Full wwPDB EM Validation Report

Jan 14, 2025 – 03:02 PM JST

PDB ID	:	8YEZ
EMDB ID	:	EMD-39205
Title	:	Human PIEZO1
Authors	:	Zhang, M.F.
Deposited on	:	2024-02-23
Resolution	:	3.30 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:

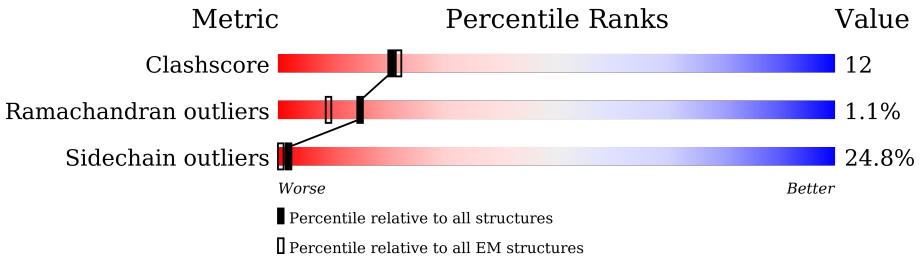
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 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	2521	10% 35% 13% · 49%
1	B	2521	11% 35% 13% · 49%
1	C	2521	10% 35% 13% · 49%

2 Entry composition

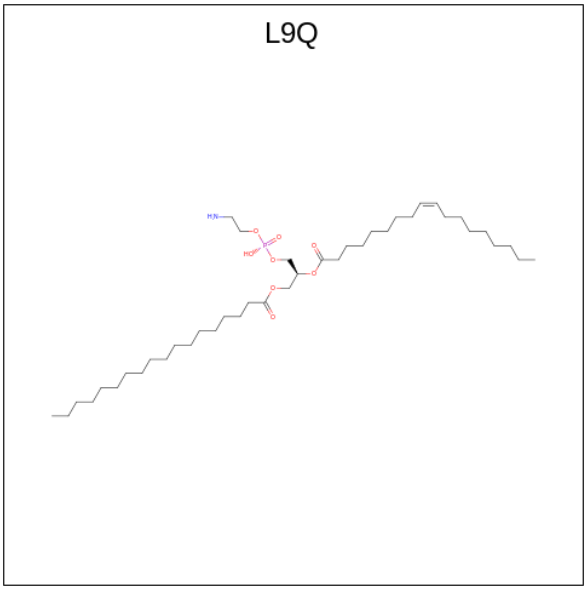
There are 2 unique types of molecules in this entry. The entry contains 31599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		
1	B	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		
1	C	1279	Total	C	N	O	S	0	0
			10431	6914	1725	1731	61		

- Molecule 2 is (1S)-2-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (three-letter code: L9Q) (formula: $C_{41}H_{80}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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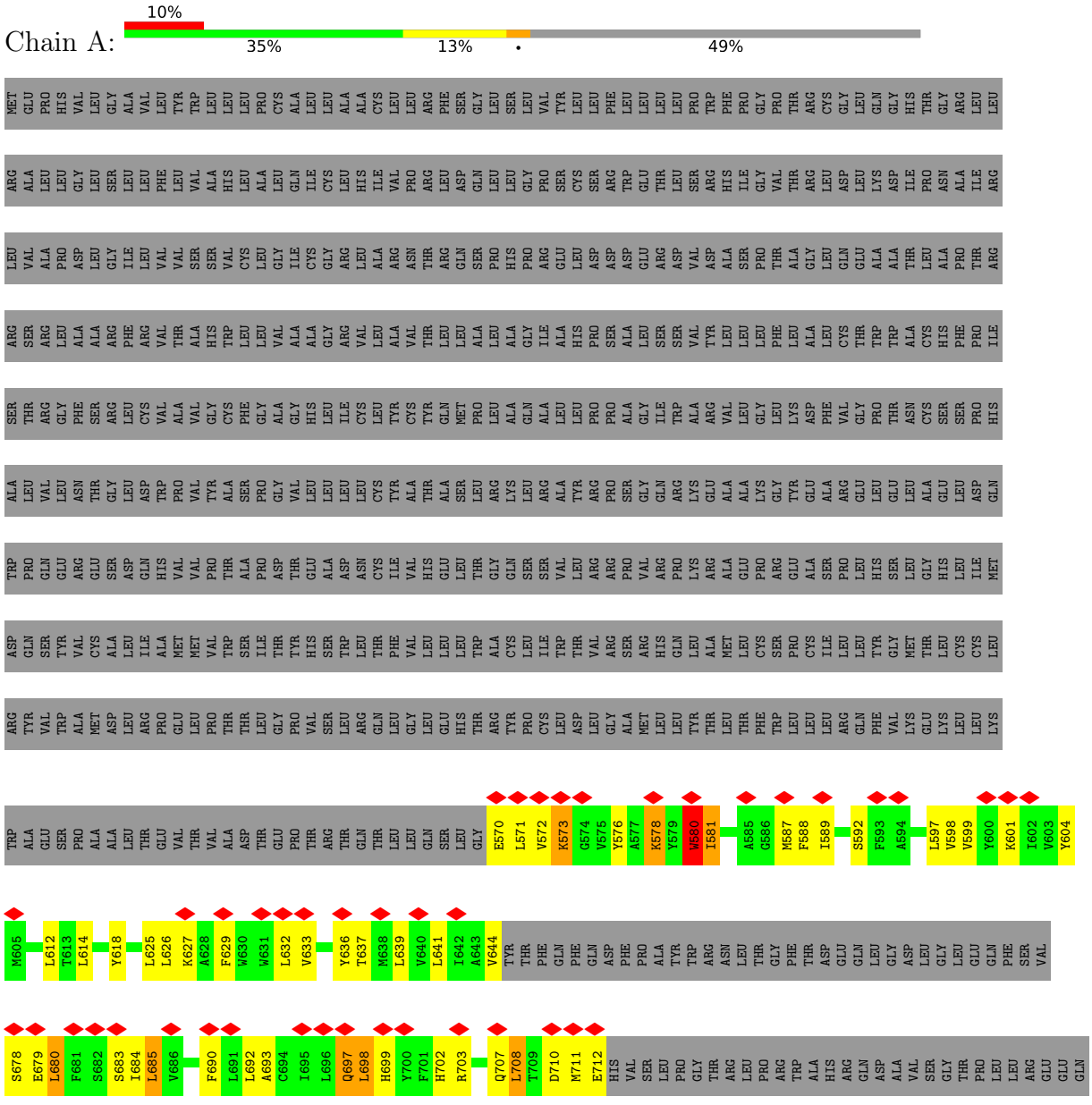
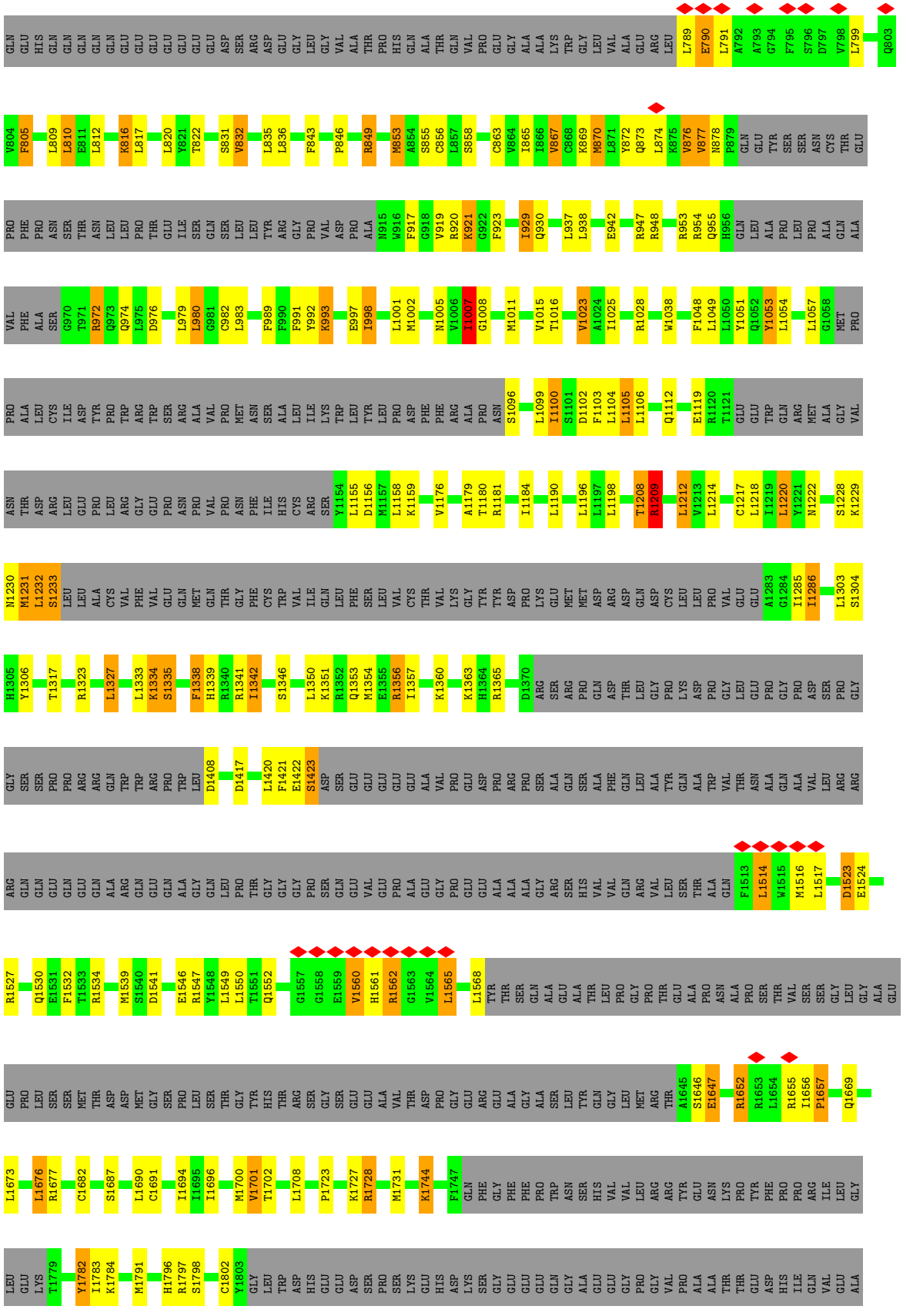
Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
2	C	1	Total	C	N	O	P	0
			51	41	1	8	1	

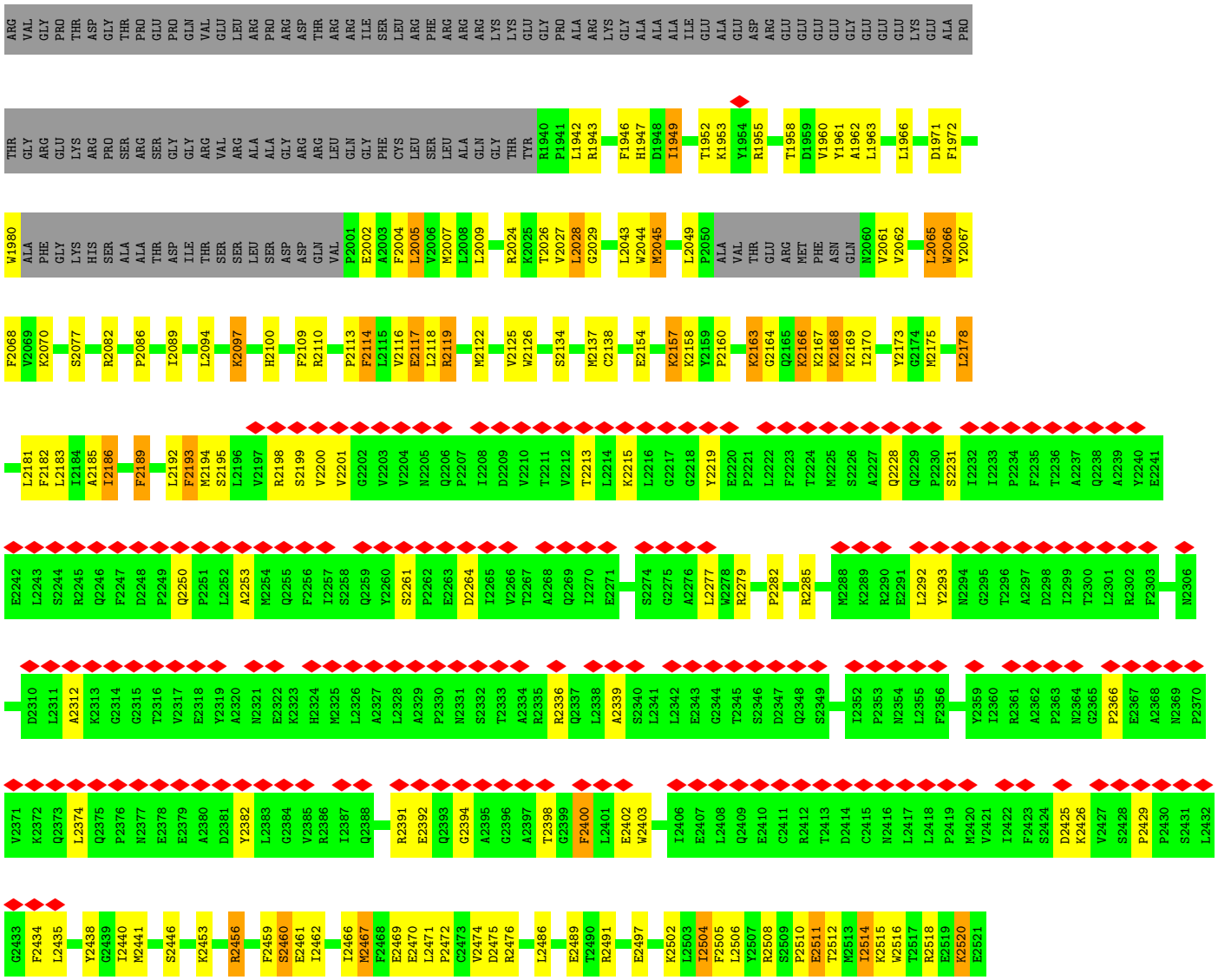
3 Residue-property plots (i)

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: Piezo-type mechanosensitive ion channel component 1

