
2:R:230:PHE:HB2	2:R:248:ILE:HB	1.99	0.44
2:S:403:LEU:HD23	2:S:408:ARG:HD3	1.98	0.44
1:B:150:TRP:HB2	1:B:170:VAL:HB	1.99	0.44
2:S:59:PHE:HE1	2:S:356:VAL:HG11	1.82	0.44
2:S:309:VAL:HG13	2:S:316:ASN:HB3	1.98	0.44
3:W:158:ILE:O	3:W:162:LEU:HG	2.17	0.44
1:B:182:LEU:HD13	1:B:237:ILE:HD11	2.00	0.44
2:R:124:PHE:HB3	2:R:162:PHE:CE2	2.53	0.44
2:R:1156:LYS:O	2:R:1160:MET:HG3	2.18	0.44
2:S:90:VAL:C	2:S:139:LEU:HD23	2.38	0.44
3:X:158:ILE:O	3:X:162:LEU:HG	2.17	0.44
2:R:1160:MET:HB3	2:R:1274:PHE:CE1	2.53	0.44
2:R:1580:VAL:O	2:R:1581:ILE:HG13	2.18	0.44
2:S:1472:ASN:O	2:S:1476:GLY:N	2.50	0.44
2:S:1815:VAL:O	2:S:1819:LEU:HG	2.17	0.44
2:S:2129:LEU:HD22	2:S:2150:LEU:HD13	1.97	0.44
3:X:508:LEU:O	3:X:512:VAL:HG23	2.18	0.44
2:R:1472:ASN:O	2:R:1476:GLY:N	2.50	0.44
2:S:1519:LEU:HD12	2:S:1522:LEU:HD12	2.00	0.44
1:B:367:VAL:HA	1:B:411:LEU:HD13	2.00	0.44
2:R:2:TRP:HH2	2:R:383:VAL:HG12	1.83	0.44
2:R:338:LEU:HA	2:R:339:PRO:HA	1.80	0.44
2:S:2:TRP:HH2	2:S:383:VAL:HG12	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:124:PHE:HB3	2:S:162:PHE:CE2	2.53	0.44
3:W:508:LEU:O	3:W:512:VAL:HG23	2.18	0.44
1:C:367:VAL:HA	1:C:411:LEU:HD13	2.00	0.44
2:R:942:PRO:HA	2:R:952:ARG:HH21	1.83	0.44
2:S:1580:VAL:O	2:S:1581:ILE:HG13	2.18	0.44
1:C:228:ASP:OD2	1:C:250:ASN:ND2	2.51	0.43
2:R:634:LEU:HD12	2:R:646:GLY:HA2	2.00	0.43
2:R:638:ASP:OD2	2:R:645:ASN:ND2	2.50	0.43
2:R:1291:MET:HG2	3:W:503:GLN:HB2	1.99	0.43
3:X:34:ILE:HG22	3:X:109:LEU:HD13	2.00	0.43
1:B:20:PHE:CE2	1:B:62:PHE:HE2	2.36	0.43
1:C:150:TRP:HB2	1:C:170:VAL:HB	2.00	0.43
1:C:306:LEU:HD22	2:S:772:THR:HG21	1.99	0.43
2:R:90:VAL:C	2:R:139:LEU:HD23	2.38	0.43
2:R:2147:PHE:HZ	2:R:2167:LEU:HD21	1.84	0.43
1:B:228:ASP:OD2	1:B:250:ASN:ND2	2.51	0.43
2:R:702:TYR:HD1	2:R:740:PHE:HB3	1.83	0.43
2:S:634:LEU:HD12	2:S:646:GLY:HA2	1.99	0.43
2:S:1094:HIS:O	2:S:1099:THR:OG1	2.36	0.43
2:S:1463:GLN:HB2	2:S:1511:LEU:HD13	1.99	0.43
1:B:393:LEU:O	1:B:397:LEU:HG	2.18	0.43
1:C:393:LEU:O	1:C:397:LEU:HG	2.18	0.43
2:S:521:LYS:NZ	2:S:543:LEU:O	2.50	0.43
3:W:34:ILE:HG22	3:W:109:LEU:HD13	2.00	0.43
3:W:206:LEU:HB3	3:W:275:ILE:HB	1.99	0.43
3:X:664:VAL:O	3:X:668:ILE:HG12	2.19	0.43
1:C:456:ASP:OD1	1:C:456:ASP:N	2.52	0.43
2:S:297:PHE:HB2	2:S:319:LEU:HD11	2.00	0.43
2:S:579:PHE:HZ	2:S:612:VAL:HG22	1.83	0.43
2:S:702:TYR:HD1	2:S:740:PHE:HB3	1.83	0.43
2:S:1139:ALA:O	2:S:1143:CYS:HB3	2.19	0.43
2:S:1156:LYS:O	2:S:1160:MET:HG3	2.18	0.43
2:S:1522:LEU:HD13	2:S:1529:MET:HB3	2.01	0.43
3:W:657:LEU:O	3:W:661:ILE:HG12	2.18	0.43
2:R:1139:ALA:O	2:R:1143:CYS:HB3	2.19	0.43
2:S:1291:MET:HG2	3:X:503:GLN:HB2	2.01	0.43
3:W:434:PRO:HB2	3:W:495:LEU:HD22	2.01	0.43
3:W:734:LEU:HD21	3:W:771:ARG:HA	2.01	0.43
1:B:298:LEU:HB3	1:B:355:LYS:HD3	2.01	0.43
1:C:20:PHE:CE2	1:C:62:PHE:HE2	2.36	0.43
2:R:59:PHE:HE1	2:R:356:VAL:HG11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:1314:GLU:OE2	2:R:1318:LYS:HE3	2.18	0.43
2:R:1471:HIS:O	2:R:1475:ALA:N	2.47	0.43
2:S:451:TRP:O	2:S:455:VAL:HG23	2.19	0.43
2:S:867:TYR:HB2	3:X:47:SER:O	2.18	0.43
3:X:753:SER:O	3:X:757:VAL:HG23	2.19	0.43
1:C:298:LEU:HB3	1:C:355:LYS:HD3	2.01	0.43
2:R:297:PHE:HB2	2:R:319:LEU:HD11	2.00	0.43
2:R:1094:HIS:O	2:R:1099:THR:OG1	2.36	0.43
2:R:1388:LEU:HG	3:W:557:HIS:CE1	2.54	0.43
2:R:1416:ILE:HG12	2:R:1436:LEU:HD23	2.01	0.43
2:R:1519:LEU:HD12	2:R:1522:LEU:HD12	2.00	0.43
2:S:614:ARG:O	2:S:669:HIS:ND1	2.40	0.43
2:S:1160:MET:HB3	2:S:1274:PHE:CE1	2.53	0.43
2:S:2060:ILE:HG13	2:S:2082:MET:CE	2.48	0.43
2:R:579:PHE:HZ	2:R:612:VAL:HG22	1.83	0.43
3:X:20:LEU:O	3:X:24:ILE:HG12	2.19	0.43
3:X:122:TYR:CZ	3:X:126:LEU:HD11	2.54	0.43
3:X:657:LEU:O	3:X:661:ILE:HG12	2.19	0.43
1:B:350:GLU:HG2	1:B:427:LYS:HB2	2.01	0.42
1:C:11:ASP:O	1:C:15:ARG:HG2	2.19	0.42
2:R:299:LEU:HD13	2:R:317:LEU:HD13	2.01	0.42
2:R:1522:LEU:HD13	2:R:1529:MET:HB3	2.01	0.42
2:R:1535:LYS:O	2:R:1539:ARG:HD3	2.19	0.42
2:S:1314:GLU:OE2	2:S:1318:LYS:HE3	2.18	0.42
1:C:478:MET:O	1:C:482:LYS:HB2	2.19	0.42
