Full wwPDB EM Validation Report ⓘ

Nov 3, 2024 – 04:22 PM EST

PDB ID	:	7K58
EMDB ID	:	EMD-22677
Title	:	Structure of outer-arm dyneins bound to microtubule with microtubule binding state 1(MTBS-1)
Authors	:	Qinhui, R.; Kai, Z.
Deposited on	:	2020-09-16
Resolution	:	4.00 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:

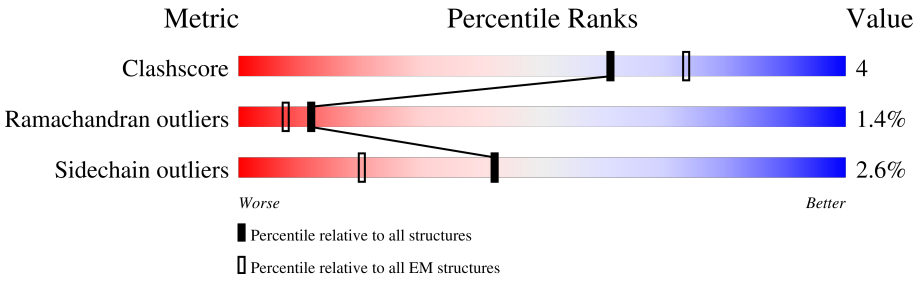
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 4.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	4615	19% 86% 9% ·
2	C	3943	22% 90% 10% ·
3	Q	192	12% 95% 5%
4	B	4588	17% 85% 12% · ·
5	I	106	26% 79% 18% ·
6	H	91	30% 90% 9% ·
7	G	96	31% 86% 14%
8	F	110	25% 82% 17% ·

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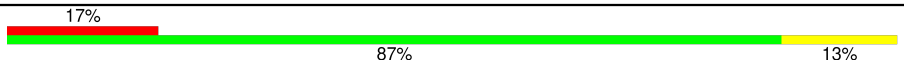
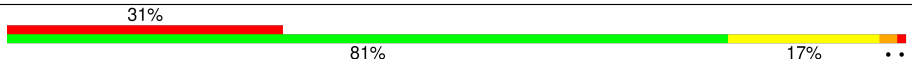
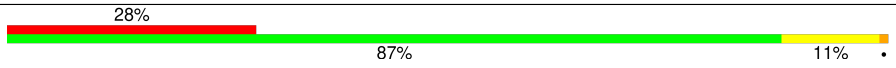
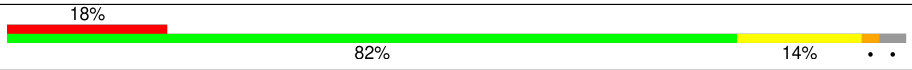
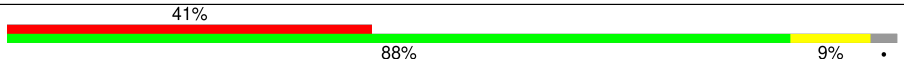
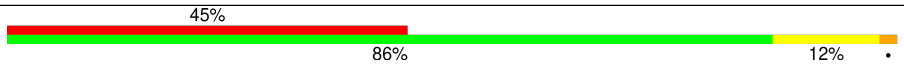
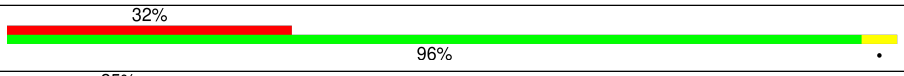
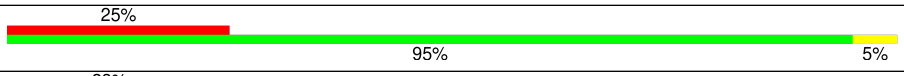
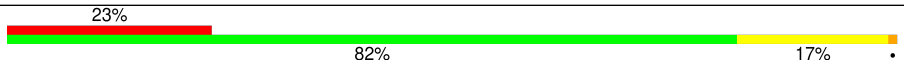
Mol	Chain	Length	Quality of chain
9	N	114	
10	O	120	
11	E	557	
12	D	595	
13	P	112	
14	L	98	
15	K	90	
16	J	95	
17	M	87	

2 Entry composition (i)

There are 20 unique types of molecules in this entry. The entry contains 117936 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	4443	33894	21519	5788	6429	158	0	0

- Molecule 2 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	3943	30436	19390	5162	5735	149	0	0

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Q	192	1002	607	202	193	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

- Molecule 4 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	B	4516	34604	21978	5928	6547	151	0	0

- Molecule 5 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	106	827	526	134	161	6	0	0

- Molecule 6 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 7 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	109	Total 541	C 323	N 109	O 109	0	0

- Molecule 14 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	98	Total 783	C 511	N 132	O 137	S 3	0	0

- Molecule 15 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	90	Total 754	C 489	N 124	O 137	S 4	0	0

- Molecule 16 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	95	Total 806	C 527	N 135	O 140	S 4	0	0

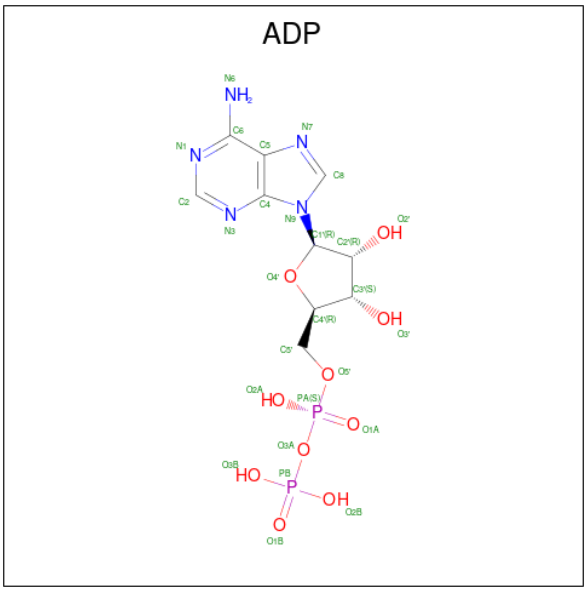
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	ALA	CYS	conflict	UNP Q22R86

- Molecule 17 is a protein called Dynein light chain.

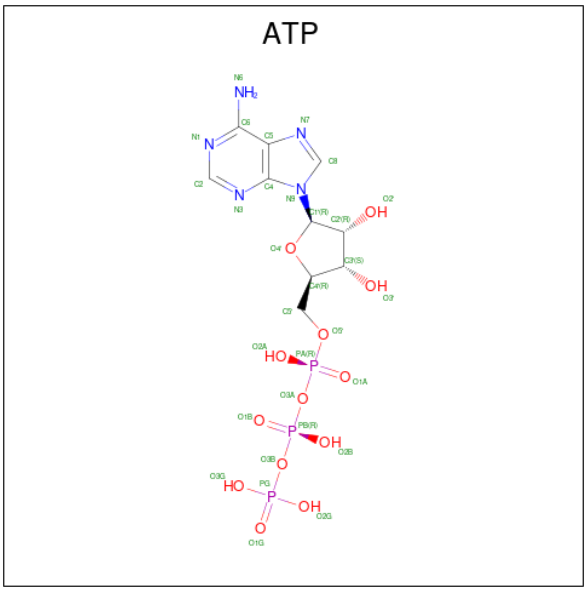
Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	87	Total 735	C 477	N 123	O 130	S 5	0	0

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
18	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
19	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

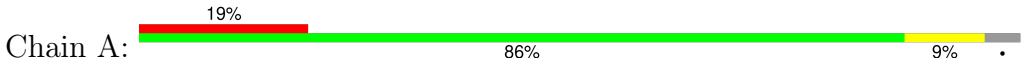
Mol	Chain	Residues	Atoms		AltConf
20	A	3	Total	Mg	0
			3	3	
20	C	3	Total	Mg	0
			3	3	
20	B	3	Total	Mg	0
			3	3	

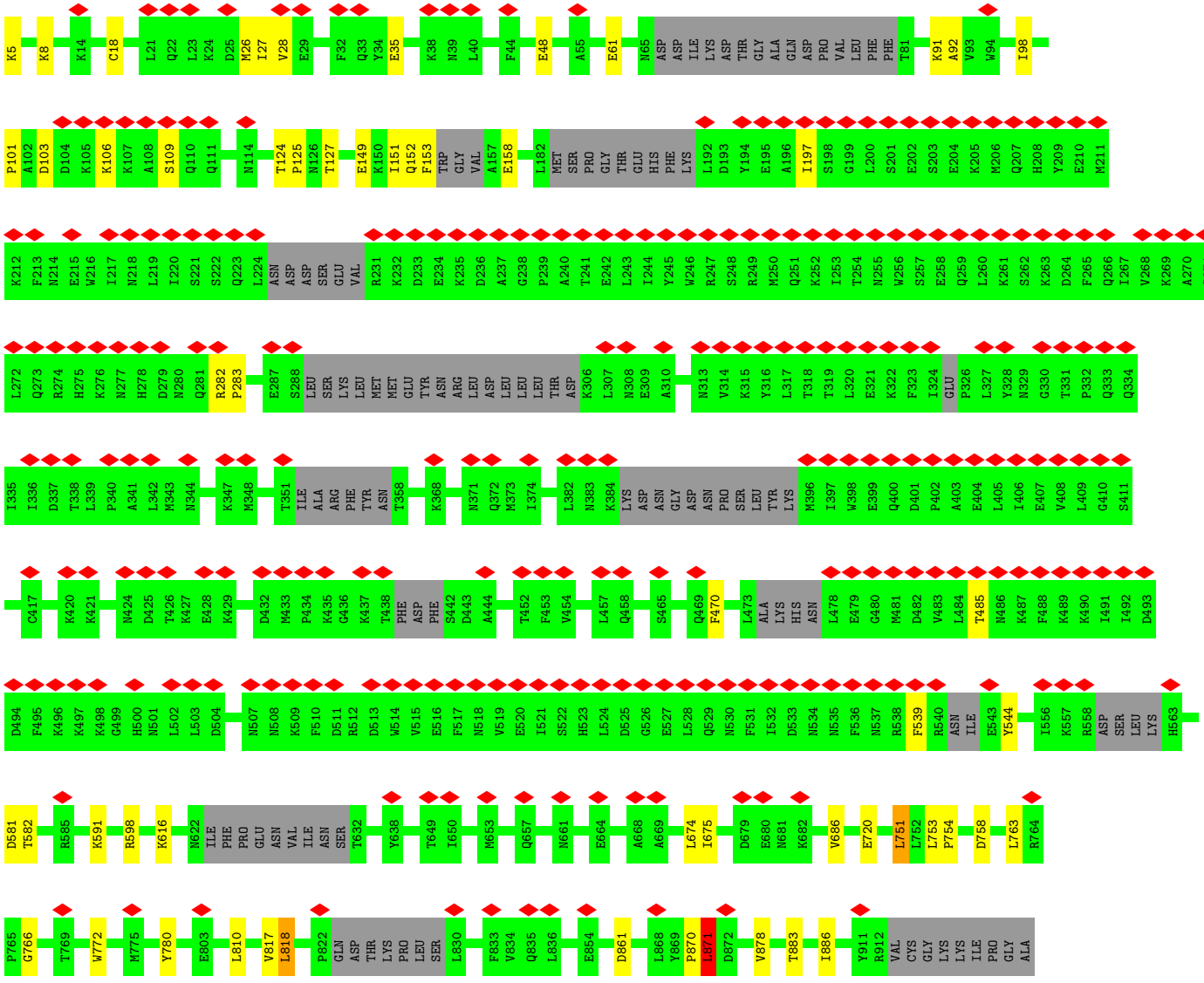
3 Residue-property plots (i)

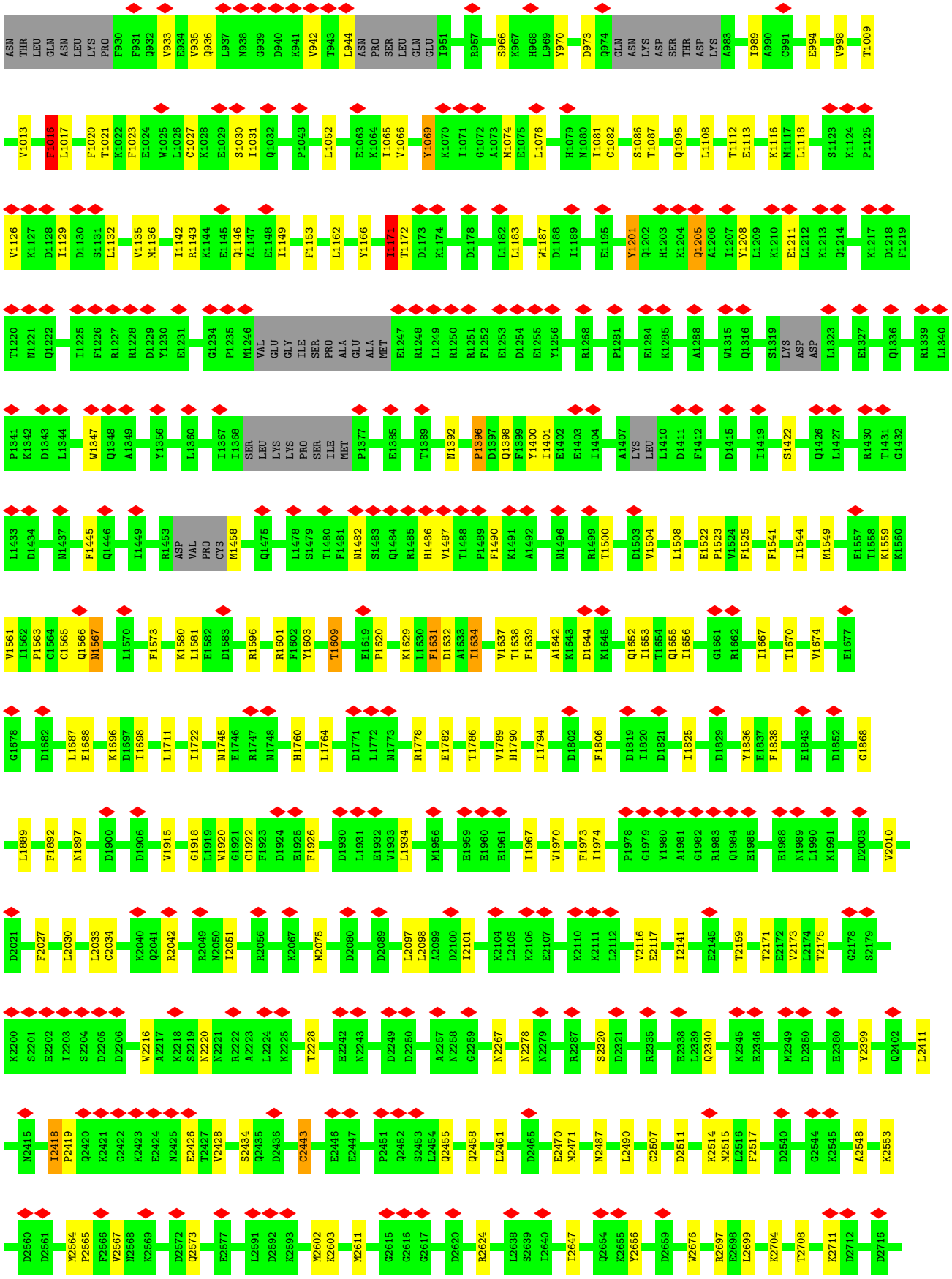
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain A:






ASN THR LEU GLN ASN LEU LYS PRO F930 F931 Q932 V933 E934 V935 Q936 L937 N938 G939 D940 K941 V942 T943 L944 ASN PRO SER LEU GLN GLU I951 R957 S966 K967 H968 L969 Y970 D973 Q974 GLN ASN LYS ASP SER THR ASP LYS A983 I989 A990 C991 E994 V998 T1009
V1013 P1016 L1017 F1020 T1021 K1022 F1023 E1024 V1025 L1026 C1027 K1028 E1029 S1030 I1031 Q1032 P1043 L1052 E1063 K1064 I1065 V1066 Y1069 K1070 I1071 G1072 A1073 M1074 E1075 L1076 H1079 N1080 I1081 C1082 S1086 T1087 Q1095 L1108 T1112 E1113 K1116 M1117 L1118 S1123 K1124 P1125
V1126 K1127 D1128 I1129 D1130 S1131 L1132 V1135 M1136 I1142 R1143 K1144 E1145 Q1146 A1147 E1148 I1149 F1153 L1162 Y1166 I1171 T1172 D1173 K1174 D1178 L1182 L1183 W1187 D1188 I1189 E1195 Y1201 Q1202 H1203 K1204 Q1205 A1206 I1207 Y1208 L1209 K1210 E1211 L1212 K1213 Q1214 K1217 D1218 F1219
T1220 N1221 Q1222 I1225 F1226 R1227 R1228 D1229 Y1230 E1231 G1234 P1235 M1246 VAL GLU GLY ILE SER PRO ALA GLU ALA MET E1247 R1248 L1249 R1250 R1251 F1252 E1253 D1254 E1255 Y1256 R1268 P1281 E1284 K1285 A1288 W1315 Q1316 S1319 LYS ASP ASP L1323 E1327 Q1336 R1339 L1340
P1341 K1342 D1343 L1344 W1347 Q1348 A1349 Y1356 L1360 I1367 I1368 SER LEU LYS LYS PRO SER ILE MET P1377 E1385 T1389 N1392 P1396 D1397 Q1398 F1399 Y1400 I1401 E1402 E1403 I1404 A1407 LYS LEU L1410 D1411 F1412 D1415 I1419 S1422 Q1426 L1427 R1430 T1431 G1432
L1433 D1434 N1437 F1445 Q1446 I1449 R1453 ASP VAL PRO CYS M1458 Q1475 L1478 S1479 T1480 F1481 N1482 S1483 Q1484 R1485 H1486 V1487 T1488 P1489 F1490 K1491 A1492 N1496 R1499 T1500 D1503 V1504 L1508 E1522 P1523 V1524 F1525 F1541 I1544 M1549 E1557 T1558 K1559 K1560
V1561 I1562 P1563 C1564 C1565 Q1566 N1567 L1570 F1573 K1580 L1581 E1582 D1583 R1596 R1601 F1602 Y1603 T1609 E1619 P1620 K1629 L1630 F1631 D1632 A1633 I1634 V1637 T1638 F1639 A1642 K1643 D1644 K1645 Q1652 I1653 T1654 Q1655 I1656 G1661 R1662 I1667 T1670 V1674 E1677
G1678 D1682 L1687 E1688 K1696 D1697 I1698 L1711 I1722 N1745 E1746 R1747 N1748 H1760 L1764 D1771 L1772 N1773 R1778 E1782 T1786 V1789 H1790 I1794 D1802 F1806 D1819 I1820 D1821 I1825 D1829 Y1836 E1837 F1838 E1843 D1852 G1868
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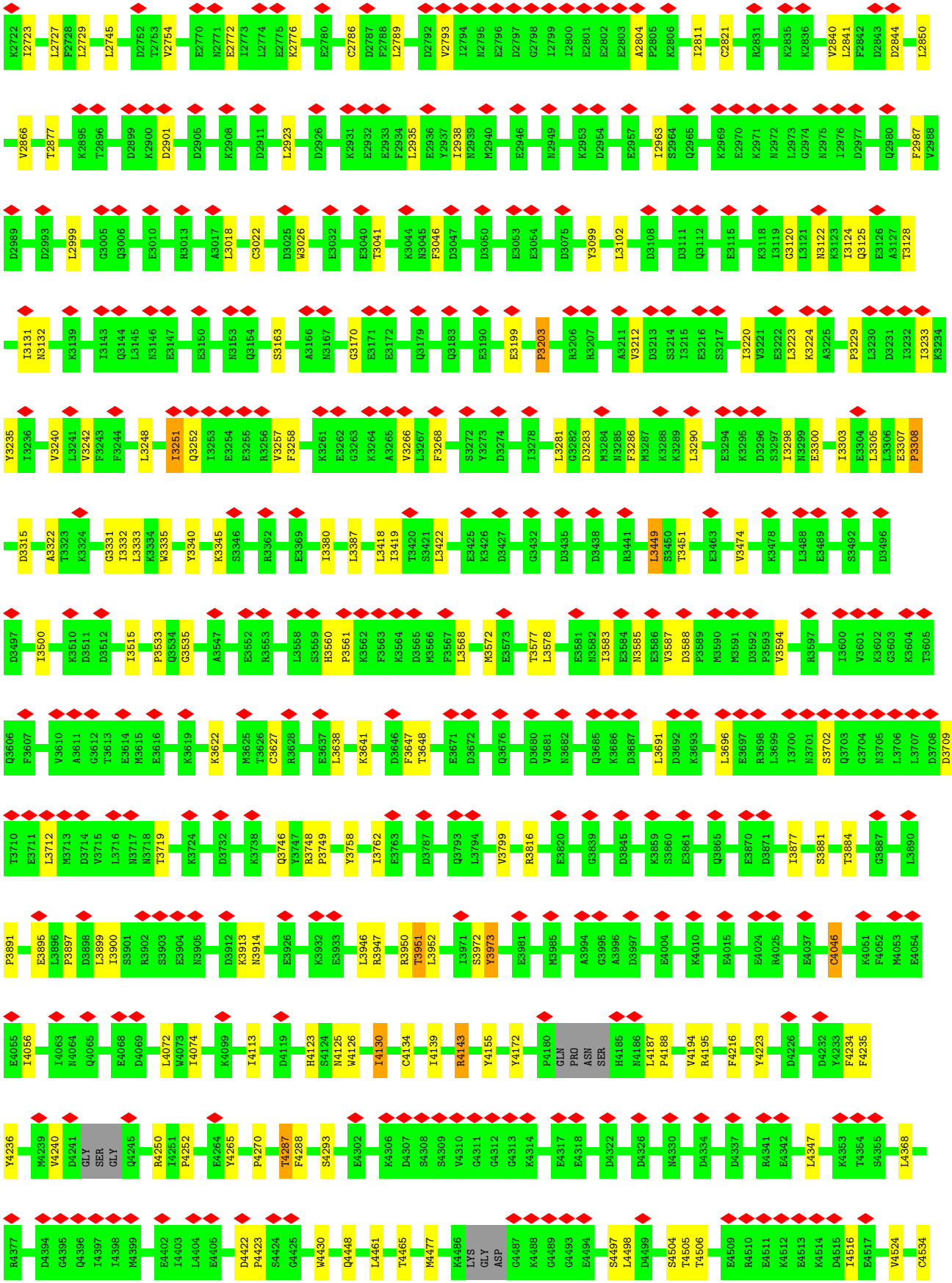
D2021 F2027 L2030 L2033 C2034 K2040 Q2041 R2042 R2049 N2050 I2051 R2056 K2067 M2075 D2080 D2089 L2097 L2098 A2099 D2100 I2101 K2104 L2105 K2106 E2107 K2110 K2111 L2112 V2116 E2117 I2141 E2145 T2159 T2171 E2172 V2173 L2174 T2175 G2178 S2179
K2200 S2201 E2202 I2203 S2204 D2205 D2206 W2216 A2217 K2218 S2219 N2220 N2221 R2222 A2223 L2224 K2225 T2228 E2242 N2243 D2249 D2250 A2257 N2258 G2259 N2267 N2278 N2279 R2287 S2320 D2321 R2335 E2338 L2339 Q2340 K2345 E2346 M2349 D2350 E2380 Y2399 Q2402 L2411
W2415 I2418 P2419 Q2420 K2421 G2422 K2423 E2424 N2425 E2426 T2427 V2428 S2434 Q2435 D2436 C2443 E2446 E2447 P2451 Q2452 S2453 L2454 Q2455 Q2458 L2461 D2465 E2470 M2471 N2487 L2490 C2507 D2511 K2514 M2515 L2516 F2517 D2540 G2544 K2545 A2548 K2553
D2560 D2561 M2564 P2565 F2566 Y2567 N2568 K2569 D2572 Q2573 E2577 L2591 D2592 K2593 M2602 K2603 M2611 G2615 G2616 G2617 D2620 R2624 L2638 S2639 I2640 I2647 Q2654 K2655 Y2656 D2659 W2676 R2697 E2698 L2699 K2704 T2708 K2711 D2712 D2716