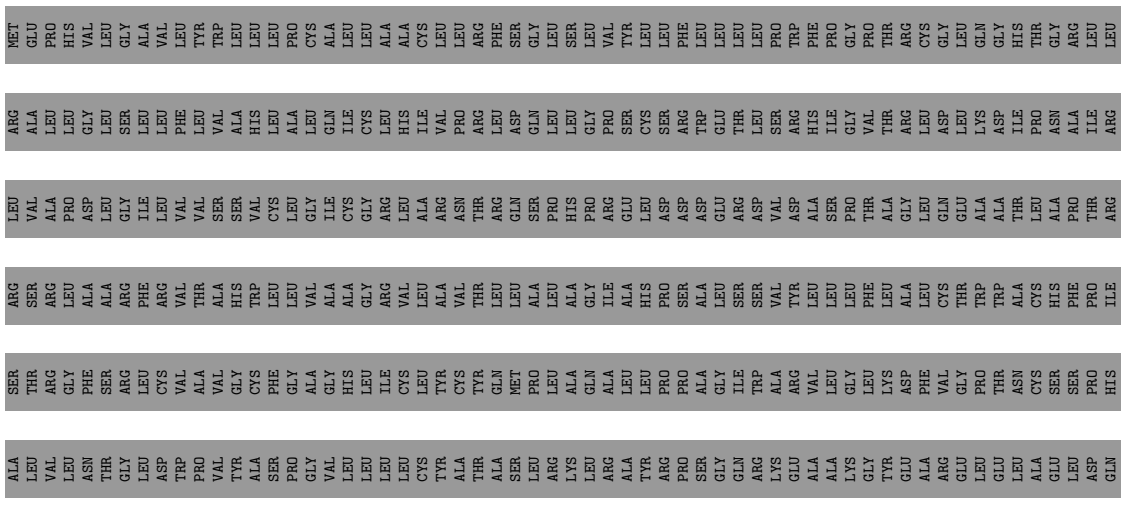


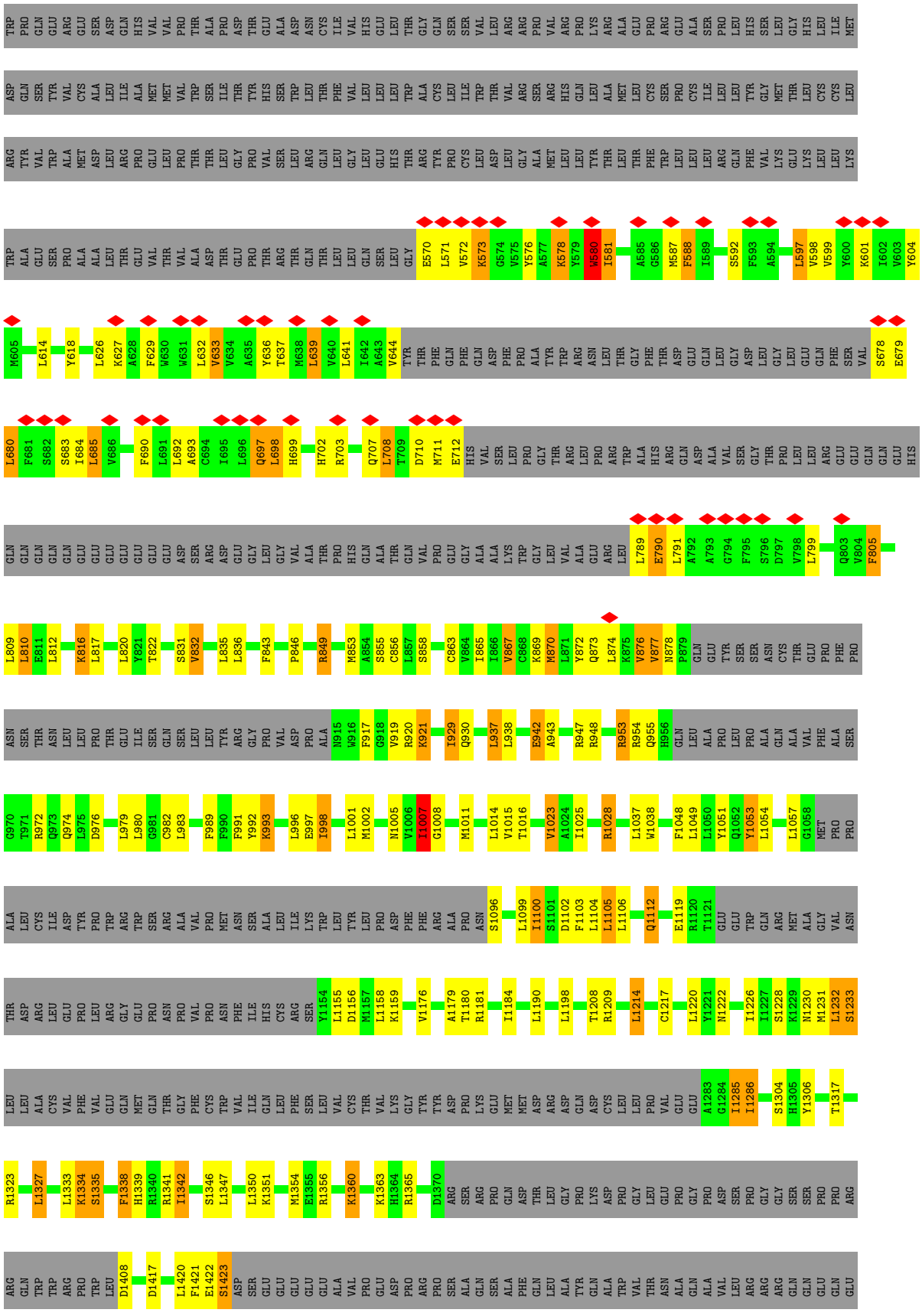


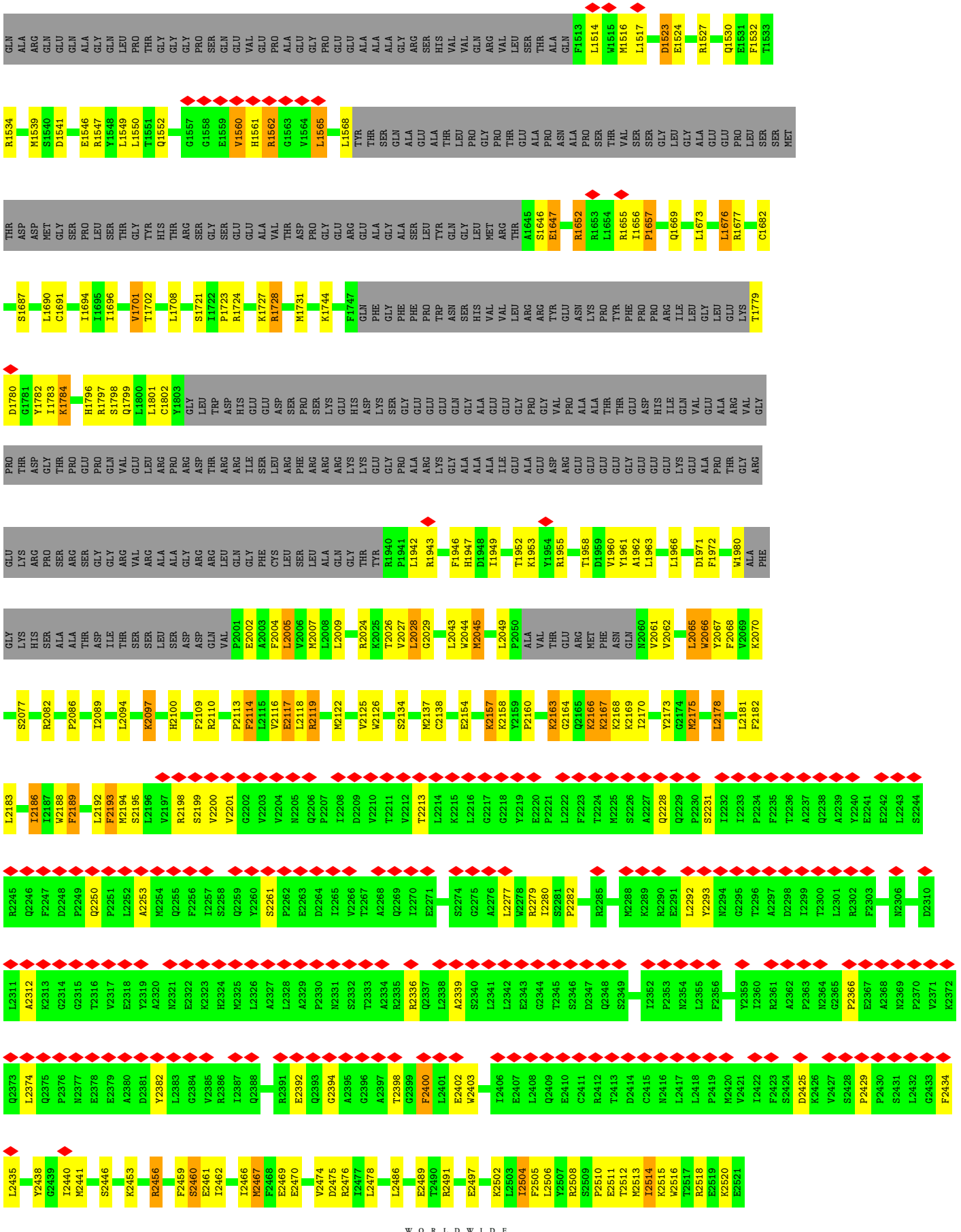


• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain B:

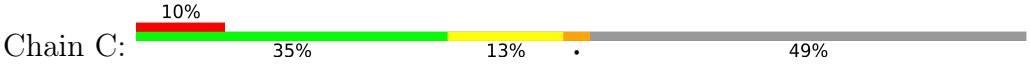


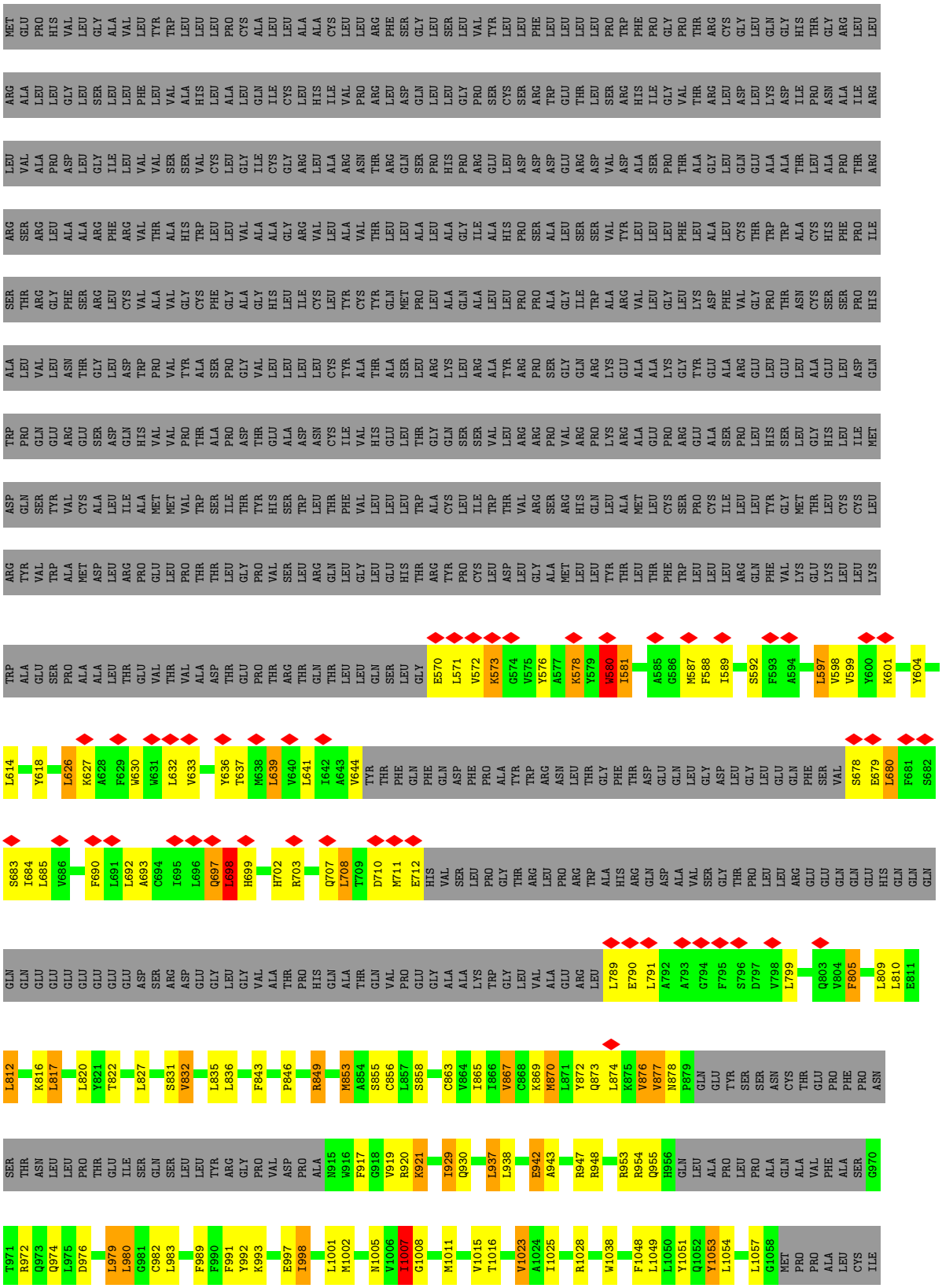


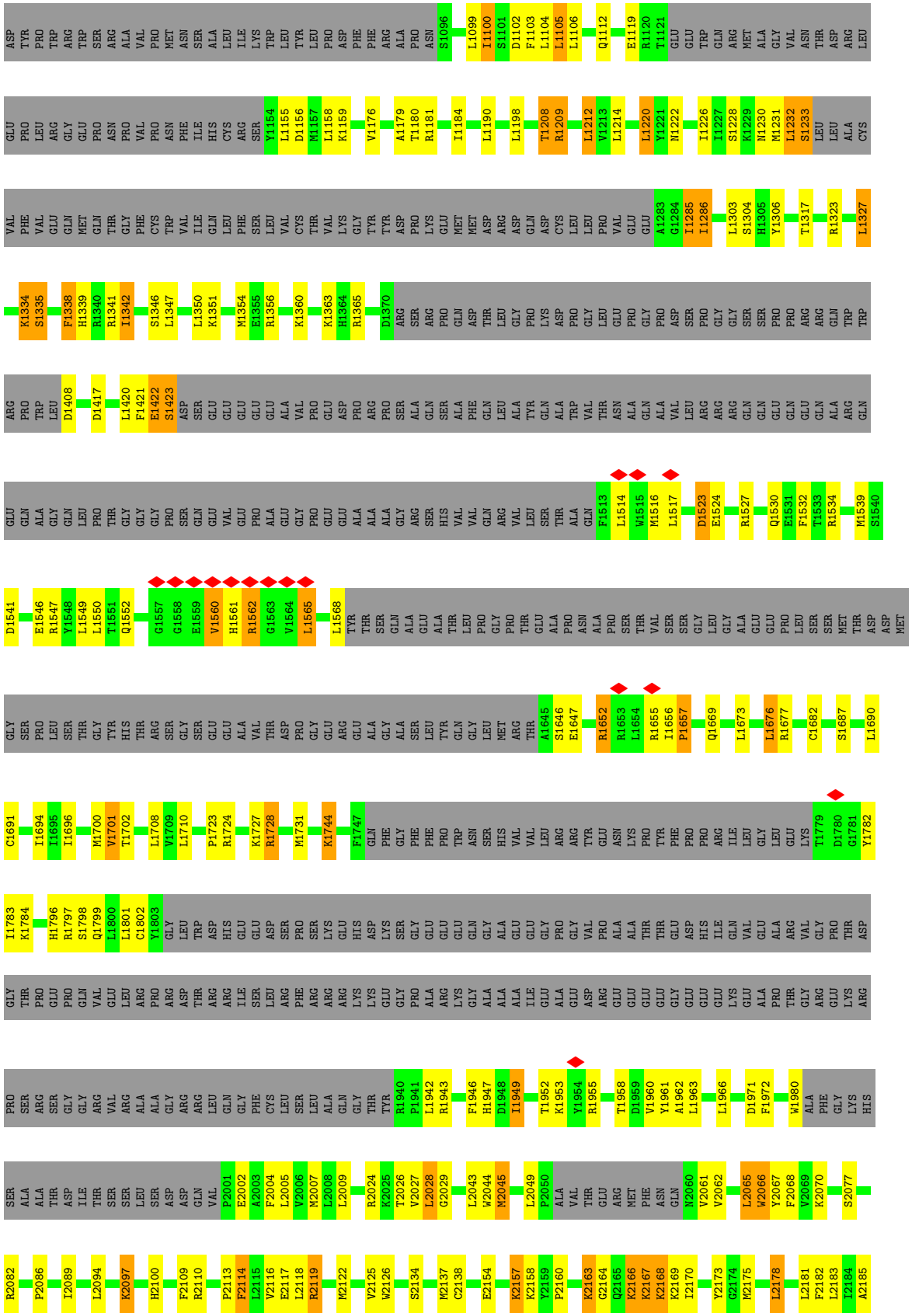


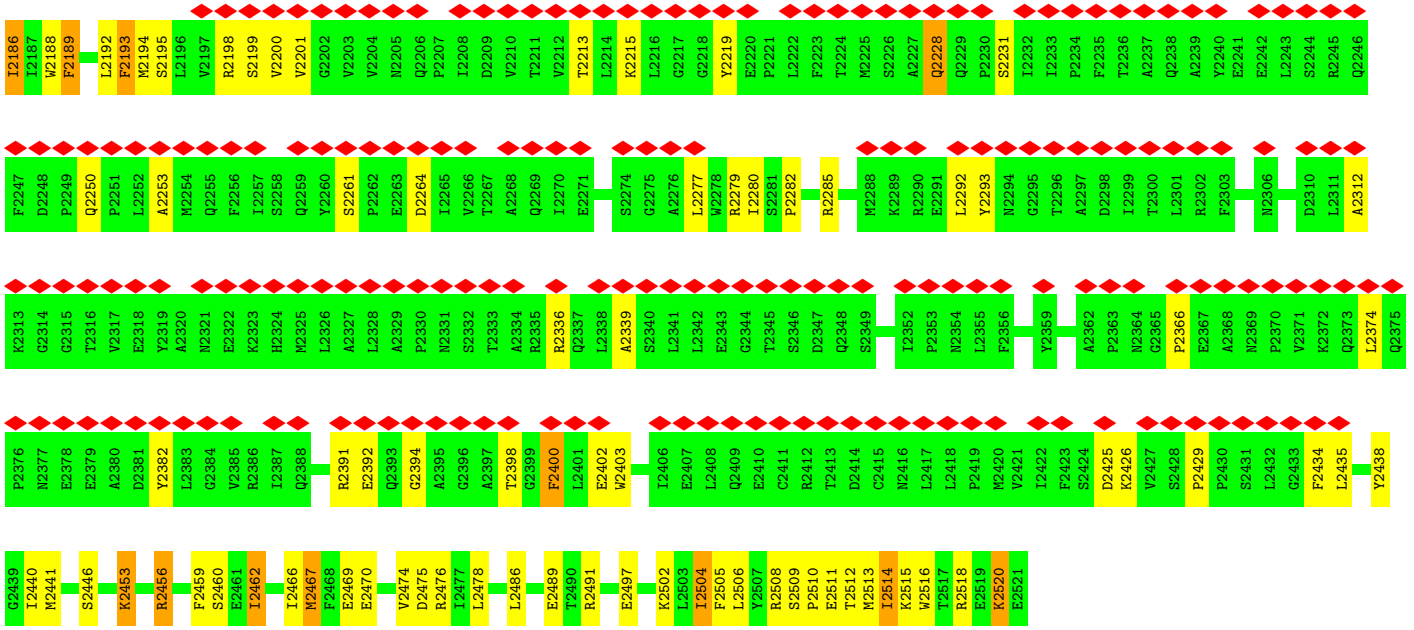
• Molecule 1: Piezo-type mechanosensitive ion channel component 1