2:R:52:ALA:HB3	2:R:356:VAL:HG22	2.02	0.42
2:R:408:ARG:HG2	2:R:411:GLU:HB2	2.01	0.42
2:S:299:LEU:HD13	2:S:317:LEU:HD13	2.01	0.42
2:S:317:LEU:HB2	2:S:338:LEU:HD12	2.02	0.42
2:S:400:LEU:HA	2:S:403:LEU:HD12	2.02	0.42
3:W:20:LEU:O	3:W:24:ILE:HG12	2.19	0.42
1:B:40:VAL:HG12	1:B:62:PHE:CD1	2.55	0.42
1:B:456:ASP:OD1	1:B:456:ASP:N	2.51	0.42
1:C:262:LEU:HD22	1:C:265:LEU:HD22	2.01	0.42
1:C:415:ILE:HB	1:C:416:PRO:HD3	2.01	0.42
2:R:1525:TYR:HB3	2:R:1586:ALA:HB3	2.01	0.42
2:S:1643:PHE:HD1	2:S:1647:LEU:HD23	1.84	0.42
1:B:478:MET:O	1:B:482:LYS:HB2	2.19	0.42
1:C:19:LYS:HG2	1:C:62:PHE:HE1	1.84	0.42
2:R:1863:ARG:O	2:R:1867:VAL:HG23	2.20	0.42
2:S:52:ALA:HB3	2:S:356:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:230:PHE:HB2	2:S:248:ILE:HB	1.99	0.42
2:S:881:LEU:HD23	2:S:894:ILE:HD13	2.01	0.42
2:S:1491:HIS:CD2	2:S:1528:GLU:HG3	2.55	0.42
3:X:576:ASP:OD1	3:X:576:ASP:N	2.52	0.42
1:B:262:LEU:HD22	1:B:265:LEU:HD22	2.01	0.42
1:C:182:LEU:HD13	1:C:237:ILE:HD11	2.00	0.42
2:R:451:TRP:O	2:R:455:VAL:HG23	2.19	0.42
2:R:517:ARG:HH22	2:R:546:GLU:HG2	1.84	0.42
2:R:1491:HIS:CD2	2:R:1528:GLU:HG3	2.55	0.42
2:R:2076:LEU:HD22	2:R:2096:LEU:HD21	2.02	0.42
2:S:1863:ARG:O	2:S:1867:VAL:HG23	2.20	0.42
2:S:2147:PHE:HZ	2:S:2167:LEU:HD21	1.84	0.42
1:B:415:ILE:HB	1:B:416:PRO:HD3	2.00	0.42
2:R:645:ASN:HA	2:R:648:GLN:HG2	2.02	0.42
2:R:878:GLU:HA	2:R:881:LEU:HD12	2.02	0.42
2:R:2060:ILE:HG13	2:R:2082:MET:CE	2.48	0.42
2:S:517:ARG:HH22	2:S:546:GLU:HG2	1.84	0.42
2:S:597:LEU:HD23	2:S:597:LEU:H	1.84	0.42
2:S:847:ARG:HG2	2:S:852:ARG:HA	2.02	0.42
2:S:2076:LEU:HD22	2:S:2096:LEU:HD21	2.02	0.42
3:W:664:VAL:O	3:W:668:ILE:HG12	2.19	0.42
1:B:19:LYS:HG2	1:B:62:PHE:HE1	1.85	0.42
1:B:111:GLY:O	1:B:115:MET:HG2	2.20	0.42
1:C:40:VAL:HG12	1:C:62:PHE:CD1	2.55	0.42
2:R:53:CYS:SG	2:R:60:ILE:HB	2.60	0.42
2:R:400:LEU:HA	2:R:403:LEU:HD12	2.02	0.42
2:R:1643:PHE:HD1	2:R:1647:LEU:HD23	1.84	0.42
2:S:31:TYR:CE2	2:S:345:TYR:HB2	2.55	0.42
1:C:113:TYR:HB2	1:C:136:LEU:HD22	2.02	0.42
2:R:31:TYR:CE2	2:R:345:TYR:HB2	2.55	0.42
2:R:695:LEU:HG	2:R:699:HIS:CD2	2.55	0.42
2:S:761:GLU:OE2	2:S:802:LYS:NZ	2.52	0.42
2:S:1535:LYS:O	2:S:1539:ARG:HD3	2.20	0.42
2:S:1623:ILE:O	2:S:1627:MET:HG2	2.20	0.42
3:W:122:TYR:CZ	3:W:126:LEU:HD11	2.54	0.42
1:C:350:GLU:HG2	1:C:427:LYS:HB2	2.01	0.42
2:R:1974:TYR:HA	2:R:1979:TRP:NE1	2.35	0.42
3:X:436:LEU:HB3	3:X:562:ARG:NH1	2.29	0.42
1:B:461:VAL:O	1:B:465:GLN:HG3	2.20	0.42
1:B:554:ILE:HG22	1:B:556:HIS:H	1.85	0.42
2:R:847:ARG:HG2	2:R:852:ARG:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:2108:LEU:HD23	2:R:2112:MET:HG3	2.01	0.42
2:S:942:PRO:HA	2:S:952:ARG:HH21	1.83	0.42
3:W:721:MET:HB2	3:W:722:PRO:HD3	2.02	0.42
3:W:753:SER:O	3:W:757:VAL:HG23	2.19	0.42
1:C:111:GLY:O	1:C:115:MET:HG2	2.20	0.41
2:R:315:THR:HG22	2:R:315:THR:O	2.20	0.41
2:R:1623:ILE:O	2:R:1627:MET:HG2	2.20	0.41
2:S:408:ARG:HG2	2:S:411:GLU:HB2	2.01	0.41
2:S:1748:THR:HG23	2:S:1804:ILE:HG12	2.02	0.41
1:B:113:TYR:HB2	1:B:136:LEU:HD22	2.02	0.41
2:R:597:LEU:HD23	2:R:597:LEU:H	1.84	0.41
2:S:1416:ILE:HG12	2:S:1436:LEU:HD23	2.01	0.41
3:X:734:LEU:HD21	3:X:771:ARG:HA	2.01	0.41
1:C:461:VAL:O	1:C:465:GLN:HG3	2.20	0.41
1:C:491:LEU:HB2	1:C:512:LEU:HD22	2.02	0.41
2:R:845:LEU:HD21	2:R:879:ASP:HB3	2.03	0.41
2:S:1508:THR:OG1	2:S:1542:GLU:OE2	2.28	0.41
2:R:881:LEU:HD23	2:R:894:ILE:HD13	2.01	0.41
2:R:1316:LYS:NZ	3:W:566:ILE:HA	2.36	0.41
2:S:53:CYS:SG	2:S:60:ILE:HB	2.60	0.41
2:S:645:ASN:HA	2:S:648:GLN:HG2	2.02	0.41
2:S:1399:ARG:HG2	3:X:465:ASN:HB3	2.03	0.41
3:X:434:PRO:HB2	3:X:495:LEU:HD22	2.01	0.41
2:R:100:LEU:HD12	2:R:141:ILE:HD11	2.02	0.41
2:R:317:LEU:HB2	2:R:338:LEU:HD12	2.02	0.41
2:R:1647:LEU:HD11	2:R:1667:ILE:HG23	2.03	0.41
2:S:757:LEU:HD21	2:S:802:LYS:HZ1	1.85	0.41
2:S:1747:GLY:HA3	2:S:1807:VAL:HG11	2.02	0.41
3:W:567:LEU:HB3	3:W:572:ALA:HB2	2.03	0.41
3:W:576:ASP:OD1	3:W:576:ASP:N	2.52	0.41
2:R:157:THR:HG22	2:R:158:TYR:H	1.85	0.41
2:S:845:LEU:HD21	2:S:879:ASP:HB3	2.03	0.41