K2722 I2723 L2727 F2728 L2729 L2745 D2752 T2753 V2754 E2770 N2771 E2772 I2773 L2774 E2775 K2776 E2780 C2786 D2787 F2788 L2789 D2792 V2793 I2794 N2795 E2796 D2797 G2798 I2799 I2800 E2801 E2802 E2803 A2804 P2805 K2806 I2811 C2821 R2831 K2835 K2836 V2840 L2841 F2842 D2843 D2844 L2850
V2866 T2877 K2895 T2896 D2899 K2900 D2901 D2905 K2908 D2911 L2923 D2926 K2931 E2932 E2933 F2934 L2935 E2936 Y2937 I2938 N2939 M2940 E2946 N2949 K2953 D2954 E2957 I2963 S2964 Q2965 K2969 E2970 K2971 N2972 L2973 G2974 N2975 I2976 D2977 Q2980 F2987 V2988
D2989 D2993 L2999 G3005 Q3006 E3010 R3013 A3017 L3018 C3022 D3025 W3026 E3032 E3040 T3041 K3044 N3045 F3046 D3047 D3050 E3053 E3054 D3075 Y3099 L3102 D3108 D3111 Q3112 E3115 K3118 I3119 G3120 L3121 N3122 K3123 I3124 Q3125 E3126 A3127 T3128
I3131 N3132 K3139 I3143 Q3144 L3145 N3146 E3147 E3150 N3153 Q3154 S3163 A3166 N3167 G3170 E3171 E3172 Q3179 Q3183 E3190 E3199 P3203 R3206 R3207 A3211 V3212 D3213 S3214 I3215 E3216 S3217 I3220 V3221 E3222 L3223 K3224 A3225 P3229 L3230 D3231 I3232 I3233 K3234
Y3235 I3236 V3240 L3241 V3242 F3243 F3244 L3248 I3251 Q3252 I3253 E3254 E3255 R3256 V3257 F3258 K3261 E3262 G3263 K3264 A3265 V3266 L3267 F3268 S3272 Y3273 D3274 I3278 L3281 G3282 D3283 M3284 N3285 F3286 M3287 K3288 K3289 L3290 E3294 K3295 D3296 S3297 I3298 N3299 E3300 I3303 E3304 L3305 L3306 E3307 P3308
D3315 A3322 T3323 K3324 G3331 I3332 L3333 K3334 W3335 Y3340 K3345 S3346 R3362 E3369 I3380 L3387 L3418 I3419 T3420 S3421 L3422 E3425 K3426 D3427 G3432 D3435 D3438 R3441 L3449 S3450 T3451 E3463 V3474 K3478 L3488 E3489 S3492 D3496
D3497 I3500 K3510 D3511 D3512 I3515 P3533 Q3534 G3535 A3547 E3552 R3553 L3558 S3559 H3560 P3561 K3562 F3563 K3564 D3565 M3566 F3567 L3568 M3572 E3573 T3577 L3578 E3581 N3582 I3583 E3584 N3585 E3586 V3587 D3588 P3589 M3590 M3591 D3592 P3593 V3594 R3597 I3600 V3601 K3602 G3603 K3604 T3605
Q3606 F3607 V3610 A3611 G3612 T3613 E3614 M3615 E3616 K3619 K3622 M3625 T3626 C3627 R3628 E3637 L3638 K3641 D3646 F3647 T3648 E3671 D3672 Q3676 D3680 V3681 N3682 Q3685 K3686 D3687 L3691 D3692 K3693 I3696 E3697 R3698 L3699 I3700 N3701 S3702 Q3703 G3704 N3705 L3706 L3707 D3708 D3709
T3710 E3711 L3712 M3713 D3714 V3715 L3716 N3717 N3718 T3719 K3724 D3732 K3738 Q3746 Y3747 R3748 P3749 Y3758 I3762 E3763 D3787 Q3793 L3794 V3799 R3816 E3820 G3839 D3845 K3859 S3860 E3861 Q3865 E3870 D3871 I3877 S3881 T3884 G3887 L3890
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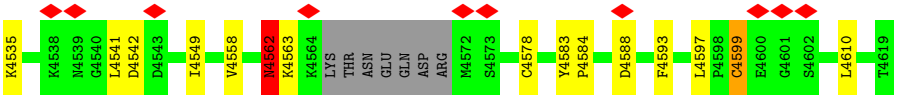
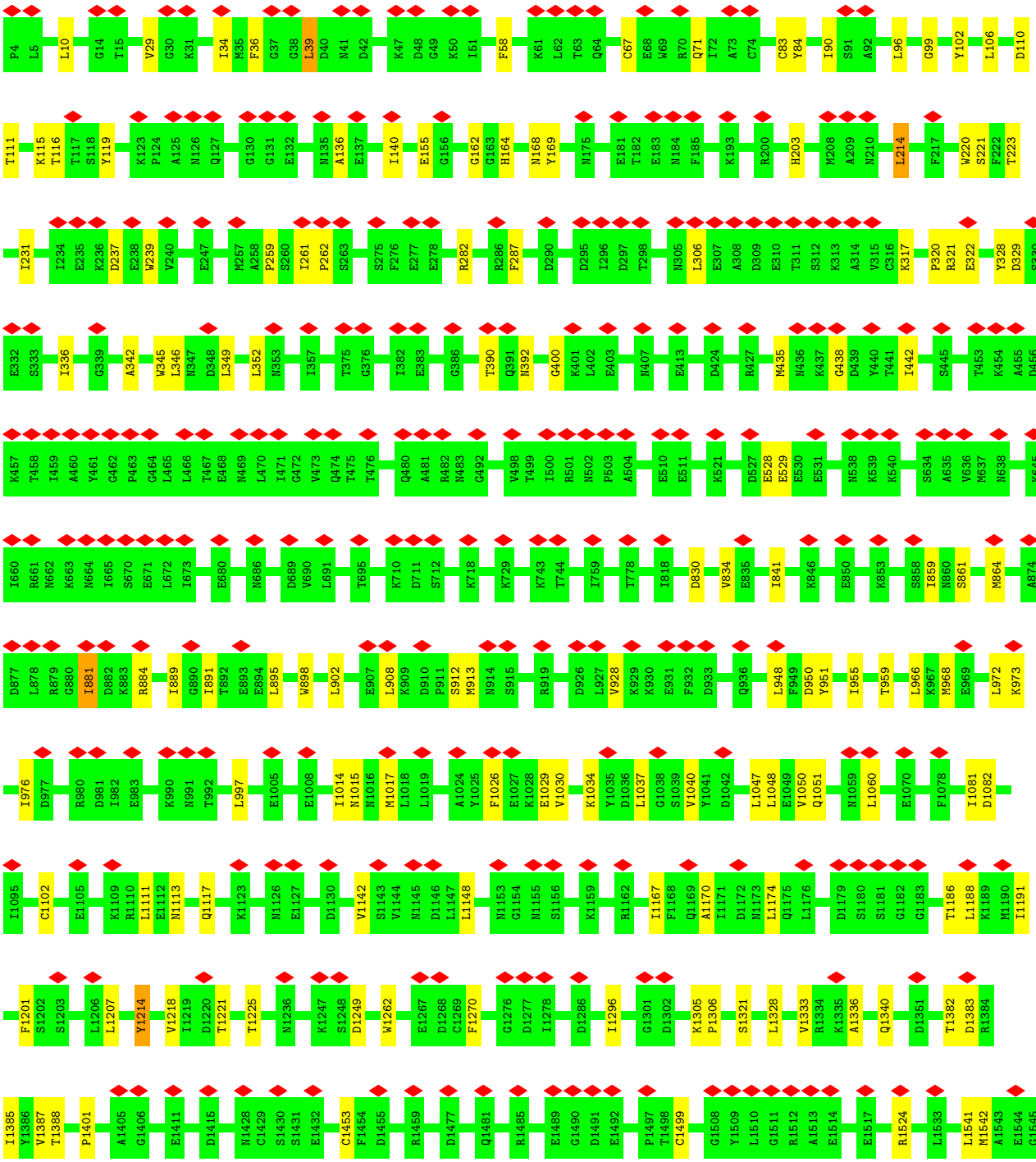
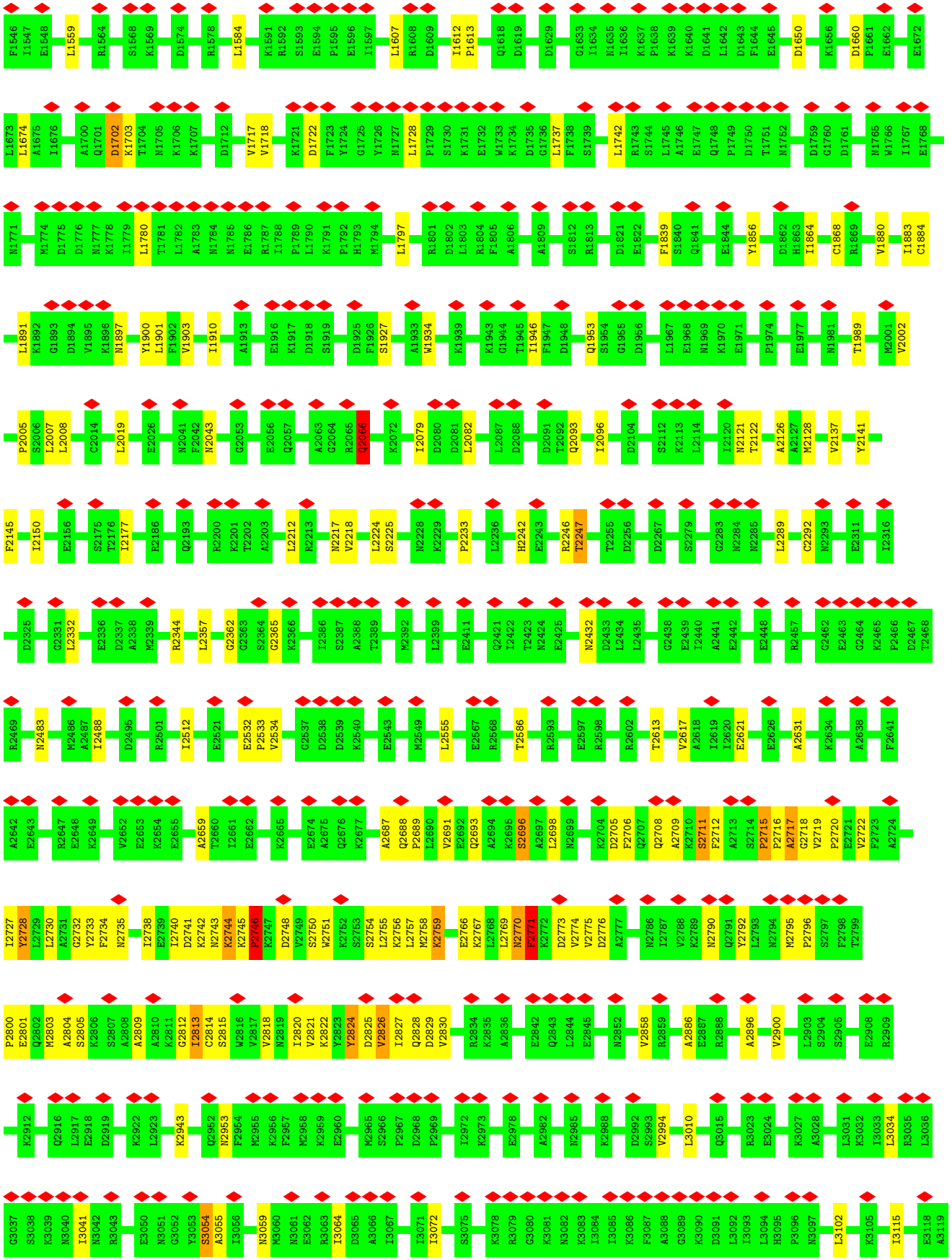


• Molecule 2: gamma heavy chain

Chain C:

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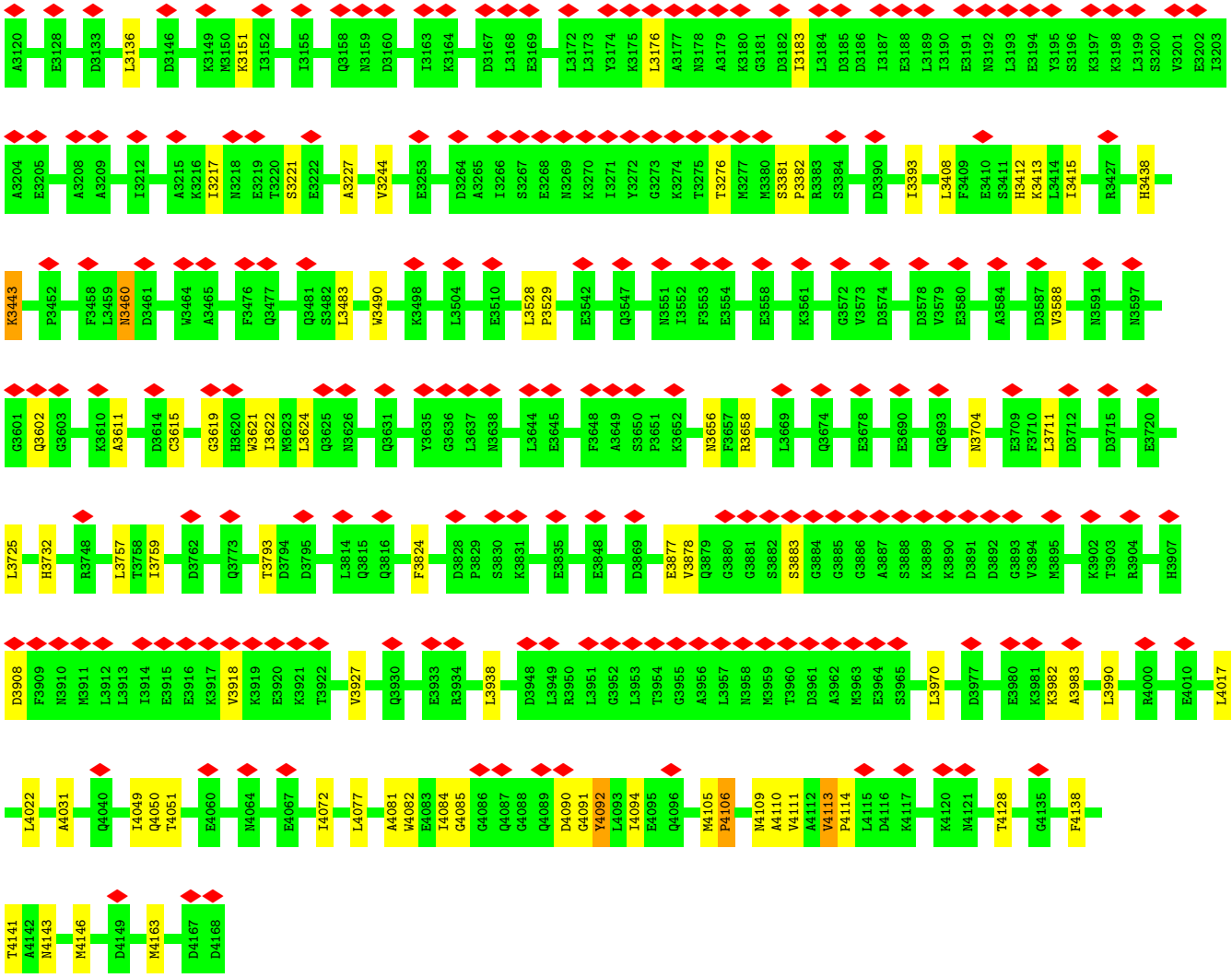
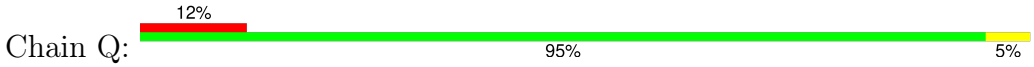
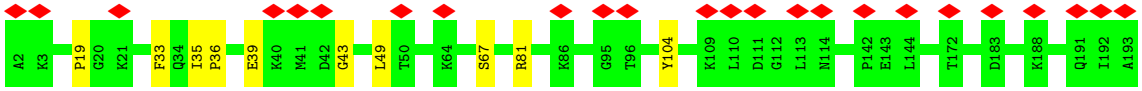
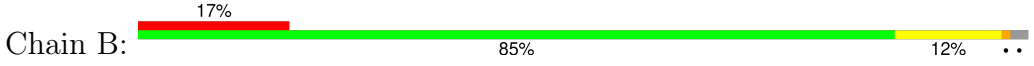


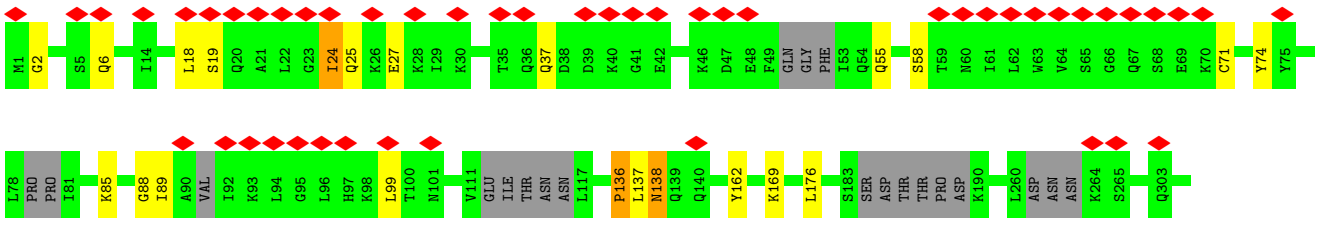
• Molecule 3: Dynein light chain 1

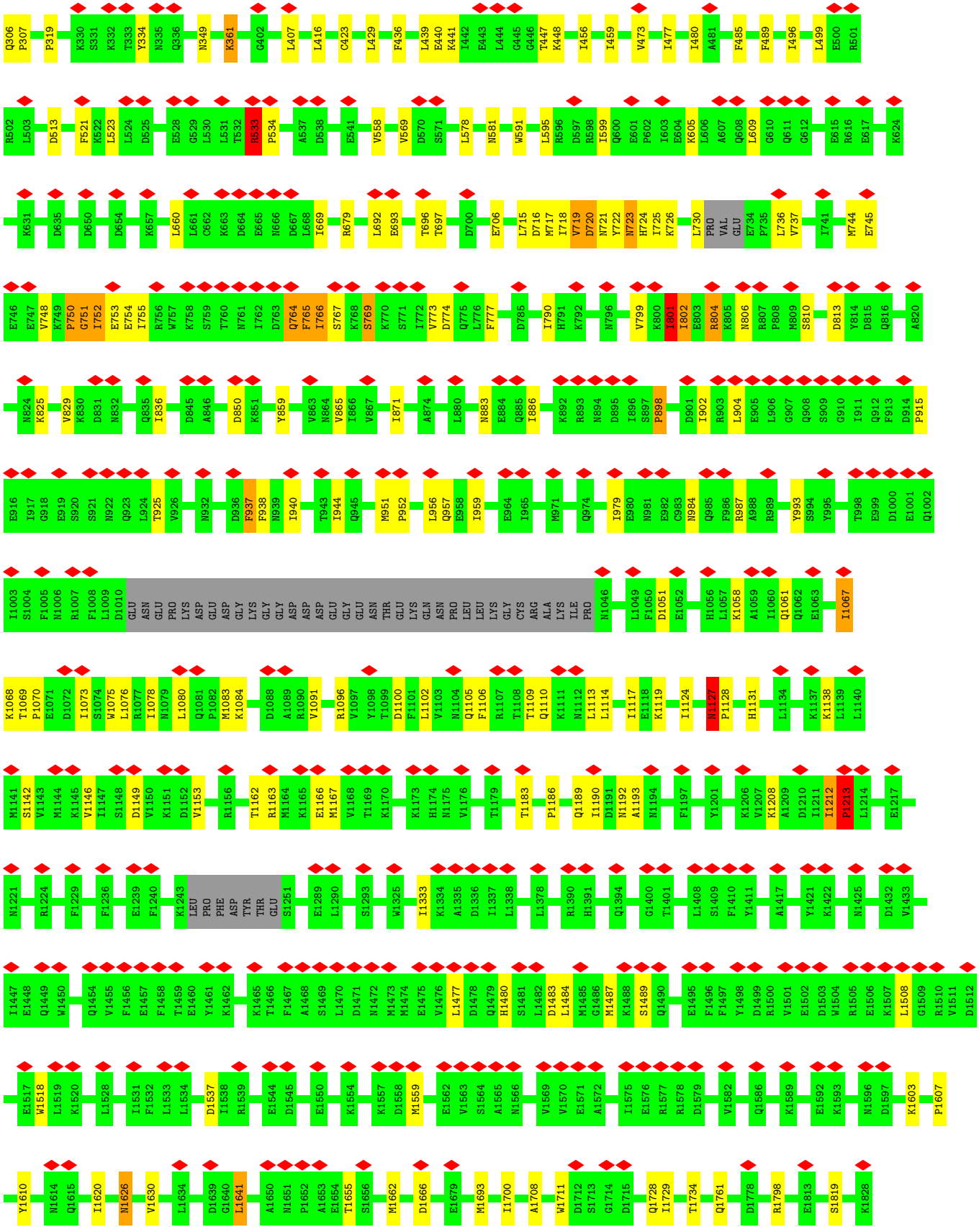




• Molecule 4: Outer arm dynein beta heavy chain



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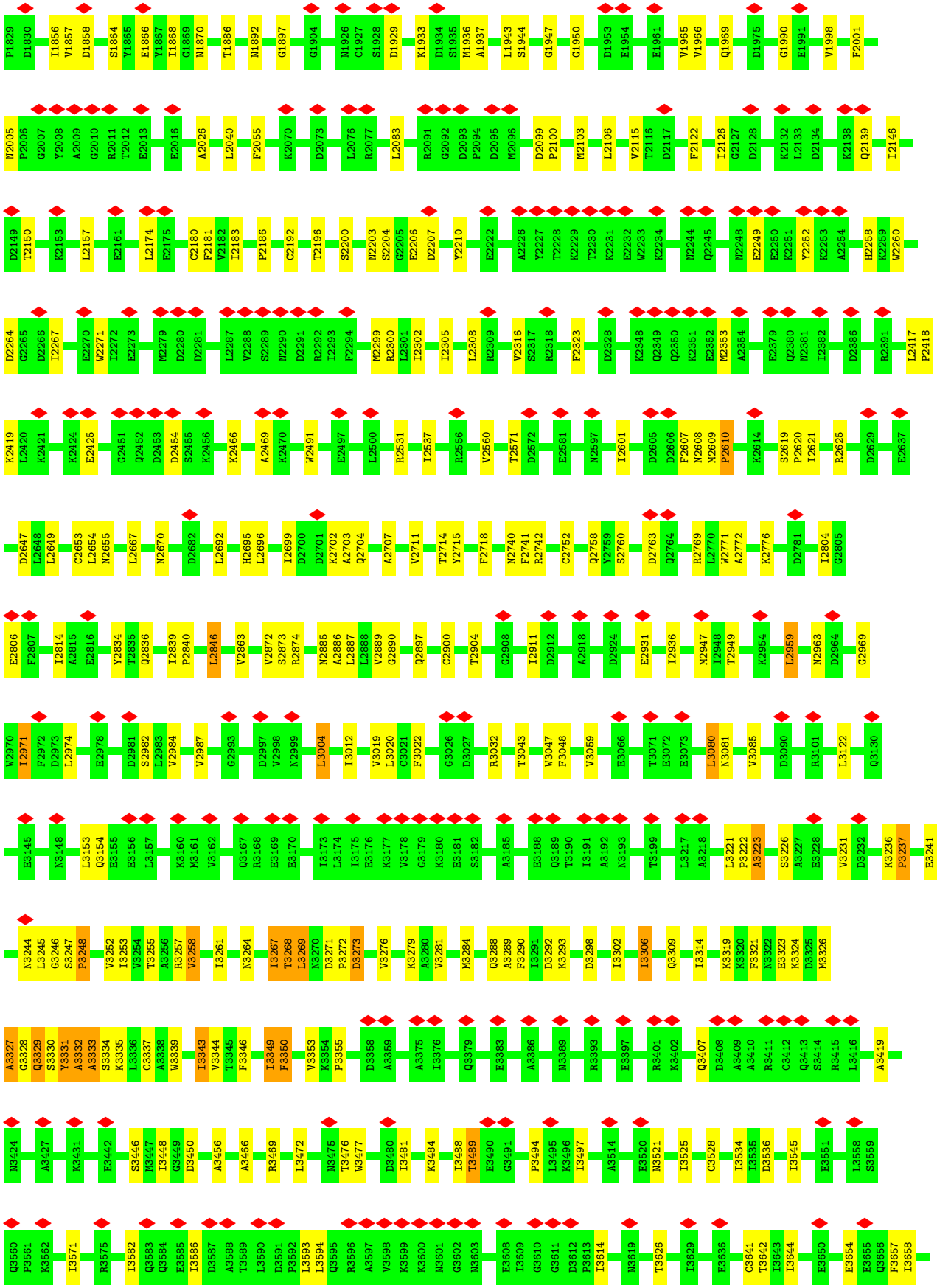
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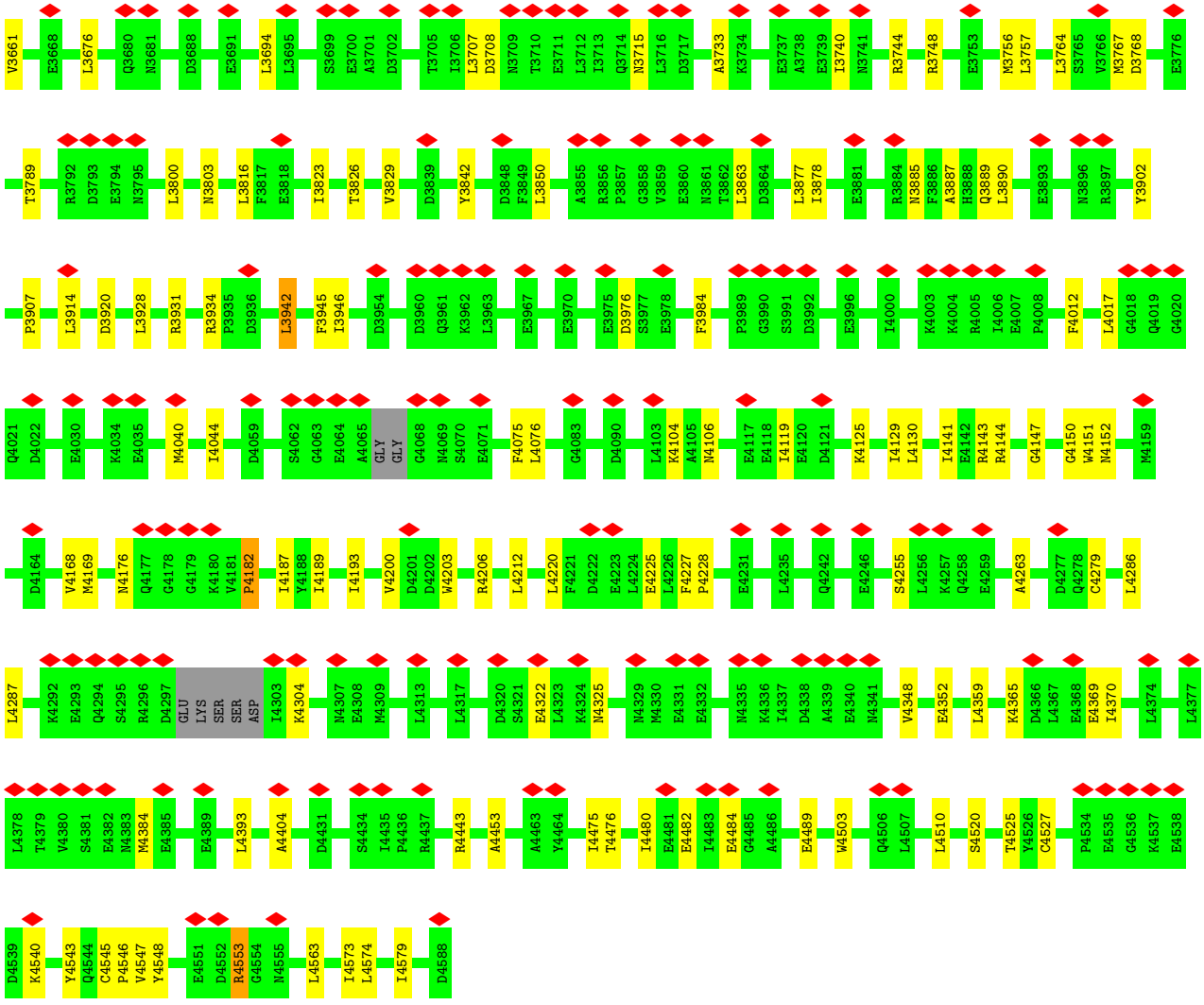
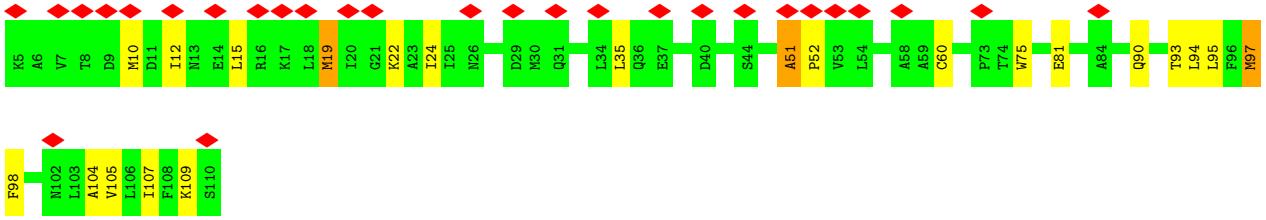


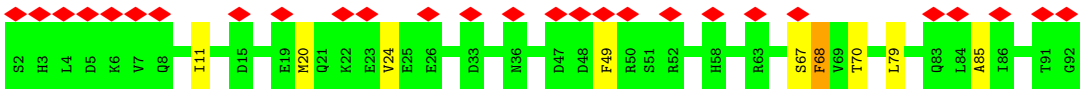
• Molecule 5: Dynein light chain

Chain I:



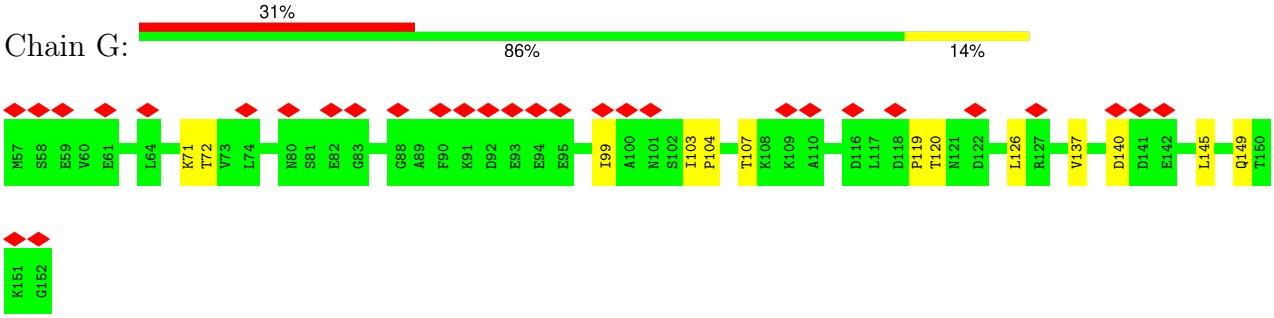
• Molecule 6: Dynein light chain

Chain H:



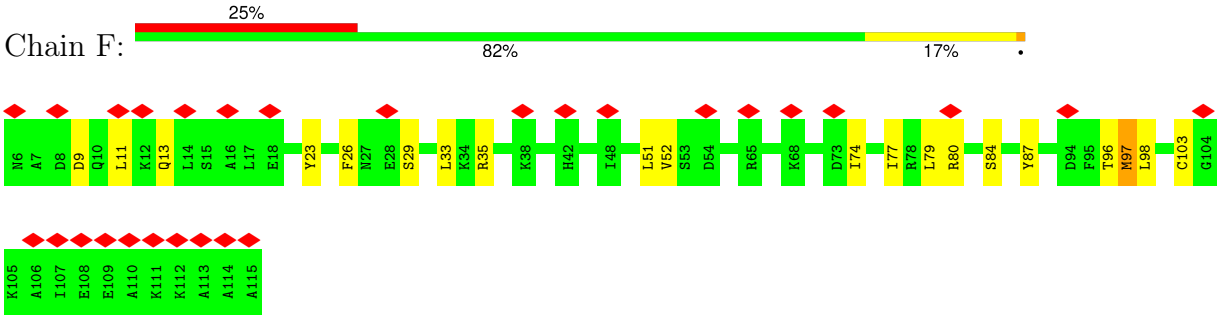
• Molecule 7: Dynein light chain roadblock

Chain G:



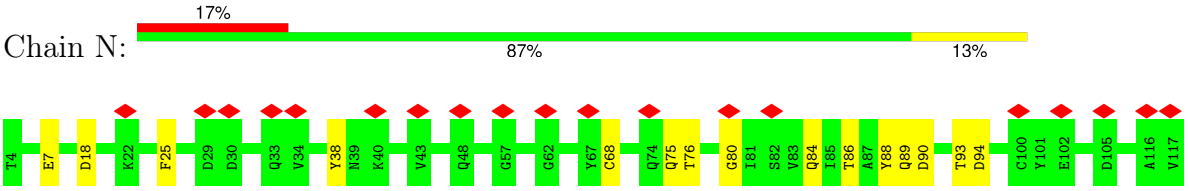
• Molecule 8: Dynein light chain roadblock-type 2 protein