Chain C:








I2186 I2187 W2188 F2189 L2192 F2193 M2194 S2195 L2196 V2197 R2198 S2199 V2200 V2201 G2202 V2203 V2204 N2205 Q2206 P2207 I2208 D2209 V2210 T2211 V2212 T2213 L2214 K2215 L2216 G2217 G2218 Y2219 E2220 P2221 L2222 F2223 T2224 M2225 S2226 A2227 Q2228 Q2229 P2230 S2231 I2232 I2233 P2234 F2235 T2236 A2237 Q2238 A2239 Y2240 E2241 E2242 L2243 S2244 R2245 Q2246
F2247 D2248 P2249 Q2250 P2251 L2252 A2253 M2254 Q2255 F2256 I2257 S2258 Q2259 Y2260 S2261 P2262 E2263 D2264 I2265 V2266 T2267 A2268 Q2269 I2270 E2271 S2274 G2275 A2276 L2277 W2278 R2279 I2280 S2281 P2282 R2285 M2288 K2289 R2290 E2291 L2292 Y2293 N2294 G2295 T2296 A2297 D2298 I2299 T2300 L2301 R2302 F2303 N2306 D2310 L2311 A2312
K2313 G2314 G2315 T2316 V2317 E2318 Y2319 A2320 N2321 E2322 K2323 H2324 M2325 L2326 A2327 L2328 A2329 P2330 N2331 S2332 T2333 A2334 R2335 R2336 Q2337 L2338 A2339 S2340 L2341 L2342 E2343 G2344 T2345 S2346 D2347 Q2348 S2349 I2352 P2353 N2354 L2355 F2356 Y2359 A2362 P2363 N2364 G2365 P2366 E2367 A2368 N2369 P2370 V2371 K2372 Q2373 L2374 Q2375
P2376 N2377 E2378 E2379 A2380 D2381 Y2382 L2383 G2384 V2385 R2386 I2387 Q2388 R2391 E2392 Q2393 G2394 A2395 G2396 A2397 T2398 G2399 F2400 L2401 E2402 W2403 I2406 E2407 L2408 Q2409 E2410 C2411 R2412 T2413 D2414 C2415 N2416 L2417 L2418 P2419 M2420 V2421 I2422 F2423 S2424 D2425 K2426 V2427 S2428 P2429 P2430 S2431 L2432 G2433 F2434 L2435 Y2438
G2439 I2440 M2441 S2446 K2453 R2456 F2459 S2460 E2461 I2462 I2466 M2467 F2468 E2469 E2470 V2474 D2475 R2476 I2477 L2478 L2486 E2489 T2490 R2491 E2497 K2502 L2503 I2504 F2505 L2506 Y2507 R2508 S2509 P2510 E2511 T2512 M2513 I2514 K2515 W2516 T2517 R2518 E2519 K2520 E2521

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	161218	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI MORGAGNI	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.095	Depositor
Minimum map value	-0.712	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	543.36, 543.36, 543.36	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.849, 0.849, 0.849	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L9Q

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	0.52	0/10690	0.65	3/14491 (0.0%)
1	B	0.52	0/10690	0.66	3/14491 (0.0%)
1	C	0.52	0/10690	0.66	3/14491 (0.0%)
All	All	0.52	0/32070	0.66	9/43473 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	2425	ASP	CB-CG-OD1	5.77	123.50	118.30
1	B	2425	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	2425	ASP	CB-CG-OD1	5.76	123.48	118.30
1	A	2382	TYR	CB-CG-CD2	-5.51	117.70	121.00
1	C	2382	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	2382	TYR	CB-CG-CD2	-5.46	117.72	121.00
1	A	2336	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	2336	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	B	2336	ARG	NE-CZ-NH1	5.33	122.97	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10431	0	10666	285	0
1	B	10431	0	10666	275	0
1	C	10431	0	10666	283	0
2	A	153	0	237	9	0
2	B	102	0	158	6	0
2	C	51	0	79	1	0
All	All	31599	0	32472	770	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 12.