3:X:567:LEU:HB3	3:X:572:ALA:HB2	2.03	0.41
2:R:667:SER:O	2:R:670:TRP:HD1	2.04	0.41
2:R:2059:LEU:HD12	2:R:2082:MET:HG2	2.02	0.41
2:S:1525:TYR:HB3	2:S:1586:ALA:HB3	2.01	0.41
2:S:2059:LEU:HD12	2:S:2082:MET:HG2	2.02	0.41
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.97	0.41
1:B:347:ASP:HB3	1:B:387:HIS:CD2	2.55	0.41
1:B:425:LEU:HD21	1:B:461:VAL:HG22	2.02	0.41
1:C:347:ASP:HB3	1:C:387:HIS:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:800:VAL:HG21	2:R:822:HIS:NE2	2.36	0.41
1:B:491:LEU:HB2	1:B:512:LEU:HD22	2.02	0.41
2:R:400:LEU:HA	2:R:403:LEU:HB2	2.03	0.41
2:S:235:PRO:HA	2:S:242:MET:HG3	2.02	0.41
2:S:601:CYS:HB2	2:S:602:PRO:HD3	2.03	0.41
2:S:695:LEU:HG	2:S:699:HIS:CD2	2.54	0.41
2:S:800:VAL:HG21	2:S:822:HIS:NE2	2.36	0.41
2:S:974:LEU:HD12	3:X:189:PHE:HB3	2.03	0.41
2:S:1368:ALA:O	2:S:1369:TRP:CG	2.74	0.41
1:C:554:ILE:HG22	1:C:556:HIS:H	1.85	0.41
2:R:822:HIS:HA	2:R:825:MET:SD	2.61	0.41
2:R:1790:SER:HA	2:S:686:ARG:HD3	2.02	0.41
2:R:2146:TYR:O	2:R:2150:LEU:N	2.40	0.41
2:S:157:THR:HG22	2:S:158:TYR:H	1.85	0.41
2:S:404:LEU:HD21	2:S:426:VAL:HG22	2.03	0.41
2:S:1242:ASN:H	2:S:1245:ASP:HB2	1.86	0.41
2:S:1740:HIS:HB3	2:S:1744:ARG:NH1	2.36	0.41
2:R:235:PRO:HA	2:R:242:MET:HG3	2.02	0.40
2:R:485:THR:O	2:R:489:MET:HG3	2.21	0.40
2:R:800:VAL:O	2:R:804:MET:HG2	2.21	0.40
2:S:1019:HIS:ND1	2:S:1055:GLN:OE1	2.55	0.40
3:W:9:LEU:O	3:W:13:GLY:N	2.54	0.40
3:X:721:MET:HB2	3:X:722:PRO:HD3	2.02	0.40
1:B:43:ILE:HD12	1:B:63:ILE:HG13	2.03	0.40
2:R:141:ILE:HG12	2:R:153:MET:HG2	2.03	0.40
2:R:835:GLU:HG2	2:R:838:LYS:NZ	2.37	0.40
2:S:315:THR:HG22	2:S:315:THR:O	2.20	0.40
2:S:800:VAL:O	2:S:804:MET:HG2	2.21	0.40
2:S:1164:LEU:HG	2:S:1274:PHE:CZ	2.57	0.40
2:S:1974:TYR:HA	2:S:1979:TRP:NE1	2.35	0.40
3:W:259:CYS:HB2	3:W:262:LEU:HG	2.04	0.40
1:B:530:LYS:HD3	1:B:547:GLN:NE2	2.37	0.40
2:R:1019:HIS:ND1	2:R:1055:GLN:OE1	2.54	0.40
2:R:1368:ALA:O	2:R:1369:TRP:CG	2.74	0.40
2:R:1747:GLY:HA3	2:R:1807:VAL:HG11	2.02	0.40
2:R:1748:THR:HG23	2:R:1804:ILE:HG12	2.02	0.40
3:W:112:LEU:HD11	3:W:154:PHE:CE1	2.57	0.40
3:X:624:LYS:HD3	3:X:627:ARG:HH21	1.87	0.40
2:S:100:LEU:HD12	2:S:141:ILE:HD11	2.02	0.40
2:S:822:HIS:HA	2:S:825:MET:SD	2.61	0.40
2:S:1518:ILE:O	2:S:1522:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:2108:LEU:HD23	2:S:2112:MET:HG3	2.02	0.40
3:X:112:LEU:HD11	3:X:154:PHE:CE1	2.57	0.40
1:C:332:VAL:O	1:C:336:VAL:HG23	2.21	0.40
2:R:71:ASP:N	2:R:71:ASP:OD1	2.52	0.40
2:R:1164:LEU:HG	2:R:1274:PHE:CZ	2.56	0.40
2:R:1643:PHE:CD1	2:R:1647:LEU:HD23	2.57	0.40
2:S:524:THR:HA	2:S:566:TYR:HE2	1.86	0.40
2:S:878:GLU:HA	2:S:881:LEU:HD12	2.02	0.40
2:S:1205:GLU:OE1	2:S:1207:GLN:NE2	2.54	0.40
2:S:1647:LEU:HD11	2:S:1667:ILE:HG23	2.03	0.40
3:W:419:ILE:HG21	3:X:478:ARG:NH1	2.36	0.40
3:X:205:GLU:OE2	3:X:276:ARG:NH1	2.55	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	B	589/591 (100%)	573 (97%)	16 (3%)	0	100	100
1	C	589/591 (100%)	573 (97%)	16 (3%)	0	100	100
2	R	2206/2464 (90%)	2136 (97%)	70 (3%)	0	100	100
2	S	2206/2464 (90%)	2137 (97%)	69 (3%)	0	100	100
3	W	777/779 (100%)	766 (99%)	11 (1%)	0	100	100
3	X	777/779 (100%)	766 (99%)	11 (1%)	0	100	100
All	All	7144/7668 (93%)	6951 (97%)	193 (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	B	542/542 (100%)	542 (100%)	0	100	100
1	C	542/542 (100%)	542 (100%)	0	100	100
2	R	1988/2204 (90%)	1986 (100%)	2 (0%)	93	97
2	S	1988/2204 (90%)	1986 (100%)	2 (0%)	93	97
3	W	710/710 (100%)	709 (100%)	1 (0%)	93	97
3	X	710/710 (100%)	709 (100%)	1 (0%)	93	97
All	All	6480/6912 (94%)	6474 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	560	ASN
2	R	863	ARG
2	S	560	ASN
2	S	863	ARG
3	W	562	ARG
3	X	562	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	547	GLN
1	B	556	HIS
1	C	547	GLN
1	C	556	HIS
2	R	1491	HIS
2	R	2023	GLN
2	S	629	GLN
2	S	1491	HIS
2	S	2023	GLN
3	W	62	GLN
3	W	452	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	X	62	GLN
3	X	452	ASN
3	X	557	HIS