Chain F:



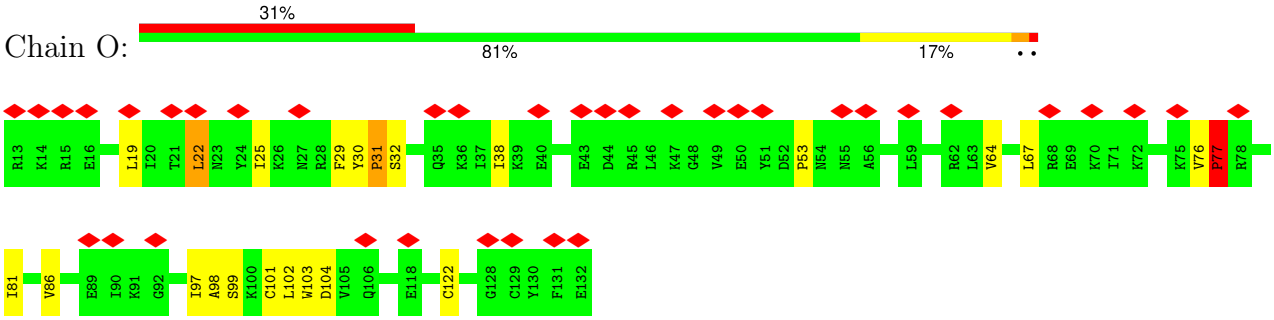
• Molecule 9: Dynein light chain tctex-type 1 protein

Chain N:



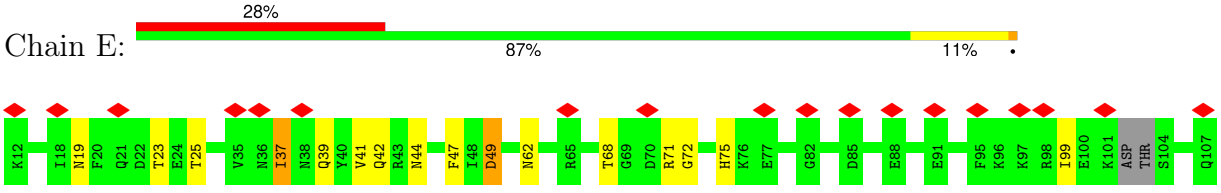
• Molecule 10: Dynein light chain 2A

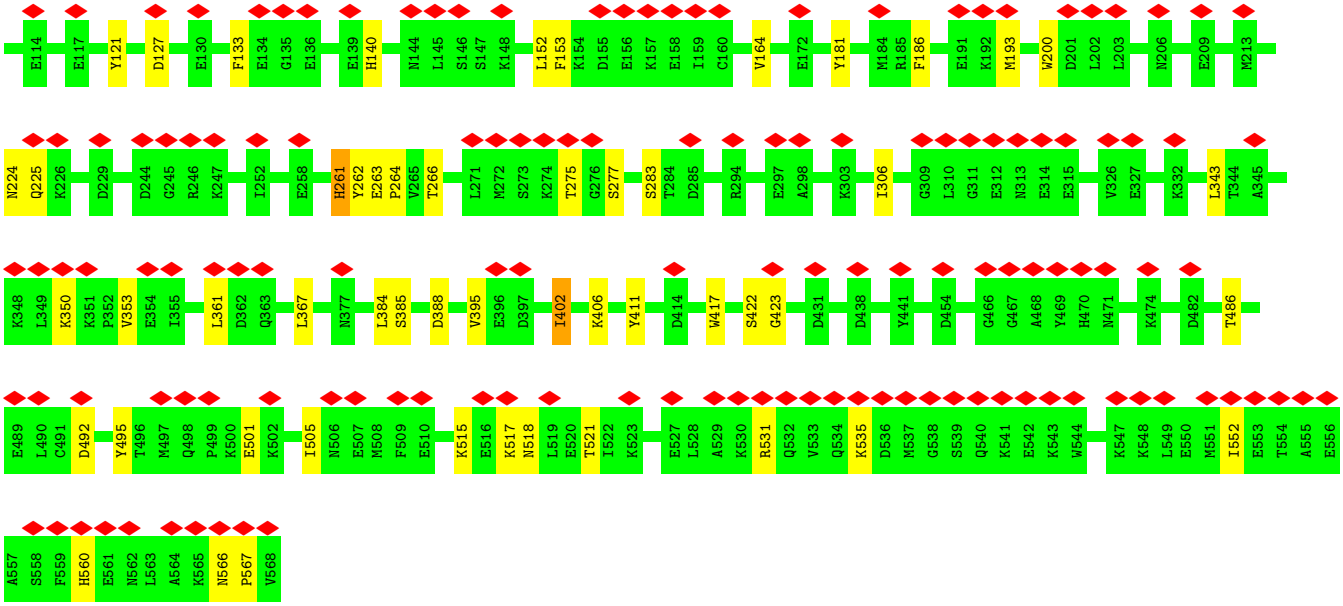
Chain O:



• Molecule 11: Flagellar outer dynein arm intermediate protein, putative

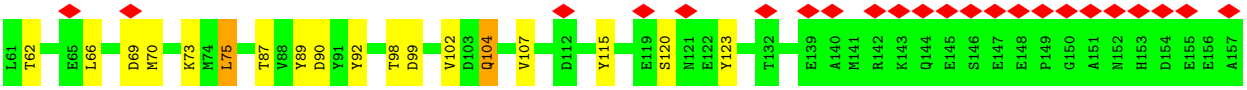
Chain E:

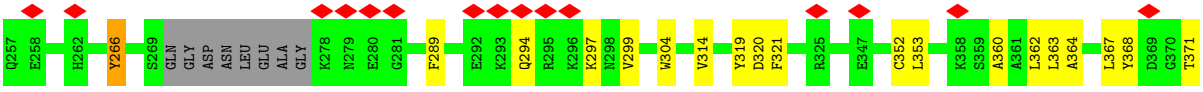


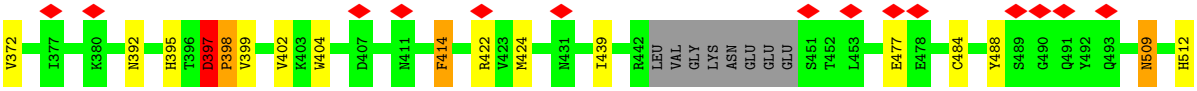


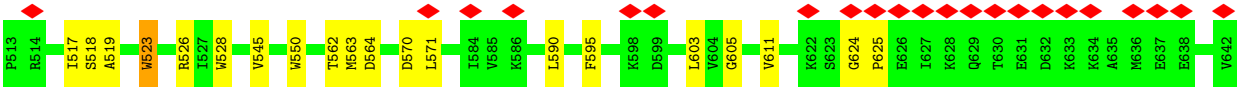
• Molecule 12: Dynein intermediate chain 2

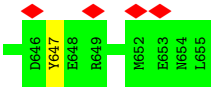
Chain D:





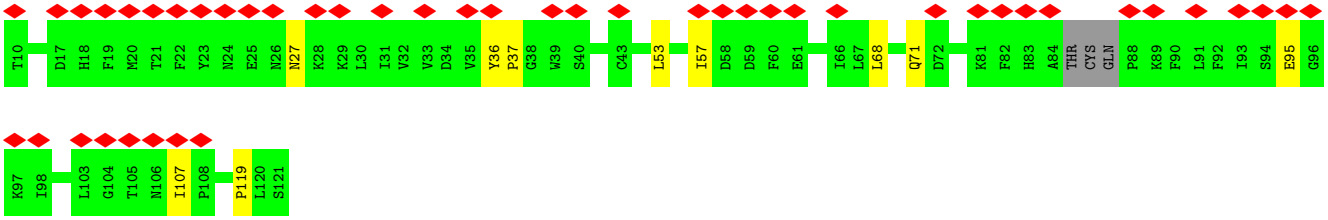






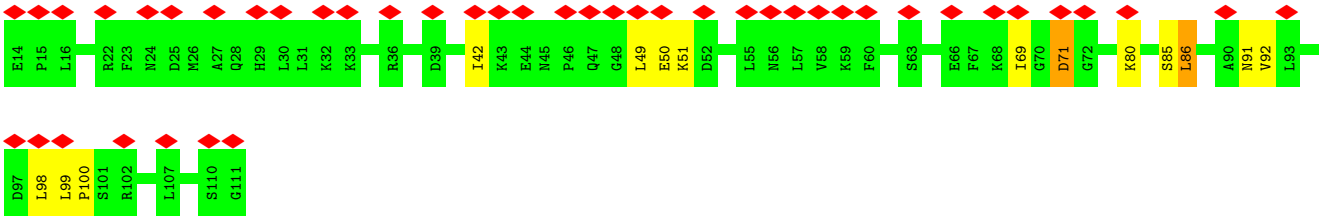
• Molecule 13: Thioredoxin

Chain P:



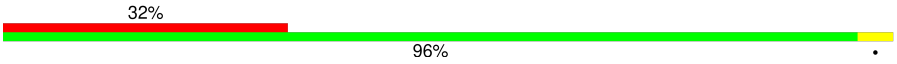
• Molecule 14: Dynein light chain

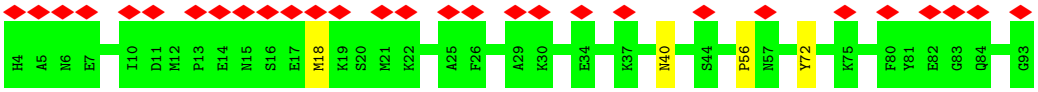
Chain L:



• Molecule 15: Dynein light chain

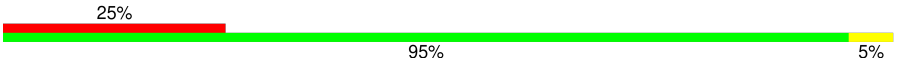
Chain K:

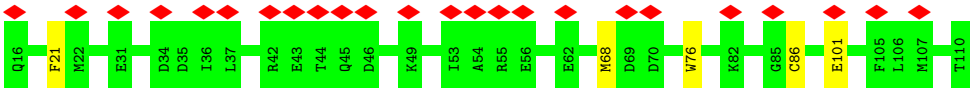




• Molecule 16: Dynein light chain

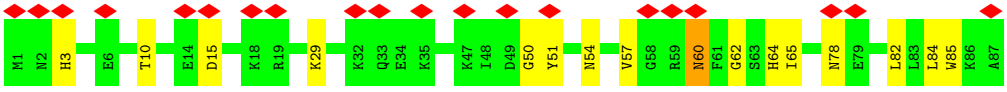
Chain J:





• Molecule 17: Dynein light chain

Chain M:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.012	Depositor
Minimum map value	0.000	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	530.5338, 477.21387, 449.22086	wwPDB
Map dimensions	398, 358, 337	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3329996, 1.3329996, 1.3329996	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