All (770) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2193:PHE:HD1	1:A:2194:MET:N	1.11	1.44
1:B:2157:LYS:NZ	1:B:2157:LYS:CB	1.70	1.44
1:C:2193:PHE:HD1	1:C:2194:MET:N	1.11	1.42
1:A:2028:LEU:CD1	1:A:2028:LEU:C	1.78	1.41
1:B:2193:PHE:HD1	1:B:2194:MET:N	1.11	1.39
1:A:2028:LEU:HD12	1:A:2029:GLY:N	1.39	1.38
1:C:2028:LEU:CD1	1:C:2028:LEU:C	1.78	1.36
1:A:2028:LEU:C	1:A:2028:LEU:HD13	1.31	1.36
1:A:2157:LYS:CB	1:A:2157:LYS:NZ	1.70	1.36
1:B:2028:LEU:HD12	1:B:2029:GLY:N	1.39	1.35
1:B:2028:LEU:CD1	1:B:2028:LEU:C	1.78	1.35
1:C:2028:LEU:HD12	1:C:2029:GLY:N	1.39	1.34
1:B:2193:PHE:CD1	1:B:2194:MET:N	1.96	1.33
1:A:2193:PHE:CD1	1:A:2194:MET:N	1.96	1.33
1:C:2193:PHE:CD1	1:C:2194:MET:N	1.96	1.33
1:C:2157:LYS:NZ	1:C:2157:LYS:CB	1.70	1.32
1:B:2137:MET:SD	1:C:2459:PHE:CE1	2.27	1.28
1:A:2137:MET:SD	1:B:2459:PHE:CE1	2.27	1.27
1:A:2459:PHE:CE1	1:C:2137:MET:SD	2.27	1.26
1:C:2028:LEU:C	1:C:2028:LEU:HD13	1.31	1.25
1:B:2028:LEU:HD13	1:B:2028:LEU:O	1.09	1.24
1:A:2028:LEU:HD13	1:A:2028:LEU:O	1.09	1.23
1:C:2193:PHE:HD1	1:C:2193:PHE:C	1.42	1.22
1:C:2028:LEU:HD13	1:C:2028:LEU:O	1.09	1.22
1:B:2193:PHE:HD1	1:B:2193:PHE:C	1.42	1.20
1:A:2193:PHE:HD1	1:A:2193:PHE:C	1.42	1.19
1:C:1783:ILE:HG22	1:C:1783:ILE:O	1.37	1.18
1:B:2028:LEU:C	1:B:2028:LEU:HD13	1.31	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2157:LYS:NZ	1:A:2157:LYS:HB3	1.41	1.15
1:B:2193:PHE:CE1	1:B:2194:MET:HG2	1.82	1.14
1:C:2193:PHE:CE1	1:C:2194:MET:HG2	1.82	1.13
1:A:2193:PHE:CE1	1:A:2194:MET:HG2	1.82	1.13
1:A:2137:MET:SD	1:B:2459:PHE:CD1	2.42	1.12
1:B:1023:VAL:O	1:B:1023:VAL:CG1	1.97	1.12
1:B:2137:MET:SD	1:C:2459:PHE:CD1	2.42	1.12
1:A:2459:PHE:CD1	1:C:2137:MET:SD	2.42	1.12
1:C:1023:VAL:CG1	1:C:1023:VAL:O	1.97	1.11
1:A:2459:PHE:HE1	1:C:2137:MET:SD	1.71	1.11
1:B:1783:ILE:O	1:B:1783:ILE:HG22	1.37	1.10
1:A:1783:ILE:HG22	1:A:1783:ILE:O	1.37	1.09
1:C:2157:LYS:NZ	1:C:2157:LYS:HB3	1.41	1.09
1:B:2157:LYS:NZ	1:B:2157:LYS:HB2	1.41	1.09
1:A:929:ILE:O	1:A:929:ILE:CG2	2.02	1.08
1:B:2137:MET:SD	1:C:2459:PHE:HE1	1.71	1.06
1:C:929:ILE:O	1:C:929:ILE:CG2	2.02	1.06
1:B:929:ILE:CG2	1:B:929:ILE:O	2.02	1.06
1:A:1023:VAL:CG1	1:A:1023:VAL:O	1.97	1.05
1:A:587:MET:SD	1:A:690:PHE:HA	1.96	1.05
1:C:2157:LYS:NZ	1:C:2157:LYS:HB2	1.41	1.05
1:B:587:MET:SD	1:B:690:PHE:HA	1.96	1.05
1:C:2028:LEU:CD1	1:C:2029:GLY:N	2.10	1.05
1:B:2028:LEU:CD1	1:B:2029:GLY:N	2.10	1.04
1:C:587:MET:SD	1:C:690:PHE:HA	1.96	1.04
1:B:2157:LYS:NZ	1:B:2157:LYS:HB3	1.41	1.04
1:A:2193:PHE:HE1	1:A:2194:MET:HG2	1.13	1.03
1:A:1023:VAL:O	1:A:1023:VAL:HG13	1.59	1.03
1:A:2157:LYS:NZ	1:A:2157:LYS:HB2	1.41	1.03
1:A:2137:MET:SD	1:B:2459:PHE:HE1	1.71	1.03
1:A:2028:LEU:CD1	1:A:2029:GLY:N	2.10	1.02
1:C:2193:PHE:HE1	1:C:2194:MET:HG2	1.13	1.02
1:A:2193:PHE:CD1	1:A:2193:PHE:C	2.18	1.02
1:C:1338:PHE:CE1	1:C:1339:HIS:CD2	2.48	1.01
1:C:1562:ARG:CD	1:C:1565:LEU:HD12	1.90	1.01
1:C:1053:TYR:O	1:C:1053:TYR:CD1	2.14	1.01
1:B:1053:TYR:O	1:B:1053:TYR:CD1	2.14	1.01
1:A:1053:TYR:O	1:A:1053:TYR:CD1	2.14	1.01
1:A:1562:ARG:CD	1:A:1565:LEU:HD12	1.90	1.01
1:B:1562:ARG:CD	1:B:1565:LEU:HD12	1.90	1.00
1:B:2193:PHE:HE1	1:B:2194:MET:HG2	1.13	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1338:PHE:HD1	1:C:1339:HIS:N	1.60	1.00
1:A:1338:PHE:CE1	1:A:1339:HIS:CD2	2.48	1.00
1:A:1338:PHE:HD1	1:A:1339:HIS:N	1.59	1.00
1:B:1338:PHE:HD1	1:B:1339:HIS:N	1.60	1.00
1:B:1338:PHE:CE1	1:B:1339:HIS:CD2	2.48	0.99
1:C:929:ILE:O	1:C:929:ILE:HG22	1.62	0.99
1:B:863:CYS:O	1:B:867:VAL:HG23	1.61	0.99
1:B:929:ILE:O	1:B:929:ILE:HG22	1.62	0.99
1:C:1338:PHE:CD1	1:C:1339:HIS:N	2.31	0.99
1:A:2505:PHE:O	1:A:2505:PHE:CD1	2.16	0.98
1:C:863:CYS:O	1:C:867:VAL:HG23	1.61	0.98
1:C:2193:PHE:CD1	1:C:2193:PHE:C	2.18	0.98
1:A:863:CYS:O	1:A:867:VAL:HG23	1.61	0.98
1:A:1338:PHE:CD1	1:A:1339:HIS:N	2.31	0.98
1:C:2193:PHE:CE1	1:C:2194:MET:CG	2.47	0.98
1:B:1023:VAL:O	1:B:1023:VAL:HG13	1.59	0.98
1:B:1338:PHE:CD1	1:B:1339:HIS:N	2.31	0.98
1:B:2193:PHE:CE1	1:B:2194:MET:CG	2.47	0.98
1:C:1023:VAL:O	1:C:1023:VAL:HG13	1.59	0.98
1:C:2505:PHE:O	1:C:2505:PHE:CD1	2.16	0.97
1:A:2193:PHE:CE1	1:A:2194:MET:CG	2.47	0.97
1:B:2505:PHE:O	1:B:2505:PHE:CD1	2.16	0.97
1:B:2504:ILE:HD11	1:C:2466:ILE:HD13	1.46	0.96
1:B:1338:PHE:HE1	1:B:1339:HIS:CD2	1.83	0.96
1:A:587:MET:HE3	1:A:693:ALA:HB3	1.44	0.96
1:C:1342:ILE:HD13	1:C:1342:ILE:N	1.80	0.96
1:A:1338:PHE:HE1	1:A:1339:HIS:CD2	1.83	0.96
1:A:2504:ILE:HD11	1:B:2466:ILE:HD13	1.46	0.96
1:A:1783:ILE:O	1:A:1783:ILE:CG2	2.12	0.96
1:B:1342:ILE:N	1:B:1342:ILE:HD13	1.80	0.95
1:A:929:ILE:O	1:A:929:ILE:HG22	1.62	0.95
1:A:1342:ILE:HD13	1:A:1342:ILE:N	1.80	0.94
1:C:1338:PHE:HE1	1:C:1339:HIS:CD2	1.84	0.94
1:B:1783:ILE:O	1:B:1783:ILE:CG2	2.12	0.93
1:A:2466:ILE:HD13	1:C:2504:ILE:HD11	1.46	0.93
1:C:2028:LEU:CD1	1:C:2028:LEU:O	2.03	0.93
1:C:2157:LYS:HB2	1:C:2157:LYS:HZ1	1.24	0.93
1:A:2157:LYS:HB2	1:A:2157:LYS:HZ1	1.27	0.93
1:B:2113:PRO:O	1:B:2114:PHE:HB2	1.69	0.92
1:C:846:PRO:HG3	1:C:1106:LEU:HD11	1.52	0.91
1:A:1356:ARG:NH2	1:A:1357:ILE:HG13	1.86	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:PRO:HG3	1:B:1106:LEU:HD11	1.52	0.91
1:B:1562:ARG:HD3	1:B:1565:LEU:HD12	1.51	0.91
1:C:2113:PRO:O	1:C:2114:PHE:HB2	1.69	0.91
1:B:587:MET:HE3	1:B:693:ALA:HB3	1.53	0.90
1:C:1562:ARG:HD3	1:C:1565:LEU:HD12	1.51	0.90
1:A:2113:PRO:O	1:A:2114:PHE:HB2	1.69	0.90
1:A:1562:ARG:HD3	1:A:1565:LEU:HD12	1.51	0.89
1:C:1783:ILE:O	1:C:1783:ILE:CG2	2.12	0.89
1:A:846:PRO:HG3	1:A:1106:LEU:HD11	1.52	0.89
1:B:2193:PHE:CD1	1:B:2193:PHE:C	2.18	0.89
1:C:587:MET:HE3	1:C:693:ALA:HB3	1.55	0.89
1:C:587:MET:HE1	1:C:693:ALA:CB	2.04	0.87
1:A:1656:ILE:HG23	1:A:1657:PRO:HD2	1.56	0.87
1:A:2312:ALA:HB2	1:B:2366:PRO:HG2	1.57	0.87
1:C:1656:ILE:HG23	1:C:1657:PRO:HD2	1.56	0.87
1:B:2312:ALA:HB2	1:C:2366:PRO:HG2	1.57	0.86
1:B:1656:ILE:HG23	1:B:1657:PRO:HD2	1.56	0.85
1:C:587:MET:CE	1:C:693:ALA:HB3	2.06	0.85
1:A:2366:PRO:HG2	1:C:2312:ALA:HB2	1.57	0.85
1:B:1338:PHE:CD1	1:B:1338:PHE:C	2.50	0.85
1:A:587:MET:CE	1:A:693:ALA:HB3	2.06	0.85
1:B:587:MET:CE	1:B:693:ALA:HB3	2.06	0.85
1:A:1338:PHE:CD1	1:A:1338:PHE:C	2.50	0.84
1:B:587:MET:HE1	1:B:693:ALA:CB	2.07	0.84
1:A:2028:LEU:CD1	1:A:2028:LEU:O	2.03	0.84
1:C:2028:LEU:HD12	1:C:2029:GLY:CA	2.08	0.84
1:C:1338:PHE:CD1	1:C:1338:PHE:C	2.50	0.84
1:A:2028:LEU:HD12	1:A:2029:GLY:CA	2.08	0.83
1:C:1560:VAL:HG12	1:C:1560:VAL:O	1.79	0.82
1:B:604:TYR:OH	1:B:637:THR:HA	1.79	0.82
1:C:604:TYR:OH	1:C:637:THR:HA	1.79	0.82
1:B:2028:LEU:HD12	1:B:2029:GLY:CA	2.08	0.81
1:C:874:LEU:HB2	1:C:877:VAL:CG2	2.10	0.81
1:A:604:TYR:OH	1:A:637:THR:HA	1.79	0.81
1:A:2403:TRP:CH2	1:B:2282:PRO:HD2	2.16	0.81
1:A:2193:PHE:HD1	1:A:2194:MET:CA	1.94	0.81
1:A:2282:PRO:HD2	1:C:2403:TRP:CH2	2.16	0.81
1:B:874:LEU:HB2	1:B:877:VAL:CG2	2.10	0.81
1:B:2403:TRP:CH2	1:C:2282:PRO:HD2	2.15	0.81
1:B:1560:VAL:HG12	1:B:1560:VAL:O	1.79	0.81
1:C:1023:VAL:O	1:C:1023:VAL:HG12	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2193:PHE:HD1	1:C:2194:MET:CA	1.94	0.81
1:B:1023:VAL:O	1:B:1023:VAL:HG12	1.80	0.81
1:B:2193:PHE:HD1	1:B:2194:MET:CA	1.94	0.81
1:A:1560:VAL:HG12	1:A:1560:VAL:O	1.79	0.80
1:C:587:MET:CE	1:C:693:ALA:CB	2.60	0.80
1:A:874:LEU:HB2	1:A:877:VAL:CG2	2.10	0.80
1:B:863:CYS:O	1:B:867:VAL:CG2	2.29	0.80
1:C:863:CYS:O	1:C:867:VAL:CG2	2.29	0.80
1:C:1342:ILE:HD13	1:C:1342:ILE:H	1.46	0.80
1:C:1656:ILE:HG23	1:C:1657:PRO:CD	2.12	0.80
1:A:1023:VAL:O	1:A:1023:VAL:HG12	1.80	0.80
1:B:2028:LEU:CD1	1:B:2028:LEU:O	2.03	0.80
1:A:587:MET:CE	1:A:693:ALA:CB	2.60	0.79
1:B:587:MET:CE	1:B:693:ALA:CB	2.60	0.79
1:A:863:CYS:O	1:A:867:VAL:CG2	2.29	0.79
1:B:1656:ILE:HG23	1:B:1657:PRO:CD	2.12	0.79
1:A:2137:MET:SD	1:B:2459:PHE:HD1	2.03	0.79
1:A:1656:ILE:HG23	1:A:1657:PRO:CD	2.12	0.78
1:B:2137:MET:SD	1:C:2459:PHE:HD1	2.03	0.78
1:B:1342:ILE:HD13	1:B:1342:ILE:H	1.45	0.78
1:A:2193:PHE:CD1	1:A:2194:MET:CA	2.66	0.78
1:A:2459:PHE:HD1	1:C:2137:MET:SD	2.03	0.78
1:C:992:TYR:OH	1:C:1119:GLU:HG2	1.84	0.78
1:B:2312:ALA:HB2	1:C:2366:PRO:CG	2.14	0.77
1:B:992:TYR:OH	1:B:1119:GLU:HG2	1.84	0.77
1:A:992:TYR:OH	1:A:1119:GLU:HG2	1.84	0.77
1:A:1701:VAL:HG12	1:A:1702:THR:N	1.99	0.77
1:A:2366:PRO:CG	1:C:2312:ALA:HB2	2.14	0.77
1:A:1342:ILE:HD13	1:A:1342:ILE:H	1.45	0.77
1:A:2312:ALA:HB2	1:B:2366:PRO:CG	2.14	0.77
1:A:1338:PHE:O	1:A:1342:ILE:CD1	2.34	0.76
1:C:1701:VAL:HG12	1:C:1702:THR:N	1.99	0.76
1:C:1338:PHE:O	1:C:1342:ILE:CD1	2.34	0.76
1:C:2193:PHE:CD1	1:C:2194:MET:CA	2.67	0.76
1:B:1338:PHE:O	1:B:1342:ILE:CD1	2.34	0.76
1:B:1701:VAL:HG12	1:B:1702:THR:N	1.99	0.76
1:A:587:MET:HE1	1:A:693:ALA:CB	2.15	0.75
1:B:2193:PHE:CD1	1:B:2194:MET:CA	2.66	0.75
1:A:929:ILE:O	1:A:929:ILE:HG23	1.86	0.75
1:C:929:ILE:O	1:C:929:ILE:HG23	1.87	0.75
1:A:1562:ARG:HD2	1:A:1565:LEU:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1562:ARG:CD	1:A:1565:LEU:CD1	2.65	0.74
1:A:2505:PHE:O	1:A:2505:PHE:HD1	1.69	0.74
1:C:1562:ARG:CD	1:C:1565:LEU:CD1	2.65	0.74
1:C:2065:LEU:O	1:C:2066:TRP:C	2.25	0.74
1:B:1562:ARG:HD2	1:B:1565:LEU:HD12	1.69	0.74
1:A:1356:ARG:HH21	1:A:1357:ILE:HG13	1.52	0.73
1:B:2065:LEU:O	1:B:2066:TRP:C	2.25	0.73
1:B:929:ILE:O	1:B:929:ILE:HG23	1.87	0.73
1:A:2065:LEU:O	1:A:2066:TRP:C	2.25	0.73
1:B:1562:ARG:CD	1:B:1565:LEU:CD1	2.64	0.73
1:C:2505:PHE:O	1:C:2505:PHE:HD1	1.69	0.72
1:B:2505:PHE:O	1:B:2505:PHE:HD1	1.69	0.72
1:B:1016:THR:HG22	1:B:1230:ASN:HD21	1.53	0.72
1:A:1016:THR:HG22	1:A:1230:ASN:HD21	1.54	0.72
1:C:1016:THR:HG22	1:C:1230:ASN:HD21	1.53	0.72
1:A:2403:TRP:CZ3	1:B:2282:PRO:HD2	2.26	0.71
1:A:2466:ILE:HD13	1:C:2504:ILE:CD1	2.21	0.71
1:A:1053:TYR:CD1	1:A:1053:TYR:C	2.63	0.70
1:A:2504:ILE:CD1	1:B:2466:ILE:HD13	2.21	0.70
1:B:1053:TYR:CD1	1:B:1053:TYR:C	2.64	0.70
1:B:2504:ILE:CD1	1:C:2466:ILE:HD13	2.21	0.70
1:A:2282:PRO:HD2	1:C:2403:TRP:CZ3	2.26	0.70
1:C:1562:ARG:HD2	1:C:1565:LEU:HD12	1.69	0.70
1:A:581:ILE:HA	1:A:697:GLN:NE2	2.07	0.70
1:B:2403:TRP:CZ3	1:C:2282:PRO:HD2	2.26	0.70
1:A:1421:PHE:HZ	1:A:2502:LYS:O	1.75	0.70
1:A:2186:ILE:O	1:A:2186:ILE:HG22	1.92	0.69
1:B:1338:PHE:O	1:B:1342:ILE:HD11	1.92	0.69
1:C:991:PHE:HE1	1:C:998:ILE:CG2	2.05	0.69
1:A:1208:THR:O	1:A:1209:ARG:C	2.31	0.69
1:A:1338:PHE:O	1:A:1342:ILE:HD11	1.92	0.69
1:B:1421:PHE:HZ	1:B:2502:LYS:O	1.75	0.69
1:C:1053:TYR:CD1	1:C:1053:TYR:C	2.64	0.69
1:C:1338:PHE:O	1:C:1342:ILE:HD11	1.92	0.69
1:A:991:PHE:HE1	1:A:998:ILE:CG2	2.05	0.69
1:A:2028:LEU:CD1	1:A:2029:GLY:CA	2.70	0.69
1:B:581:ILE:HA	1:B:697:GLN:NE2	2.07	0.69
1:C:1421:PHE:HZ	1:C:2502:LYS:O	1.75	0.69
1:B:991:PHE:HE1	1:B:998:ILE:CG2	2.05	0.69
1:C:581:ILE:HA	1:C:697:GLN:NE2	2.07	0.69
1:C:2028:LEU:CD1	1:C:2029:GLY:CA	2.70	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2186:ILE:HG22	1:B:2186:ILE:O	1.92	0.68
1:B:1342:ILE:N	1:B:1342:ILE:CD1	2.53	0.67
1:C:2186:ILE:HG22	1:C:2186:ILE:O	1.92	0.67
1:B:2028:LEU:CD1	1:B:2029:GLY:CA	2.70	0.67
1:C:2186:ILE:O	1:C:2186:ILE:CG2	2.43	0.67
1:A:2456:ARG:NH2	1:C:2110:ARG:O	2.28	0.67
1:B:2189:PHE:CD1	1:B:2189:PHE:C	2.69	0.66
1:A:2065:LEU:O	1:A:2067:TYR:N	2.29	0.66
1:A:2110:ARG:O	1:B:2456:ARG:NH2	2.28	0.66
1:C:2189:PHE:CD1	1:C:2189:PHE:C	2.69	0.66
1:B:1562:ARG:HD3	1:B:1565:LEU:CD1	2.25	0.66
1:B:2186:ILE:O	1:B:2186:ILE:CG2	2.43	0.66
1:A:2189:PHE:CD1	1:A:2189:PHE:C	2.69	0.66
1:B:2065:LEU:O	1:B:2067:TYR:N	2.29	0.66
1:B:2110:ARG:O	1:C:2456:ARG:NH2	2.28	0.66
1:C:2065:LEU:O	1:C:2067:TYR:N	2.29	0.65
1:A:2186:ILE:O	1:A:2186:ILE:CG2	2.43	0.65
1:A:2113:PRO:O	1:A:2114:PHE:CB	2.43	0.64
1:C:874:LEU:HB2	1:C:877:VAL:HG21	1.80	0.64
1:A:1961:TYR:O	1:A:1962:ALA:C	2.37	0.63
1:B:1568:LEU:HG	1:B:1652:ARG:HG3	1.81	0.63
1:B:2113:PRO:O	1:B:2114:PHE:CB	2.43	0.63
1:B:874:LEU:HB2	1:B:877:VAL:HG21	1.80	0.63
1:A:874:LEU:HB2	1:A:877:VAL:HG21	1.80	0.63
1:B:1961:TYR:O	1:B:1962:ALA:C	2.37	0.62