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

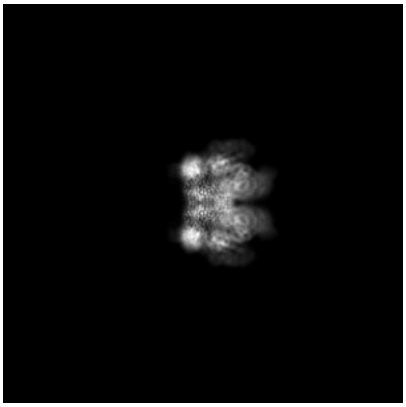
This section contains visualisations of the EMDB entry EMD-14120. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

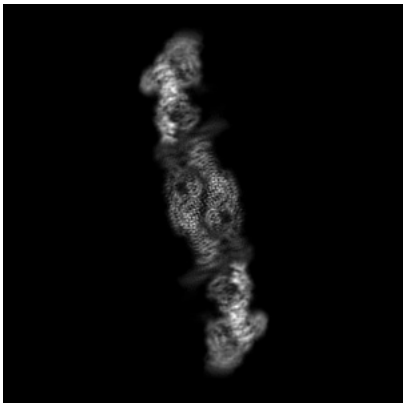
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



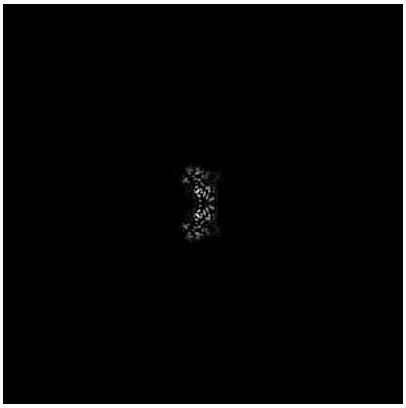
Z

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

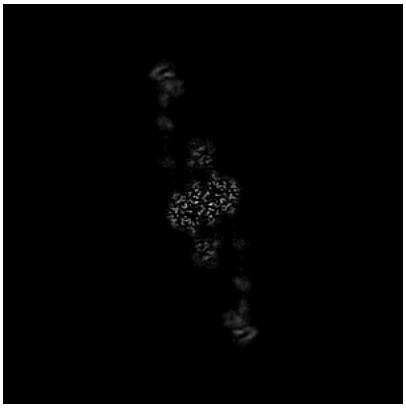
6.2 Central slices

6.2.1 Primary map

X Index: 150



Y Index: 150



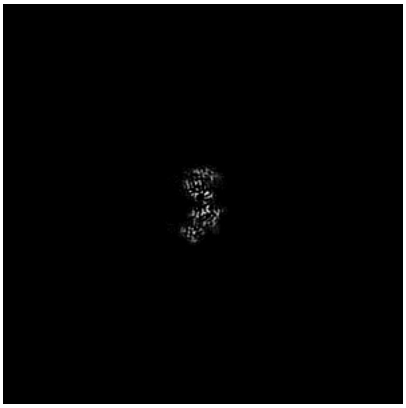
Z Index: 150

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

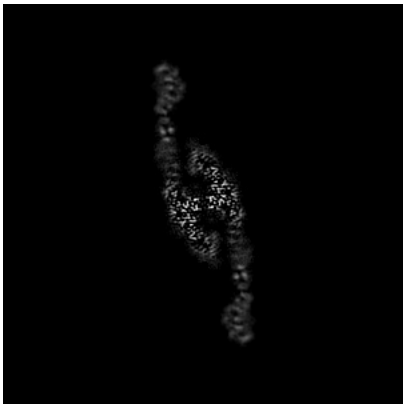
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 159