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	0.69	0/34464	0.78	1/46623 (0.0%)
2	C	0.68	0/31038	0.77	1/42003 (0.0%)
3	Q	0.86	0/1005	0.84	0/1388
4	B	0.69	1/35205 (0.0%)	0.80	3/47647 (0.0%)
5	I	0.69	0/838	0.77	0/1131
6	H	0.67	0/767	0.76	0/1031
7	G	0.69	0/755	0.77	0/1018
8	F	0.68	0/875	0.77	0/1178
9	N	0.69	0/867	0.79	0/1179
10	O	0.67	0/1004	0.80	0/1349
11	E	0.67	0/4522	0.78	0/6114
12	D	0.66	0/4772	0.78	1/6458 (0.0%)
13	P	0.87	0/538	0.86	0/746
14	L	0.66	0/800	0.76	0/1076
15	K	0.66	0/776	0.73	0/1038
16	J	0.63	0/831	0.74	0/1118
17	M	0.65	0/752	0.76	0/1006
All	All	0.69	1/119809 (0.0%)	0.78	6/162103 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	C	0	3
4	B	0	4
11	E	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	730	LEU	C-O	5.23	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	3248	PRO	N-CA-CB	-6.26	95.71	102.60
4	B	533	ARG	CB-CA-C	6.19	122.77	110.40
4	B	1127	ASN	CB-CA-C	5.71	121.82	110.40
12	D	397	ASP	CB-CA-C	5.18	120.76	110.40
1	A	1016	PHE	CB-CA-C	5.13	120.66	110.40
2	C	2824	TYR	CB-CA-C	-5.12	100.15	110.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
4	B	1864	SER	Peptide
4	B	2466	LYS	Peptide
4	B	3319	LYS	Peptide
4	B	3536	ASP	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide
2	C	528	GLU	Peptide
11	E	406	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33894	0	32288	250	0
2	C	30436	0	29392	239	0
3	Q	1002	0	501	6	0
4	B	34604	0	33094	332	0
5	I	827	0	829	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	12	0
10	O	986	0	1002	12	0
11	E	4423	0	4291	40	0
12	D	4664	0	4484	57	0
13	P	541	0	220	2	0
14	L	783	0	811	10	0
15	K	754	0	716	3	0
16	J	806	0	772	1	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112434	961	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (961) 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)
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.26
4:B:764:GLN:O	4:B:766:ILE:N	1.79	1.12
4:B:750:PRO:O	4:B:752:ILE:N	1.89	1.05
4:B:3255:THR:OG1	4:B:3337:CYS:SG	2.13	1.02
2:C:2826:VAL:O	2:C:2829:ASP:N	1.96	0.97
4:B:902:ILE:HD11	4:B:1076:LEU:HD11	1.47	0.94
4:B:765:PHE:O	4:B:766:ILE:C	2.00	0.94
4:B:751:GLY:O	4:B:754:GLU:N	2.01	0.92
4:B:716:ASP:O	4:B:717:MET:C	2.11	0.88
4:B:750:PRO:O	4:B:751:GLY:C	2.09	0.88
9:N:38:TYR:CB	9:N:75:GLN:HE22	1.89	0.85
2:C:1014:ILE:HD11	2:C:1037:LEU:HD12	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2887:LEU:HD13	4:B:3020:LEU:HD11	1.62	0.82
2:C:2659:ALA:HB1	2:C:2858:VAL:HG22	1.65	0.79
4:B:660:LEU:CB	4:B:755:ILE:HD12	2.13	0.79
2:C:2066:GLN:HE21	2:C:2066:GLN:HA	1.48	0.79
4:B:349:ASN:HA	4:B:416:LEU:HD21	1.64	0.78
9:N:76:THR:HG21	11:E:39:GLN:HE22	1.47	0.78
4:B:715:LEU:O	4:B:716:ASP:C	2.22	0.77
2:C:10:LEU:HD12	2:C:349:LEU:HD23	1.66	0.77
12:D:397:ASP:HB3	12:D:398:PRO:HD3	1.67	0.77
2:C:2687:ALA:HB1	2:C:2830:VAL:HG22	1.66	0.76
1:A:1016:PHE:CZ	1:A:1069:TYR:HB2	2.22	0.75
4:B:993:TYR:OH	4:B:1067:ILE:HG21	1.88	0.74
4:B:3253:ILE:O	4:B:3253:ILE:HG22	1.88	0.73
1:A:933:VAL:HG11	1:A:944:LEU:HD12	1.68	0.73
2:C:2613:THR:HG21	2:C:3176:LEU:HD22	1.70	0.73
2:C:2717:ALA:HB1	2:C:2803:MET:SD	2.29	0.73
11:E:395:VAL:CG2	11:E:402:ILE:HD12	2.18	0.72
2:C:2812:GLY:O	2:C:2815:SER:N	2.23	0.71
4:B:2621:ILE:HG23	4:B:2667:LEU:CD1	2.20	0.71
2:C:898:TRP:O	2:C:902:LEU:HD13	1.90	0.71
2:C:2766:GLU:O	2:C:2769:LEU:N	2.23	0.71
4:B:719:VAL:O	4:B:720:ASP:C	2.29	0.70
1:A:3212:VAL:HG13	1:A:3335:TRP:NE1	2.06	0.70
2:C:2617:VAL:CG1	2:C:2900:VAL:HG22	2.21	0.70
4:B:751:GLY:O	4:B:753:GLU:N	2.24	0.69
4:B:764:GLN:O	4:B:767:SER:N	2.26	0.69
2:C:2617:VAL:HG22	2:C:3183:ILE:HD13	1.74	0.69
4:B:660:LEU:CB	4:B:752:ILE:HG23	2.22	0.69
4:B:2696:LEU:HD12	4:B:2707:ALA:HB2	1.74	0.69
4:B:3331:TYR:O	4:B:3334:SER:N	2.26	0.69
2:C:2812:GLY:O	2:C:2815:SER:OG	2.08	0.68
1:A:3583:ILE:HG22	1:A:3627:CYS:HA	1.74	0.68
1:A:1500:THR:HG23	1:A:1566:GLN:HE22	1.58	0.68
4:B:3273:ASP:O	4:B:3276:VAL:N	2.24	0.68
9:N:38:TYR:CB	9:N:75:GLN:NE2	2.57	0.68
2:C:3970:LEU:HD23	2:C:3990:LEU:HD21	1.75	0.68
1:A:1016:PHE:CZ	1:A:1076:LEU:HD12	2.30	0.67
2:C:972:LEU:HD21	2:C:1017:MET:CE	2.25	0.67
2:C:2177:ILE:HG22	2:C:2233:PRO:HA	1.77	0.67
2:C:2790:ASN:CB	2:C:2821:VAL:HG22	2.25	0.66
1:A:751:LEU:HG	1:A:886:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2443:CYS:O	1:A:2443:CYS:SG	2.53	0.66
2:C:834:VAL:HG22	2:C:881:ILE:HD11	1.78	0.66
11:E:395:VAL:HG21	11:E:402:ILE:HD12	1.78	0.66
2:C:39:LEU:HD12	2:C:345:TRP:CZ2	2.31	0.66
4:B:1102:LEU:HD23	4:B:1105:GLN:HB2	1.78	0.65
4:B:4168:VAL:HG11	4:B:4189:ILE:HG21	1.77	0.65
1:A:1631:PHE:HB2	1:A:1634:ILE:CG2	2.27	0.65
4:B:904:LEU:HG	4:B:1083:MET:HB2	1.77	0.65
4:B:3289:ALA:O	4:B:3292:ASP:HB2	1.97	0.65
1:A:1013:VAL:HG13	1:A:1076:LEU:HD11	1.78	0.65
1:A:1634:ILE:HD13	1:A:1656:ILE:HG23	1.78	0.65
2:C:2801:GLU:O	2:C:2804:ALA:HB3	1.96	0.64
4:B:2157:LEU:HB2	19:B:4701:ATP:N1	2.12	0.64
5:I:94:LEU:HD21	12:D:195:ILE:HD13	1.79	0.64
1:A:1926:PHE:HB3	1:A:1974:ILE:HG23	1.80	0.64
4:B:3332:ALA:O	4:B:3335:LYS:N	2.31	0.64
1:A:3128:THR:HG22	1:A:3422:LEU:HB3	1.80	0.64
1:A:3702:SER:CB	1:A:3712:LEU:HD11	2.28	0.64
4:B:871:ILE:HD11	4:B:944:ILE:HD11	1.79	0.63
1:A:3212:VAL:HG13	1:A:3335:TRP:CD1	2.34	0.63
1:A:2418:ILE:HG22	1:A:2419:PRO:HD2	1.80	0.63
4:B:3878:ILE:HD11	4:B:3887:ALA:HB2	1.81	0.63
2:C:1081:ILE:HD11	2:C:1117:GLN:CB	2.29	0.62
12:D:167:ASN:O	12:D:168:TYR:CD2	2.51	0.62
1:A:3290:LEU:HD22	1:A:3335:TRP:CZ2	2.33	0.62
2:C:1880:VAL:HA	2:C:1883:ILE:HD12	1.79	0.62
7:G:107:THR:HG21	7:G:137:VAL:HG11	1.81	0.62
1:A:2171:THR:O	1:A:2175:THR:HG23	1.99	0.62
1:A:1392:ASN:O	1:A:1396:PRO:N	2.33	0.62
4:B:764:GLN:O	4:B:765:PHE:O	2.17	0.62
4:B:2984:VAL:HG13	4:B:3004:LEU:HD12	1.81	0.62
2:C:2722:VAL:HG12	2:C:2813:ILE:HD13	1.82	0.61
2:C:2790:ASN:HB2	2:C:2821:VAL:HG22	1.82	0.61
11:E:531:ARG:O	11:E:535:LYS:N	2.31	0.61
12:D:397:ASP:CB	12:D:398:PRO:HD3	2.29	0.61
1:A:4287:THR:HG22	1:A:4549:ILE:HD12	1.82	0.61
1:A:1458:MET:SD	1:A:1549:MET:HA	2.39	0.61
2:C:1718:VAL:HG21	2:C:1737:LEU:HD21	1.82	0.61
4:B:3314:ILE:CD1	4:B:3344:VAL:HG21	2.30	0.61
5:I:51:ALA:HB1	5:I:52:PRO:CD	2.30	0.61
8:F:80:ARG:NH2	8:F:103:CYS:SG	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:PHE:CZ	1:A:1508:LEU:HD21	2.36	0.61
1:A:1806:PHE:CD1	1:A:4194:VAL:HG22	2.36	0.61
5:I:24:ILE:HD11	12:D:207:ALA:HB1	1.82	0.61
1:A:91:LYS:CB	4:B:136:PRO:CB	2.79	0.60
4:B:723:ASN:O	4:B:726:LYS:N	2.34	0.60
4:B:3327:ALA:O	4:B:3329:GLN:N	2.34	0.60
4:B:3525:ILE:HG22	4:B:3644:ILE:HD13	1.82	0.60
1:A:4056:ILE:HD11	1:A:4072:LEU:HD21	1.82	0.60
5:I:51:ALA:HB1	5:I:52:PRO:HD2	1.83	0.60
10:O:102:LEU:HD12	12:D:75:LEU:HD12	1.84	0.60
11:E:423:GLY:HA2	11:E:505:ILE:HD12	1.82	0.60
4:B:1102:LEU:HA	4:B:1105:GLN:HB2	1.83	0.60
12:D:352:CYS:SG	12:D:402:VAL:N	2.74	0.60
1:A:3533:PRO:HD3	1:A:3648:THR:HG22	1.83	0.60
4:B:764:GLN:C	4:B:766:ILE:N	2.51	0.60
1:A:1396:PRO:O	1:A:1400:TYR:N	2.34	0.60
1:A:3914:ASN:O	1:A:3950:ARG:NH1	2.34	0.60
2:C:2738:ILE:HG22	2:C:2746:PRO:HD3	1.83	0.60
4:B:3528:CYS:SG	4:B:3642:THR:HG21	2.42	0.59
4:B:765:PHE:O	4:B:766:ILE:O	2.19	0.59
4:B:1061:GLN:HE21	4:B:1091:VAL:HG12	1.67	0.59
4:B:3327:ALA:HA	4:B:3334:SER:HB2	1.84	0.59
2:C:1333:VAL:HG12	2:C:1340:GLN:HE21	1.68	0.59
4:B:4206:ARG:NH2	4:B:4573:ILE:HD13	2.17	0.59
1:A:539:PHE:HA	1:A:544:TYR:CB	2.33	0.59
1:A:1066:VAL:HB	1:A:1069:TYR:CE1	2.38	0.59
1:A:1789:VAL:HG21	1:A:2010:VAL:HG22	1.83	0.59
1:A:3895:GLU:O	1:A:3899:LEU:HD13	2.02	0.59
2:C:1186:THR:O	2:C:1188:LEU:N	2.35	0.59
4:B:2174:LEU:HD11	4:B:2302:ILE:HD11	1.85	0.59
2:C:2217:ASN:HD22	2:C:2247:THR:HG23	1.68	0.59
4:B:3326:MET:O	4:B:3327:ALA:C	2.40	0.59
11:E:306:ILE:HG23	11:E:343:LEU:HD12	1.85	0.59
1:A:1632:ASP:HB2	1:A:1892:PHE:CD1	2.37	0.59
2:C:2722:VAL:CG1	2:C:2813:ILE:HD13	2.33	0.59
2:C:2821:VAL:O	2:C:2825:ASP:N	2.36	0.58
4:B:829:VAL:HG11	4:B:940:ILE:HG23	1.83	0.58
4:B:3081:ASN:HD21	4:B:3484:LYS:HD3	1.69	0.58
4:B:3324:LYS:O	4:B:3327:ALA:N	2.37	0.58
1:A:2042:ARG:HG3	1:A:2278:ASN:HA	1.84	0.58
4:B:3764:LEU:HD11	4:B:3816:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:102:LEU:CD1	12:D:75:LEU:HD12	2.34	0.58
4:B:3472:LEU:O	4:B:3476:THR:OG1	2.21	0.58
1:A:1031:ILE:HG21	1:A:1095:GLN:HG3	1.85	0.58
2:C:1081:ILE:HD11	2:C:1117:GLN:HB3	1.86	0.58
2:C:3732:HIS:CG	2:C:3757:LEU:HD12	2.39	0.58
4:B:3153:LEU:HD13	4:B:3707:LEU:HD11	1.83	0.58
2:C:1559:LEU:HD23	2:C:1607:LEU:HD21	1.86	0.58
2:C:2555:LEU:HD22	2:C:2953:ASN:HD22	1.68	0.58
4:B:2740:ASN:O	4:B:2742:ARG:N	2.37	0.57
10:O:98:ALA:HA	12:D:107:VAL:HA	1.86	0.57
1:A:3223:LEU:HD11	1:A:3332:ILE:CD1	2.34	0.57
4:B:773:VAL:O	4:B:777:PHE:HB2	2.05	0.57
1:A:1013:VAL:HG12	1:A:1017:LEU:HD12	1.86	0.57
1:A:4599:CYS:O	1:A:4599:CYS:SG	2.63	0.57
2:C:2631:ALA:HB1	2:C:2886:ALA:HB1	1.85	0.57
1:A:936:GLN:HA	1:A:1081:ILE:CB	2.34	0.57
1:A:3223:LEU:HD21	1:A:3332:ILE:CD1	2.35	0.57
4:B:1110:GLN:O	4:B:1114:LEU:HG	2.05	0.57
4:B:2703:ALA:HB2	4:B:2763:ASP:HB2	1.87	0.57
1:A:2786:CYS:HB3	1:A:2850:LEU:HD22	1.87	0.57
2:C:2534:VAL:HG21	2:C:2586:THR:HG22	1.86	0.57
12:D:571:LEU:HB3	12:D:647:TYR:CE2	2.40	0.57
1:A:2033:LEU:CD2	1:A:4498:LEU:HD23	2.34	0.57
4:B:2264:ASP:O	4:B:2625:ARG:NH2	2.38	0.56
4:B:2040:LEU:CD1	4:B:2083:LEU:HD22	2.35	0.56
4:B:3267:ILE:HG23	4:B:3271:ASP:HB2	1.88	0.56
2:C:136:ALA:HB2	2:C:168:ASN:HA	1.87	0.56
4:B:4370:ILE:HD13	4:B:4384:MET:HB3	1.87	0.56
17:M:65:ILE:HD13	17:M:85:TRP:CH2	2.40	0.56
4:B:3829:VAL:HG11	4:B:3946:ILE:HD13	1.86	0.56
1:A:1065:ILE:HG21	1:A:1082:CYS:SG	2.46	0.56
4:B:3267:ILE:HD12	4:B:3279:LYS:CD	2.35	0.56
4:B:3984:PHE:CE2	4:B:4076:LEU:HD11	2.40	0.56
1:A:1525:PHE:HB2	1:A:1541:PHE:HD2	1.70	0.56
2:C:1900:TYR:O	2:C:1903:VAL:N	2.38	0.56
9:N:38:TYR:O	9:N:75:GLN:NE2	2.39	0.56
1:A:1544:ILE:HG12	1:A:1580:LYS:HG2	1.88	0.55
1:A:2216:TRP:O	1:A:2220:ASN:ND2	2.38	0.55
4:B:3085:VAL:HG21	4:B:3456:ALA:HB1	1.89	0.55
4:B:3984:PHE:CD2	4:B:4076:LEU:HD11	2.40	0.55
12:D:294:GLN:HE21	12:D:297:LYS:HE2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ILE:HD12	2:C:116:THR:HG22	1.88	0.55
2:C:2659:ALA:CB	2:C:2858:VAL:HG22	2.35	0.55
4:B:1477:LEU:HD22	4:B:1508:LEU:HD22	1.89	0.55
14:L:42:ILE:HD12	14:L:98:LEU:HD12	1.89	0.55
1:A:3018:LEU:O	1:A:3022:CYS:SG	2.64	0.55
1:A:3709:ASP:HB3	1:A:3712:LEU:HD12	1.87	0.55
2:C:2790:ASN:HB3	2:C:2821:VAL:HG22	1.88	0.55
1:A:1631:PHE:CZ	1:A:1687:LEU:HD22	2.41	0.55
1:A:2030:LEU:HB2	1:A:2101:ILE:HD13	1.87	0.55
2:C:3460:ASN:N	2:C:3460:ASN:HD22	2.05	0.55
1:A:1500:THR:O	1:A:1504:VAL:HG23	2.06	0.55
1:A:3099:TYR:HA	1:A:3451:THR:HG21	1.88	0.55
2:C:881:ILE:O	2:C:881:ILE:HG22	2.07	0.55
2:C:913:MET:CE	2:C:959:THR:HG22	2.37	0.55
1:A:942:VAL:HG21	1:A:1021:THR:HG22	1.89	0.55
4:B:319:PRO:CB	11:E:552:ILE:HG22	2.36	0.55
4:B:3257:ARG:O	4:B:3258:VAL:C	2.45	0.55
12:D:75:LEU:HD23	12:D:75:LEU:N	2.22	0.55
2:C:2822:LYS:O	2:C:2826:VAL:HG23	2.07	0.55
12:D:174:GLN:HA	17:M:62:GLY:HA2	1.89	0.55
1:A:3220:ILE:HD11	1:A:3290:LEU:HD12	1.88	0.54
2:C:955:ILE:O	2:C:959:THR:HG23	2.07	0.54
4:B:1937:ALA:HB2	4:B:1969:GLN:HE22	1.72	0.54
9:N:90:ASP:O	9:N:93:THR:OG1	2.25	0.54
4:B:1484:LEU:HD12	4:B:1508:LEU:HD12	1.90	0.54
1:A:4125:ASN:HD21	1:A:4187:LEU:HG	1.73	0.54
1:A:4505:THR:HG22	1:A:4558:VAL:HG12	1.90	0.54
2:C:1541:LEU:HD13	2:C:1584:LEU:HD22	1.88	0.54
4:B:162:TYR:CB	4:B:176:LEU:CB	2.85	0.54
4:B:3902:TYR:O	4:B:3934:ARG:NH1	2.40	0.54
4:B:3658:ILE:HD11	4:B:3748:ARG:HE	1.72	0.54
5:I:90:GLN:HB2	5:I:93:THR:HG21	1.90	0.54
1:A:1504:VAL:HG22	1:A:1565:CYS:HB3	1.89	0.54
2:C:972:LEU:HD21	2:C:1017:MET:SD	2.48	0.54
2:C:2007:LEU:HD11	2:C:2128:MET:HE2	1.89	0.54
4:B:3020:LEU:HD13	4:B:3022:PHE:CZ	2.42	0.54
4:B:3586:ILE:HG21	4:B:3594:LEU:HD11	1.88	0.54
4:B:3314:ILE:HD12	4:B:3344:VAL:HG21	1.90	0.54
2:C:2008:LEU:HD23	2:C:2150:ILE:HD11	1.89	0.54
4:B:2846:LEU:HD11	4:B:2872:VAL:HG11	1.90	0.54
14:L:80:LYS:HB2	17:M:60:ASN:HD21	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3124:ILE:O	1:A:3128:THR:HG23	2.07	0.54
1:A:3500:ILE:HD12	1:A:3515:ILE:HG23	1.89	0.54
4:B:718:ILE:HD11	4:B:773:VAL:HG21	1.89	0.54
1:A:2745:LEU:HD11	1:A:2754:VAL:HG21	1.89	0.53
1:A:3913:LYS:O	1:A:3947:ARG:NH1	2.40	0.53
7:G:149:GLN:HE22	12:D:252:VAL:HA	1.74	0.53
12:D:364:ALA:HB2	12:D:404:TRP:NE1	2.23	0.53
4:B:2122:PHE:CE2	4:B:2126:ILE:HD11	2.42	0.53
4:B:2621:ILE:HG23	4:B:2667:LEU:HD13	1.90	0.53
11:E:384:LEU:HD23	11:E:417:TRP:CE2	2.43	0.53
1:A:3170:GLY:HA2	1:A:3380:ILE:HD13	1.91	0.53
2:C:214:LEU:C	2:C:214:LEU:HD22	2.29	0.53
1:A:1016:PHE:CE2	1:A:1069:TYR:HB2	2.43	0.53
1:A:3235:TYR:OH	1:A:3258:PHE:CD1	2.60	0.53
12:D:66:LEU:HB2	12:D:70:MET:HB2	1.91	0.53
1:A:2418:ILE:CG2	1:A:2428:VAL:HG22	2.38	0.53
1:A:3449:LEU:HD21	1:A:3474:VAL:HG22	1.90	0.53
4:B:716:ASP:O	4:B:719:VAL:N	2.41	0.53
4:B:1102:LEU:HD23	4:B:1105:GLN:CB	2.39	0.53
1:A:4234:PHE:O	1:A:4236:TYR:N	2.42	0.53
4:B:3085:VAL:HG23	4:B:3477:TRP:CE2	2.43	0.53
2:C:912:SER:HA	2:C:966:LEU:HD22	1.91	0.53
2:C:1207:LEU:HD13	2:C:1214:TYR:CE1	2.44	0.53
1:A:1445:PHE:CE1	1:A:1561:VAL:HG13	2.43	0.53
1:A:2411:LEU:HD12	1:A:2428:VAL:HG21	1.90	0.53
4:B:744:MET:HE1	4:B:773:VAL:HG23	1.90	0.53
12:D:89:TYR:CD1	15:K:56:PRO:HB3	2.44	0.53
2:C:2128:MET:HE1	2:C:2137:VAL:HG21	1.90	0.53
2:C:4084:ILE:HD11	2:C:4106:PRO:HG3	1.91	0.53
2:C:1017:MET:HE2	2:C:1030:VAL:HB	1.91	0.52
2:C:4051:THR:HG21	2:C:4143:ASN:HD22	1.74	0.52
2:C:4077:LEU:HD13	2:C:4105:MET:HG2	1.90	0.52
4:B:361:LYS:HA	4:B:477:ILE:HG23	1.90	0.52
4:B:569:VAL:HG13	4:B:578:LEU:HD11	1.91	0.52
12:D:519:ALA:HB1	12:D:545:VAL:CG1	2.39	0.52
1:A:2567:VAL:HG22	1:A:2573:GLN:HG3	1.90	0.52
2:C:4017:LEU:HD21	2:C:4022:LEU:HD11	1.91	0.52
4:B:769:SER:O	4:B:773:VAL:N	2.41	0.52
4:B:2608:ASN:ND2	4:B:2655:ASN:O	2.42	0.52
4:B:3332:ALA:O	4:B:3333:ALA:C	2.48	0.52
1:A:1129:ILE:HD11	1:A:1211:GLU:HB3	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:90:ILE:HD11	2:C:96:LEU:HD23	1.90	0.52
4:B:2863:VAL:HG21	4:B:3059:VAL:HA	1.91	0.52
1:A:1634:ILE:HD13	1:A:1656:ILE:CG2	2.39	0.52
1:A:3220:ILE:CD1	1:A:3290:LEU:HD12	2.40	0.52
2:C:2896:ALA:O	2:C:2900:VAL:HG23	2.10	0.52
1:A:1482:ASN:HA	1:A:1487:VAL:HG11	1.92	0.52
1:A:1825:ILE:HD12	1:A:1889:LEU:HA	1.91	0.52
1:A:2935:LEU:HD12	1:A:2938:ILE:HD11	1.91	0.52
2:C:2096:ILE:HD11	2:C:2141:TYR:CD2	2.45	0.52
2:C:3227:ALA:HA	2:C:3393:ILE:HG22	1.91	0.52
4:B:1212:ILE:HG22	4:B:1213:PRO:HD3	1.91	0.52
1:A:2676:TRP:CD2	1:A:2699:LEU:HD21	2.45	0.52
4:B:533:ARG:HB3	4:B:534:PRO:CD	2.39	0.52
4:B:1109:THR:O	4:B:1113:LEU:HG	2.10	0.52
4:B:1117:ILE:HG12	4:B:1190:ILE:HD11	1.91	0.52
4:B:3331:TYR:O	4:B:3332:ALA:C	2.47	0.52
1:A:1052:LEU:HB3	1:A:1166:TYR:CE2	2.45	0.52
2:C:2177:ILE:CG2	2:C:2233:PRO:HA	2.39	0.52
4:B:2150:THR:HG22	4:B:2203:ASN:HD22	1.75	0.52
1:A:1487:VAL:HA	1:A:1490:PHE:CZ	2.44	0.52
1:A:3229:PRO:HB2	1:A:3233:ILE:HG23	1.92	0.52
4:B:4545:CYS:SG	4:B:4579:ILE:HD13	2.50	0.52
12:D:509:ASN:HD21	12:D:512:HIS:HB3	1.74	0.52
4:B:825:LYS:O	4:B:829:VAL:HG23	2.10	0.52
4:B:3020:LEU:HD13	4:B:3022:PHE:CE2	2.45	0.52
4:B:3789:THR:HG22	4:B:3803:ASN:HD22	1.75	0.52
9:N:88:TYR:HA	11:E:23:THR:HG22	1.91	0.52
10:O:38:ILE:HG22	10:O:67:LEU:HD11	1.91	0.52
17:M:65:ILE:HG21	17:M:85:TRP:CE2	2.45	0.52
2:C:2066:GLN:HE21	2:C:2066:GLN:CA	2.17	0.52
2:C:2659:ALA:HB1	2:C:2858:VAL:CG2	2.39	0.52
2:C:2751:TRP:O	2:C:2754:SER:HB3	2.10	0.52
5:I:12:ILE:HG23	7:G:120:THR:HG23	1.91	0.52
7:G:99:ILE:HG23	7:G:103:ILE:HD12	1.91	0.52
10:O:76:VAL:N	10:O:77:PRO:CD	2.73	0.52
1:A:1609:THR:HG21	1:A:1629:LYS:HE3	1.91	0.51
1:A:3702:SER:HB3	1:A:3712:LEU:HD11	1.91	0.51
4:B:1149:ASP:O	4:B:1153:VAL:N	2.43	0.51
1:A:1422:SER:HB2	1:A:1486:HIS:CE1	2.45	0.51
1:A:2676:TRP:CE2	1:A:2699:LEU:HD21	2.45	0.51
1:A:3170:GLY:HA3	1:A:3380:ILE:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:765:PHE:O	4:B:767:SER:N	2.43	0.51
8:F:26:PHE:CE2	8:F:52:VAL:HG11	2.46	0.51
1:A:3132:ASN:N	1:A:3419:ILE:HD11	2.25	0.51
2:C:2693:GLN:O	2:C:2696:SER:OG	2.20	0.51
4:B:1069:THR:HB	4:B:1070:PRO:HD2	1.92	0.51
4:B:2696:LEU:HD23	4:B:2699:ILE:HD12	1.91	0.51
4:B:2695:HIS:CG	4:B:2695:HIS:O	2.63	0.51
1:A:935:VAL:HG22	1:A:1017:LEU:HD21	1.92	0.51
2:C:1856:TYR:HA	2:C:1934:TRP:HH2	1.75	0.51
4:B:716:ASP:O	4:B:718:ILE:N	2.43	0.51
4:B:721:ASN:OD1	4:B:777:PHE:CE2	2.63	0.51
4:B:979:ILE:HD12	4:B:1075:TRP:CZ3	2.45	0.51
4:B:3694:LEU:HD22	4:B:3715:ASN:HD22	1.76	0.51
1:A:2564:MET:N	1:A:2565:PRO:HD2	2.26	0.51
1:A:3533:PRO:CD	1:A:3648:THR:HG22	2.41	0.51
4:B:871:ILE:HG21	4:B:959:ILE:HD11	1.93	0.51
4:B:1641:LEU:HD13	4:B:1662:MET:HB2	1.93	0.51
4:B:2711:VAL:HA	4:B:2714:THR:HG22	1.91	0.51
7:G:71:LYS:HG3	7:G:72:THR:HG23	1.91	0.51
12:D:120:SER:OG	12:D:123:TYR:N	2.38	0.51
1:A:3163:SER:HA	1:A:3387:LEU:HD13	1.91	0.51
2:C:834:VAL:CG2	2:C:881:ILE:HD11	2.40	0.51
2:C:1864:ILE:HD11	2:C:1910:ILE:HG23	1.91	0.51
2:C:4138:PHE:CE1	2:C:4141:THR:HA	2.46	0.51
4:B:804:ARG:NH1	4:B:898:PRO:O	2.44	0.51
4:B:3085:VAL:HG23	4:B:3477:TRP:CZ2	2.45	0.51
2:C:2755:LEU:O	2:C:2758:MET:N	2.41	0.51
4:B:2005:ASN:N	4:B:2005:ASN:HD22	2.09	0.51
12:D:603:LEU:HD22	12:D:611:VAL:HG12	1.91	0.51
13:P:53:LEU:O	13:P:57:ILE:N	2.44	0.51
1:A:4240:VAL:HG11	1:A:4270:PRO:HG2	1.93	0.51
1:A:2490:LEU:HD11	1:A:2611:MET:HG2	1.93	0.50
1:A:3131:ILE:HD12	1:A:3422:LEU:HD11	1.93	0.50
4:B:591:TRP:CD1	11:E:411:TYR:OH	2.63	0.50
14:L:86:LEU:HD12	17:M:54:ASN:HB3	1.93	0.50
2:C:3064:ILE:HG13	2:C:3115:ILE:HD12	1.94	0.50
10:O:19:LEU:HA	10:O:22:LEU:HD21	1.91	0.50
1:A:1563:PRO:O	1:A:1567:ASN:N	2.44	0.50
1:A:1135:VAL:HG13	1:A:1201:TYR:OH	2.10	0.50
1:A:883:THR:HA	1:A:886:ILE:HD12	1.94	0.50
1:A:1634:ILE:HD11	1:A:1637:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3322:ALA:HB2	1:A:3333:LEU:HD12	1.94	0.50
4:B:3446:SER:HB2	4:B:3489:THR:HG23	1.94	0.50
4:B:4359:LEU:HD22	4:B:4404:ALA:HB2	1.94	0.50
11:E:42:GLN:HE22	14:L:91:ASN:ND2	2.09	0.50
1:A:675:ILE:HG22	1:A:686:VAL:HA	1.94	0.50
2:C:1296:ILE:HD11	2:C:1542:MET:SD	2.52	0.50
4:B:2099:ASP:HB2	4:B:2100:PRO:HD3	1.94	0.50
1:A:1183:LEU:C	1:A:1183:LEU:HD23	2.32	0.50
4:B:993:TYR:OH	4:B:1067:ILE:HD13	2.12	0.50
4:B:2619:SER:N	4:B:2620:PRO:HD2	2.27	0.50
12:D:545:VAL:HA	12:D:562:THR:HG22	1.94	0.50
4:B:715:LEU:O	4:B:717:MET:N	2.45	0.49
4:B:904:LEU:HG	4:B:1083:MET:CB	2.42	0.49
1:A:1126:VAL:HG21	1:A:1135:VAL:HG11	1.93	0.49
1:A:4583:TYR:HB3	1:A:4584:PRO:HD2	1.94	0.49
2:C:968:MET:HB2	2:C:1026:PHE:CZ	2.48	0.49
2:C:2659:ALA:HB1	2:C:2858:VAL:HG13	1.94	0.49
4:B:669:ILE:CD1	4:B:752:ILE:HD11	2.42	0.49
4:B:2267:ILE:HG22	4:B:2271:TRP:HZ3	1.78	0.49
1:A:1868:GLY:O	1:A:1973:PHE:HA	2.11	0.49
2:C:1221:THR:O	2:C:1225:THR:HG23	2.12	0.49
2:C:1989:THR:HG23	2:C:2019:LEU:HD22	1.94	0.49
1:A:3331:GLY:O	1:A:3335:TRP:N	2.45	0.49
2:C:972:LEU:HD13	2:C:1029:GLU:HG2	1.94	0.49
4:B:558:VAL:HG11	4:B:599:ILE:HD11	1.94	0.49
12:D:299:VAL:HG11	12:D:605:GLY:HA3	1.93	0.49
12:D:519:ALA:HB1	12:D:545:VAL:HG12	1.94	0.49
1:A:3248:LEU:HB2	3:Q:104:TYR:CE1	2.48	0.49
2:C:1047:LEU:HG	2:C:1111:LEU:HD11	1.94	0.49
2:C:2002:VAL:HG12	2:C:2002:VAL:O	2.13	0.49
2:C:2617:VAL:CG2	2:C:3183:ILE:HD13	2.40	0.49
9:N:89:GLN:HG2	9:N:94:ASP:HB2	1.94	0.49
1:A:2793:VAL:HG23	1:A:2804:ALA:HB2	1.95	0.49
1:A:2840:VAL:HG22	18:A:4901:ADP:HN62	1.78	0.49
4:B:1128:PRO:HG2	4:B:1131:HIS:CG	2.48	0.49
2:C:2212:LEU:HD11	18:C:4401:ADP:H8	1.77	0.49
4:B:3223:ALA:HB1	4:B:3349:ILE:HD13	1.94	0.49
11:E:41:VAL:HG22	11:E:42:GLN:HG3	1.95	0.49
1:A:1915:VAL:HA	1:A:1970:VAL:HG21	1.94	0.49
4:B:696:THR:HG22	4:B:697:THR:HG23	1.95	0.49
1:A:1522:GLU:HG3	1:A:1523:PRO:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2117:GLU:HG2	1:A:2141:ILE:HD11	1.94	0.49
1:A:3691:LEU:HB3	1:A:3719:THR:HG22	1.94	0.49
1:A:3748:ARG:HB3	1:A:3749:PRO:HD3	1.95	0.49
4:B:2936:ILE:HG22	4:B:3012:ILE:HD13	1.95	0.48
1:A:3242:VAL:HA	1:A:3248:LEU:HD11	1.95	0.48
2:C:2709:ALA:HA	2:C:2758:MET:SD	2.53	0.48
4:B:1075:TRP:CE3	4:B:1076:LEU:HB3	2.48	0.48
4:B:1708:ALA:HA	4:B:1711:TRP:NE1	2.28	0.48
4:B:2769:ARG:CD	4:B:2836:GLN:HE22	2.26	0.48
4:B:1212:ILE:HB	4:B:1213:PRO:HD2	1.94	0.48
4:B:1666:ASP:HB2	4:B:1870:ASN:HD21	1.79	0.48
4:B:3245:LEU:O	4:B:3247:SER:N	2.46	0.48
9:N:76:THR:CG2	11:E:39:GLN:HE22	2.23	0.48
1:A:4461:LEU:HD21	1:A:4516:ILE:HG21	1.95	0.48
2:C:2128:MET:HE1	2:C:2137:VAL:CG2	2.42	0.48
2:C:2740:ILE:HG22	2:C:2741:ASP:H	1.78	0.48
4:B:1058:LYS:HG3	4:B:1166:GLU:O	2.12	0.48
4:B:1897:GLY:O	4:B:2001:PHE:HA	2.14	0.48
4:B:2769:ARG:HD2	4:B:2836:GLN:HE22	1.79	0.48
8:F:87:TYR:HB3	8:F:98:LEU:HD11	1.94	0.48
11:E:133:PHE:HZ	12:D:360:ALA:HB3	1.78	0.48
1:A:2938:ILE:HD12	1:A:2999:LEU:HD21	1.95	0.48
2:C:1188:LEU:HD21	2:C:1218:VAL:HG22	1.94	0.48
2:C:2734:PHE:CE2	2:C:2767:LYS:HG3	2.49	0.48
4:B:1944:SER:HA	4:B:1998:VAL:HG11	1.96	0.48
2:C:1081:ILE:HD11	2:C:1117:GLN:HB2	1.96	0.48
2:C:2800:PRO:HG3	2:C:2818:VAL:HG21	1.95	0.48
2:C:2826:VAL:O	2:C:2828:GLN:N	2.47	0.48
4:B:4348:VAL:HG21	4:B:4453:ALA:HB2	1.96	0.48
1:A:1889:LEU:HD12	1:A:1920:TRP:CZ2	2.49	0.48
2:C:2687:ALA:HB1	2:C:2830:VAL:CG2	2.40	0.48
4:B:2299:MET:HE3	4:B:2300:ARG:O	2.13	0.48
4:B:4359:LEU:HD22	4:B:4404:ALA:CB	2.43	0.48
1:A:3223:LEU:HD11	1:A:3332:ILE:HD11	1.94	0.48
6:H:70:THR:HG23	11:E:68:THR:HB	1.95	0.48
12:D:87:THR:HG22	12:D:98:THR:HA	1.95	0.48
2:C:1047:LEU:O	2:C:1051:GLN:HG3	2.14	0.48
2:C:2734:PHE:HE2	2:C:2767:LYS:HG3	1.79	0.48
4:B:2308:LEU:HD23	4:B:2316:VAL:HG22	1.96	0.48
6:H:67:SER:O	11:E:72:GLY:HA2	2.14	0.48
1:A:2418:ILE:HG22	1:A:2419:PRO:CD	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:29:VAL:CG1	2:C:116:THR:HG21	2.44	0.48
2:C:214:LEU:O	2:C:231:ILE:HA	2.14	0.48
2:C:972:LEU:HD11	2:C:1017:MET:HE3	1.95	0.48
2:C:1262:TRP:CE2	2:C:1321:SER:HB2	2.49	0.48
2:C:1270:PHE:CG	2:C:1336:ALA:HB2	2.49	0.48
2:C:1385:ILE:HA	2:C:1388:THR:HG22	1.96	0.48
4:B:3657:PHE:O	4:B:3661:VAL:HG23	2.14	0.48
2:C:1060:LEU:HD21	2:C:1148:LEU:HD13	1.95	0.47
2:C:1856:TYR:CE2	2:C:1903:VAL:HG22	2.49	0.47
4:B:521:PHE:CE2	4:B:605:LYS:HB3	2.49	0.47
4:B:2804:ILE:O	4:B:2806:GLU:N	2.47	0.47
4:B:2987:VAL:HG12	4:B:2987:VAL:O	2.14	0.47
4:B:3236:LYS:N	4:B:3237:PRO:HD2	2.28	0.47
4:B:3350:PHE:HA	4:B:3353:VAL:HG12	1.95	0.47
4:B:3676:LEU:HD21	4:B:3733:ALA:HB2	1.95	0.47
4:B:3878:ILE:CD1	4:B:3887:ALA:HB2	2.43	0.47
1:A:1118:LEU:HD12	1:A:1142:ILE:HG13	1.96	0.47
1:A:2511:ASP:HB2	1:A:2514:LYS:HB2	1.96	0.47
1:A:3303:ILE:HD11	1:A:3340:TYR:CE2	2.48	0.47
2:C:4128:THR:HA	2:C:4163:MET:O	2.14	0.47
4:B:720:ASP:O	4:B:721:ASN:C	2.52	0.47
4:B:979:ILE:CD1	4:B:1075:TRP:CZ3	2.97	0.47
4:B:2040:LEU:HD13	4:B:2083:LEU:HD22	1.96	0.47
4:B:2210:TYR:HA	4:B:2260:TRP:O	2.14	0.47
4:B:2758:GLN:HE22	4:B:2834:TYR:H	1.62	0.47
2:C:2082:LEU:HD11	2:C:2096:ILE:CD1	2.44	0.47
2:C:2719:VAL:HG13	2:C:2720:PRO:HD3	1.94	0.47
2:C:2758:MET:O	2:C:2759:LYS:C	2.52	0.47
4:B:447:THR:OG1	4:B:448:LYS:N	2.47	0.47
4:B:883:ASN:HA	4:B:886:ILE:HG22	1.95	0.47
4:B:915:PRO:HA	4:B:925:THR:HA	1.96	0.47
9:N:84:GLN:HB2	10:O:64:VAL:HG21	1.95	0.47
2:C:3412:HIS:HA	2:C:3415:ILE:HD12	1.96	0.47
4:B:938:PHE:HB3	4:B:956:LEU:HD13	1.95	0.47
5:I:75:TRP:CE3	5:I:109:LYS:HB2	2.49	0.47
1:A:1634:ILE:HD11	1:A:1637:VAL:CG2	2.44	0.47
1:A:3577:THR:HG22	1:A:3622:LYS:HB2	1.95	0.47
2:C:2688:GLN:N	2:C:2689:PRO:CD	2.78	0.47
2:C:2795:MET:N	2:C:2796:PRO:CD	2.78	0.47
5:I:97:MET:O	5:I:105:VAL:HB	2.15	0.47
2:C:2617:VAL:HG22	2:C:3183:ILE:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2730:LEU:HD23	2:C:2738:ILE:HD13	1.97	0.47
2:C:2740:ILE:HG13	2:C:2744:LYS:HB3	1.97	0.47
4:B:3740:ILE:O	4:B:3744:ARG:N	2.48	0.47
4:B:3863:LEU:N	4:B:3863:LEU:HD22	2.29	0.47
10:O:30:TYR:N	10:O:31:PRO:CD	2.78	0.47
1:A:766:GLY:HA3	1:A:780:TYR:CE1	2.50	0.47
1:A:1108:LEU:O	1:A:1112:THR:N	2.42	0.47