1:C:1562:ARG:HD3	1:C:1565:LEU:CD1	2.25	0.62
1:A:1356:ARG:NH2	1:A:1357:ILE:CG1	2.59	0.62
1:C:2113:PRO:O	1:C:2114:PHE:CB	2.43	0.62
1:A:581:ILE:HB	1:A:697:GLN:NE2	2.15	0.61
1:C:1568:LEU:HG	1:C:1652:ARG:HG3	1.81	0.61
1:C:581:ILE:HB	1:C:697:GLN:NE2	2.15	0.61
1:C:1342:ILE:N	1:C:1342:ILE:CD1	2.53	0.61
1:B:581:ILE:HB	1:B:697:GLN:NE2	2.15	0.61
1:B:581:ILE:HA	1:B:697:GLN:HE21	1.65	0.61
1:B:2126:TRP:CZ3	1:C:2173:TYR:CE1	2.89	0.61
1:A:2173:TYR:CE1	1:C:2126:TRP:CZ3	2.89	0.61
1:C:1560:VAL:O	1:C:1560:VAL:CG1	2.49	0.61
1:A:581:ILE:HA	1:A:697:GLN:HE21	1.65	0.60
1:A:1656:ILE:CG2	1:A:1657:PRO:CD	2.79	0.60
1:C:581:ILE:HA	1:C:697:GLN:HE21	1.65	0.60
1:A:1568:LEU:HG	1:A:1652:ARG:HG3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:PHE:CD1	1:C:805:PHE:C	2.73	0.60
1:C:1338:PHE:CD1	1:C:1339:HIS:CD2	2.89	0.60
1:A:1338:PHE:CD1	1:A:1339:HIS:CD2	2.89	0.60
1:B:587:MET:HE1	1:B:693:ALA:HB2	1.84	0.60
1:B:2193:PHE:CE1	1:B:2194:MET:HG3	2.36	0.60
1:B:876:VAL:CG2	1:B:876:VAL:O	2.50	0.60
1:B:1560:VAL:O	1:B:1560:VAL:CG1	2.49	0.60
1:A:1562:ARG:HD3	1:A:1565:LEU:CD1	2.25	0.60
1:B:1338:PHE:CD1	1:B:1339:HIS:CD2	2.89	0.59
1:B:1656:ILE:CG2	1:B:1657:PRO:CD	2.79	0.59
1:B:805:PHE:CD1	1:B:805:PHE:C	2.73	0.59
1:C:876:VAL:CG2	1:C:876:VAL:O	2.50	0.59
1:A:2126:TRP:CZ3	1:B:2173:TYR:CE1	2.89	0.59
1:C:1656:ILE:CG2	1:C:1657:PRO:CD	2.79	0.59
1:B:1423:SER:OG	1:B:1423:SER:O	2.20	0.59
1:C:587:MET:HE1	1:C:693:ALA:HB2	1.81	0.59
1:A:876:VAL:O	1:A:876:VAL:CG2	2.50	0.58
1:A:1334:LYS:HG3	1:A:1335:SER:N	2.18	0.58
1:A:1228:SER:O	1:A:1230:ASN:N	2.36	0.58
1:C:1961:TYR:O	1:C:1962:ALA:C	2.37	0.58
1:A:1423:SER:O	1:A:1423:SER:OG	2.20	0.58
1:C:1728:ARG:NH1	1:C:1728:ARG:HG2	2.18	0.58
1:A:1728:ARG:NH1	1:A:1728:ARG:HG2	2.18	0.57
1:C:580:TRP:HE1	1:C:697:GLN:HB2	1.70	0.57
1:B:1334:LYS:HG3	1:B:1335:SER:N	2.18	0.57
1:A:580:TRP:HE1	1:A:697:GLN:HB2	1.70	0.57
1:C:2193:PHE:CE1	1:C:2194:MET:HG3	2.36	0.57
1:A:1560:VAL:O	1:A:1560:VAL:CG1	2.49	0.57
1:B:580:TRP:HE1	1:B:697:GLN:HB2	1.70	0.57
1:B:1728:ARG:HG2	1:B:1728:ARG:NH1	2.18	0.57
1:A:874:LEU:CB	1:A:877:VAL:CG2	2.82	0.57
1:C:874:LEU:CB	1:C:877:VAL:CG2	2.82	0.57
1:A:991:PHE:HE1	1:A:998:ILE:HG21	1.70	0.56
1:A:2394:GLY:HA3	1:B:2398:THR:HG21	1.87	0.56
1:B:2028:LEU:CD1	1:B:2029:GLY:HA2	2.35	0.56
1:C:1212:LEU:HD11	1:C:1303:LEU:HD11	1.87	0.56
1:A:805:PHE:C	1:A:805:PHE:CD1	2.73	0.56
1:B:991:PHE:HE1	1:B:998:ILE:HG21	1.70	0.56
1:A:1103:PHE:O	1:A:1104:LEU:C	2.43	0.56
1:A:2392:GLU:CB	1:B:2282:PRO:HG2	2.36	0.56
1:B:2178:LEU:CD2	1:B:2182:PHE:CZ	2.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2398:THR:HG21	1:C:2394:GLY:HA3	1.87	0.56
1:A:629:PHE:O	1:A:633:VAL:HG23	2.06	0.56
1:C:2509:SER:HB3	1:C:2512:THR:HG22	1.86	0.56
1:A:805:PHE:CD1	1:A:805:PHE:O	2.59	0.56
1:A:2178:LEU:CD2	1:A:2182:PHE:CZ	2.89	0.56
1:A:2193:PHE:CE1	1:A:2194:MET:HG3	2.36	0.56
1:C:2178:LEU:CD2	1:C:2182:PHE:CZ	2.89	0.56
1:C:1701:VAL:CG1	1:C:1702:THR:N	2.69	0.56
1:A:1228:SER:O	1:A:1229:LYS:C	2.44	0.56
1:A:2282:PRO:HG2	1:C:2392:GLU:CB	2.36	0.56
1:B:581:ILE:CA	1:B:697:GLN:NE2	2.69	0.56
1:C:805:PHE:CD1	1:C:805:PHE:O	2.59	0.56
1:B:1523:ASP:HB3	1:B:1527:ARG:HH21	1.71	0.55
1:A:2028:LEU:CD1	1:A:2029:GLY:HA2	2.35	0.55
1:C:581:ILE:CA	1:C:697:GLN:NE2	2.69	0.55
1:C:1423:SER:O	1:C:1423:SER:OG	2.20	0.55
1:B:805:PHE:CD1	1:B:805:PHE:O	2.59	0.55
1:B:2277:LEU:HD11	1:C:2279:ARG:O	2.07	0.55
1:C:1334:LYS:HG3	1:C:1335:SER:N	2.18	0.55
1:A:1523:ASP:HB3	1:A:1527:ARG:HH21	1.72	0.55
1:A:2173:TYR:HE1	1:C:2126:TRP:CZ3	2.25	0.55
1:B:2394:GLY:HA3	1:C:2398:THR:HG21	1.87	0.55
1:C:991:PHE:HE1	1:C:998:ILE:HG21	1.70	0.55
1:C:1523:ASP:HB3	1:C:1527:ARG:HH21	1.71	0.55
1:A:2277:LEU:HD11	1:B:2279:ARG:O	2.06	0.55
1:C:2028:LEU:CD1	1:C:2029:GLY:HA2	2.35	0.55
1:A:581:ILE:CA	1:A:697:GLN:NE2	2.69	0.55
1:B:2126:TRP:CZ3	1:C:2173:TYR:HE1	2.25	0.55
1:B:2392:GLU:CB	1:C:2282:PRO:HG2	2.35	0.55
1:A:1342:ILE:N	1:A:1342:ILE:CD1	2.53	0.55
1:C:1103:PHE:O	1:C:1104:LEU:C	2.43	0.55
1:C:1687:SER:HB2	1:C:1796:HIS:ND1	2.22	0.55
1:A:1656:ILE:CG2	1:A:1657:PRO:HD2	2.35	0.54
1:B:2114:PHE:CD1	1:C:2183:LEU:HD22	2.42	0.54
1:A:2126:TRP:CZ3	1:B:2173:TYR:HE1	2.25	0.54
1:B:1103:PHE:O	1:B:1104:LEU:C	2.43	0.54
1:A:2114:PHE:CD1	1:B:2183:LEU:HD22	2.42	0.54
1:B:874:LEU:CB	1:B:877:VAL:CG2	2.82	0.54
1:A:1212:LEU:HD11	1:A:1303:LEU:HD11	1.88	0.54
1:B:1728:ARG:HG2	1:B:1728:ARG:HH11	1.73	0.54
1:A:2183:LEU:HD22	1:C:2114:PHE:CD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2466:ILE:HG23	1:A:2470:GLU:HG3	1.90	0.53
1:B:1103:PHE:O	1:B:1105:LEU:N	2.42	0.53
1:A:2183:LEU:HD22	1:C:2114:PHE:CE1	2.43	0.53
1:B:1687:SER:HB2	1:B:1796:HIS:ND1	2.22	0.53
1:B:2466:ILE:HG23	1:B:2470:GLU:HG3	1.90	0.53
1:A:1687:SER:HB2	1:A:1796:HIS:ND1	2.22	0.53
1:C:2466:ILE:HG23	1:C:2470:GLU:HG3	1.90	0.53
1:B:2114:PHE:CE1	1:C:2183:LEU:HD22	2.43	0.53
1:C:1728:ARG:HG2	1:C:1728:ARG:HH11	1.73	0.53
1:A:1338:PHE:HE1	1:A:1339:HIS:CG	2.27	0.53
1:A:1728:ARG:HG2	1:A:1728:ARG:HH11	1.73	0.53
1:A:2114:PHE:CE1	1:B:2183:LEU:HD22	2.43	0.53
1:B:641:LEU:HB2	1:B:684:ILE:HG23	1.91	0.53
1:A:1103:PHE:O	1:A:1105:LEU:N	2.42	0.52
1:C:641:LEU:HB2	1:C:684:ILE:HG23	1.91	0.52
1:B:1053:TYR:O	1:B:1053:TYR:HD1	1.88	0.52
1:C:1103:PHE:O	1:C:1105:LEU:N	2.42	0.52
1:A:578:LYS:HD2	1:A:708:LEU:HG	1.92	0.52
1:A:641:LEU:HB2	1:A:684:ILE:HG23	1.91	0.52
1:B:992:TYR:CZ	1:B:1119:GLU:HG2	2.45	0.52
1:A:2173:TYR:HH	1:C:2126:TRP:HZ3	1.54	0.51
1:C:870:MET:C	1:C:872:TYR:H	2.13	0.51
1:C:992:TYR:CZ	1:C:1119:GLU:HG2	2.45	0.51
1:C:832:VAL:HG23	1:C:917:PHE:HA	1.92	0.51
1:B:578:LYS:HD2	1:B:708:LEU:HG	1.91	0.51
1:B:2510:PRO:HG2	1:C:2510:PRO:HG2	1.92	0.51
1:A:1228:SER:C	1:A:1230:ASN:N	2.62	0.51
1:A:2510:PRO:HG2	1:B:2510:PRO:HG2	1.92	0.51
1:C:1053:TYR:O	1:C:1053:TYR:CG	2.62	0.51
1:B:1656:ILE:CG2	1:B:1657:PRO:HD2	2.35	0.51
1:A:870:MET:C	1:A:872:TYR:H	2.13	0.51
1:A:1356:ARG:HH22	1:A:1357:ILE:CG1	2.24	0.51
1:A:2514:ILE:HG23	1:C:2508:ARG:NH2	2.26	0.51
1:A:587:MET:HE1	1:A:693:ALA:HB2	1.92	0.51
1:A:2508:ARG:NH2	1:B:2514:ILE:HG23	2.26	0.51
1:B:2508:ARG:NH2	1:C:2514:ILE:HG23	2.26	0.51
1:A:1338:PHE:HD1	1:A:1339:HIS:H	1.55	0.51
1:B:1728:ARG:HH11	1:B:1728:ARG:CG	2.24	0.51
1:C:1208:THR:O	1:C:1209:ARG:C	2.48	0.51
1:C:578:LYS:HD2	1:C:708:LEU:HG	1.92	0.51
1:C:1728:ARG:HH11	1:C:1728:ARG:CG	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:870:MET:C	1:B:872:TYR:H	2.13	0.51
1:A:832:VAL:HG23	1:A:917:PHE:HA	1.92	0.50
1:A:992:TYR:CZ	1:A:1119:GLU:HG2	2.45	0.50
1:B:989:PHE:HB3	1:B:992:TYR:HB3	1.93	0.50
1:B:1338:PHE:O	1:B:1342:ILE:HG12	2.12	0.50
1:A:1049:LEU:HD13	1:A:1102:ASP:HB3	1.93	0.50
1:A:1338:PHE:O	1:A:1342:ILE:HG12	2.12	0.50
1:A:2510:PRO:HG2	1:C:2510:PRO:HG2	1.92	0.50
1:C:1338:PHE:O	1:C:1342:ILE:HG12	2.12	0.50
1:B:2400:PHE:HB3	1:B:2402:GLU:HG3	1.93	0.50
1:A:989:PHE:HB3	1:A:992:TYR:HB3	1.93	0.50
1:B:832:VAL:HG23	1:B:917:PHE:HA	1.92	0.50
1:B:1053:TYR:O	1:B:1053:TYR:CG	2.62	0.50
1:B:1049:LEU:HD13	1:B:1102:ASP:HB3	1.93	0.50
1:C:1049:LEU:HD13	1:C:1102:ASP:HB3	1.93	0.50
1:C:2400:PHE:HB3	1:C:2402:GLU:HG3	1.93	0.50
1:A:2193:PHE:HE1	1:A:2194:MET:CG	1.96	0.49
1:B:2065:LEU:O	1:B:2068:PHE:N	2.45	0.49
1:B:1053:TYR:C	1:B:1053:TYR:HD1	2.15	0.49
1:C:604:TYR:HH	1:C:637:THR:HA	1.77	0.49
1:A:865:ILE:HG22	1:A:869:LYS:HD2	1.95	0.49
1:A:1728:ARG:HH11	1:A:1728:ARG:CG	2.24	0.49
1:C:2193:PHE:CD1	1:C:2194:MET:HA	2.47	0.49
1:A:1338:PHE:CD1	1:A:1339:HIS:CA	2.95	0.49
1:A:2065:LEU:O	1:A:2068:PHE:N	2.45	0.49
1:C:604:TYR:OH	1:C:637:THR:CA	2.57	0.49
1:C:1347:LEU:HD23	1:C:1347:LEU:HA	1.60	0.49
1:A:1053:TYR:O	1:A:1053:TYR:CG	2.62	0.49
1:B:991:PHE:CE1	1:B:998:ILE:CG2	2.93	0.49
1:B:1338:PHE:CD1	1:B:1339:HIS:CA	2.95	0.49
2:B:2601:L9Q:H15	2:B:2601:L9Q:H18	1.40	0.49
1:C:2065:LEU:O	1:C:2068:PHE:N	2.45	0.49
1:A:2117:GLU:H	1:A:2117:GLU:HG2	1.42	0.49
1:B:629:PHE:O	1:B:633:VAL:HG23	2.13	0.49
1:C:989:PHE:HB3	1:C:992:TYR:HB3	1.93	0.49
1:A:2065:LEU:C	1:A:2067:TYR:N	2.66	0.48
1:A:2400:PHE:HB3	1:A:2402:GLU:HG3	1.93	0.48
1:A:708:LEU:HD13	1:A:708:LEU:HA	1.64	0.48
1:C:1338:PHE:CD1	1:C:1339:HIS:CA	2.95	0.48
1:A:993:LYS:HB3	1:A:993:LYS:HE3	1.40	0.48
1:A:1196:LEU:CD1	1:A:1218:LEU:HD22	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1656:ILE:CG2	1:A:1657:PRO:N	2.76	0.48
1:B:865:ILE:HG22	1:B:869:LYS:HD2	1.95	0.48
1:B:2193:PHE:CE1	1:B:2194:MET:CA	2.96	0.48
1:B:1338:PHE:HD1	1:B:1339:HIS:H	1.56	0.48
1:B:1342:ILE:H	1:B:1342:ILE:CD1	2.09	0.48
1:B:1656:ILE:CG2	1:B:1657:PRO:N	2.76	0.48
1:C:1338:PHE:HE1	1:C:1339:HIS:CG	2.27	0.48
1:C:1656:ILE:CG2	1:C:1657:PRO:N	2.76	0.48
1:A:2504:ILE:HD12	1:A:2504:ILE:HA	1.66	0.48
1:C:2193:PHE:CE1	1:C:2194:MET:CA	2.96	0.48
1:A:2193:PHE:CE1	1:A:2194:MET:CA	2.96	0.48
1:C:1342:ILE:H	1:C:1342:ILE:CD1	2.09	0.48
1:B:2504:ILE:HD11	1:C:2466:ILE:CD1	2.33	0.47
1:C:708:LEU:HD13	1:C:708:LEU:HA	1.64	0.47
1:A:1562:ARG:HD3	1:A:1562:ARG:HA	1.35	0.47
2:A:2601:L9Q:H17A	2:A:2601:L9Q:H20	1.51	0.47
1:C:2065:LEU:C	1:C:2067:TYR:N	2.66	0.47
2:B:2602:L9Q:H33	2:B:2602:L9Q:H36	1.65	0.47
1:C:991:PHE:CE1	1:C:998:ILE:CG2	2.93	0.47
1:A:2193:PHE:CD1	1:A:2194:MET:HA	2.47	0.47
1:A:2506:LEU:HD12	1:A:2512:THR:HG23	1.97	0.47
1:B:2117:GLU:HG3	1:C:2459:PHE:CD2	2.49	0.47
1:C:865:ILE:HG22	1:C:869:LYS:HD2	1.94	0.47
1:A:2163:LYS:HE3	1:A:2163:LYS:HB2	1.25	0.47
1:A:2166:LYS:HB2	1:A:2166:LYS:HE2	1.38	0.47
1:A:2504:ILE:HD11	1:B:2466:ILE:CD1	2.33	0.47
1:A:993:LYS:H	1:A:993:LYS:HG2	1.39	0.47
1:A:1232:LEU:O	1:A:1233:SER:CB	2.63	0.47
1:B:2193:PHE:CD1	1:B:2194:MET:HA	2.47	0.47
1:C:2097:LYS:HB2	1:C:2097:LYS:HE2	1.62	0.47
1:B:1338:PHE:HE1	1:B:1339:HIS:CG	2.27	0.47
1:C:991:PHE:CE1	1:C:998:ILE:HG21	2.50	0.47
1:A:1053:TYR:C	1:A:1053:TYR:HD1	2.15	0.47
1:C:2166:LYS:HE2	1:C:2166:LYS:HB2	1.38	0.47
1:C:980:LEU:HD12	1:C:980:LEU:HA	1.68	0.47
1:C:1338:PHE:O	1:C:1342:ILE:CG1	2.63	0.47
1:C:2506:LEU:HD12	1:C:2512:THR:HG23	1.97	0.47
1:A:604:TYR:OH	1:A:637:THR:CA	2.57	0.46
1:A:1338:PHE:O	1:A:1342:ILE:CG1	2.63	0.46
1:A:1408:ASP:OD1	1:B:2160:PRO:HB3	2.15	0.46
1:A:2459:PHE:CD2	1:C:2117:GLU:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2511:GLU:HA	1:A:2514:ILE:HG13	1.97	0.46
1:B:2045:MET:HE3	1:B:2045:MET:HB3	1.86	0.46
1:B:2504:ILE:HD12	1:B:2504:ILE:HA	1.66	0.46
1:C:1232:LEU:O	1:C:1233:SER:CB	2.63	0.46
1:B:2119:ARG:HE	1:B:2119:ARG:HB3	1.59	0.46
1:B:604:TYR:OH	1:B:637:THR:CA	2.57	0.46
1:A:1353:GLN:O	1:A:1356:ARG:HG3	2.16	0.46
1:C:2502:LYS:HE3	1:C:2502:LYS:HB3	1.72	0.46
1:B:1408:ASP:OD1	1:C:2160:PRO:HB3	2.15	0.46
2:A:2601:L9Q:H18	2:A:2601:L9Q:H15	1.40	0.46
1:B:1007:ILE:HG23	1:B:1015:VAL:HG13	1.98	0.46
1:B:1647:GLU:H	1:B:1647:GLU:HG3	1.40	0.46
1:B:2097:LYS:HE2	1:B:2097:LYS:HB2	1.62	0.46
1:A:980:LEU:HD12	1:A:980:LEU:HA	1.68	0.46
1:B:1232:LEU:O	1:B:1233:SER:CB	2.63	0.46
1:C:805:PHE:O	1:C:805:PHE:HD1	1.99	0.46
1:C:874:LEU:HB2	1:C:877:VAL:HG22	1.97	0.46
1:A:680:LEU:H	1:A:680:LEU:HG	1.38	0.46
1:B:2478:LEU:HD12	1:B:2478:LEU:HA	1.80	0.46
1:B:2506:LEU:HD12	1:B:2512:THR:HG23	1.97	0.46
1:A:587:MET:HE2	1:A:587:MET:HB2	1.51	0.46
1:A:1782:TYR:HD1	1:A:1782:TYR:H	1.63	0.46
1:B:581:ILE:CA	1:B:697:GLN:HE22	2.29	0.46
1:B:993:LYS:H	1:B:993:LYS:HG2	1.39	0.46
1:B:2065:LEU:C	1:B:2067:TYR:N	2.66	0.46
1:A:604:TYR:HH	1:A:637:THR:HA	1.77	0.46
1:A:1647:GLU:H	1:A:1647:GLU:HG3	1.40	0.46
1:B:991:PHE:CE1	1:B:998:ILE:HG21	2.50	0.46
1:C:581:ILE:CA	1:C:697:GLN:HE22	2.29	0.46
1:C:2478:LEU:HD12	1:C:2478:LEU:HA	1.80	0.46
1:A:849:ARG:H	1:A:849:ARG:HG2	1.53	0.45
1:A:2126:TRP:HZ3	1:B:2173:TYR:HH	1.61	0.45
1:A:2164:GLY:HA2	1:C:2497:GLU:OE1	2.16	0.45
2:A:2602:L9Q:H36	2:A:2602:L9Q:H33	1.65	0.45
1:B:685:LEU:HD12	1:B:685:LEU:HA	1.81	0.45
1:B:2497:GLU:OE1	1:C:2164:GLY:HA2	2.16	0.45
1:C:1179:ALA:HB2	1:C:1190:LEU:HD21	1.98	0.45
1:C:2193:PHE:HE1	1:C:2194:MET:CG	1.96	0.45
1:A:816:LYS:H	1:A:816:LYS:HG2	1.52	0.45