Y Index: 155



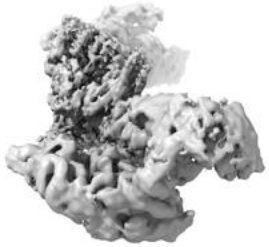
Z Index: 144

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 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

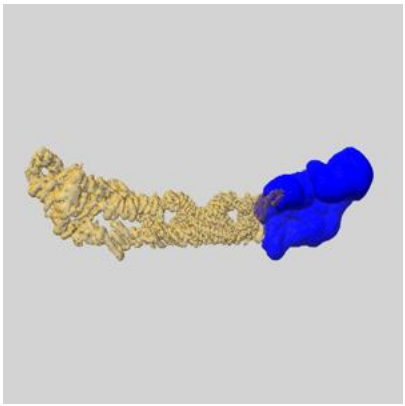
6.5 Mask visualisation (i)

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

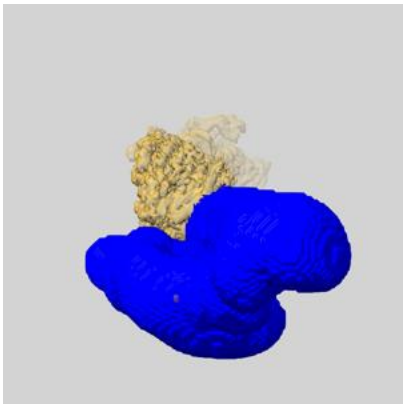
A mask typically either:

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

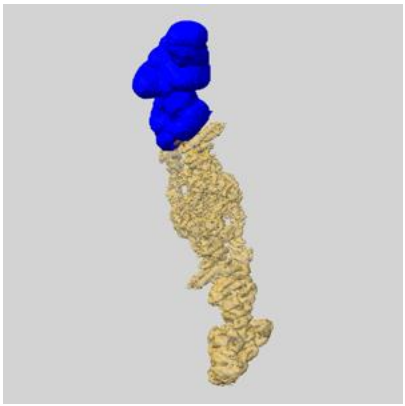
6.5.1 emd_14120_msk_1.map (i)



X

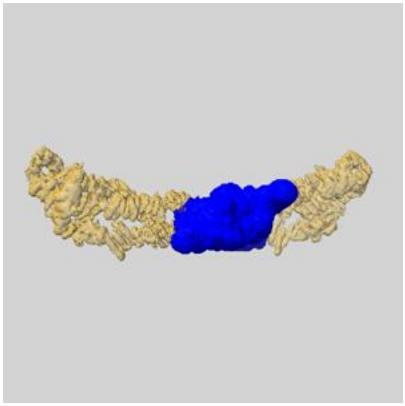


Y

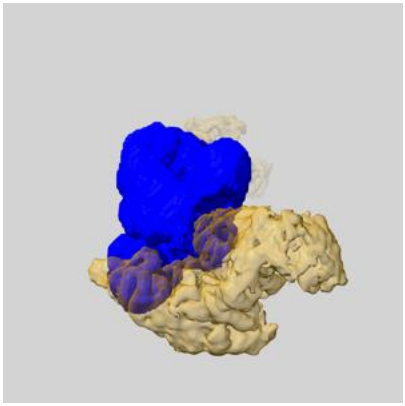


Z

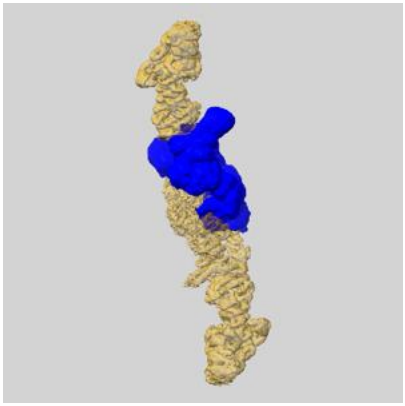
6.5.2 emd_14120_msk_2.map (i)