1:A:1487:VAL:HG23	1:A:1490:PHE:CE1	2.50	0.47
1:A:1687:LEU:C	1:A:1687:LEU:HD23	2.35	0.47
1:A:1760:HIS:O	1:A:1764:LEU:HG	2.15	0.47
1:A:2866:VAL:HG11	1:A:3026:TRP:CZ3	2.50	0.47
2:C:10:LEU:HD11	2:C:67:CYS:HB3	1.96	0.47
2:C:39:LEU:HD23	2:C:83:CYS:SG	2.55	0.47
2:C:306:LEU:HD11	2:C:317:LYS:HG2	1.96	0.47
2:C:1864:ILE:HD11	2:C:1910:ILE:CG2	2.44	0.47
2:C:3151:LYS:CE	2:C:3217:ILE:HD11	2.45	0.47
2:C:4113:VAL:HG12	2:C:4114:PRO:HD2	1.97	0.47
4:B:898:PRO:HD3	4:B:1073:ILE:HG21	1.96	0.47
4:B:3255:THR:CB	4:B:3337:CYS:SG	3.02	0.47
4:B:4017:LEU:HD12	4:B:4044:ILE:HD13	1.97	0.47
11:E:423:GLY:N	11:E:501:GLU:OE1	2.47	0.47
2:C:58:PHE:CD2	2:C:71:GLN:HB3	2.50	0.47
2:C:884:ARG:HA	2:C:889:ILE:HD11	1.97	0.47
2:C:3938:LEU:HD12	2:C:3982:LYS:HD3	1.95	0.47
4:B:3284:MET:SD	4:B:3290:PHE:CD1	3.08	0.47
4:B:736:LEU:HD12	4:B:859:TYR:HB2	1.96	0.47
4:B:2115:VAL:HG12	4:B:2323:PHE:CE2	2.50	0.47
8:F:33:LEU:HD11	11:E:99:ILE:HG21	1.96	0.47
2:C:2738:ILE:HD12	2:C:2740:ILE:O	2.14	0.47
4:B:459:ILE:HG23	4:B:499:LEU:HD11	1.97	0.47
4:B:1819:SER:HA	4:B:1857:VAL:HG13	1.96	0.47
6:H:20:MET:O	6:H:24:VAL:HG23	2.15	0.47
1:A:1149:ILE:HG21	1:A:1187:TRP:CZ2	2.50	0.46
2:C:2770:ASN:O	2:C:2773:ASP:N	2.45	0.46
4:B:2890:GLY:HA3	4:B:3048:PHE:HB2	1.97	0.46
4:B:2897:GLN:HA	4:B:2947:MET:CE	2.46	0.46
4:B:2971:ILE:HG23	4:B:2974:LEU:HB2	1.98	0.46
4:B:3290:PHE:O	4:B:3293:LYS:N	2.48	0.46
1:A:2515:MET:HA	1:A:2553:LYS:O	2.16	0.46
2:C:3072:ILE:HD12	2:C:3102:LEU:HD11	1.97	0.46
4:B:721:ASN:OD1	4:B:777:PHE:CD2	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1114:LEU:HA	4:B:1117:ILE:HD12	1.96	0.46
7:G:145:LEU:HD22	12:D:248:MET:HG3	1.96	0.46
1:A:61:GLU:CB	1:A:98:ILE:O	2.63	0.46
1:A:92:ALA:O	1:A:124:THR:CB	2.63	0.46
2:C:2698:LEU:HD21	2:C:2820:ILE:CA	2.46	0.46
3:Q:43:GLY:HA3	3:Q:67:SER:CB	2.45	0.46
4:B:591:TRP:HD1	11:E:411:TYR:OH	1.97	0.46
4:B:1620:ILE:HG23	4:B:1630:VAL:HG13	1.97	0.46
4:B:2200:SER:O	4:B:2204:SER:N	2.48	0.46
4:B:3887:ALA:O	4:B:3890:LEU:N	2.48	0.46
5:I:12:ILE:HG21	7:G:119:PRO:HG2	1.98	0.46
8:F:74:ILE:HD12	8:F:77:ILE:HD11	1.97	0.46
11:E:75:HIS:CG	11:E:75:HIS:O	2.68	0.46
11:E:152:LEU:HD22	11:E:486:THR:HG22	1.97	0.46
12:D:564:ASP:HA	12:D:590:LEU:HD13	1.98	0.46
1:A:1113:GLU:O	1:A:1116:LYS:N	2.49	0.46
1:A:2723:ILE:HG21	1:A:2776:LYS:HE2	1.98	0.46
1:A:4422:ASP:HB2	1:A:4423:PRO:HD2	1.96	0.46
2:C:29:VAL:HG11	2:C:116:THR:HG21	1.97	0.46
4:B:447:THR:OG1	4:B:513:ASP:HB3	2.14	0.46
4:B:3241:GLU:O	4:B:3244:ASN:N	2.49	0.46
4:B:3268:THR:HG22	4:B:3269:LEU:HD12	1.97	0.46
16:J:68:MET:HB3	16:J:76:TRP:CD1	2.51	0.46
1:A:1667:ILE:HD12	1:A:1838:PHE:CD1	2.51	0.46
1:A:3257:VAL:HG21	1:A:3266:VAL:HG13	1.98	0.46
1:A:3286:PHE:CE2	1:A:3290:LEU:HD11	2.50	0.46
2:C:2532:GLU:N	2:C:2533:PRO:HD2	2.31	0.46
2:C:2708:GLN:HE21	2:C:2809:ALA:HA	1.80	0.46
4:B:1483:ASP:O	4:B:1487:MET:N	2.47	0.46
4:B:3343:ILE:O	4:B:3346:PHE:HB3	2.16	0.46
2:C:3483:LEU:HD12	2:C:3490:TRP:CD1	2.50	0.46
4:B:1708:ALA:HA	4:B:1711:TRP:CD1	2.51	0.46
4:B:1943:LEU:HD11	4:B:1950:GLY:HA3	1.98	0.46
11:E:224:ASN:HD21	11:E:277:SER:CB	2.27	0.46
1:A:1009:THR:HB	1:A:1074:MET:SD	2.56	0.46
1:A:1013:VAL:HG13	1:A:1076:LEU:CD1	2.45	0.46
1:A:2027:PHE:CE2	1:A:2051:ILE:HG23	2.50	0.46
1:A:3877:ILE:HD11	1:A:3900:ILE:HD13	1.98	0.46
4:B:3339:TRP:CZ2	4:B:3343:ILE:HD12	2.51	0.46
17:M:3:HIS:CE1	17:M:78:ASN:HD22	2.33	0.46
2:C:169:TYR:HB3	4:B:865:VAL:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:24:ILE:O	4:B:25:GLN:CB	2.64	0.46
11:E:261:HIS:CE1	11:E:283:SER:HB3	2.51	0.46
12:D:162:LEU:O	12:D:162:LEU:HD23	2.16	0.46
1:A:2116:VAL:HG23	1:A:2173:VAL:HG11	1.98	0.45
1:A:3897:PRO:HA	1:A:3900:ILE:HG22	1.97	0.45
2:C:973:LYS:HA	2:C:976:ILE:HD12	1.98	0.45
2:C:1728:LEU:HD12	2:C:1728:LEU:O	2.16	0.45
2:C:3276:THR:HG23	2:C:3656:ASN:HA	1.98	0.45
4:B:3258:VAL:HG11	4:B:3321:PHE:CZ	2.51	0.45
4:B:3850:LEU:O	4:B:3931:ARG:NH2	2.43	0.45
12:D:367:LEU:HD12	12:D:368:TYR:O	2.16	0.45
12:D:517:ILE:HG12	12:D:550:TRP:CE2	2.51	0.45
1:A:3268:PHE:CD1	3:Q:35:ILE:CB	2.99	0.45
1:A:3307:GLU:N	1:A:3308:PRO:HD2	2.30	0.45
2:C:106:LEU:N	2:C:106:LEU:HD12	2.31	0.45
2:C:2365:GLY:HA2	18:C:4801:ADP:O3'	2.16	0.45
4:B:3154:GLN:CB	4:B:3419:ALA:HB1	2.46	0.45
4:B:4206:ARG:CZ	4:B:4573:ILE:HD13	2.47	0.45
11:E:566:ASN:HB2	11:E:567:PRO:HD2	1.98	0.45
12:D:372:VAL:HG13	12:D:414:PHE:CZ	2.51	0.45
1:A:1087:THR:O	1:A:1087:THR:HG22	2.17	0.45
1:A:1522:GLU:N	1:A:1523:PRO:CD	2.80	0.45
1:A:4477:MET:HG3	1:A:4524:VAL:HG23	1.98	0.45
1:A:4534:CYS:SG	1:A:4535:LYS:N	2.90	0.45
2:C:859:ILE:CB	2:C:864:MET:SD	3.04	0.45
2:C:2332:LEU:HD13	18:C:4801:ADP:O2'	2.16	0.45
4:B:1102:LEU:O	4:B:1106:PHE:N	2.35	0.45
4:B:1127:ASN:CB	4:B:1128:PRO:CD	2.94	0.45
4:B:2839:ILE:N	4:B:2840:PRO:HD2	2.32	0.45
4:B:3264:ASN:HB2	4:B:3306:ILE:HD11	1.97	0.45
4:B:4475:ILE:HD13	4:B:4525:THR:HG23	1.98	0.45
1:A:1601:ARG:NE	1:A:1688:GLU:OE1	2.49	0.45
1:A:1638:THR:HG21	1:A:1655:GLN:HE21	1.81	0.45
1:A:2340:GLN:NE2	1:A:2399:TYR:OH	2.50	0.45
1:A:3102:LEU:HD23	1:A:3451:THR:HG23	1.97	0.45
1:A:4139:ILE:HD13	1:A:4223:TYR:OH	2.16	0.45
2:C:221:SER:O	2:C:282:ARG:NH1	2.49	0.45
2:C:1382:THR:HA	2:C:1385:ILE:HG22	1.99	0.45
2:C:1524:ARG:HH22	2:C:3759:ILE:HG21	1.81	0.45
2:C:1674:LEU:HD21	2:C:1797:LEU:HD11	1.98	0.45
2:C:2705:ASP:O	2:C:2708:GLN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3481:ILE:HG21	4:B:3488:ILE:CD1	2.46	0.45
5:I:10:MET:HB3	5:I:15:LEU:HD21	1.98	0.45
1:A:1634:ILE:CD1	1:A:1656:ILE:HG23	2.44	0.45
1:A:2704:LYS:O	1:A:2708:THR:HG23	2.16	0.45
1:A:3709:ASP:CB	1:A:3712:LEU:HD12	2.47	0.45
1:A:4562:ASN:CG	1:A:4562:ASN:O	2.54	0.45
2:C:2621:GLU:HG3	2:C:2900:VAL:HG21	1.98	0.45
5:I:95:LEU:HD23	5:I:107:ILE:HD11	1.97	0.45
1:A:1825:ILE:HG21	1:A:1889:LEU:CD2	2.47	0.45
2:C:1142:VAL:HG21	2:C:1167:ILE:HD13	1.97	0.45
2:C:2770:ASN:O	2:C:2771:PHE:C	2.55	0.45
4:B:3823:ILE:HG23	4:B:4286:LEU:HD12	1.99	0.45
4:B:4322:GLU:HB3	4:B:4325:ASN:HB3	1.98	0.45
11:E:153:PHE:HB3	11:E:200:TRP:CE2	2.52	0.45
1:A:2548:ALA:HB2	1:A:2603:LYS:HG2	1.99	0.45
1:A:3120:GLY:HA2	1:A:3696:LEU:HD13	1.98	0.45
1:A:4347:LEU:CD1	1:A:4368:LEU:HD23	2.47	0.45
2:C:102:TYR:O	2:C:106:LEU:HB2	2.16	0.45
4:B:2959:LEU:O	4:B:2959:LEU:HD13	2.17	0.45
4:B:3826:THR:HG22	4:B:3942:LEU:HD22	1.97	0.45
4:B:4543:TYR:CE2	4:B:4545:CYS:HB3	2.52	0.45
7:G:103:ILE:N	7:G:104:PRO:HD2	2.31	0.45
11:E:164:VAL:HG22	11:E:181:TYR:CE1	2.52	0.45
12:D:75:LEU:HD23	12:D:75:LEU:H	1.81	0.45
1:A:2877:THR:HG21	1:A:2923:LEU:HD13	1.98	0.45
2:C:2708:GLN:CD	2:C:2813:ILE:HD11	2.37	0.45
4:B:1189:GLN:HA	4:B:1192:ASN:ND2	2.32	0.45
4:B:3481:ILE:HG21	4:B:3488:ILE:HD12	1.99	0.45
4:B:3914:LEU:O	4:B:3914:LEU:HG	2.17	0.45
1:A:5:LYS:CB	1:A:48:GLU:HA	2.46	0.45
1:A:1696:LYS:HA	1:A:1836:TYR:CE1	2.52	0.45
1:A:4562:ASN:O	1:A:4562:ASN:ND2	2.50	0.45
2:C:1612:ILE:N	2:C:1613:PRO:HD2	2.32	0.45
2:C:2792:TYR:O	2:C:2796:PRO:HG3	2.17	0.45
2:C:1927:SER:CB	2:C:1946:ILE:HG21	2.47	0.45
4:B:3264:ASN:CB	4:B:3306:ILE:HD11	2.47	0.45
12:D:66:LEU:HD21	12:D:73:LYS:HG2	1.98	0.45
1:A:470:PHE:CB	1:A:485:THR:CB	2.95	0.44
1:A:2866:VAL:HG11	1:A:3026:TRP:CH2	2.52	0.44
1:A:3298:ILE:HG22	1:A:3300:GLU:HG3	1.99	0.44
1:A:3877:ILE:HG13	1:A:3946:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:364:ALA:HB1	12:D:414:PHE:CE1	2.52	0.44
1:A:944:LEU:HD23	1:A:944:LEU:N	2.33	0.44
1:A:1525:PHE:HB2	1:A:1541:PHE:CD2	2.51	0.44
1:A:2033:LEU:HD23	1:A:2097:LEU:HD22	1.99	0.44
1:A:4056:ILE:CD1	1:A:4072:LEU:HD21	2.47	0.44
2:C:928:VAL:HA	2:C:951:TYR:CE1	2.53	0.44
2:C:4082:TRP:CZ2	2:C:4091:GLY:HA3	2.52	0.44
4:B:2904:THR:HG21	4:B:2911:ILE:HB	1.98	0.44
4:B:3326:MET:O	4:B:3327:ALA:O	2.34	0.44
1:A:753:LEU:N	1:A:754:PRO:HD2	2.32	0.44
1:A:1171:ILE:HD13	1:A:1171:ILE:H	1.82	0.44
1:A:1790:HIS:CE1	1:A:1794:ILE:HD11	2.52	0.44
2:C:1174:LEU:CD1	2:C:1191:ILE:HG22	2.47	0.44
2:C:2218:VAL:HG23	2:C:2247:THR:HG21	1.99	0.44
4:B:2889:VAL:HG11	4:B:3047:TRP:CZ3	2.53	0.44
1:A:870:PRO:C	1:A:871:LEU:HD13	2.37	0.44
1:A:1205:GLN:HA	1:A:1208:TYR:HB3	1.99	0.44
1:A:4252:PRO:HG3	1:A:4265:TYR:CG	2.52	0.44
2:C:2357:LEU:HD12	2:C:2512:ILE:HG22	1.99	0.44
2:C:2708:GLN:HG2	2:C:2809:ALA:HB1	2.00	0.44
2:C:2771:PHE:O	2:C:2774:VAL:N	2.51	0.44
4:B:436:PHE:CZ	4:B:499:LEU:HD23	2.52	0.44
5:I:98:PHE:HB3	5:I:104:ALA:HA	1.99	0.44
1:A:3240:VAL:HG22	1:A:3335:TRP:CE3	2.52	0.44
1:A:3746:GLN:O	1:A:3799:VAL:HG21	2.18	0.44
1:A:4143:ARG:NH1	1:A:4610:LEU:O	2.50	0.44
4:B:902:ILE:HD11	4:B:1076:LEU:CD1	2.34	0.44
12:D:162:LEU:HD23	12:D:162:LEU:C	2.38	0.44
14:L:69:ILE:HG22	14:L:69:ILE:O	2.18	0.44
1:A:2602:MET:SD	1:A:2602:MET:N	2.90	0.44
2:C:2096:ILE:HD13	2:C:2137:VAL:HG11	2.00	0.44
2:C:2705:ASP:O	2:C:2706:PHE:C	2.56	0.44
2:C:2800:PRO:HA	2:C:2814:CYS:HB3	1.99	0.44
4:B:3081:ASN:HD21	4:B:3484:LYS:CD	2.30	0.44
4:B:473:VAL:O	4:B:473:VAL:HG13	2.18	0.44
12:D:397:ASP:CB	12:D:398:PRO:CD	2.96	0.44
1:A:3131:ILE:HD12	1:A:3422:LEU:CD1	2.48	0.44
2:C:1839:PHE:CE1	2:C:1891:LEU:HD11	2.53	0.44
4:B:745:GLU:HA	4:B:748:VAL:HG12	1.99	0.44
11:E:140:HIS:CE1	12:D:362:LEU:HD21	2.53	0.44
1:A:1162:LEU:C	1:A:1162:LEU:HD23	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1790:HIS:NE2	1:A:1794:ILE:HD11	2.32	0.44
1:A:4172:TYR:CD2	1:A:4195:ARG:NH2	2.86	0.44
2:C:3611:ALA:O	2:C:3615:CYS:SG	2.71	0.44
4:B:3223:ALA:HB1	4:B:3349:ILE:CD1	2.47	0.44
11:E:62:ASN:HB2	15:K:40:ASN:HB2	2.00	0.44
1:A:3252:GLN:HE22	3:Q:36:PRO:HA	1.82	0.43
2:C:336:ILE:HG22	2:C:349:LEU:HD11	1.99	0.43
4:B:902:ILE:HB	4:B:1078:ILE:HA	2.00	0.43
4:B:951:MET:N	4:B:952:PRO:HD2	2.33	0.43
4:B:3654:GLU:O	4:B:3658:ILE:HG13	2.18	0.43
12:D:174:GLN:HE22	14:L:49:LEU:HB3	1.82	0.43
1:A:1143:ARG:CZ	12:D:169:ASN:ND2	2.81	0.43
1:A:4046:CYS:SG	1:A:4074:ILE:HG23	2.58	0.43
2:C:2242:HIS:HB2	2:C:2289:LEU:CD1	2.48	0.43
2:C:3381:SER:N	2:C:3382:PRO:HD2	2.33	0.43
1:A:4287:THR:HG22	1:A:4549:ILE:CD1	2.47	0.43
2:C:259:PRO:HD2	2:C:328:TYR:CE2	2.53	0.43
2:C:3244:VAL:HB	2:C:3878:VAL:HG22	2.00	0.43
4:B:1051:ASP:HB3	4:B:1162:THR:HG21	1.99	0.43
4:B:2267:ILE:HG22	4:B:2271:TRP:CZ3	2.53	0.43
1:A:2656:TYR:CG	1:A:2711:LYS:HD2	2.53	0.43
2:C:321:ARG:HA	2:C:342:ALA:HB2	2.01	0.43
2:C:2079:ILE:HG21	2:C:2082:LEU:HD13	2.00	0.43
2:C:3010:LEU:HA	2:C:3102:LEU:HB2	2.00	0.43
4:B:751:GLY:O	4:B:752:ILE:C	2.56	0.43
4:B:1761:GLN:HE22	4:B:1798:ARG:HG3	1.84	0.43
4:B:2897:GLN:HA	4:B:2947:MET:HE2	2.00	0.43
6:H:85:ALA:HB2	11:E:75:HIS:CD2	2.53	0.43
11:E:49:ASP:HA	14:L:85:SER:HA	1.99	0.43
1:A:1653:ILE:HB	1:A:1674:VAL:HB	2.01	0.43
1:A:3223:LEU:HD21	1:A:3332:ILE:HD11	2.01	0.43
2:C:2708:GLN:CG	2:C:2809:ALA:HB1	2.49	0.43
2:C:3528:LEU:N	2:C:3529:PRO:CD	2.82	0.43
4:B:744:MET:CE	4:B:773:VAL:HG23	2.48	0.43
4:B:1142:SER:O	4:B:1146:VAL:HG23	2.18	0.43
17:M:84:LEU:HD12	17:M:84:LEU:C	2.38	0.43
1:A:2727:LEU:HD22	1:A:2772:GLU:HG2	1.99	0.43
1:A:2840:VAL:HG11	1:A:3041:THR:HG21	2.00	0.43
1:A:3333:LEU:HD23	1:A:3333:LEU:HA	1.92	0.43
2:C:1742:LEU:HD12	2:C:1780:LEU:HD22	1.99	0.43
2:C:2357:LEU:C	2:C:2357:LEU:HD13	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:737:VAL:HG13	4:B:737:VAL:O	2.17	0.43
4:B:1700:ILE:CG2	4:B:1729:ILE:HD13	2.47	0.43
12:D:304:TRP:CZ2	12:D:603:LEU:HD12	2.53	0.43
12:D:624:GLY:N	12:D:625:PRO:CD	2.82	0.43
14:L:99:LEU:N	14:L:100:PRO:HD2	2.33	0.43
1:A:2159:THR:HG22	1:A:2624:ARG:HD2	2.01	0.43
4:B:790:ILE:HG12	4:B:836:ILE:HG23	2.00	0.43
4:B:2704:GLN:O	4:B:2707:ALA:N	2.31	0.43
4:B:4510:LEU:HD22	4:B:4563:LEU:HD11	1.99	0.43
10:O:19:LEU:O	10:O:19:LEU:HD23	2.19	0.43
1:A:966:SER:HB3	1:A:989:ILE:HD12	1.99	0.43
2:C:2687:ALA:CB	2:C:2830:VAL:HG22	2.44	0.43
2:C:3438:HIS:ND1	2:C:3443:LYS:HB2	2.34	0.43
4:B:724:HIS:O	4:B:724:HIS:CD2	2.72	0.43
4:B:3252:VAL:HG22	4:B:3333:ALA:HB2	2.00	0.43
4:B:3267:ILE:HD12	4:B:3279:LYS:HD3	2.00	0.43
4:B:3494:PRO:HA	4:B:3497:ILE:HG22	2.00	0.43
1:A:2821:CYS:HB3	1:A:2841:LEU:HD13	2.01	0.43
1:A:3587:VAL:HG11	1:A:3638:LEU:HD13	2.00	0.43
2:C:1702:ASP:OD1	2:C:1703:LYS:N	2.51	0.43
2:C:2727:ILE:HD13	2:C:2745:LYS:HD3	2.01	0.43
2:C:4072:ILE:HD12	2:C:4110:ALA:HB2	2.00	0.43
2:C:4084:ILE:HG22	2:C:4085:GLY:N	2.34	0.43
12:D:92:TYR:CG	17:M:29:LYS:HB3	2.53	0.43
1:A:4541:LEU:HD21	1:A:4597:LEU:HD13	2.00	0.43
2:C:913:MET:HE1	2:C:959:THR:HG22	2.00	0.43
2:C:2212:LEU:C	2:C:2212:LEU:HD13	2.39	0.43
2:C:2728:TYR:O	2:C:2728:TYR:CG	2.71	0.43
4:B:1728:GLN:HE21	4:B:1868:ILE:HD12	1.83	0.43
4:B:2192:CYS:O	4:B:2196:THR:HG23	2.19	0.43
4:B:3122:LEU:HD11	4:B:3448:ILE:HG12	2.01	0.43
12:D:353:LEU:HG	12:D:363:LEU:HD21	2.01	0.43
1:A:994:GLU:O	1:A:998:VAL:HG23	2.18	0.42
1:A:1596:ARG:HD3	1:A:1603:TYR:CD1	2.54	0.42
1:A:1782:GLU:O	1:A:1786:THR:HG23	2.19	0.42
1:A:3199:GLU:O	1:A:3203:PRO:HD2	2.19	0.42
1:A:3568:LEU:C	1:A:3568:LEU:HD23	2.40	0.42
1:A:3884:THR:HA	1:A:3891:PRO:HA	2.01	0.42
2:C:164:HIS:CE1	4:B:957:GLN:HG3	2.53	0.42
2:C:287:PHE:HB3	2:C:320:PRO:HB2	2.01	0.42
2:C:4081:ALA:N	2:C:4094:ILE:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1819:SER:HA	4:B:1857:VAL:CG1	2.48	0.42
4:B:1858:ASP:O	4:B:1892:ASN:ND2	2.52	0.42
4:B:4287:LEU:HD11	4:B:4393:LEU:HG	2.01	0.42
5:I:93:THR:HB	5:I:109:LYS:HB3	2.00	0.42
1:A:3131:ILE:HG21	1:A:3418:LEU:HB3	2.00	0.42
1:A:3224:LYS:HA	1:A:3281:LEU:HD11	2.00	0.42
2:C:3408:LEU:HD23	2:C:3413:LYS:HA	2.01	0.42
4:B:1933:LYS:HG3	4:B:1965:VAL:HG11	2.01	0.42
9:N:68:CYS:HA	10:O:101:CYS:HA	2.01	0.42
1:A:3305:LEU:CD2	3:Q:81:ARG:CB	2.97	0.42
4:B:58:SER:H	4:B:71:CYS:CB	2.32	0.42
4:B:1075:TRP:CZ3	4:B:1076:LEU:HD13	2.53	0.42
4:B:2531:ARG:C	4:B:2649:LEU:HD21	2.40	0.42
11:E:492:ASP:HA	11:E:495:TYR:CE2	2.54	0.42
12:D:509:ASN:HA	12:D:550:TRP:CD1	2.54	0.42
12:D:526:ARG:HB2	12:D:528:TRP:CH2	2.54	0.42
1:A:3251:ILE:HG22	1:A:3252:GLN:N	2.34	0.42
1:A:3816:ARG:HA	1:A:3973:TYR:CE1	2.54	0.42
2:C:997:LEU:HB2	2:C:1051:GLN:HE22	1.85	0.42
2:C:1328:LEU:HG	2:C:1333:VAL:HG21	2.02	0.42
2:C:2082:LEU:HG	2:C:2137:VAL:HG21	2.00	0.42
2:C:2093:GLN:HB2	2:C:2096:ILE:HG22	2.00	0.42
2:C:2691:VAL:HG22	2:C:2827:ILE:HG13	2.00	0.42
2:C:2715:PRO:HG2	2:C:2719:VAL:HB	2.02	0.42
2:C:2792:TYR:O	2:C:2796:PRO:HD3	2.19	0.42
5:I:12:ILE:HG23	7:G:120:THR:CG2	2.49	0.42
5:I:15:LEU:HD22	12:D:212:ILE:HD13	2.01	0.42
9:N:86:THR:HG22	11:E:25:THR:HG22	2.01	0.42
1:A:2455:GLN:HB2	1:A:2458:GLN:HE21	1.85	0.42
1:A:4113:ILE:HD11	1:A:4134:CYS:SG	2.59	0.42
1:A:4123:HIS:NE2	1:A:4188:PRO:HD3	2.34	0.42
2:C:972:LEU:HD21	2:C:1017:MET:HE1	2.00	0.42
2:C:1040:VAL:HA	2:C:1102:CYS:SG	2.59	0.42
2:C:3276:THR:OG1	2:C:3658:ARG:NH2	2.53	0.42
4:B:429:LEU:HD22	4:B:496:ILE:HD12	2.00	0.42
4:B:3269:LEU:O	4:B:3269:LEU:HD22	2.19	0.42
5:I:19:MET:HB2	5:I:22:LYS:HG2	2.01	0.42
1:A:598:ARG:HD3	12:D:319:TYR:CE1	2.55	0.42
2:C:2943:LYS:HB3	2:C:2994:VAL:HG11	2.01	0.42
2:C:4049:ILE:HD11	2:C:4110:ALA:HB1	2.01	0.42
4:B:1212:ILE:HG22	4:B:1213:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:3885:ASN:O	4:B:3889:GLN:HG2	2.19	0.42
17:M:57:VAL:HG22	17:M:82:LEU:HG	2.01	0.42
2:C:115:LYS:O	2:C:119:TYR:N	2.53	0.42
2:C:162:GLY:HA2	2:C:203:HIS:CE1	2.55	0.42
2:C:261:ILE:N	2:C:262:PRO:HD2	2.34	0.42
2:C:830:ASP:O	2:C:834:VAL:HG23	2.18	0.42
2:C:1328:LEU:HG	2:C:1333:VAL:HG11	2.02	0.42
4:B:719:VAL:O	4:B:722:TYR:HB3	2.19	0.42
4:B:1119:LYS:HB3	4:B:1138:LYS:HD3	2.02	0.42
4:B:1192:ASN:OD1	4:B:1193:ALA:N	2.52	0.42
6:H:68:PHE:HA	11:E:71:ARG:O	2.20	0.42
12:D:183:ARG:HB2	15:K:72:TYR:HE2	1.83	0.42
1:A:1620:PRO:HB2	1:A:1639:PHE:CE1	2.54	0.42
1:A:1926:PHE:CE2	1:A:1934:LEU:HD22	2.54	0.42
2:C:913:MET:HE3	2:C:959:THR:HG22	2.02	0.42
2:C:1191:ILE:HG23	2:C:1201:PHE:CE2	2.54	0.42
2:C:2082:LEU:HD11	2:C:2096:ILE:HD13	2.02	0.42
4:B:439:LEU:HD21	4:B:456:ILE:HG23	2.01	0.42
4:B:459:ILE:HG23	4:B:499:LEU:CD1	2.50	0.42
4:B:1936:MET:HG2	4:B:1966:VAL:HG22	2.01	0.42
4:B:2417:LEU:N	4:B:2418:PRO:HD2	2.35	0.42
4:B:3223:ALA:O	4:B:3226:SER:OG	2.37	0.42
4:B:4106:ASN:HD21	4:B:4141:ILE:HB	1.85	0.42
6:H:11:ILE:HG22	6:H:79:LEU:HB3	2.01	0.42
1:A:1027:CYS:O	1:A:1027:CYS:SG	2.78	0.42
1:A:1143:ARG:NH1	12:D:169:ASN:ND2	2.67	0.42
1:A:2697:ARG:NH1	18:A:4701:ADP:O3B	2.36	0.42
2:C:2742:LYS:HG3	2:C:2743:ASN:HD22	1.85	0.42
4:B:669:ILE:HD13	4:B:752:ILE:HD11	2.01	0.42
8:F:97:MET:HG3	8:F:98:LEU:N	2.35	0.42
14:L:92:VAL:HG12	14:L:92:VAL:O	2.20	0.42
1:A:3308:PRO:HB3	3:Q:33:PHE:CB	2.50	0.42
2:C:2007:LEU:HD13	2:C:2126:ALA:HB3	2.02	0.42
2:C:2719:VAL:CG1	2:C:2720:PRO:HD3	2.50	0.42
2:C:3927:VAL:HG21	2:C:4031:ALA:HB2	2.02	0.42
4:B:1626:ASN:ND2	4:B:1655:THR:HG21	2.35	0.42
4:B:2667:LEU:O	4:B:2670:ASN:N	2.53	0.42
4:B:2776:LYS:NZ	4:B:2814:ILE:HG23	2.35	0.42
4:B:3268:THR:HG23	4:B:3309:GLN:OE1	2.20	0.42
12:D:422:ARG:NH2	12:D:424:MET:SD	2.92	0.42
1:A:1205:GLN:HG2	12:D:166:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2246:ARG:CD	2:C:2344:ARG:HG2	2.50	0.41
2:C:2803:MET:HB3	2:C:2814:CYS:SG	2.60	0.41
2:C:2826:VAL:C	2:C:2828:GLN:N	2.74	0.41
4:B:441:LYS:O	11:E:518:ASN:ND2	2.53	0.41
4:B:2692:LEU:O	4:B:2695:HIS:N	2.52	0.41
4:B:2900:CYS:SG	4:B:3019:VAL:HG11	2.60	0.41
4:B:3582:ILE:HG23	4:B:3582:ILE:O	2.19	0.41
11:E:367:LEU:N	11:E:388:ASP:OD2	2.53	0.41
12:D:314:VAL:HG21	12:D:611:VAL:HG21	2.01	0.41
1:A:151:ILE:O	1:A:153:PHE:N	2.53	0.41
2:C:1047:LEU:O	2:C:1050:VAL:HG22	2.21	0.41
4:B:447:THR:HG21	4:B:513:ASP:C	2.41	0.41
4:B:1109:THR:C	4:B:1113:LEU:HG	2.41	0.41
4:B:1693:MET:HE1	4:B:1866:GLU:HG2	2.01	0.41
4:B:2886:ALA:HB3	4:B:3019:VAL:HG22	2.02	0.41
4:B:3582:ILE:HG23	4:B:3626:THR:HG22	2.02	0.41
4:B:4119:ILE:HD12	4:B:4130:LEU:HD13	2.01	0.41
9:N:88:TYR:N	10:O:81:ILE:O	2.54	0.41
1:A:3758:TYR:CE2	1:A:3762:ILE:HD11	2.55	0.41
1:A:4126:TRP:CZ2	1:A:4130:ILE:HD11	2.55	0.41
2:C:908:LEU:CD1	2:C:948:LEU:HD13	2.50	0.41
2:C:2066:GLN:CA	2:C:2066:GLN:NE2	2.83	0.41
4:B:4143:ARG:NH2	4:B:4574:LEU:O	2.51	0.41
5:I:35:LEU:HD22	5:I:95:LEU:HD13	2.01	0.41
11:E:517:LYS:O	11:E:521:THR:HG23	2.20	0.41
2:C:841:ILE:HG13	2:C:891:ILE:HD13	2.02	0.41
2:C:2711:SER:HB2	2:C:2755:LEU:HD23	2.02	0.41
4:B:1163:ARG:O	4:B:1167:MET:N	2.53	0.41
11:E:42:GLN:HE22	14:L:91:ASN:HD21	1.68	0.41
12:D:66:LEU:N	12:D:66:LEU:HD22	2.35	0.41
1:A:8:LYS:CB	1:A:109:SER:HA	2.51	0.41
1:A:3572:MET:HE1	1:A:3594:VAL:HG13	2.02	0.41
1:A:3951:THR:OG1	1:A:4293:SER:HB2	2.21	0.41
2:C:895:LEU:C	2:C:895:LEU:HD23	2.41	0.41
2:C:3622:ILE:HD11	2:C:3624:LEU:HD21	2.03	0.41
4:B:137:LEU:O	4:B:138:ASN:CB	2.69	0.41
4:B:984:ASN:HA	4:B:987:ARG:HD3	2.03	0.41
4:B:1068:LYS:CB	4:B:1084:LYS:HE2	2.50	0.41
4:B:2055:PHE:CE1	4:B:2106:LEU:HD21	2.55	0.41
4:B:3571:ILE:HD11	4:B:3593:LEU:HD22	2.03	0.41
4:B:4040:MET:HG2	4:B:4075:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:E:121:TYR:HB3	12:D:266:TYR:OH	2.19	0.41
2:C:2005:PRO:HB2	2:C:2145:PHE:CD1	2.55	0.41
2:C:2812:GLY:O	2:C:2815:SER:CB	2.69	0.41
4:B:1886:THR:HA	4:B:4193:ILE:HG23	2.02	0.41
4:B:2180:CYS:SG	4:B:2181:PHE:N	2.94	0.41
4:B:2560:VAL:HG13	4:B:2601:ILE:HD13	2.02	0.41
4:B:3080:LEU:HD12	4:B:3484:LYS:HE2	2.03	0.41
4:B:3255:THR:HG23	4:B:3337:CYS:SG	2.61	0.41
8:F:11:LEU:HD22	8:F:23:TYR:CE1	2.56	0.41
4:B:801:ILE:HG22	4:B:802:ILE:N	2.36	0.41
4:B:1061:GLN:HG2	4:B:1091:VAL:CG1	2.50	0.41
1:A:1642:ALA:HB2	1:A:1652:GLN:HB3	2.03	0.41
1:A:2507:CYS:SG	1:A:2517:PHE:CE1	3.13	0.41
2:C:1383:ASP:O	2:C:1387:VAL:HG23	2.20	0.41
4:B:2026:ALA:HB1	4:B:4200:VAL:HG12	2.02	0.41
4:B:2183:ILE:HG22	4:B:2305:ILE:HB	2.03	0.41
4:B:2537:ILE:HA	4:B:2654:LEU:O	2.21	0.41
4:B:2771:TRP:O	4:B:2772:ALA:C	2.59	0.41
12:D:102:VAL:HG23	12:D:104:GLN:HB2	2.03	0.41
13:P:27:ASN:HA	13:P:95:GLU:HA	2.03	0.41
1:A:1638:THR:HB	1:A:1655:GLN:HG2	2.03	0.41
1:A:1918:GLY:HA3	1:A:1967:ILE:HG21	2.02	0.41
2:C:1048:LEU:C	2:C:1048:LEU:HD13	2.42	0.41
2:C:3034:LEU:HB3	2:C:3041:ILE:HG22	2.02	0.41
2:C:3054:SER:OG	2:C:3055:ALA:N	2.50	0.41
2:C:3136:LEU:HD21	2:C:3221:SER:HB2	2.02	0.41
2:C:3460:ASN:N	2:C:3460:ASN:ND2	2.67	0.41
2:C:3588:VAL:HG11	2:C:3621:TRP:CD2	2.56	0.41
4:B:523:LEU:C	4:B:523:LEU:HD23	2.41	0.41
4:B:558:VAL:HG13	4:B:595:LEU:HD22	2.03	0.41
4:B:725:ILE:HD13	4:B:725:ILE:HA	1.94	0.41
4:B:937:PHE:CD1	4:B:937:PHE:N	2.88	0.41
4:B:1603:LYS:HB3	4:B:1610:TYR:CE2	2.56	0.41
4:B:2157:LEU:HD21	4:B:2196:THR:CG2	2.51	0.41
4:B:3271:ASP:CG	4:B:3272:PRO:HD2	2.41	0.41
4:B:3594:LEU:HD22	4:B:3641:CYS:SG	2.61	0.41
4:B:3826:THR:HG22	4:B:3942:LEU:CD2	2.51	0.41
4:B:3877:LEU:HD13	4:B:3928:LEU:CD1	2.51	0.41
4:B:3907:PRO:HG3	4:B:3934:ARG:HD3	2.03	0.41
4:B:4220:LEU:O	4:B:4220:LEU:HD23	2.21	0.41
4:B:4227:PHE:CD1	4:B:4263:ALA:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:D:439:ILE:HD13	12:D:484:CYS:HB3	2.01	0.41
1:A:1108:LEU:HD23	1:A:1108:LEU:HA	1.95	0.41
1:A:1698:ILE:HG21	1:A:1722:ILE:HD13	2.03	0.41
2:C:3711:LEU:HD21	2:C:3725:LEU:HD23	2.02	0.41
4:B:722:TYR:O	4:B:723:ASN:O	2.39	0.41
4:B:2695:HIS:O	4:B:2695:HIS:CD2	2.74	0.41
6:H:24:VAL:HG22	6:H:49:PHE:HZ	1.86	0.41
1:A:1541:PHE:HA	1:A:1544:ILE:HB	2.03	0.40
1:A:2963:ILE:HD13	1:A:2987:PHE:HB2	2.03	0.40
2:C:1305:LYS:N	2:C:1306:PRO:CD	2.84	0.40
4:B:1080:LEU:HD12	4:B:1080:LEU:N	2.36	0.40
4:B:1096:ARG:O	4:B:1100:ASP:N	2.46	0.40
4:B:2609:MET:N	4:B:2610:PRO:HD2	2.35	0.40
4:B:2715:TYR:O	4:B:2718:PHE:N	2.54	0.40
4:B:4129:ILE:HG23	4:B:4169:MET:SD	2.61	0.40
8:F:79:LEU:HB2	8:F:87:TYR:HB2	2.02	0.40
1:A:3322:ALA:CB	1:A:3333:LEU:HD12	2.51	0.40
1:A:4347:LEU:HD11	1:A:4368:LEU:HD23	2.02	0.40
4:B:679:ARG:HB2	11:E:186:PHE:HE2	1.85	0.40
4:B:2040:LEU:HD12	4:B:2040:LEU:HA	1.90	0.40
4:B:3306:ILE:O	4:B:3309:GLN:N	2.54	0.40
4:B:4187:ILE:O	4:B:4212:LEU:HD21	2.21	0.40
7:G:126:LEU:HD13	8:F:79:LEU:HD23	2.02	0.40
1:A:1143:ARG:O	1:A:1146:GLN:HB3	2.21	0.40
4:B:1480:HIS:O	4:B:1484:LEU:HG	2.21	0.40
4:B:3534:ILE:CD1	4:B:3545:ILE:HD11	2.51	0.40
4:B:3767:MET:HG3	4:B:3768:ASP:N	2.35	0.40
4:B:3829:VAL:HG11	4:B:3946:ILE:CD1	2.52	0.40
1:A:1967:ILE:O	1:A:1970:VAL:HG23	2.21	0.40
1:A:2461:LEU:HD11	1:A:2647:ILE:CG1	2.52	0.40
1:A:3560:HIS:CG	1:A:3561:PRO:HD2	2.56	0.40
1:A:3638:LEU:HA	1:A:3641:LYS:HE3	2.02	0.40
2:C:1015:ASN:OD1	2:C:1034:LYS:NZ	2.53	0.40
2:C:1839:PHE:HE1	2:C:1891:LEU:HD11	1.86	0.40
4:B:55:GLN:O	4:B:85:LYS:HA	2.22	0.40
4:B:2146:ILE:O	4:B:2150:THR:HG23	2.22	0.40
4:B:3281:VAL:O	4:B:3284:MET:N	2.55	0.40
4:B:4203:TRP:CE3	4:B:4546:PRO:HG3	2.57	0.40
4:B:4480:ILE:HG22	4:B:4480:ILE:O	2.21	0.40
1:A:2789:LEU:HD21	1:A:2811:ILE:HD13	2.03	0.40
1:A:3132:ASN:CA	1:A:3419:ILE:HD11	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:2775:VAL:HG22	2:C:2824:TYR:CE1	2.56	0.40
2:C:4109:ASN:O	2:C:4111:VAL:HG23	2.22	0.40
4:B:2885:ASN:HB2	4:B:3043:THR:HG22	2.03	0.40
4:B:4548:TYR:CD2	4:B:4553:ARG:HD2	2.57	0.40
10:O:86:VAL:HG11	10:O:97:ILE:HD13	2.04	0.40
11:E:263:GLU:HB3	11:E:264:PRO:CD	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	4381/4615 (95%)	4081 (93%)	257 (6%)	43 (1%)	13 47
2	C	3915/3943 (99%)	3583 (92%)	283 (7%)	49 (1%)	10 42
3	Q	190/192 (99%)	163 (86%)	24 (13%)	3 (2%)	8 38
4	B	4488/4588 (98%)	4019 (90%)	382 (8%)	87 (2%)	6 35
5	I	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	13 47
6	H	89/91 (98%)	83 (93%)	6 (7%)	0	100 100
7	G	92/96 (96%)	87 (95%)	5 (5%)	0	100 100
8	F	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14 49
9	N	112/114 (98%)	92 (82%)	17 (15%)	3 (3%)	4 29
10	O	118/120 (98%)	104 (88%)	9 (8%)	5 (4%)	2 22
11	E	551/557 (99%)	496 (90%)	51 (9%)	4 (1%)	19 55
12	D	569/595 (96%)	510 (90%)	51 (9%)	8 (1%)	9 40
13	P	103/112 (92%)	86 (84%)	11 (11%)	6 (6%)	1 17
14	L	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	13 47
15	K	88/90 (98%)	79 (90%)	9 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
16	J	93/95 (98%)	84 (90%)	8 (9%)	1 (1%)	12 45
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	5 31
All	All	15182/15609 (97%)	13821 (91%)	1147 (8%)	214 (1%)	12 40