1:B:1179:ALA:HB2	1:B:1190:LEU:HD21	1.98	0.45
1:C:2070:LYS:HD2	1:C:2070:LYS:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:SER:O	1:A:1096:SER:OG	2.34	0.45
1:A:2279:ARG:O	1:C:2277:LEU:HG	2.16	0.45
1:A:2497:GLU:OE1	1:B:2164:GLY:HA2	2.16	0.45
1:B:993:LYS:HE3	1:B:993:LYS:HB3	1.40	0.45
1:B:1214:LEU:HD13	1:B:1214:LEU:HA	1.65	0.45
1:B:1334:LYS:HE3	1:B:1334:LYS:HB2	1.77	0.45
1:B:2193:PHE:CE1	1:B:2194:MET:HA	2.52	0.45
1:C:581:ILE:CB	1:C:697:GLN:NE2	2.79	0.45
1:C:1690:LEU:O	1:C:1691:CYS:C	2.55	0.45
1:C:2045:MET:HE3	1:C:2045:MET:HB3	1.77	0.45
1:C:2193:PHE:CE1	1:C:2194:MET:HA	2.52	0.45
1:A:581:ILE:CA	1:A:697:GLN:HE22	2.29	0.45
1:A:1744:LYS:HB2	1:A:1744:LYS:HE2	1.37	0.45
1:A:2160:PRO:HB3	1:C:1408:ASP:OD1	2.15	0.45
1:B:953:ARG:HE	1:B:953:ARG:HB2	1.57	0.45
1:B:2163:LYS:HE3	1:B:2163:LYS:HB2	1.25	0.45
1:A:805:PHE:O	1:A:805:PHE:HD1	1.99	0.45
1:A:1007:ILE:HG23	1:A:1015:VAL:HG13	1.98	0.45
1:A:2168:LYS:H	1:A:2168:LYS:HG2	1.34	0.45
2:A:2603:L9Q:H18	2:A:2603:L9Q:H15	1.40	0.45
1:C:2154:GLU:O	1:C:2158:LYS:HG3	2.17	0.45
1:A:2193:PHE:CE1	1:A:2194:MET:HA	2.52	0.45
1:A:2293:TYR:CE2	1:A:2339:ALA:HB1	2.51	0.45
1:C:630:TRP:HB2	1:C:698:LEU:CD1	2.47	0.45
1:C:1562:ARG:HD3	1:C:1562:ARG:HA	1.35	0.45
1:C:1334:LYS:CG	1:C:1335:SER:N	2.80	0.45
1:C:1656:ILE:CG2	1:C:1657:PRO:HD2	2.35	0.45
1:C:2504:ILE:HA	1:C:2504:ILE:HD12	1.66	0.45
1:A:1100:ILE:H	1:A:1100:ILE:HG13	1.48	0.45
2:A:2602:L9Q:H21A	2:A:2602:L9Q:H24A	1.29	0.45
1:B:1338:PHE:O	1:B:1342:ILE:CG1	2.63	0.45
1:B:2502:LYS:HE3	1:B:2502:LYS:HB3	1.72	0.45
1:C:1338:PHE:CE1	1:C:1339:HIS:CG	3.03	0.45
1:C:2293:TYR:CE2	1:C:2339:ALA:HB1	2.51	0.45
1:A:1220:LEU:HD13	1:A:1220:LEU:HA	1.75	0.45
1:B:2293:TYR:CE2	1:B:2339:ALA:HB1	2.51	0.45
1:C:937:LEU:HD22	1:C:937:LEU:HA	1.75	0.45
1:C:2167:LYS:HE2	1:C:2167:LYS:HB2	1.42	0.45
1:A:2292:LEU:HB3	1:A:2339:ALA:HB2	1.99	0.44
1:B:581:ILE:CB	1:B:697:GLN:NE2	2.79	0.44
1:B:1333:LEU:HD23	1:B:1333:LEU:HA	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1214:LEU:HD12	1:C:1214:LEU:HA	1.78	0.44
1:A:790:GLU:H	1:A:790:GLU:HG2	1.49	0.44
1:A:874:LEU:HD23	1:A:874:LEU:HA	1.88	0.44
1:A:1053:TYR:O	1:A:1053:TYR:HD1	1.88	0.44
1:B:1334:LYS:CG	1:B:1335:SER:N	2.80	0.44
1:B:1347:LEU:HD23	1:B:1347:LEU:HA	1.60	0.44
1:B:2505:PHE:O	1:B:2505:PHE:CG	2.60	0.44
1:C:1007:ILE:HG23	1:C:1015:VAL:HG13	1.98	0.44
1:C:1100:ILE:H	1:C:1100:ILE:HG13	1.48	0.44
1:A:2164:GLY:N	1:C:2497:GLU:OE1	2.51	0.44
1:B:597:LEU:H	1:B:597:LEU:HG	1.51	0.44
1:B:869:LYS:CB	1:B:929:ILE:HD11	2.48	0.44
1:B:1014:LEU:HD23	1:B:1014:LEU:HA	1.79	0.44
1:B:1226:ILE:HA	1:B:1285:ILE:HD11	1.99	0.44
1:C:2163:LYS:HB2	1:C:2163:LYS:HE3	1.30	0.44
1:C:2505:PHE:O	1:C:2505:PHE:CG	2.60	0.44
1:A:1179:ALA:HB2	1:A:1190:LEU:HD21	1.98	0.44
1:A:2097:LYS:HB2	1:A:2097:LYS:HE2	1.62	0.44
1:B:805:PHE:O	1:B:805:PHE:HD1	1.99	0.44
1:B:2154:GLU:O	1:B:2158:LYS:HG3	2.17	0.44
1:B:2292:LEU:HB3	1:B:2339:ALA:HB2	2.00	0.44
1:C:2119:ARG:HE	1:C:2119:ARG:HB3	1.59	0.44
1:A:991:PHE:CE1	1:A:998:ILE:HG21	2.50	0.44
1:B:876:VAL:O	1:B:876:VAL:HG23	2.18	0.44
1:B:1286:ILE:H	1:B:1286:ILE:HG13	1.52	0.44
2:B:2601:L9Q:H39	2:B:2601:L9Q:H42	1.81	0.44
1:C:869:LYS:CB	1:C:929:ILE:HD11	2.48	0.44
1:C:2292:LEU:HB3	1:C:2339:ALA:HB2	1.99	0.44
1:A:581:ILE:CB	1:A:697:GLN:NE2	2.79	0.44
1:A:2154:GLU:O	1:A:2158:LYS:HG3	2.17	0.44
1:B:1327:LEU:N	1:B:1327:LEU:HD23	2.33	0.44
1:B:2167:LYS:HB2	1:B:2167:LYS:HE2	1.42	0.44
1:C:2186:ILE:HD12	1:C:2186:ILE:HA	1.78	0.44
1:C:2228:GLN:HE21	1:C:2228:GLN:HB3	1.64	0.44
1:A:1159:LYS:HE2	1:A:1306:TYR:CE2	2.53	0.44
1:B:604:TYR:HH	1:B:637:THR:HA	1.78	0.44
1:B:996:LEU:HD23	1:B:996:LEU:HA	1.86	0.44
1:B:2497:GLU:OE1	1:C:2164:GLY:N	2.51	0.44
1:C:576:TYR:HA	1:C:580:TRP:HB3	1.99	0.44
1:C:1159:LYS:HE2	1:C:1306:TYR:CE2	2.53	0.44
1:C:1949:ILE:H	1:C:1949:ILE:HG13	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1690:LEU:O	1:A:1691:CYS:C	2.55	0.44
1:B:790:GLU:H	1:B:790:GLU:HG2	1.49	0.44
1:B:2178:LEU:HD23	1:B:2182:PHE:CZ	2.53	0.44
1:A:1676:LEU:HD13	1:A:1676:LEU:HA	1.66	0.43
1:C:1103:PHE:C	1:C:1105:LEU:N	2.70	0.43
1:A:2173:TYR:OH	1:C:2126:TRP:HZ3	2.00	0.43
1:B:573:LYS:HB2	1:B:573:LYS:HE2	1.79	0.43
1:B:708:LEU:HD13	1:B:708:LEU:HA	1.64	0.43
1:C:1327:LEU:HD23	1:C:1327:LEU:N	2.33	0.43
1:A:991:PHE:CE1	1:A:998:ILE:CG2	2.93	0.43
1:A:2178:LEU:HD23	1:A:2182:PHE:CZ	2.53	0.43
1:A:2497:GLU:OE1	1:B:2164:GLY:N	2.51	0.43
2:A:2601:L9Q:H39	2:A:2601:L9Q:H42	1.81	0.43
1:B:849:ARG:H	1:B:849:ARG:HG2	1.53	0.43
1:B:1159:LYS:HE2	1:B:1306:TYR:CE2	2.53	0.43
1:C:1053:TYR:C	1:C:1053:TYR:HD1	2.15	0.43
1:C:1226:ILE:HA	1:C:1285:ILE:HD11	1.99	0.43
1:B:2511:GLU:HA	1:B:2514:ILE:HG13	2.00	0.43
1:C:630:TRP:O	1:C:633:VAL:HB	2.18	0.43
1:A:876:VAL:O	1:A:876:VAL:HG23	2.18	0.43
1:A:2126:TRP:HZ3	1:B:2173:TYR:OH	2.00	0.43
1:A:2520:LYS:H	1:A:2520:LYS:HG3	1.53	0.43
1:B:1676:LEU:HD13	1:B:1676:LEU:HA	1.66	0.43
1:B:2070:LYS:HD2	1:B:2070:LYS:HA	1.81	0.43
1:A:576:TYR:HA	1:A:580:TRP:HB3	1.99	0.43
1:A:685:LEU:HD12	1:A:685:LEU:HA	1.81	0.43
1:A:869:LYS:CB	1:A:929:ILE:HD11	2.48	0.43
1:A:972:ARG:HA	1:A:972:ARG:HD2	1.68	0.43
1:A:1334:LYS:CG	1:A:1335:SER:N	2.80	0.43
1:B:1037:LEU:HD12	1:B:1037:LEU:HA	1.92	0.43
1:B:2166:LYS:HE2	1:B:2166:LYS:HB2	1.38	0.43
1:C:849:ARG:H	1:C:849:ARG:HG2	1.53	0.43
1:C:1656:ILE:HG22	1:C:1657:PRO:N	2.34	0.43
1:A:581:ILE:CB	1:A:697:GLN:HE22	2.32	0.43
1:B:1656:ILE:HG22	1:B:1657:PRO:N	2.34	0.43
1:B:1690:LEU:O	1:B:1691:CYS:C	2.55	0.43
1:C:2168:LYS:H	1:C:2168:LYS:HG2	1.33	0.43
1:C:2462:ILE:H	1:C:2462:ILE:HG13	1.59	0.43
1:A:810:LEU:HD23	1:A:810:LEU:HA	1.81	0.43
1:A:1327:LEU:N	1:A:1327:LEU:HD23	2.33	0.43
1:A:2467:MET:HA	1:C:2508:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:LEU:H	1:B:680:LEU:HG	1.39	0.43
1:C:1212:LEU:HD23	1:C:1212:LEU:HA	1.76	0.43
1:A:1103:PHE:C	1:A:1105:LEU:N	2.70	0.43
1:B:1103:PHE:C	1:B:1105:LEU:N	2.70	0.43
1:C:853:MET:HE3	1:C:853:MET:HB3	1.86	0.43
1:A:1700:MET:HE3	1:A:1700:MET:HB3	1.94	0.43
2:A:2602:L9Q:H26A	2:A:2602:L9Q:H23	1.58	0.43
1:B:581:ILE:CB	1:B:697:GLN:HE22	2.32	0.43
1:B:1096:SER:O	1:B:1096:SER:OG	2.34	0.43
1:B:587:MET:HE2	1:B:587:MET:HB2	1.52	0.42
1:C:589:ILE:H	1:C:589:ILE:HG13	1.71	0.42
1:C:876:VAL:O	1:C:876:VAL:HG23	2.18	0.42
1:C:1334:LYS:HE3	1:C:1334:LYS:HB2	1.77	0.42
1:C:1676:LEU:HD13	1:C:1676:LEU:HA	1.66	0.42
1:A:874:LEU:HB2	1:A:877:VAL:HG22	1.97	0.42
1:B:576:TYR:HA	1:B:580:TRP:HB3	1.99	0.42
1:A:1333:LEU:HD23	1:A:1333:LEU:HA	1.74	0.42
1:A:1656:ILE:HG22	1:A:1657:PRO:N	2.34	0.42
1:A:2173:TYR:CD1	1:C:2125:VAL:CG1	3.03	0.42
1:C:2195:SER:HA	1:C:2198:ARG:HD2	2.01	0.42
1:A:2125:VAL:CG1	1:B:2173:TYR:CD1	3.03	0.42
1:A:2460:SER:HB3	1:A:2461:GLU:H	1.75	0.42
1:B:1104:LEU:HD23	1:B:1104:LEU:HA	1.86	0.42
1:B:1360:LYS:HE2	1:B:1360:LYS:HB2	1.90	0.42
1:B:2175:MET:HE2	1:B:2175:MET:HB2	1.85	0.42
1:B:2467:MET:HE2	1:B:2467:MET:HB2	1.81	0.42
1:C:1422:GLU:HB3	1:C:1423:SER:H	1.43	0.42
1:C:2178:LEU:HD23	1:C:2182:PHE:CZ	2.53	0.42
1:A:873:GLN:HE22	1:A:921:LYS:HA	1.84	0.42
1:B:2125:VAL:CG1	1:C:2173:TYR:CD1	3.02	0.42
1:B:2195:SER:HA	1:B:2198:ARG:HD2	2.01	0.42
1:C:1946:PHE:O	1:C:1947:HIS:C	2.58	0.42
1:A:589:ILE:H	1:A:589:ILE:HG13	1.72	0.42
1:A:1356:ARG:HH22	1:A:1357:ILE:HG13	1.75	0.42
1:A:2045:MET:HE3	1:A:2045:MET:HB3	1.86	0.42
2:A:2602:L9Q:H28A	2:A:2602:L9Q:H25	1.76	0.42
1:B:873:GLN:HE22	1:B:921:LYS:HA	1.84	0.42
1:B:937:LEU:HD22	1:B:937:LEU:HA	1.75	0.42
1:B:1562:ARG:HD3	1:B:1562:ARG:HA	1.35	0.42
1:B:2126:TRP:HZ3	1:C:2173:TYR:OH	2.00	0.42
1:C:1220:LEU:HD13	1:C:1220:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2253:ALA:HB1	1:C:2374:LEU:HD23	2.02	0.42
1:A:1231:MET:HE2	1:A:1231:MET:HB2	1.95	0.42
1:A:1946:PHE:O	1:A:1947:HIS:C	2.58	0.42
1:A:1949:ILE:H	1:A:1949:ILE:HG13	1.49	0.42
1:A:2186:ILE:HD12	1:A:2186:ILE:HA	1.78	0.42
1:A:2466:ILE:CD1	1:C:2504:ILE:HD11	2.33	0.42
1:B:639:LEU:HD13	1:B:639:LEU:HA	1.76	0.42
1:B:1232:LEU:O	1:B:1233:SER:HB3	2.19	0.42
1:B:2126:TRP:HZ3	1:C:2173:TYR:HH	1.62	0.42
1:A:1159:LYS:HE2	1:A:1306:TYR:HE2	1.85	0.42
1:A:1286:ILE:H	1:A:1286:ILE:HG13	1.52	0.42
1:A:2070:LYS:HD2	1:A:2070:LYS:HA	1.81	0.42
1:A:2253:ALA:HB1	1:A:2374:LEU:HD23	2.02	0.42
1:B:816:LYS:H	1:B:816:LYS:HG2	1.53	0.42
1:C:581:ILE:HB	1:C:697:GLN:HE22	1.85	0.42
1:A:2119:ARG:HE	1:A:2119:ARG:HB3	1.59	0.42
1:A:2508:ARG:HG2	1:B:2467:MET:HA	2.01	0.42
1:B:1338:PHE:CE1	1:B:1339:HIS:CG	3.03	0.42
1:C:581:ILE:CB	1:C:697:GLN:HE22	2.32	0.42
1:C:680:LEU:H	1:C:680:LEU:HG	1.38	0.42
1:B:810:LEU:HD23	1:B:810:LEU:HA	1.81	0.41
1:C:639:LEU:HD13	1:C:639:LEU:HA	1.76	0.41
1:C:979:LEU:HD13	1:C:979:LEU:HA	1.85	0.41
1:C:1710:LEU:HA	1:C:1710:LEU:HD23	1.80	0.41
1:A:1232:LEU:O	1:A:1233:SER:HB3	2.19	0.41
1:A:2195:SER:HA	1:A:2198:ARG:HD2	2.01	0.41
1:B:1568:LEU:HD12	1:B:1568:LEU:HA	1.93	0.41
2:B:2601:L9Q:H20	2:B:2601:L9Q:H17A	1.51	0.41
1:C:597:LEU:H	1:C:597:LEU:HG	1.51	0.41
1:C:2513:MET:HE2	1:C:2513:MET:HB2	1.86	0.41
1:A:1342:ILE:H	1:A:1342:ILE:CD1	2.09	0.41
1:C:1744:LYS:HB2	1:C:1744:LYS:HE2	1.37	0.41
1:C:2520:LYS:H	1:C:2520:LYS:HG3	1.53	0.41
1:B:2508:ARG:HG2	1:C:2467:MET:HA	2.01	0.41
1:C:873:GLN:HE22	1:C:921:LYS:HA	1.84	0.41
1:A:1196:LEU:HD11	1:A:1218:LEU:HD22	2.03	0.41
1:B:2253:ALA:HB1	1:B:2374:LEU:HD23	2.02	0.41
1:B:2513:MET:HE2	1:B:2513:MET:HB2	1.84	0.41
1:C:2511:GLU:HA	1:C:2514:ILE:HG13	2.01	0.41
1:C:1159:LYS:HE2	1:C:1306:TYR:HE2	1.85	0.41
1:C:1700:MET:HE3	1:C:1700:MET:HB3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1338:PHE:CE1	1:A:1339:HIS:CG	3.03	0.41
1:B:1100:ILE:H	1:B:1100:ILE:HG13	1.48	0.41
1:C:1007:ILE:H	1:C:1007:ILE:HG13	1.62	0.41
1:B:1159:LYS:HE2	1:B:1306:TYR:HE2	1.85	0.41
1:C:874:LEU:HD23	1:C:874:LEU:HA	1.88	0.41
1:C:942:GLU:CG	1:C:943:ALA:N	2.84	0.41
1:A:573:LYS:HB2	1:A:573:LYS:HE2	1.79	0.41
1:A:612:LEU:HD23	1:A:612:LEU:HA	1.80	0.41
1:A:2005:LEU:HD11	1:B:2188:TRP:NE1	2.36	0.41
1:A:2285:ARG:HH22	1:A:2391:ARG:HH21	1.69	0.41
1:A:2471:LEU:HA	1:A:2472:PRO:HD3	1.93	0.41
1:B:874:LEU:HD23	1:B:874:LEU:HA	1.88	0.41
1:B:942:GLU:CG	1:B:943:ALA:N	2.84	0.41
2:B:2602:L9Q:H24A	2:B:2602:L9Q:H21A	1.29	0.41
1:C:817:LEU:HD22	1:C:817:LEU:HA	1.72	0.41
1:C:827:LEU:HD23	1:C:827:LEU:HA	1.85	0.41
1:C:1286:ILE:H	1:C:1286:ILE:HG13	1.52	0.41
1:C:1338:PHE:HD1	1:C:1339:HIS:H	1.55	0.41
1:C:2453:LYS:HZ3	1:C:2453:LYS:HG3	1.74	0.41
1:A:1791:MET:HE2	1:A:1791:MET:HB2	1.86	0.41
2:A:2603:L9Q:H20	2:A:2603:L9Q:H17A	1.51	0.41
1:B:588:PHE:CZ	1:B:633:VAL:HG21	2.56	0.41
1:B:1112:GLN:HE21	1:B:1112:GLN:HB3	1.70	0.41
1:C:2264:ASP:OD2	1:C:2426:LYS:HE3	2.21	0.41
1:A:2215:LYS:HE2	1:A:2219:TYR:O	2.21	0.40
1:A:2264:ASP:OD2	1:A:2426:LYS:HE3	2.21	0.40
1:B:1946:PHE:O	1:B:1947:HIS:C	2.58	0.40
1:B:2460:SER:HB3	1:B:2461:GLU:H	1.75	0.40
1:C:1232:LEU:O	1:C:1233:SER:HB3	2.19	0.40
1:C:2185:ALA:C	1:C:2186:ILE:HD13	2.42	0.40
1:C:2215:LYS:HE2	1:C:2219:TYR:O	2.21	0.40
1:A:853:MET:HE3	1:A:853:MET:HB3	1.84	0.40
2:B:2602:L9Q:H23	2:B:2602:L9Q:H26A	1.58	0.40
1:B:1799:GLN:C	1:B:1801:LEU:H	2.25	0.40
1:C:812:LEU:H	1:C:812:LEU:HG	1.64	0.40
1:C:1799:GLN:C	1:C:1801:LEU:H	2.25	0.40
1:C:573:LYS:HB2	1:C:573:LYS:HE2	1.79	0.40
2:C:2601:L9Q:H33	2:C:2601:L9Q:H36	1.64	0.40
1:A:1514:LEU:HD12	1:A:1514:LEU:HA	1.87	0.40
1:A:2185:ALA:C	1:A:2186:ILE:HD13	2.42	0.40
1:A:2508:ARG:HG3	1:B:2466:ILE:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1028:ARG:H	1:B:1028:ARG:HG3	1.58	0.40
1:B:1784:LYS:H	1:B:1784:LYS:HG3	1.75	0.40
1:B:2005:LEU:HD11	1:C:2188:TRP:NE1	2.36	0.40
1:C:2285:ARG:HH22	1:C:2391:ARG:HH21	1.69	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	1249/2521 (50%)	1126 (90%)	109 (9%)	14 (1%)	12	40
1	B	1249/2521 (50%)	1128 (90%)	107 (9%)	14 (1%)	12	40
1	C	1249/2521 (50%)	1128 (90%)	107 (9%)	14 (1%)	12	40
All	All	3747/7563 (50%)	3382 (90%)	323 (9%)	42 (1%)	15	40