X



Y

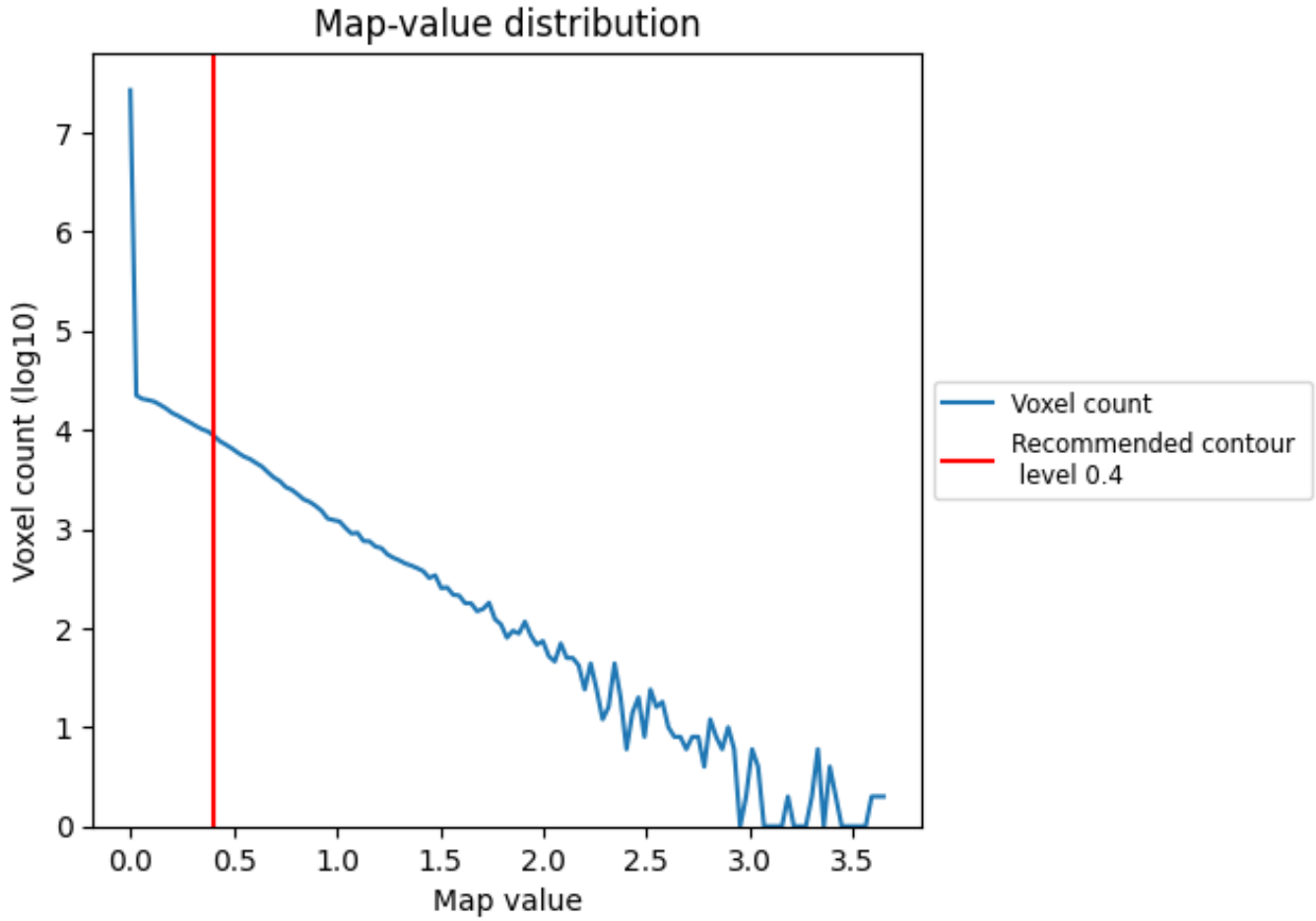


Z

7 Map analysis

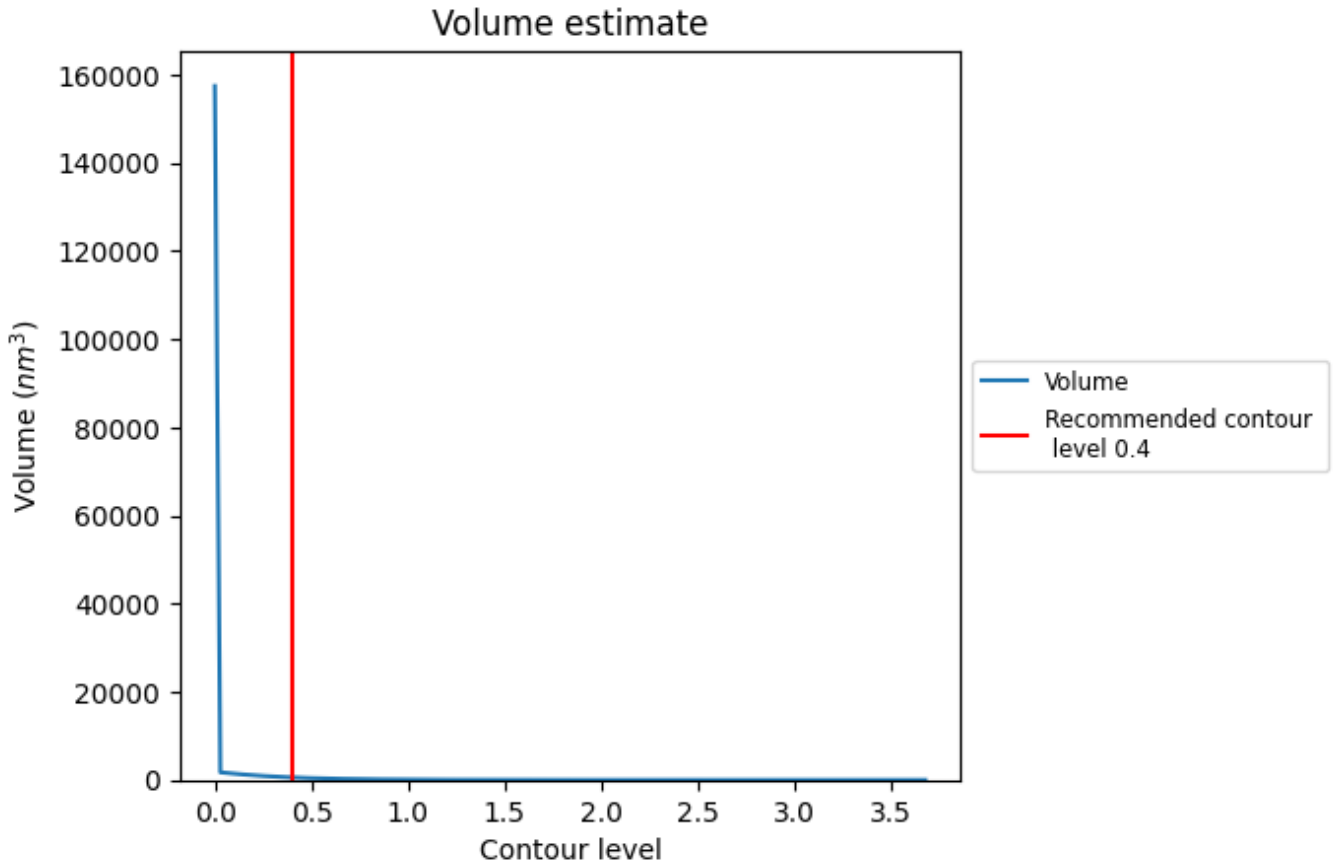
This section contains the results of statistical analysis of the map.

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.