All (214) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	ILE
1	A	4235	PHE
2	C	435	MET
2	C	529	GLU
2	C	2733	TYR
2	C	2744	LYS
2	C	3054	SER
2	C	3443	LYS
3	Q	19	PRO
3	Q	39	GLU
4	B	6	GLN
4	B	37	GLN
4	B	533	ARG
4	B	692	LEU
4	B	750	PRO
4	B	765	PHE
4	B	1127	ASN
4	B	2249	GLU
4	B	2741	PHE
4	B	2760	SER
4	B	3248	PRO
4	B	3267	ILE
4	B	3329	GLN
4	B	3331	TYR
4	B	3333	ALA
9	N	7	GLU
10	O	29	PHE
11	E	37	ILE
12	D	397	ASP
13	P	37	PRO

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Mol	Chain	Res	Type
13	P	107	ILE
13	P	119	PRO
17	M	51	TYR
1	A	27	ILE
1	A	28	VAL
1	A	158	GLU
1	A	282	ARG
1	A	720	GLU
1	A	1670	THR
1	A	4430	TRP
1	A	4563	LYS
2	C	140	ILE
2	C	155	GLU
2	C	322	GLU
2	C	400	GLY
2	C	861	SER
2	C	1170	ALA
2	C	1901	LEU
2	C	2718	GLY
2	C	2759	LYS
2	C	2771	PHE
2	C	3619	GLY
2	C	4106	PRO
3	Q	49	LEU
4	B	18	LEU
4	B	19	SER
4	B	24	ILE
4	B	27	GLU
4	B	74	TYR
4	B	136	PRO
4	B	138	ASN
4	B	307	PRO
4	B	720	ASP
4	B	723	ASN
4	B	751	GLY
4	B	752	ILE
4	B	799	VAL
4	B	801	ILE
4	B	1124	ILE
4	B	1947	GLY
4	B	1990	GLY
4	B	2353	MET

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Mol	Chain	Res	Type
4	B	3323	GLU
4	B	3327	ALA
4	B	3328	GLY
4	B	3332	ALA
4	B	4152	ASN
4	B	4228	PRO
4	B	4484	GLU
4	B	4489	GLU
4	B	4527	CYS
5	I	51	ALA
10	O	31	PRO
11	E	19	ASN
11	E	350	LYS
12	D	168	TYR
12	D	563	MET
13	P	36	TYR
17	M	50	GLY
1	A	18	CYS
1	A	103	ASP
1	A	149	GLU
1	A	283	PRO
1	A	818	LEU
1	A	970	TYR
1	A	1172	THR
1	A	1347	TRP
1	A	1396	PRO
2	C	223	THR
2	C	237	ASP
2	C	390	THR
2	C	1214	TYR
2	C	2362	GLY
2	C	2716	PRO
2	C	2732	GLY
2	C	2735	ASN
2	C	2746	PRO
2	C	2750	SER
2	C	2770	ASN
2	C	2805	SER
2	C	4092	TYR
4	B	361	LYS
4	B	764	GLN
4	B	774	ASP

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Mol	Chain	Res	Type
4	B	806	ASN
4	B	898	PRO
4	B	2252	TYR
4	B	2571	THR
4	B	2969	GLY
4	B	3246	GLY
4	B	4225	GLU
9	N	25	PHE
11	E	275	THR
12	D	236	MET
1	A	26	MET
1	A	127	THR
1	A	152	GLN
1	A	591	LYS
1	A	1030	SER
1	A	1897	ASN
1	A	3585	ASN
1	A	4562	ASN
1	A	4599	CYS
2	C	84	TYR
2	C	1897	ASN
2	C	2247	THR
2	C	2756	LYS
2	C	3983	ALA
4	B	169	LYS
4	B	334	TYR
4	B	1333	ILE
4	B	1489	SER
4	B	1856	ILE
4	B	2469	ALA
4	B	2491	TRP
4	B	3223	ALA
4	B	3237	PRO
4	B	3268	THR
4	B	3273	ASP
12	D	231	LYS
12	D	523	TRP
13	P	68	LEU
13	P	71	GLN
14	L	71	ASP
16	J	101	GLU
1	A	101	PRO

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Mol	Chain	Res	Type
1	A	106	LYS
1	A	3972	SER
2	C	392	ASN
2	C	881	ILE
2	C	1082	ASP
2	C	2066	GLN
2	C	4090	ASP
4	B	89	ILE
4	B	99	LEU
4	B	306	GLN
4	B	719	VAL
4	B	1626	ASN
4	B	1641	LEU
4	B	2207	ASP
4	B	3302	ILE
4	B	3306	ILE
4	B	3466	ALA
4	B	4144	ARG
4	B	4182	PRO
10	O	77	PRO
12	D	321	PHE
12	D	398	PRO
1	A	772	TRP
1	A	878	VAL
1	A	1398	GLN
1	A	1745	ASN
2	C	438	GLY
4	B	407	LEU
4	B	2702	LYS
4	B	3221	LEU
8	F	29	SER
1	A	817	VAL
1	A	1171	ILE
1	A	1401	ILE
4	B	2	GLY
9	N	80	GLY
10	O	53	PRO
1	A	3535	GLY
2	C	442	ILE
2	C	2813	ILE
4	B	1212	ILE
4	B	1213	PRO

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Mol	Chain	Res	Type
2	C	99	GLY
2	C	1401	PRO
4	B	3258	VAL
4	B	3261	ILE
4	B	4150	GLY
2	C	2826	VAL
4	B	88	GLY
4	B	2186	PRO
4	B	4147	GLY
10	O	25	ILE
2	C	1717	VAL
2	C	2715	PRO

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	3420/4191 (82%)	3338 (98%)	82 (2%)	44 63
2	C	3149/3501 (90%)	3095 (98%)	54 (2%)	56 72
3	Q	10/176 (6%)	10 (100%)	0	100 100
4	B	3497/4138 (84%)	3399 (97%)	98 (3%)	38 59
5	I	91/91 (100%)	87 (96%)	4 (4%)	24 47
6	H	82/82 (100%)	81 (99%)	1 (1%)	67 78
7	G	86/87 (99%)	85 (99%)	1 (1%)	67 78
8	F	93/93 (100%)	86 (92%)	7 (8%)	11 33
9	N	85/102 (83%)	84 (99%)	1 (1%)	67 78
10	O	106/108 (98%)	99 (93%)	7 (7%)	14 37
11	E	484/496 (98%)	467 (96%)	17 (4%)	31 53
12	D	507/545 (93%)	482 (95%)	25 (5%)	21 44
14	L	87/87 (100%)	83 (95%)	4 (5%)	23 46
15	K	80/80 (100%)	79 (99%)	1 (1%)	65 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
16	J	81/81 (100%)	79 (98%)	2 (2%)	42 62
17	M	78/78 (100%)	74 (95%)	4 (5%)	20 43
All	All	11936/13936 (86%)	11628 (97%)	308 (3%)	42 61

All (308) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	581	ASP
1	A	582	THR
1	A	616	LYS
1	A	674	LEU
1	A	751	LEU
1	A	758	ASP
1	A	763	LEU
1	A	810	LEU
1	A	818	LEU
1	A	861	ASP
1	A	871	LEU
1	A	1016	PHE
1	A	1020	PHE
1	A	1023	PHE
1	A	1069	TYR
1	A	1086	SER
1	A	1132	LEU
1	A	1136	MET
1	A	1153	PHE
1	A	1171	ILE
1	A	1201	TYR
1	A	1205	GLN
1	A	1559	LYS
1	A	1567	ASN
1	A	1573	PHE
1	A	1581	LEU
1	A	1609	THR
1	A	1631	PHE
1	A	1634	ILE
1	A	1644	ASP
1	A	1711	LEU
1	A	1778	ARG
1	A	1922	CYS
1	A	2034	CYS

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Mol	Chain	Res	Type
1	A	2075	MET
1	A	2098	LEU
1	A	2228	THR
1	A	2267	ASN
1	A	2320	SER
1	A	2418	ILE
1	A	2426	GLU
1	A	2434	SER
1	A	2443	CYS
1	A	2470	GLU
1	A	2471	MET
1	A	2487	ASN
1	A	2729	LEU
1	A	2844	ASP
1	A	2901	ASP
1	A	3046	PHE
1	A	3122	ASN
1	A	3125	GLN
1	A	3203	PRO
1	A	3283	ASP
1	A	3308	PRO
1	A	3315	ASP
1	A	3345	LYS
1	A	3449	LEU
1	A	3578	LEU
1	A	3588	ASP
1	A	3647	PHE
1	A	3881	SER
1	A	3951	THR
1	A	3952	LEU
1	A	3973	TYR
1	A	4046	CYS
1	A	4130	ILE
1	A	4143	ARG
1	A	4155	TYR
1	A	4216	PHE
1	A	4287	THR
1	A	4288	PHE
1	A	4448	GLN
1	A	4465	THR
1	A	4497	SER
1	A	4504	SER

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Mol	Chain	Res	Type
1	A	4506	THR
1	A	4542	ASP
1	A	4562	ASN
1	A	4578	CYS
1	A	4588	ASP
1	A	4593	PHE
2	C	36	PHE
2	C	39	LEU
2	C	110	ASP
2	C	111	THR
2	C	214	LEU
2	C	220	TRP
2	C	239	TRP
2	C	329	ASP
2	C	346	LEU
2	C	352	LEU
2	C	950	ASP
2	C	1113	ASN
2	C	1249	ASP
2	C	1453	CYS
2	C	1499	CYS
2	C	1650	ASP
2	C	1660	ASP
2	C	1702	ASP
2	C	1722	ASP
2	C	1868	CYS
2	C	1884	CYS
2	C	1953	GLN
2	C	2043	ASN
2	C	2066	GLN
2	C	2121	ASN
2	C	2122	THR
2	C	2224	LEU
2	C	2225	SER
2	C	2292	CYS
2	C	2432	ASN
2	C	2483	ASN
2	C	2488	ILE
2	C	2696	SER
2	C	2711	SER
2	C	2712	PHE
2	C	2728	TYR

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Mol	Chain	Res	Type
2	C	2748	ASP
2	C	2757	LEU
2	C	2771	PHE
2	C	2776	ASP
2	C	3059	ASN
2	C	3460	ASN
2	C	3602	GLN
2	C	3704	ASN
2	C	3793	THR
2	C	3824	PHE
2	C	3877	GLU
2	C	3883	SER
2	C	3908	ASP
2	C	3918	VAL
2	C	4050	GLN
2	C	4092	TYR
2	C	4113	VAL
2	C	4146	MET
4	B	423	CYS
4	B	440	GLU
4	B	480	ILE
4	B	485	PHE
4	B	489	PHE
4	B	581	ASN
4	B	609	LEU
4	B	693	GLU
4	B	706	GLU
4	B	766	ILE
4	B	769	SER
4	B	801	ILE
4	B	802	ILE
4	B	804	ARG
4	B	810	SER
4	B	813	ASP
4	B	850	ASP
4	B	937	PHE
4	B	1067	ILE
4	B	1183	THR
4	B	1186	PRO
4	B	1208	LYS
4	B	1213	PRO
4	B	1518	TRP

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Mol	Chain	Res	Type
4	B	1537	ASP
4	B	1559	MET
4	B	1607	PRO
4	B	1734	THR
4	B	1929	ASP
4	B	2103	MET
4	B	2139	GLN
4	B	2206	GLU
4	B	2258	HIS
4	B	2419	LYS
4	B	2425	GLU
4	B	2454	ASP
4	B	2607	PHE
4	B	2610	PRO
4	B	2647	ASP
4	B	2653	CYS
4	B	2752	CYS
4	B	2846	LEU
4	B	2873	SER
4	B	2874	ARG
4	B	2931	GLU
4	B	2949	THR
4	B	2959	LEU
4	B	2963	ASN
4	B	2971	ILE
4	B	2982	SER
4	B	3004	LEU
4	B	3032	ARG
4	B	3080	LEU
4	B	3222	PRO
4	B	3231	VAL
4	B	3269	LEU
4	B	3288	GLN
4	B	3298	ASP
4	B	3330	SER
4	B	3343	ILE
4	B	3349	ILE
4	B	3350	PHE
4	B	3355	PRO
4	B	3407	GLN
4	B	3450	ASP
4	B	3469	ARG

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Mol	Chain	Res	Type
4	B	3489	THR
4	B	3521	ASN
4	B	3614	ILE
4	B	3708	ASP
4	B	3756	MET
4	B	3757	LEU
4	B	3800	LEU
4	B	3842	TYR
4	B	3920	ASP
4	B	3942	LEU
4	B	3945	PHE
4	B	3976	ASP
4	B	4012	PHE
4	B	4104	LYS
4	B	4125	LYS
4	B	4151	TRP
4	B	4176	ASN
4	B	4182	PRO
4	B	4255	SER
4	B	4279	CYS
4	B	4304	LYS
4	B	4352	GLU
4	B	4365	LYS
4	B	4369	GLU
4	B	4443	ARG
4	B	4476	THR
4	B	4482	GLU
4	B	4503	TRP
4	B	4520	SER
4	B	4540	LYS
4	B	4547	VAL
4	B	4553	ARG
5	I	19	MET
5	I	60	CYS
5	I	81	GLU
5	I	97	MET
6	H	68	PHE
7	G	140	ASP
8	F	9	ASP
8	F	13	GLN
8	F	35	ARG
8	F	51	LEU

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Mol	Chain	Res	Type
8	F	84	SER
8	F	96	THR
8	F	97	MET
9	N	18	ASP
10	O	22	LEU
10	O	32	SER
10	O	77	PRO
10	O	99	SER
10	O	103	TRP
10	O	104	ASP
10	O	122	CYS
11	E	37	ILE
11	E	44	ASN
11	E	47	PHE
11	E	49	ASP
11	E	127	ASP
11	E	193	MET
11	E	225	GLN
11	E	261	HIS
11	E	262	TYR
11	E	266	THR
11	E	353	VAL
11	E	361	LEU
11	E	385	SER
11	E	402	ILE
11	E	422	SER
11	E	515	LYS
11	E	560	HIS
12	D	62	THR
12	D	69	ASP
12	D	75	LEU
12	D	90	ASP
12	D	99	ASP
12	D	104	GLN
12	D	115	TYR
12	D	169	ASN
12	D	172	GLU
12	D	177	ASN
12	D	266	TYR
12	D	289	PHE
12	D	320	ASP
12	D	371	THR

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Mol	Chain	Res	Type
12	D	392	ASN
12	D	395	HIS
12	D	399	VAL
12	D	414	PHE
12	D	477	GLU
12	D	488	TYR
12	D	509	ASN
12	D	518	SER
12	D	523	TRP
12	D	570	ASP
12	D	595	PHE
14	L	50	GLU
14	L	51	LYS
14	L	71	ASP
14	L	86	LEU
15	K	18	MET
16	J	21	PHE
16	J	86	CYS
17	M	10	THR
17	M	15	ASP
17	M	60	ASN
17	M	64	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (143) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	599	ASN
1	A	687	ASN
1	A	804	ASN
1	A	837	GLN
1	A	1114	GLN
1	A	1205	GLN
1	A	1276	GLN
1	A	1566	GLN
1	A	1567	ASN
1	A	1585	GLN
1	A	1624	GLN
1	A	1666	ASN
1	A	1690	ASN
1	A	1718	GLN
1	A	1728	GLN
1	A	1940	GLN

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Mol	Chain	Res	Type
1	A	2095	ASN
1	A	2251	ASN
1	A	2279	ASN
1	A	2340	GLN
1	A	2369	GLN
1	A	2373	GLN
1	A	2458	GLN
1	A	2479	GLN
1	A	2487	ASN
1	A	2508	ASN
1	A	2628	GLN
1	A	2889	GLN
1	A	3113	GLN
1	A	3122	ASN
1	A	3252	GLN
1	A	3311	ASN
1	A	3343	HIS
1	A	3606	GLN
1	A	3746	GLN
1	A	3888	GLN
1	A	4088	GLN
1	A	4125	ASN
1	A	4137	HIS
1	A	4330	ASN
1	A	4479	GLN
1	A	4574	ASN
2	C	17	GLN
2	C	168	ASN
2	C	1051	GLN
2	C	1113	ASN
2	C	1238	GLN
2	C	1300	GLN
2	C	1428	ASN
2	C	1765	ASN
2	C	1888	GLN
2	C	1981	ASN
2	C	2066	GLN
2	C	2142	GLN
2	C	2207	HIS
2	C	2217	ASN
2	C	2483	ASN
2	C	2778	ASN

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Mol	Chain	Res	Type
2	C	2784	ASN
2	C	2819	ASN
2	C	2951	ASN
2	C	2953	ASN
2	C	3004	ASN
2	C	3460	ASN
2	C	3654	HIS
2	C	3674	GLN
2	C	3791	HIS
2	C	3870	GLN
2	C	3958	ASN
2	C	4050	GLN
2	C	4068	ASN
2	C	4143	ASN
4	B	672	ASN
4	B	721	ASN
4	B	724	HIS
4	B	764	GLN
4	B	775	GLN
4	B	832	ASN
4	B	883	ASN
4	B	923	GLN
4	B	957	GLN
4	B	975	ASN
4	B	1079	ASN
4	B	1081	GLN
4	B	1728	GLN
4	B	1761	GLN
4	B	1807	GLN
4	B	1870	ASN
4	B	1956	ASN
4	B	1969	GLN
4	B	2005	ASN
4	B	2038	ASN
4	B	2148	GLN
4	B	2203	ASN
4	B	2325	ASN
4	B	2462	ASN
4	B	2476	GLN
4	B	2504	GLN
4	B	2591	ASN
4	B	2608	ASN