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1723	PRO
1	C	626	LEU
1	C	1723	PRO
1	A	1657	PRO
1	A	2429	PRO
1	B	1657	PRO
1	B	2280	ILE
1	B	2429	PRO
1	C	1657	PRO
1	C	2280	ILE
1	C	2429	PRO
1	A	1209	ARG
1	A	1422	GLU

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Mol	Chain	Res	Type
1	B	626	LEU
1	B	1422	GLU
1	C	1422	GLU
1	A	578	LYS
1	A	698	LEU
1	A	1008	GLY
1	A	1723	PRO
1	A	2114	PHE
1	B	578	LYS
1	B	698	LEU
1	B	1008	GLY
1	B	2114	PHE
1	C	578	LYS
1	C	698	LEU
1	C	1008	GLY
1	C	2114	PHE
1	A	580	TRP
1	A	2066	TRP
1	B	580	TRP
1	B	2066	TRP
1	C	580	TRP
1	C	2066	TRP
1	A	923	PHE
1	A	2086	PRO
1	B	2086	PRO
1	C	2086	PRO
1	A	1007	ILE
1	B	1007	ILE
1	C	1007	ILE

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	1116/2172 (51%)	839 (75%)	277 (25%)	0 2
1	B	1116/2172 (51%)	837 (75%)	279 (25%)	0 2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	1116/2172 (51%)	842 (75%)	274 (25%)	0 2
All	All	3348/6516 (51%)	2518 (75%)	830 (25%)	2 2

All (830) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	570	GLU
1	A	571	LEU
1	A	572	VAL
1	A	573	LYS
1	A	580	TRP
1	A	581	ILE
1	A	588	PHE
1	A	592	SER
1	A	597	LEU
1	A	598	VAL
1	A	599	VAL
1	A	601	LYS
1	A	614	LEU
1	A	618	TYR
1	A	625	LEU
1	A	626	LEU
1	A	627	LYS
1	A	632	LEU
1	A	636	TYR
1	A	639	LEU
1	A	644	VAL
1	A	678	SER
1	A	679	GLU
1	A	680	LEU
1	A	683	SER
1	A	685	LEU
1	A	692	LEU
1	A	697	GLN
1	A	698	LEU
1	A	699	HIS
1	A	702	HIS
1	A	703	ARG
1	A	707	GLN
1	A	708	LEU
1	A	710	ASP
1	A	711	MET

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Mol	Chain	Res	Type
1	A	712	GLU
1	A	789	LEU
1	A	790	GLU
1	A	791	LEU
1	A	799	LEU
1	A	805	PHE
1	A	809	LEU
1	A	810	LEU
1	A	812	LEU
1	A	816	LYS
1	A	817	LEU
1	A	820	LEU
1	A	822	THR
1	A	831	SER
1	A	832	VAL
1	A	835	LEU
1	A	836	LEU
1	A	843	PHE
1	A	849	ARG
1	A	853	MET
1	A	855	SER
1	A	856	CYS
1	A	858	SER
1	A	867	VAL
1	A	870	MET
1	A	876	VAL
1	A	877	VAL
1	A	878	ASN
1	A	919	VAL
1	A	920	ARG
1	A	921	LYS
1	A	929	ILE
1	A	930	GLN
1	A	937	LEU
1	A	938	LEU
1	A	942	GLU
1	A	947	ARG
1	A	948	ARG
1	A	953	ARG
1	A	954	ARG
1	A	955	GLN
1	A	972	ARG

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Mol	Chain	Res	Type
1	A	974	GLN
1	A	976	ASP
1	A	979	LEU
1	A	980	LEU
1	A	982	CYS
1	A	983	LEU
1	A	993	LYS
1	A	997	GLU
1	A	998	ILE
1	A	1001	LEU
1	A	1002	MET
1	A	1005	ASN
1	A	1007	ILE
1	A	1011	MET
1	A	1023	VAL
1	A	1025	ILE
1	A	1028	ARG
1	A	1038	TRP
1	A	1048	PHE
1	A	1051	TYR
1	A	1053	TYR
1	A	1054	LEU
1	A	1057	LEU
1	A	1099	LEU
1	A	1100	ILE
1	A	1105	LEU
1	A	1112	GLN
1	A	1155	LEU
1	A	1156	ASP
1	A	1158	LEU
1	A	1176	VAL
1	A	1180	THR
1	A	1181	ARG
1	A	1184	ILE
1	A	1198	LEU
1	A	1208	THR
1	A	1209	ARG
1	A	1212	LEU
1	A	1214	LEU
1	A	1217	CYS
1	A	1220	LEU
1	A	1222	ASN

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Mol	Chain	Res	Type
1	A	1231	MET
1	A	1232	LEU
1	A	1233	SER
1	A	1285	ILE
1	A	1286	ILE
1	A	1304	SER
1	A	1317	THR
1	A	1323	ARG
1	A	1327	LEU
1	A	1334	LYS
1	A	1335	SER
1	A	1338	PHE
1	A	1341	ARG
1	A	1342	ILE
1	A	1346	SER
1	A	1350	LEU
1	A	1351	LYS
1	A	1354	MET
1	A	1356	ARG
1	A	1360	LYS
1	A	1363	LYS
1	A	1365	ARG
1	A	1417	ASP
1	A	1420	LEU
1	A	1423	SER
1	A	1514	LEU
1	A	1516	MET
1	A	1517	LEU
1	A	1523	ASP
1	A	1524	GLU
1	A	1530	GLN
1	A	1532	PHE
1	A	1534	ARG
1	A	1539	MET
1	A	1541	ASP
1	A	1546	GLU
1	A	1547	ARG
1	A	1549	LEU
1	A	1550	LEU
1	A	1552	GLN
1	A	1560	VAL
1	A	1561	HIS

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Mol	Chain	Res	Type
1	A	1562	ARG
1	A	1565	LEU
1	A	1646	SER
1	A	1647	GLU
1	A	1652	ARG
1	A	1655	ARG
1	A	1669	GLN
1	A	1673	LEU
1	A	1676	LEU
1	A	1677	ARG
1	A	1682	CYS
1	A	1694	ILE
1	A	1696	ILE
1	A	1701	VAL
1	A	1708	LEU
1	A	1727	LYS
1	A	1728	ARG
1	A	1731	MET
1	A	1744	LYS
1	A	1782	TYR
1	A	1784	LYS
1	A	1797	ARG
1	A	1798	SER
1	A	1802	CYS
1	A	1942	LEU
1	A	1943	ARG
1	A	1949	ILE
1	A	1952	THR
1	A	1953	LYS
1	A	1955	ARG
1	A	1958	THR
1	A	1960	VAL
1	A	1963	LEU
1	A	1966	LEU
1	A	1971	ASP
1	A	1972	PHE
1	A	1980	TRP
1	A	2002	GLU
1	A	2004	PHE
1	A	2005	LEU
1	A	2007	MET
1	A	2009	LEU

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Mol	Chain	Res	Type
1	A	2024	ARG
1	A	2026	THR
1	A	2027	VAL
1	A	2028	LEU
1	A	2043	LEU
1	A	2044	TRP
1	A	2045	MET
1	A	2049	LEU
1	A	2061	VAL
1	A	2062	VAL
1	A	2065	LEU
1	A	2077	SER
1	A	2082	ARG
1	A	2089	ILE
1	A	2094	LEU
1	A	2097	LYS
1	A	2100	HIS
1	A	2109	PHE
1	A	2116	VAL
1	A	2117	GLU
1	A	2118	LEU
1	A	2119	ARG
1	A	2122	MET
1	A	2134	SER
1	A	2138	CYS
1	A	2157	LYS
1	A	2163	LYS
1	A	2166	LYS
1	A	2167	LYS
1	A	2168	LYS
1	A	2169	LYS
1	A	2170	ILE
1	A	2175	MET
1	A	2178	LEU
1	A	2181	LEU
1	A	2186	ILE
1	A	2189	PHE
1	A	2192	LEU
1	A	2193	PHE
1	A	2199	SER
1	A	2200	VAL
1	A	2201	VAL