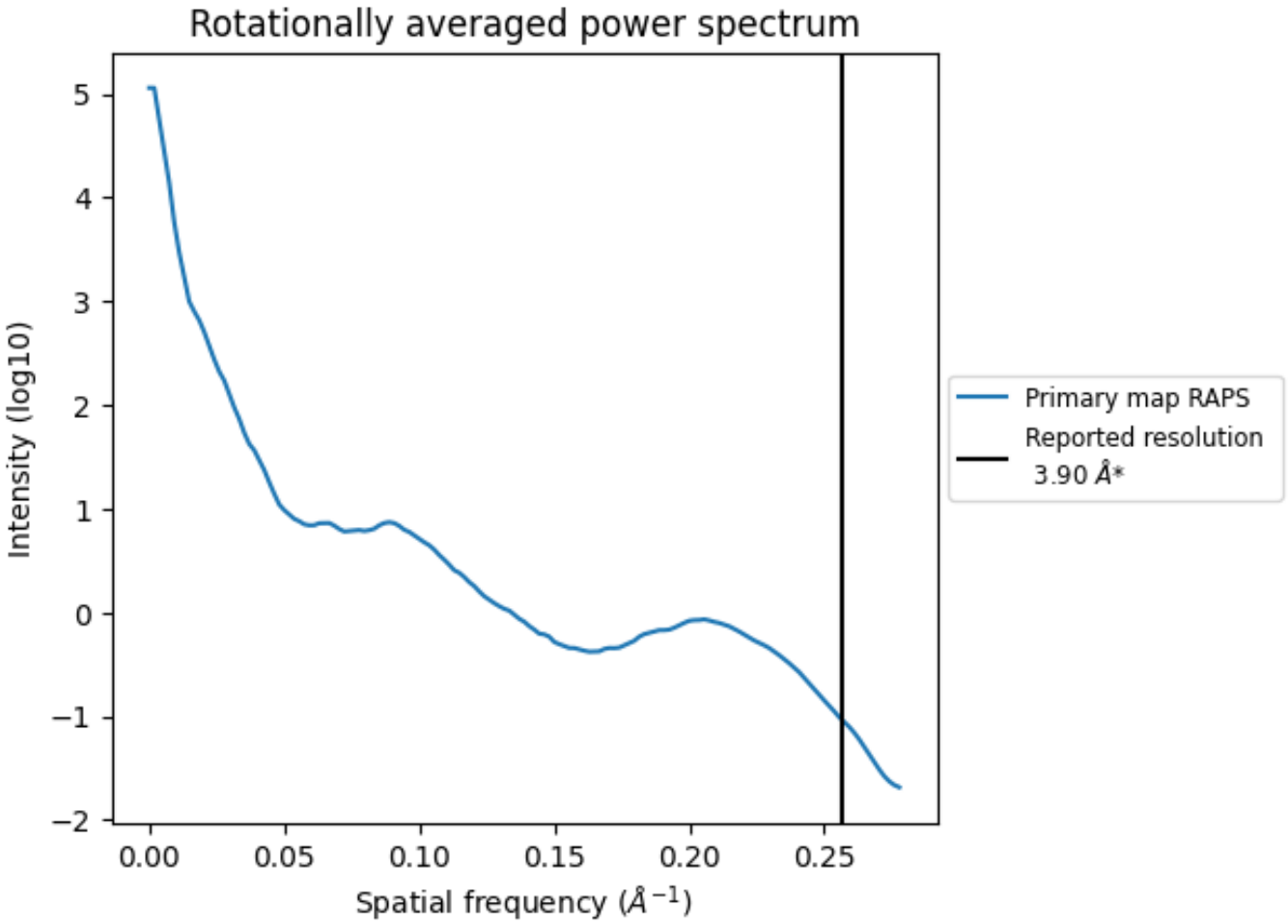
7.2 Volume estimate



The volume at the recommended contour level is 571 nm^3; this corresponds to an approximate mass of 516 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)