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Mol	Chain	Res	Type
4	B	2656	GLN
4	B	2836	GLN
4	B	2897	GLN
4	B	3042	ASN
4	B	3081	ASN
4	B	3093	ASN
4	B	3288	GLN
4	B	3407	GLN
4	B	3521	ASN
4	B	3715	ASN
4	B	3772	GLN
4	B	3803	ASN
4	B	3879	ASN
4	B	4097	ASN
4	B	4106	ASN
4	B	4176	ASN
4	B	4177	GLN
5	I	100	ASN
6	H	36	ASN
7	G	129	GLN
7	G	149	GLN
9	N	75	GLN
11	E	31	GLN
11	E	39	GLN
11	E	42	GLN
11	E	52	ASN
11	E	122	GLN
11	E	224	ASN
11	E	237	ASN
11	E	379	ASN
11	E	481	GLN
12	D	64	GLN
12	D	167	ASN
12	D	177	ASN
12	D	294	GLN
12	D	298	ASN
12	D	324	GLN
12	D	413	ASN
14	L	28	GLN
14	L	64	GLN
16	J	87	GLN
17	M	3	HIS

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Mol	Chain	Res	Type
17	M	78	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	ADP	C	4801	20	24,29,29	0.72	0	29,45,45	1.04	2 (6%)
18	ADP	B	5501	20	24,29,29	0.75	0	29,45,45	0.93	2 (6%)
19	ATP	C	4201	20	28,33,33	0.70	0	34,52,52	0.78	1 (2%)
18	ADP	A	4701	20	24,29,29	0.74	0	29,45,45	0.79	1 (3%)
18	ADP	C	4401	20	24,29,29	0.75	1 (4%)	29,45,45	1.25	3 (10%)
18	ADP	A	4901	-	24,29,29	0.75	0	29,45,45	1.04	2 (6%)
18	ADP	B	5601	20	24,29,29	0.74	0	29,45,45	0.69	1 (3%)
19	ATP	B	4701	20	28,33,33	0.71	0	34,52,52	0.85	1 (2%)
19	ATP	A	4801	20	28,33,33	0.70	0	34,52,52	0.79	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	ADP	C	4801	20	-	4/12/32/32	0/3/3/3
18	ADP	B	5501	20	-	5/12/32/32	0/3/3/3
19	ATP	C	4201	20	-	4/18/38/38	0/3/3/3
18	ADP	A	4701	20	-	5/12/32/32	0/3/3/3
18	ADP	C	4401	20	-	5/12/32/32	0/3/3/3
18	ADP	A	4901	-	-	1/12/32/32	0/3/3/3
18	ADP	B	5601	20	-	2/12/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/18/38/38	0/3/3/3
19	ATP	A	4801	20	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4401	ADP	C8-N7	-2.02	1.31	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	C	4401	ADP	C4'-O4'-C1'	-4.32	105.97	109.92
18	A	4901	ADP	C4'-O4'-C1'	-3.85	106.40	109.92
18	C	4801	ADP	C4'-O4'-C1'	-3.63	106.60	109.92
18	C	4401	ADP	C1'-N9-C4	2.72	131.41	126.64
19	B	4701	ATP	C5-C6-N6	2.45	124.04	120.31
19	A	4801	ATP	C5-C6-N6	2.25	123.73	120.31
18	C	4801	ADP	C5-C6-N6	2.22	123.69	120.31
18	B	5601	ADP	C5-C6-N6	2.17	123.62	120.31
19	C	4201	ATP	C5-C6-N6	2.17	123.62	120.31
18	B	5501	ADP	C5-C6-N6	2.15	123.58	120.31
18	B	5501	ADP	O3B-PB-O3A	2.12	111.76	104.64
18	A	4701	ADP	C5-C6-N6	2.07	123.46	120.31
18	A	4901	ADP	C5-C6-N6	2.07	123.46	120.31
18	C	4401	ADP	C5-C6-N6	2.05	123.44	120.31

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4401	ADP	C5'-O5'-PA-O1A
18	C	4401	ADP	C5'-O5'-PA-O2A
18	C	4401	ADP	C5'-O5'-PA-O3A
18	C	4801	ADP	O4'-C4'-C5'-O5'
18	B	5501	ADP	PB-O3A-PA-O5'
18	B	5501	ADP	C5'-O5'-PA-O1A
18	B	5501	ADP	C5'-O5'-PA-O2A
18	B	5501	ADP	C5'-O5'-PA-O3A
19	C	4201	ATP	C5'-O5'-PA-O1A
19	C	4201	ATP	C5'-O5'-PA-O3A
18	C	4401	ADP	C3'-C4'-C5'-O5'
18	C	4401	ADP	O4'-C4'-C5'-O5'
18	C	4801	ADP	C3'-C4'-C5'-O5'
19	A	4801	ATP	O4'-C4'-C5'-O5'
18	B	5601	ADP	PA-O3A-PB-O2B
19	A	4801	ATP	C3'-C4'-C5'-O5'
18	B	5501	ADP	C4'-C5'-O5'-PA
19	A	4801	ATP	PB-O3A-PA-O2A
18	A	4701	ADP	O4'-C4'-C5'-O5'
18	B	5601	ADP	C4'-C5'-O5'-PA
18	C	4801	ADP	PB-O3A-PA-O1A
18	A	4901	ADP	C4'-C5'-O5'-PA
18	A	4701	ADP	PA-O3A-PB-O1B
18	A	4701	ADP	PA-O3A-PB-O2B
19	A	4801	ATP	PB-O3B-PG-O2G
19	A	4801	ATP	PB-O3A-PA-O1A
19	C	4201	ATP	PG-O3B-PB-O2B
19	C	4201	ATP	O4'-C4'-C5'-O5'
18	A	4701	ADP	C4'-C5'-O5'-PA
18	C	4801	ADP	PB-O3A-PA-O2A

There are no ring outliers.

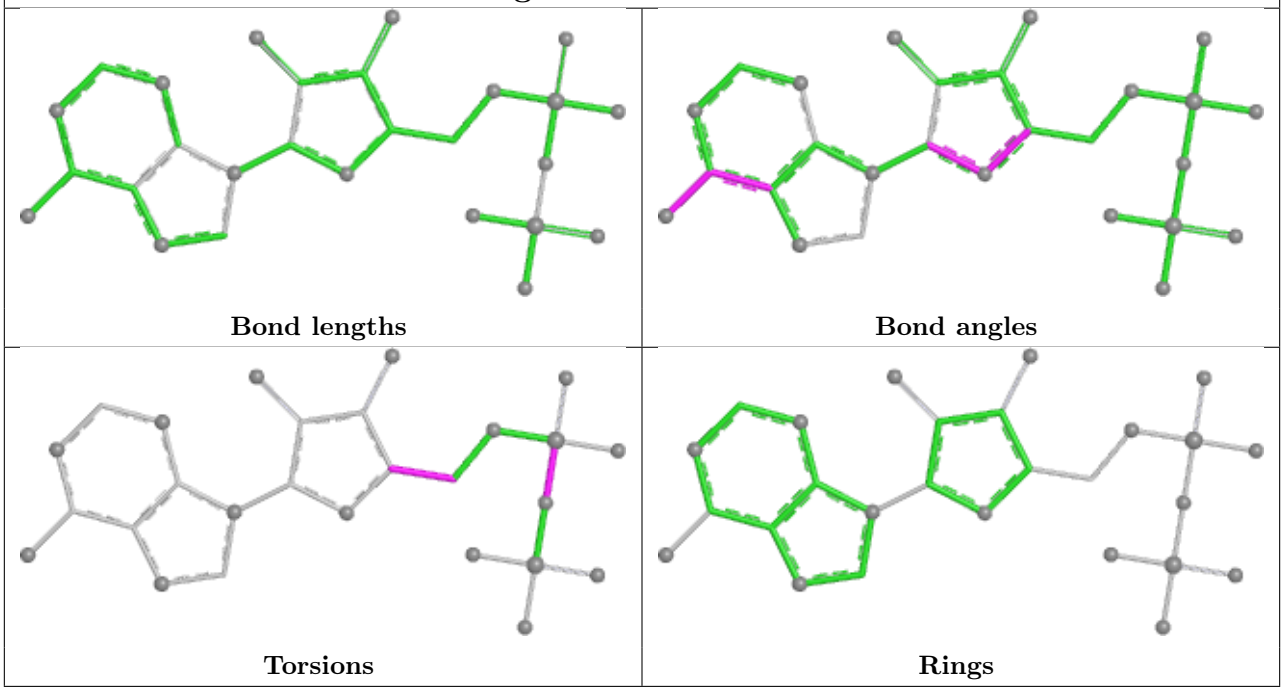
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4801	ADP	2	0
18	A	4701	ADP	1	0
18	C	4401	ADP	1	0
18	A	4901	ADP	1	0
19	B	4701	ATP	1	0

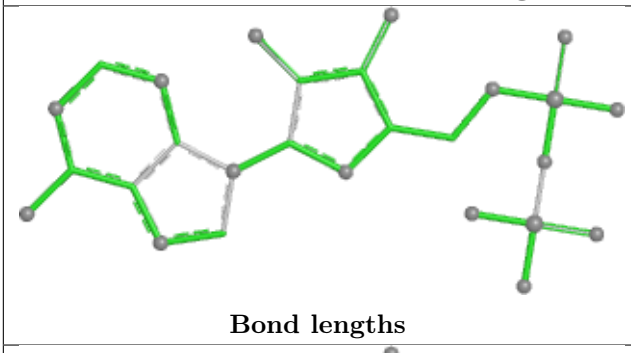
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

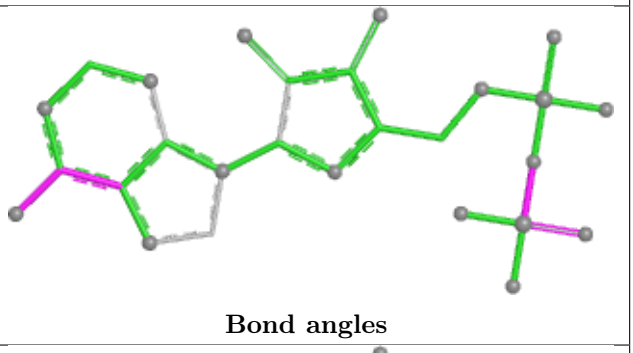
Ligand ADP C 4801



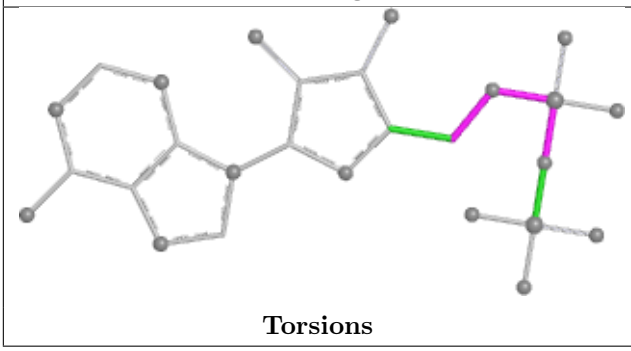
Ligand ADP B 5501



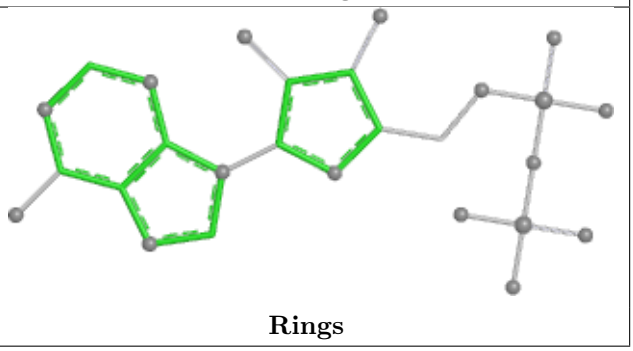
Bond lengths



Bond angles

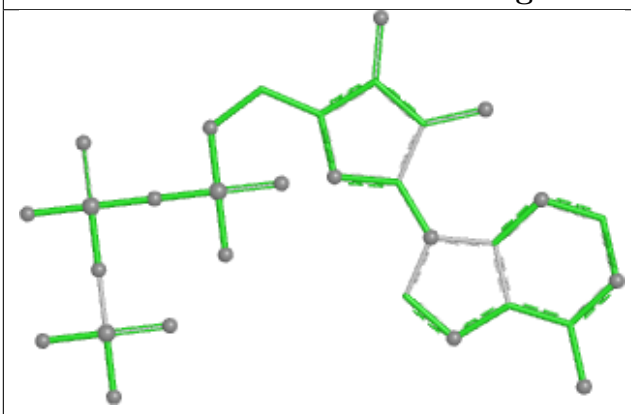


Torsions

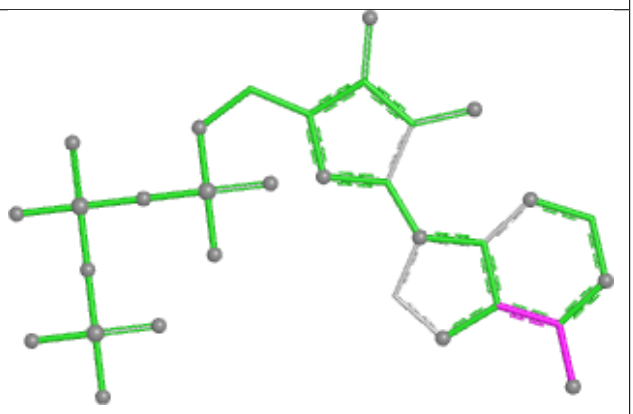


Rings

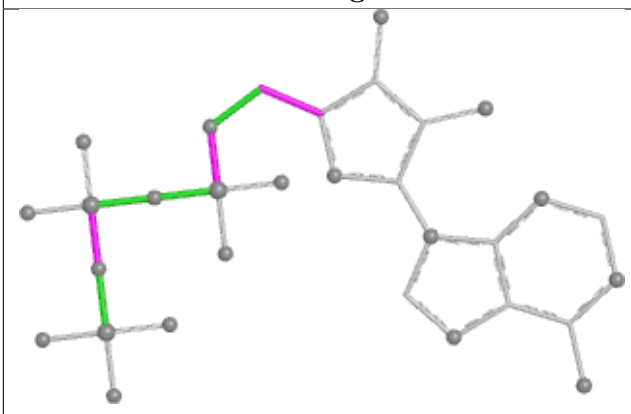
Ligand ATP C 4201



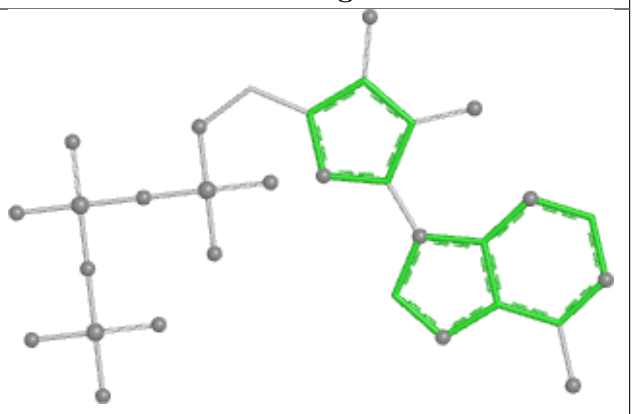
Bond lengths



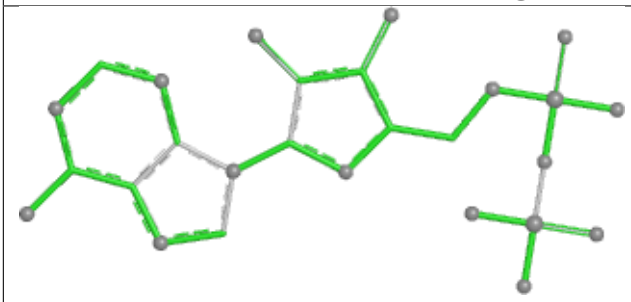
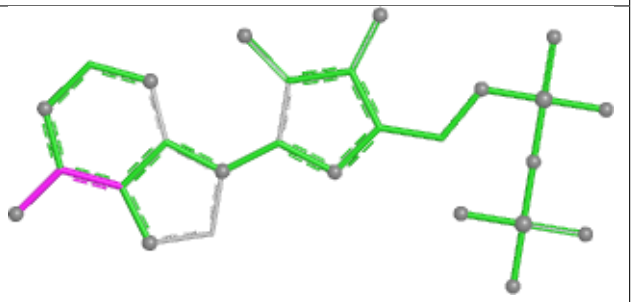
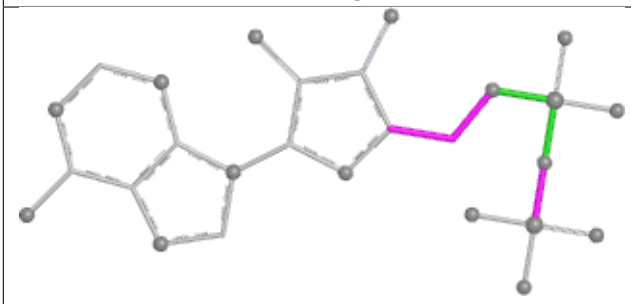
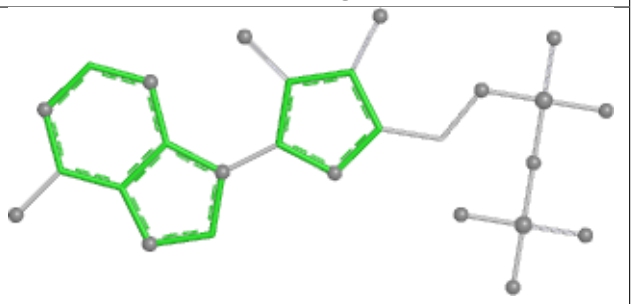
Bond angles

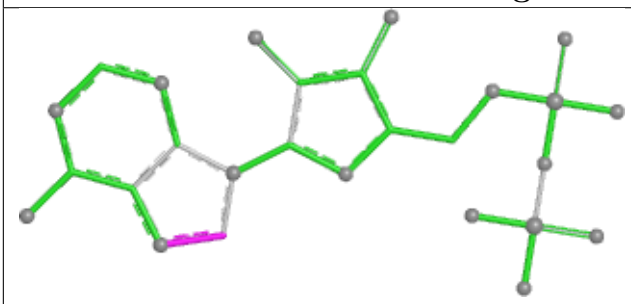
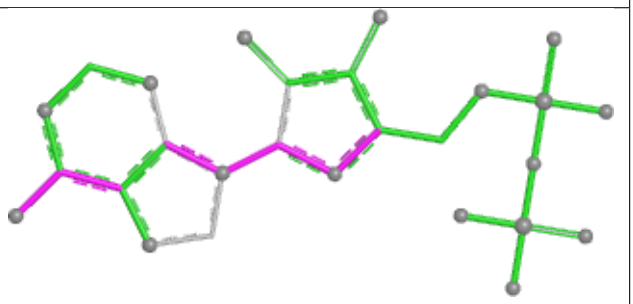
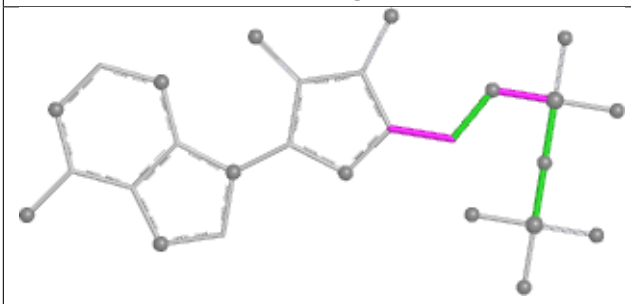
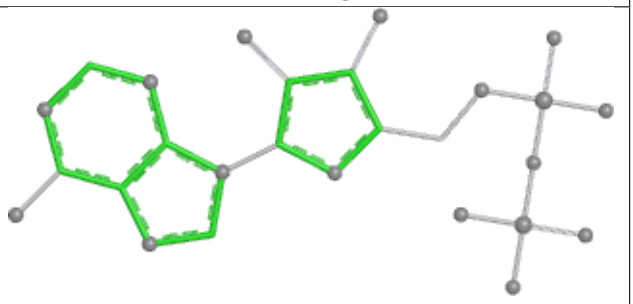


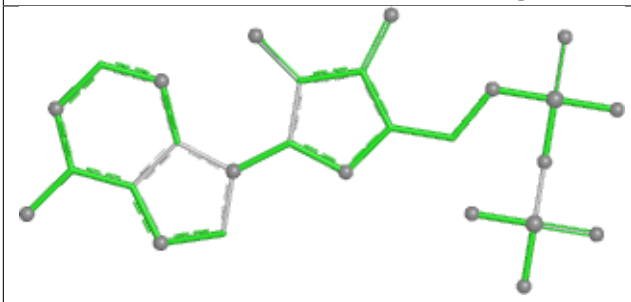
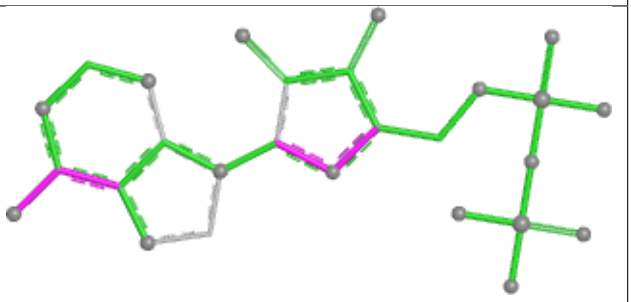
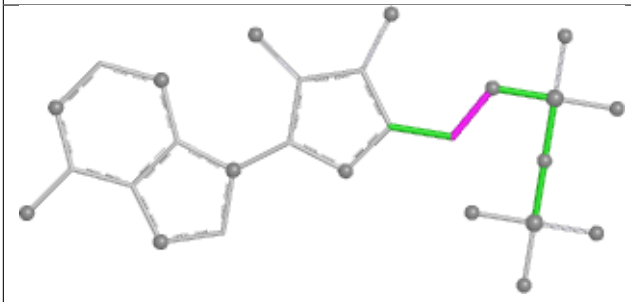
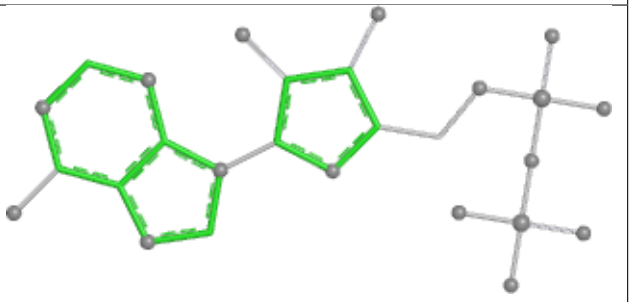
Torsions

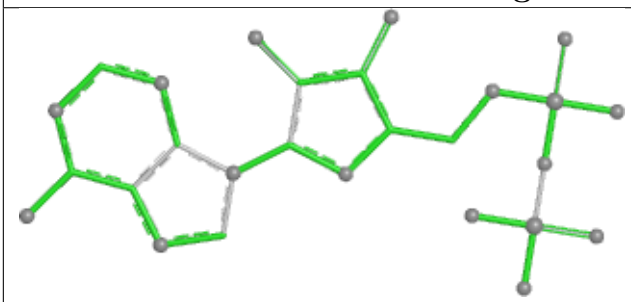
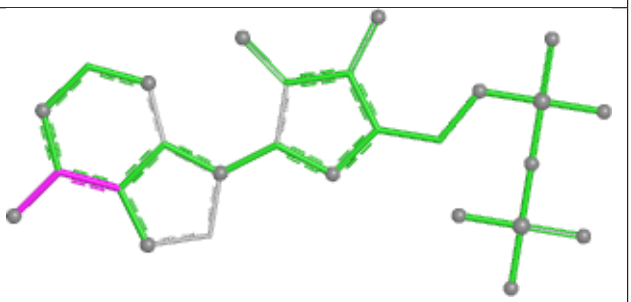
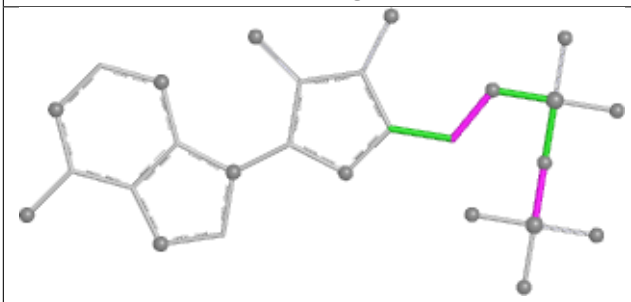
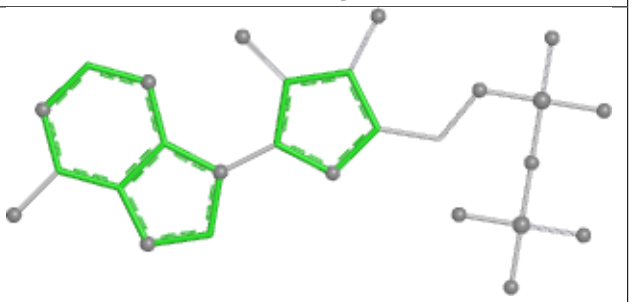


Rings

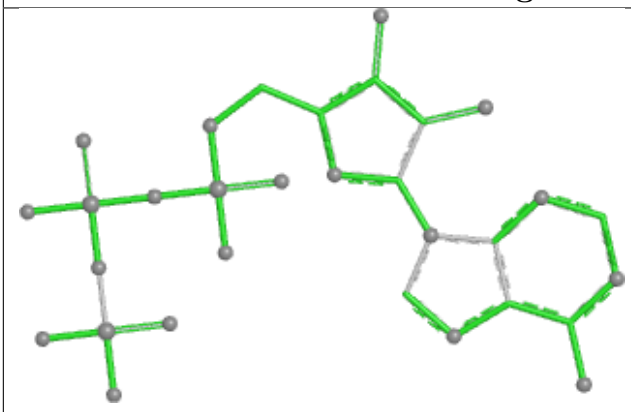
Ligand ADP A 4701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 4401	
 Bond lengths	 Bond angles
 Torsions	 Rings

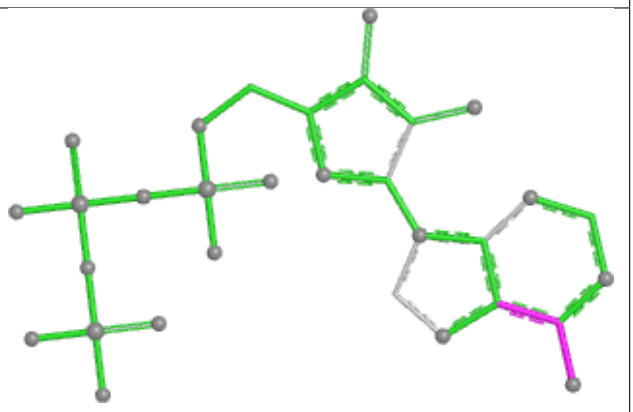
Ligand ADP A 4901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 5601	
 Bond lengths	 Bond angles
 Torsions	 Rings

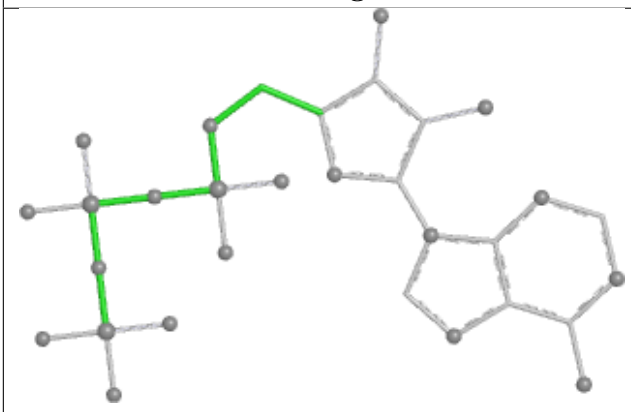
Ligand ATP B 4701



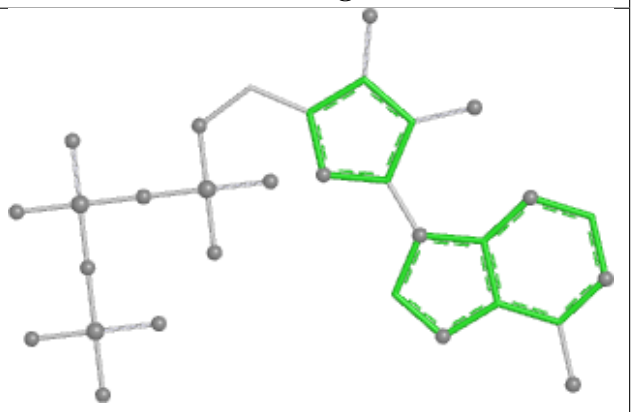
Bond lengths



Bond angles

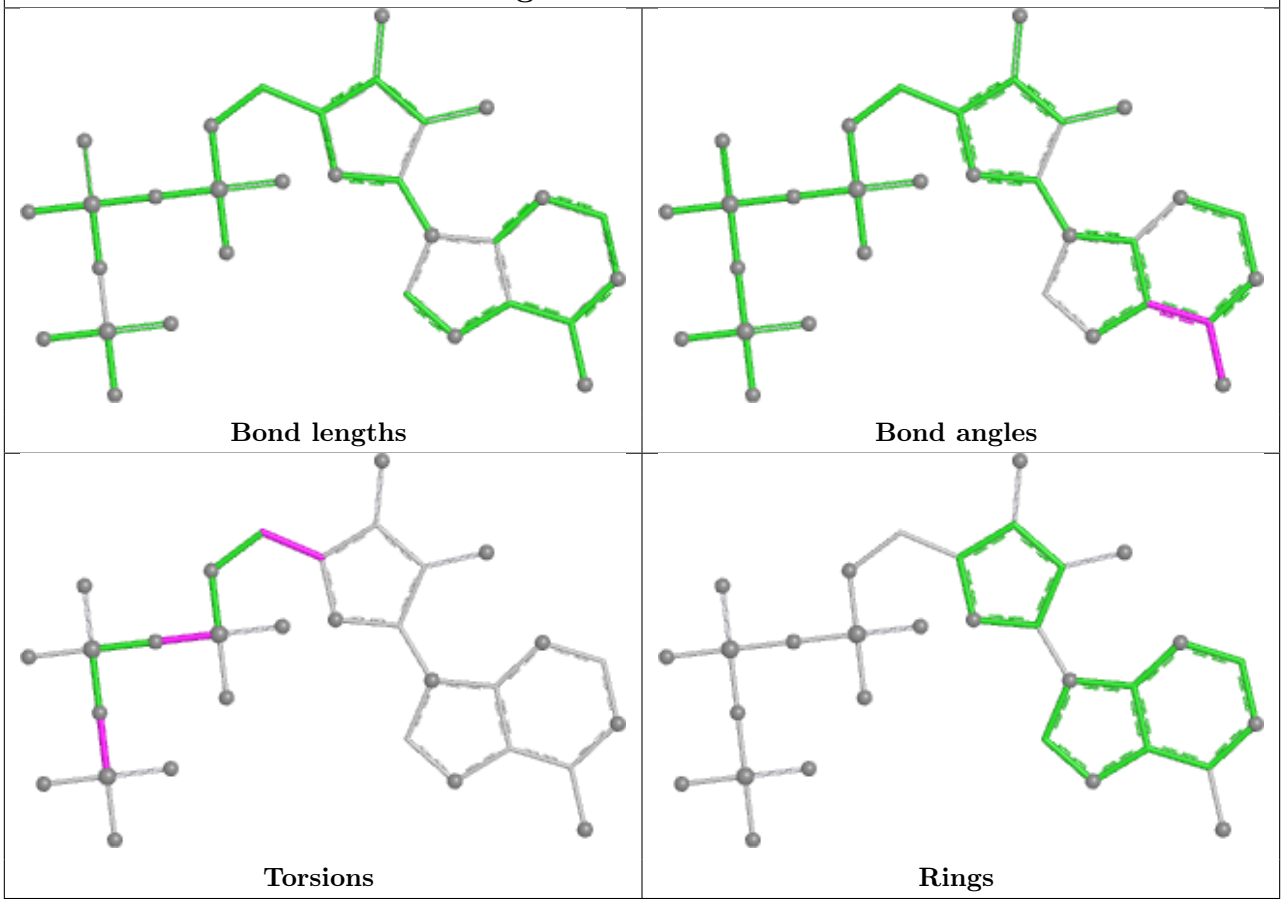


Torsions



Rings

Ligand ATP A 4801



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	13
1	A	6
4	B	2
12	D	2
13	P	1
7	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3277:MET	C	3380:MET	N	42.35
1	C	809:ARG	C	818:ILE	N	14.24
1	A	1235:PRO	C	1246:MET	N	12.91
1	C	665:ILE	C	670:SER	N	11.42
1	C	449:TYR	C	453:THR	N	10.61
1	C	546:LYS	C	629:ASN	N	8.50
1	C	360:PRO	C	364:ILE	N	7.00
1	C	483:ASN	C	492:GLY	N	6.36
1	C	1061:PHE	C	1066:GLU	N	6.36
1	C	773:PHE	C	776:TYR	N	4.39
1	A	4489:GLY	C	4493:GLY	N	4.28
1	B	25:GLN	C	26:LYS	N	3.78
1	D	216:HIS	C	217:GLN	N	3.67
1	C	706:LYS	C	710:LYS	N	3.60
1	A	53:ILE	C	54:PHE	N	3.57
1	C	2780:VAL	C	2783:ALA	N	3.50
1	A	115:ASP	C	116:ASN	N	3.46
1	A	40:LEU	C	41:LEU	N	3.39
1	A	24:LYS	C	25:ASP	N	3.36
1	P	15:SER	C	16:GLU	N	3.31
1	C	305:ASN	C	306:LEU	N	3.20
1	G	58:SER	C	59:GLU	N	3.19
1	D	238:SER	C	239:THR	N	3.15
1	C	1186:THR	C	1188:LEU	N	2.99
1	B	994:SER	C	995:TYR	N	2.89

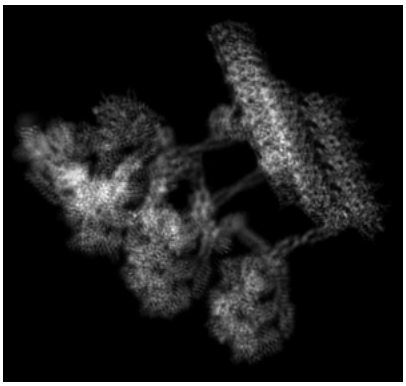
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22677. These allow visual inspection of the internal detail of the map and identification of artifacts.

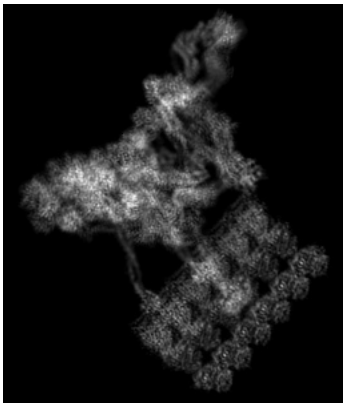
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

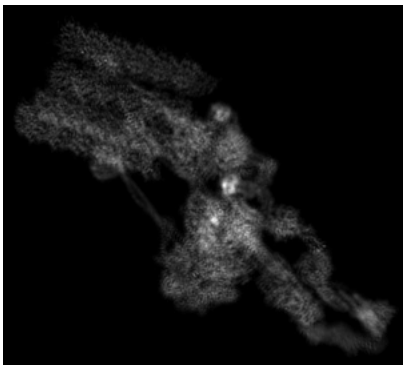
6.1.1 Primary map



X



Y

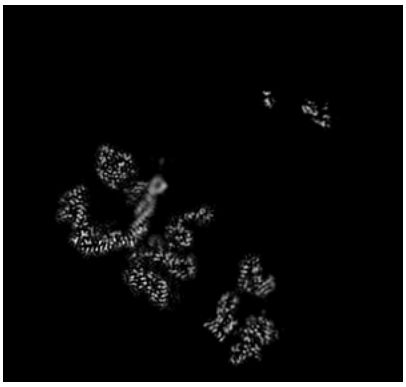


Z

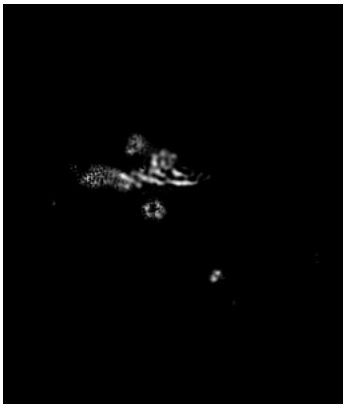
The images above show the map projected in three orthogonal directions.

6.2 Central slices

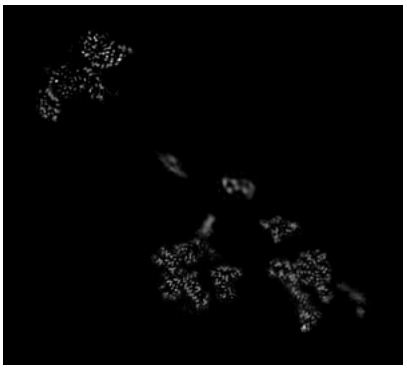
6.2.1 Primary map



X Index: 199



Y Index: 179

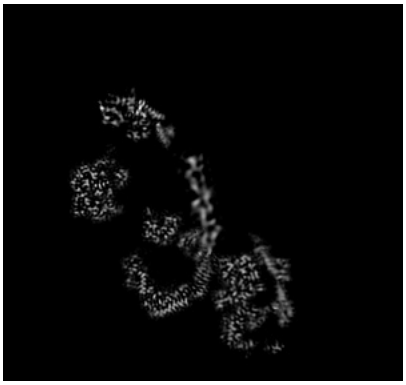


Z Index: 168

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

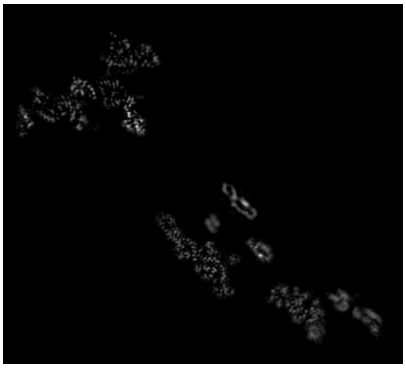
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 222

Y Index: 223

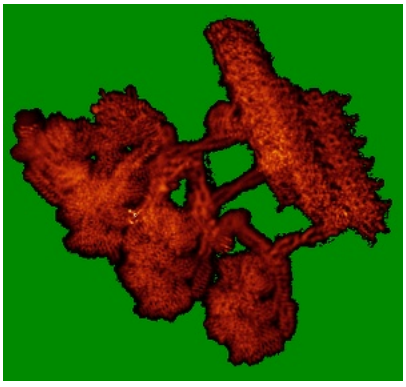


Z Index: 191

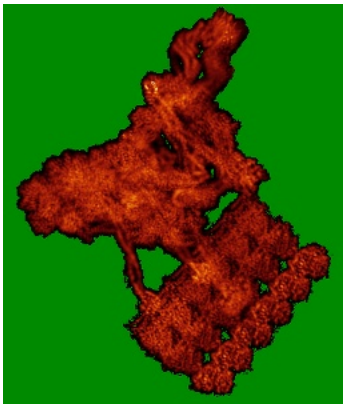
The images above show the largest variance slices of the map in three orthogonal directions.

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

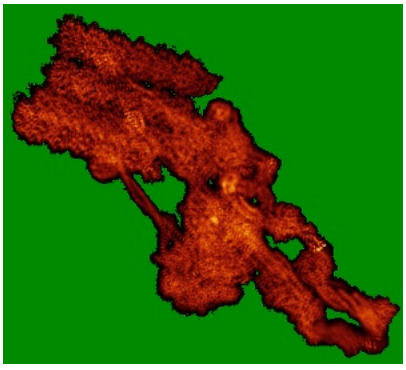
6.4.1 Primary map



X



Y

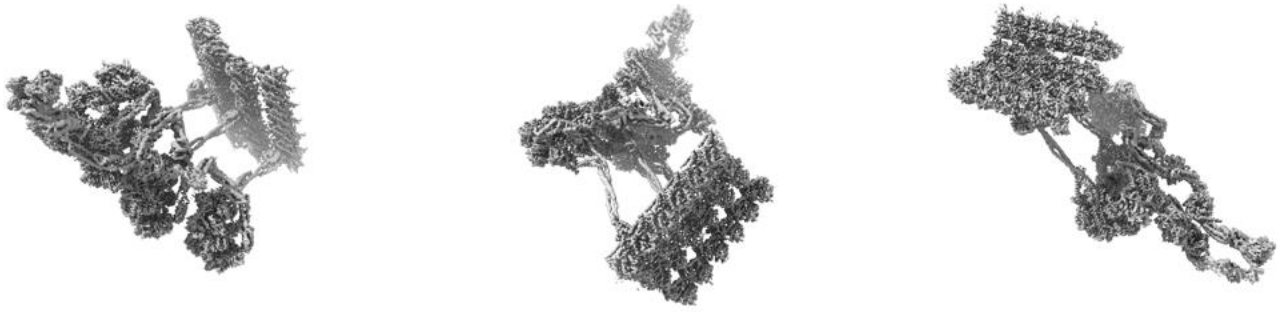


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

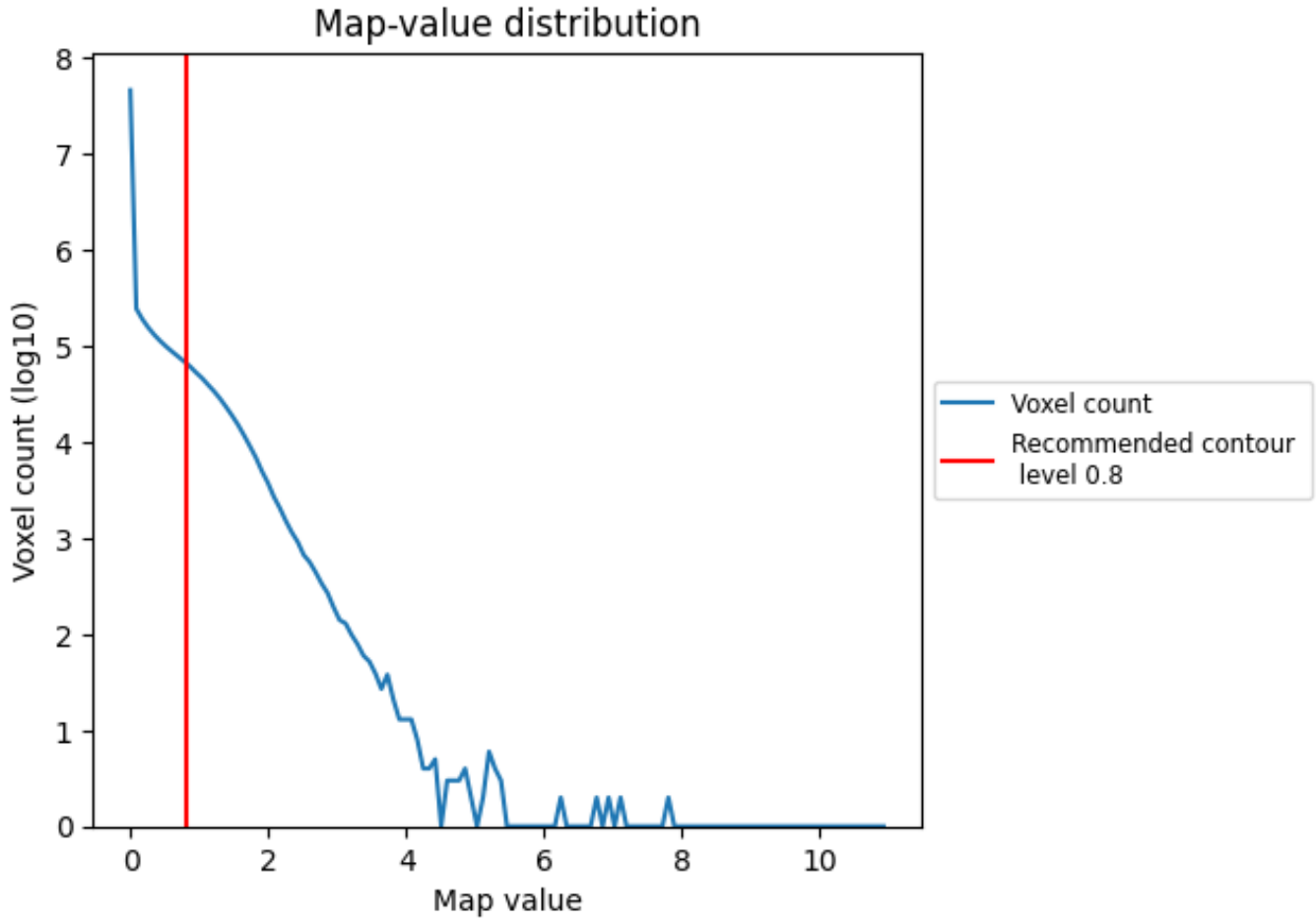
6.6 Mask visualisation (i)

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

7 Map analysis

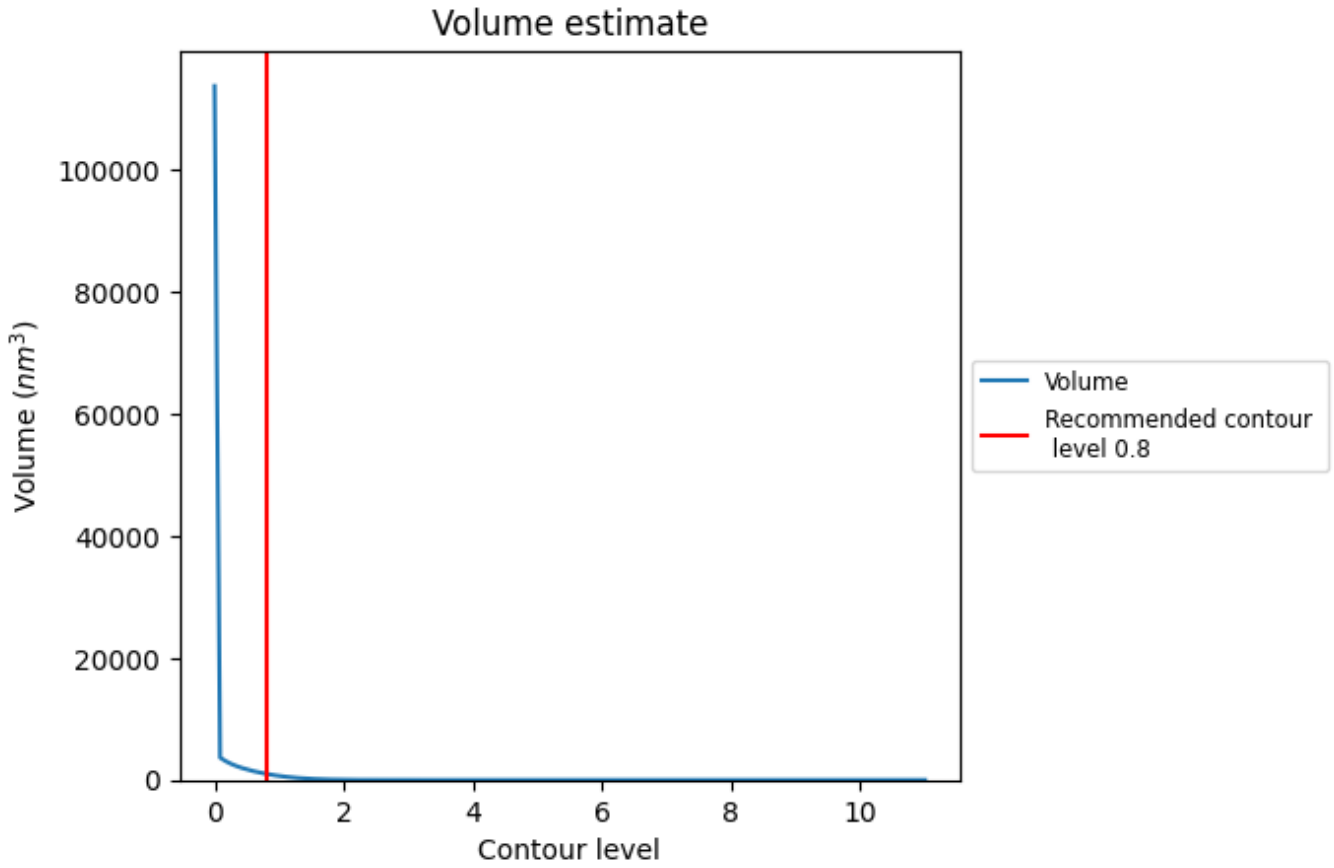
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

7.2 Volume estimate



The volume at the recommended contour level is 1003 nm^3; this corresponds to an approximate mass of 906 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

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

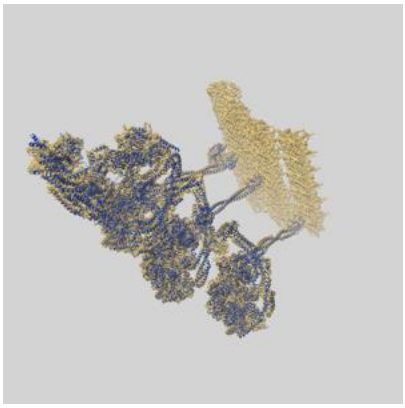
8 Fourier-Shell correlation (i)

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

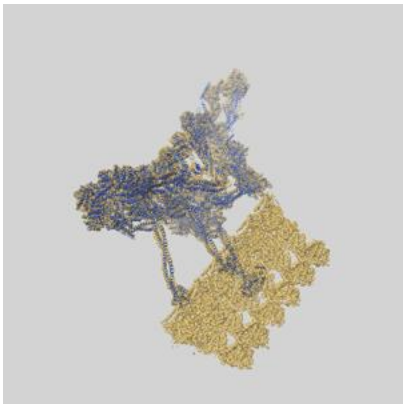
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22677 and PDB model 7K58. Per-residue inclusion information can be found in section 3 on page 9.

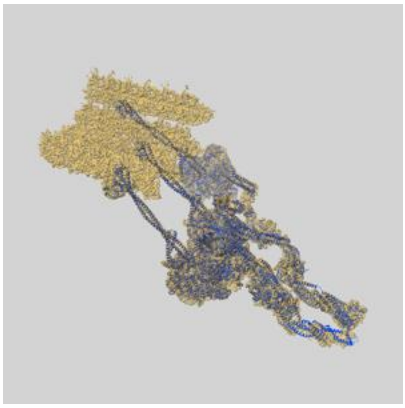
9.1 Map-model overlay



X



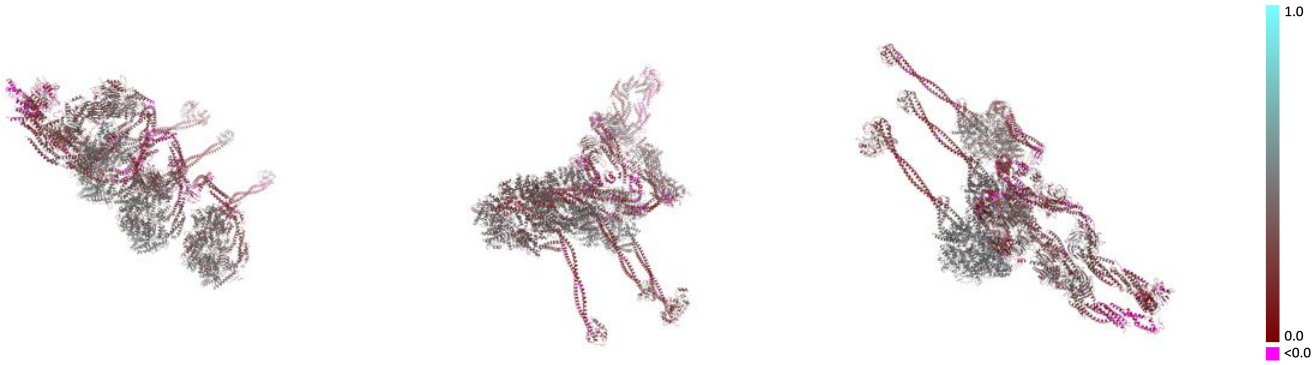
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.8 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.

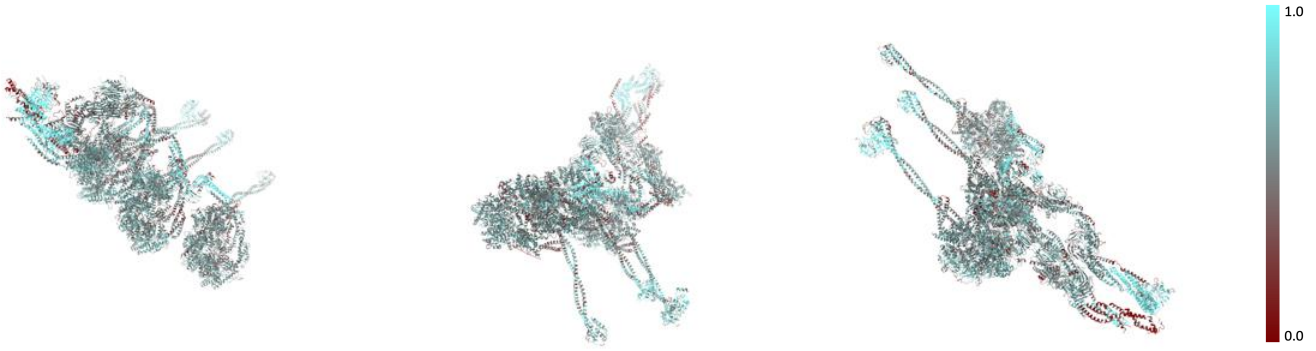
9.2 Q-score mapped to coordinate model (i)



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.

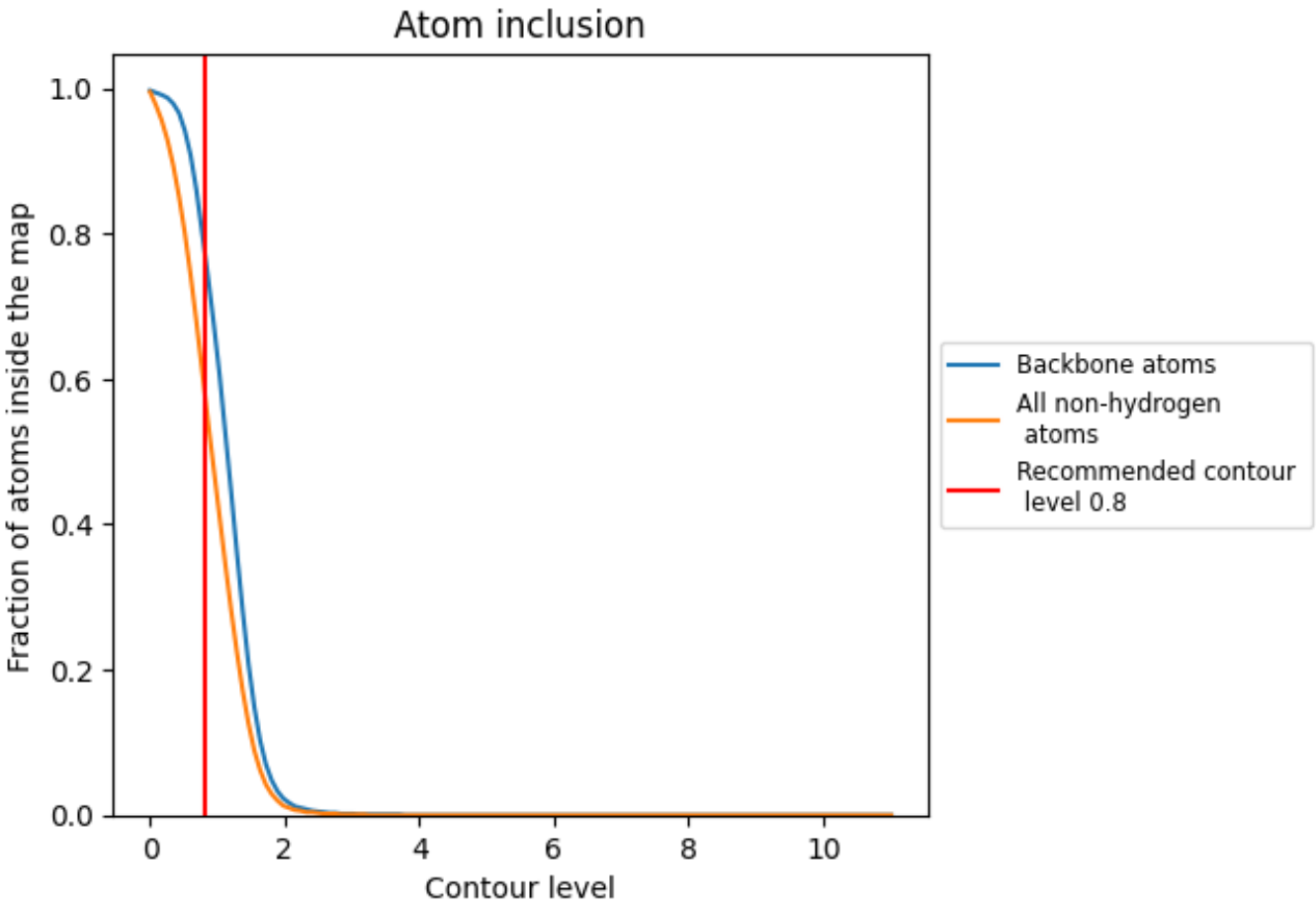
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.8).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5890	0.3570
A	0.6020	0.3820
B	0.6170	0.3590
C	0.5700	0.3380
D	0.5990	0.3420
E	0.5230	0.3550
F	0.5180	0.3830
G	0.4550	0.3710
H	0.4860	0.3550
I	0.5260	0.3180
J	0.5370	0.3860
K	0.4750	0.3630
L	0.4140	0.3650
M	0.5180	0.3810
N	0.5700	0.2740
O	0.5110	0.2540
P	0.5560	0.1490
Q	0.7990	0.3230