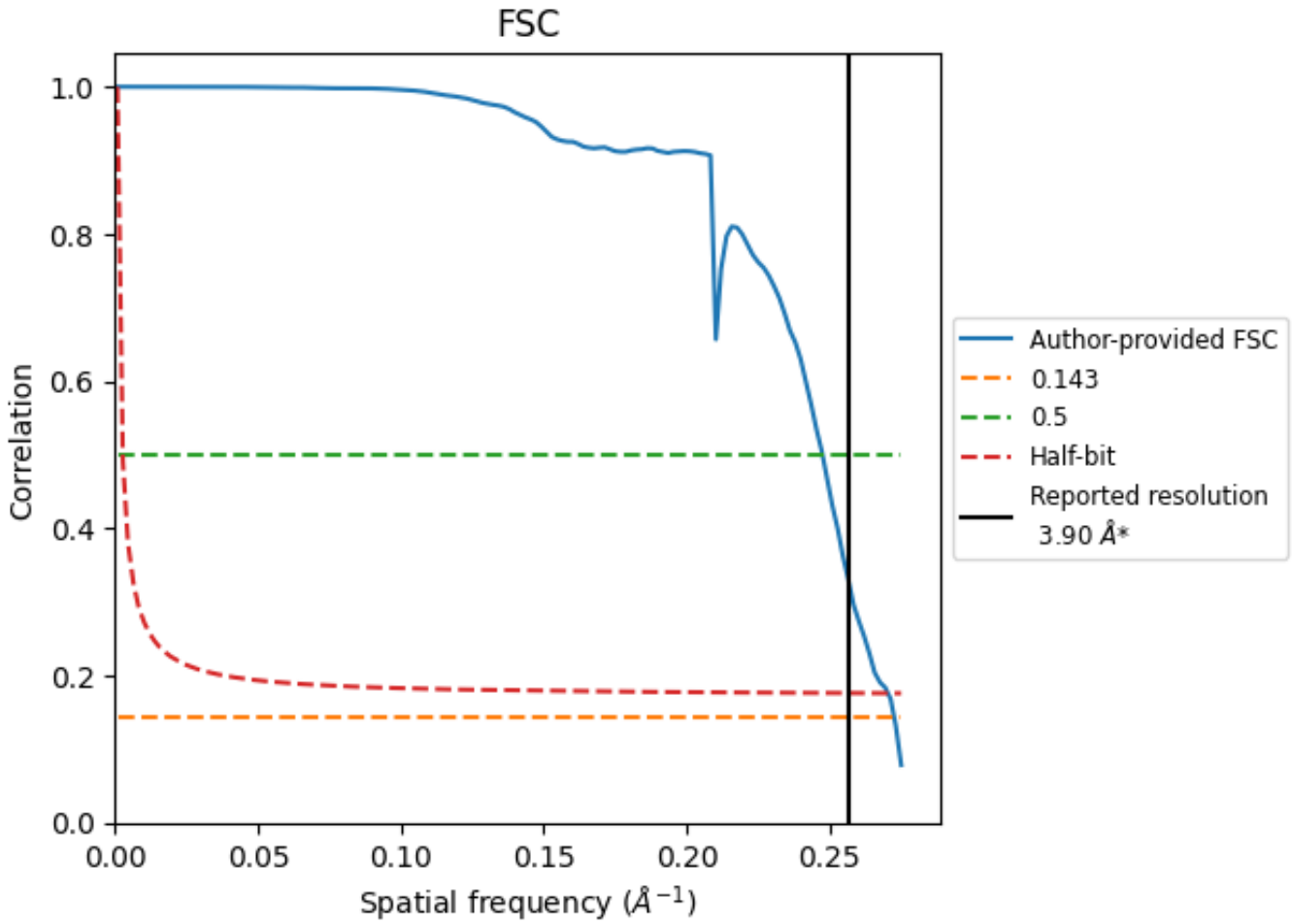


*Reported resolution corresponds to spatial frequency of 0.256 Å^{-1}

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

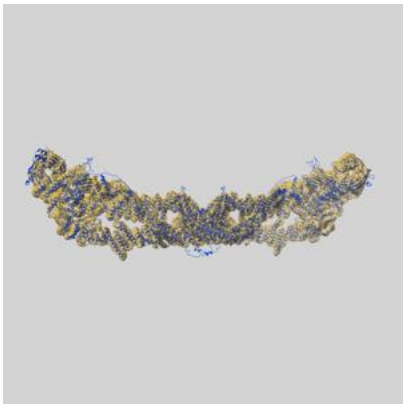
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.67	4.04	3.70
Unmasked-calculated*	-	-	-

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

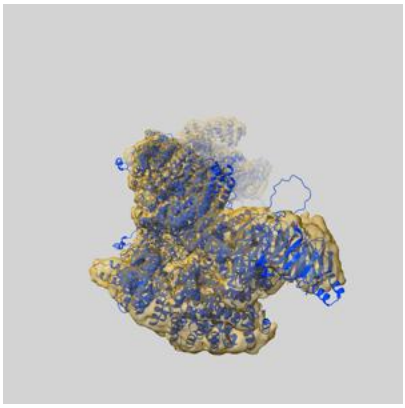
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14120 and PDB model 7QPG. Per-residue inclusion information can be found in section 3 on page 5.

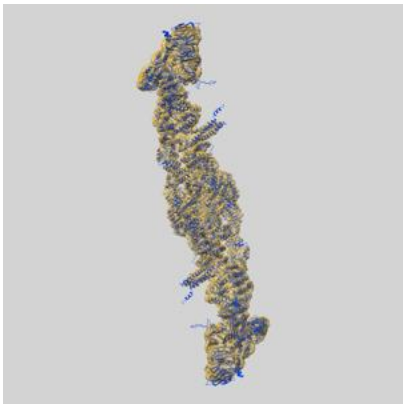
9.1 Map-model overlay



X



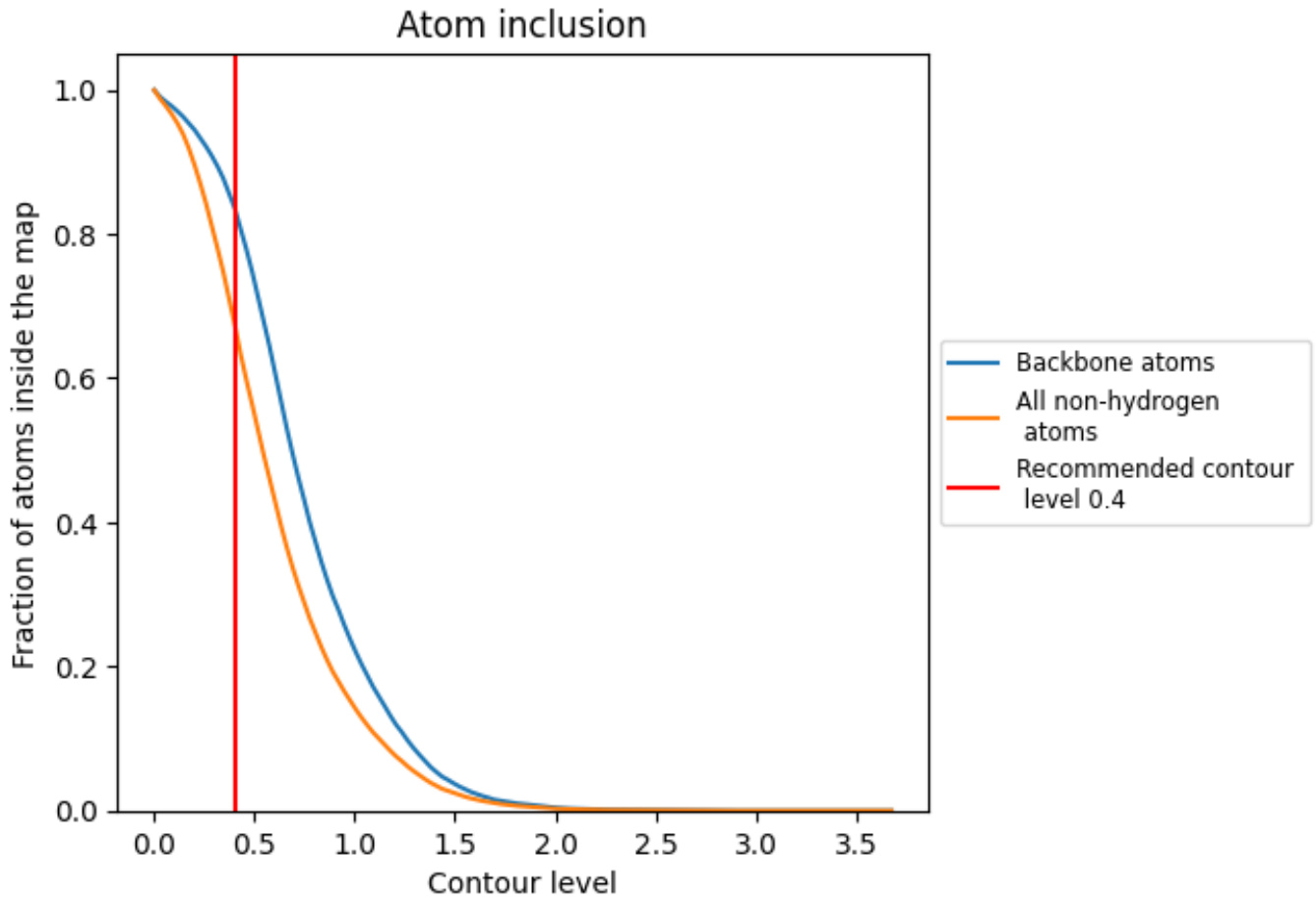
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.