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Mol	Chain	Res	Type
1	A	2213	THR
1	A	2228	GLN
1	A	2231	SER
1	A	2250	GLN
1	A	2261	SER
1	A	2400	PHE
1	A	2434	PHE
1	A	2435	LEU
1	A	2438	TYR
1	A	2440	ILE
1	A	2441	MET
1	A	2446	SER
1	A	2453	LYS
1	A	2456	ARG
1	A	2460	SER
1	A	2462	ILE
1	A	2467	MET
1	A	2469	GLU
1	A	2474	VAL
1	A	2475	ASP
1	A	2476	ARG
1	A	2486	LEU
1	A	2489	GLU
1	A	2491	ARG
1	A	2504	ILE
1	A	2511	GLU
1	A	2514	ILE
1	A	2515	LYS
1	A	2516	TRP
1	A	2518	ARG
1	A	2520	LYS
1	B	570	GLU
1	B	571	LEU
1	B	572	VAL
1	B	573	LYS
1	B	580	TRP
1	B	581	ILE
1	B	588	PHE
1	B	592	SER
1	B	597	LEU
1	B	598	VAL
1	B	599	VAL

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Mol	Chain	Res	Type
1	B	601	LYS
1	B	614	LEU
1	B	618	TYR
1	B	627	LYS
1	B	632	LEU
1	B	633	VAL
1	B	636	TYR
1	B	639	LEU
1	B	644	VAL
1	B	678	SER
1	B	679	GLU
1	B	680	LEU
1	B	683	SER
1	B	685	LEU
1	B	692	LEU
1	B	697	GLN
1	B	698	LEU
1	B	699	HIS
1	B	702	HIS
1	B	703	ARG
1	B	707	GLN
1	B	708	LEU
1	B	710	ASP
1	B	711	MET
1	B	712	GLU
1	B	789	LEU
1	B	790	GLU
1	B	791	LEU
1	B	799	LEU
1	B	805	PHE
1	B	809	LEU
1	B	810	LEU
1	B	812	LEU
1	B	816	LYS
1	B	817	LEU
1	B	820	LEU
1	B	822	THR
1	B	831	SER
1	B	832	VAL
1	B	835	LEU
1	B	836	LEU
1	B	843	PHE

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Mol	Chain	Res	Type
1	B	849	ARG
1	B	853	MET
1	B	855	SER
1	B	856	CYS
1	B	858	SER
1	B	867	VAL
1	B	870	MET
1	B	876	VAL
1	B	877	VAL
1	B	878	ASN
1	B	919	VAL
1	B	920	ARG
1	B	921	LYS
1	B	929	ILE
1	B	930	GLN
1	B	937	LEU
1	B	938	LEU
1	B	942	GLU
1	B	947	ARG
1	B	948	ARG
1	B	953	ARG
1	B	954	ARG
1	B	955	GLN
1	B	972	ARG
1	B	974	GLN
1	B	976	ASP
1	B	979	LEU
1	B	980	LEU
1	B	982	CYS
1	B	983	LEU
1	B	993	LYS
1	B	997	GLU
1	B	998	ILE
1	B	1001	LEU
1	B	1002	MET
1	B	1005	ASN
1	B	1007	ILE
1	B	1011	MET
1	B	1023	VAL
1	B	1025	ILE
1	B	1028	ARG
1	B	1038	TRP

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Mol	Chain	Res	Type
1	B	1048	PHE
1	B	1051	TYR
1	B	1053	TYR
1	B	1054	LEU
1	B	1057	LEU
1	B	1099	LEU
1	B	1100	ILE
1	B	1105	LEU
1	B	1112	GLN
1	B	1155	LEU
1	B	1156	ASP
1	B	1158	LEU
1	B	1176	VAL
1	B	1180	THR
1	B	1181	ARG
1	B	1184	ILE
1	B	1198	LEU
1	B	1208	THR
1	B	1209	ARG
1	B	1214	LEU
1	B	1217	CYS
1	B	1220	LEU
1	B	1222	ASN
1	B	1228	SER
1	B	1231	MET
1	B	1232	LEU
1	B	1233	SER
1	B	1285	ILE
1	B	1286	ILE
1	B	1304	SER
1	B	1317	THR
1	B	1323	ARG
1	B	1327	LEU
1	B	1334	LYS
1	B	1335	SER
1	B	1338	PHE
1	B	1341	ARG
1	B	1342	ILE
1	B	1346	SER
1	B	1350	LEU
1	B	1351	LYS
1	B	1354	MET

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Mol	Chain	Res	Type
1	B	1356	ARG
1	B	1360	LYS
1	B	1363	LYS
1	B	1365	ARG
1	B	1417	ASP
1	B	1420	LEU
1	B	1423	SER
1	B	1514	LEU
1	B	1516	MET
1	B	1517	LEU
1	B	1523	ASP
1	B	1524	GLU
1	B	1530	GLN
1	B	1532	PHE
1	B	1534	ARG
1	B	1539	MET
1	B	1541	ASP
1	B	1546	GLU
1	B	1547	ARG
1	B	1549	LEU
1	B	1550	LEU
1	B	1552	GLN
1	B	1560	VAL
1	B	1561	HIS
1	B	1562	ARG
1	B	1565	LEU
1	B	1646	SER
1	B	1647	GLU
1	B	1652	ARG
1	B	1655	ARG
1	B	1669	GLN
1	B	1673	LEU
1	B	1676	LEU
1	B	1677	ARG
1	B	1682	CYS
1	B	1694	ILE
1	B	1696	ILE
1	B	1701	VAL
1	B	1708	LEU
1	B	1721	SER
1	B	1724	ARG
1	B	1727	LYS

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Mol	Chain	Res	Type
1	B	1728	ARG
1	B	1731	MET
1	B	1744	LYS
1	B	1779	THR
1	B	1780	ASP
1	B	1782	TYR
1	B	1784	LYS
1	B	1797	ARG
1	B	1798	SER
1	B	1802	CYS
1	B	1942	LEU
1	B	1943	ARG
1	B	1949	ILE
1	B	1952	THR
1	B	1953	LYS
1	B	1955	ARG
1	B	1958	THR
1	B	1960	VAL
1	B	1963	LEU
1	B	1966	LEU
1	B	1971	ASP
1	B	1972	PHE
1	B	1980	TRP
1	B	2002	GLU
1	B	2004	PHE
1	B	2005	LEU
1	B	2007	MET
1	B	2009	LEU
1	B	2024	ARG
1	B	2026	THR
1	B	2027	VAL
1	B	2028	LEU
1	B	2043	LEU
1	B	2044	TRP
1	B	2045	MET
1	B	2049	LEU
1	B	2061	VAL
1	B	2062	VAL
1	B	2065	LEU
1	B	2077	SER
1	B	2082	ARG
1	B	2089	ILE

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Mol	Chain	Res	Type
1	B	2094	LEU
1	B	2097	LYS
1	B	2100	HIS
1	B	2109	PHE
1	B	2116	VAL
1	B	2117	GLU
1	B	2118	LEU
1	B	2119	ARG
1	B	2122	MET
1	B	2134	SER
1	B	2138	CYS
1	B	2157	LYS
1	B	2163	LYS
1	B	2166	LYS
1	B	2167	LYS
1	B	2168	LYS
1	B	2169	LYS
1	B	2170	ILE
1	B	2175	MET
1	B	2178	LEU
1	B	2181	LEU
1	B	2186	ILE
1	B	2189	PHE
1	B	2192	LEU
1	B	2193	PHE
1	B	2199	SER
1	B	2200	VAL
1	B	2201	VAL
1	B	2213	THR
1	B	2228	GLN
1	B	2231	SER
1	B	2250	GLN
1	B	2261	SER
1	B	2400	PHE
1	B	2434	PHE
1	B	2435	LEU
1	B	2438	TYR
1	B	2440	ILE
1	B	2441	MET
1	B	2446	SER
1	B	2453	LYS
1	B	2456	ARG

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Mol	Chain	Res	Type
1	B	2460	SER
1	B	2462	ILE
1	B	2467	MET
1	B	2469	GLU
1	B	2474	VAL
1	B	2475	ASP
1	B	2476	ARG
1	B	2486	LEU
1	B	2489	GLU
1	B	2491	ARG
1	B	2504	ILE
1	B	2514	ILE
1	B	2515	LYS
1	B	2516	TRP
1	B	2518	ARG
1	B	2520	LYS
1	C	570	GLU
1	C	571	LEU
1	C	572	VAL
1	C	573	LYS
1	C	580	TRP
1	C	581	ILE
1	C	588	PHE
1	C	592	SER
1	C	597	LEU
1	C	598	VAL
1	C	599	VAL
1	C	601	LYS
1	C	614	LEU
1	C	618	TYR
1	C	626	LEU
1	C	627	LYS
1	C	632	LEU
1	C	636	TYR
1	C	639	LEU
1	C	644	VAL
1	C	678	SER
1	C	679	GLU
1	C	680	LEU
1	C	683	SER
1	C	685	LEU
1	C	692	LEU

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Mol	Chain	Res	Type
1	C	697	GLN
1	C	698	LEU
1	C	699	HIS
1	C	702	HIS
1	C	703	ARG
1	C	707	GLN
1	C	708	LEU
1	C	710	ASP
1	C	711	MET
1	C	712	GLU
1	C	789	LEU
1	C	790	GLU
1	C	791	LEU
1	C	799	LEU
1	C	805	PHE
1	C	809	LEU
1	C	810	LEU
1	C	812	LEU
1	C	816	LYS
1	C	817	LEU
1	C	820	LEU
1	C	822	THR
1	C	831	SER
1	C	832	VAL
1	C	835	LEU
1	C	836	LEU
1	C	843	PHE
1	C	849	ARG
1	C	853	MET
1	C	855	SER
1	C	856	CYS
1	C	858	SER
1	C	867	VAL
1	C	870	MET
1	C	876	VAL
1	C	877	VAL
1	C	878	ASN
1	C	919	VAL
1	C	920	ARG
1	C	921	LYS
1	C	929	ILE
1	C	930	GLN

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Mol	Chain	Res	Type
1	C	937	LEU
1	C	938	LEU
1	C	942	GLU
1	C	947	ARG
1	C	948	ARG
1	C	953	ARG
1	C	954	ARG
1	C	955	GLN
1	C	972	ARG
1	C	974	GLN
1	C	976	ASP
1	C	979	LEU
1	C	980	LEU
1	C	982	CYS
1	C	983	LEU
1	C	993	LYS
1	C	997	GLU
1	C	998	ILE
1	C	1001	LEU
1	C	1002	MET
1	C	1005	ASN
1	C	1007	ILE
1	C	1011	MET
1	C	1023	VAL
1	C	1025	ILE
1	C	1028	ARG
1	C	1038	TRP
1	C	1048	PHE
1	C	1051	TYR
1	C	1053	TYR
1	C	1054	LEU
1	C	1057	LEU
1	C	1099	LEU
1	C	1100	ILE
1	C	1105	LEU
1	C	1112	GLN
1	C	1155	LEU
1	C	1156	ASP
1	C	1158	LEU
1	C	1176	VAL
1	C	1180	THR
1	C	1181	ARG

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Mol	Chain	Res	Type
1	C	1184	ILE
1	C	1198	LEU
1	C	1208	THR
1	C	1209	ARG
1	C	1212	LEU
1	C	1220	LEU
1	C	1222	ASN
1	C	1228	SER
1	C	1231	MET
1	C	1232	LEU
1	C	1233	SER
1	C	1285	ILE
1	C	1286	ILE
1	C	1304	SER
1	C	1317	THR
1	C	1323	ARG
1	C	1327	LEU
1	C	1334	LYS
1	C	1335	SER
1	C	1338	PHE
1	C	1341	ARG
1	C	1342	ILE
1	C	1346	SER
1	C	1350	LEU
1	C	1351	LYS
1	C	1354	MET
1	C	1356	ARG
1	C	1360	LYS
1	C	1363	LYS
1	C	1365	ARG
1	C	1417	ASP
1	C	1420	LEU
1	C	1423	SER
1	C	1514	LEU
1	C	1516	MET
1	C	1517	LEU
1	C	1523	ASP
1	C	1524	GLU
1	C	1530	GLN
1	C	1532	PHE
1	C	1534	ARG
1	C	1539	MET

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Mol	Chain	Res	Type
1	C	1541	ASP
1	C	1546	GLU
1	C	1547	ARG
1	C	1549	LEU
1	C	1550	LEU
1	C	1552	GLN
1	C	1560	VAL
1	C	1561	HIS
1	C	1562	ARG
1	C	1565	LEU
1	C	1646	SER
1	C	1647	GLU
1	C	1652	ARG
1	C	1655	ARG
1	C	1669	GLN
1	C	1673	LEU
1	C	1676	LEU
1	C	1677	ARG
1	C	1682	CYS
1	C	1694	ILE
1	C	1696	ILE
1	C	1701	VAL
1	C	1708	LEU
1	C	1724	ARG
1	C	1727	LYS
1	C	1728	ARG
1	C	1731	MET
1	C	1744	LYS
1	C	1782	TYR
1	C	1784	LYS
1	C	1797	ARG
1	C	1798	SER
1	C	1802	CYS
1	C	1942	LEU
1	C	1943	ARG
1	C	1949	ILE
1	C	1952	THR
1	C	1953	LYS
1	C	1955	ARG
1	C	1958	THR
1	C	1960	VAL
1	C	1963	LEU

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Mol	Chain	Res	Type
1	C	1966	LEU
1	C	1971	ASP
1	C	1972	PHE
1	C	1980	TRP
1	C	2002	GLU
1	C	2004	PHE
1	C	2005	LEU
1	C	2007	MET
1	C	2009	LEU
1	C	2024	ARG
1	C	2026	THR
1	C	2027	VAL
1	C	2028	LEU
1	C	2043	LEU
1	C	2044	TRP
1	C	2045	MET
1	C	2049	LEU
1	C	2061	VAL
1	C	2062	VAL
1	C	2065	LEU
1	C	2077	SER
1	C	2082	ARG
1	C	2089	ILE
1	C	2094	LEU
1	C	2097	LYS
1	C	2100	HIS
1	C	2109	PHE
1	C	2116	VAL
1	C	2118	LEU
1	C	2119	ARG
1	C	2122	MET
1	C	2134	SER
1	C	2138	CYS
1	C	2157	LYS
1	C	2163	LYS
1	C	2166	LYS
1	C	2167	LYS
1	C	2168	LYS
1	C	2169	LYS
1	C	2170	ILE
1	C	2175	MET
1	C	2178	LEU

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Mol	Chain	Res	Type
1	C	2181	LEU
1	C	2186	ILE
1	C	2189	PHE
1	C	2192	LEU
1	C	2193	PHE
1	C	2199	SER
1	C	2200	VAL
1	C	2201	VAL
1	C	2213	THR
1	C	2228	GLN
1	C	2231	SER
1	C	2250	GLN
1	C	2261	SER
1	C	2400	PHE
1	C	2434	PHE
1	C	2435	LEU
1	C	2438	TYR
1	C	2440	ILE
1	C	2441	MET
1	C	2446	SER
1	C	2453	LYS
1	C	2456	ARG
1	C	2460	SER
1	C	2462	ILE
1	C	2467	MET
1	C	2469	GLU
1	C	2474	VAL
1	C	2475	ASP
1	C	2476	ARG
1	C	2486	LEU
1	C	2489	GLU
1	C	2491	ARG
1	C	2504	ILE
1	C	2514	ILE
1	C	2515	LYS
1	C	2516	TRP
1	C	2518	ARG
1	C	2520	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	697	GLN
1	A	699	HIS
1	A	977	GLN
1	A	1112	GLN
1	A	1230	ASN
1	A	1339	HIS
1	A	2064	GLN
1	A	2228	GLN
1	B	697	GLN
1	B	699	HIS
1	B	977	GLN
1	B	1230	ASN
1	B	1339	HIS
1	B	2064	GLN
1	B	2228	GLN
1	C	697	GLN
1	C	699	HIS
1	C	977	GLN
1	C	1112	GLN
1	C	1230	ASN
1	C	1339	HIS
1	C	2064	GLN
1	C	2228	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	L9Q	A	2602	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	A	2603	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)
2	L9Q	C	2601	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	B	2601	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)
2	L9Q	B	2602	-	50,50,50	1.03	3 (6%)	53,55,55	1.17	4 (7%)
2	L9Q	A	2601	-	50,50,50	1.05	3 (6%)	53,55,55	1.10	3 (5%)

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
2	L9Q	A	2602	-	-	37/54/54/54	-
2	L9Q	A	2603	-	-	33/54/54/54	-
2	L9Q	C	2601	-	-	37/54/54/54	-
2	L9Q	B	2601	-	-	33/54/54/54	-
2	L9Q	B	2602	-	-	37/54/54/54	-
2	L9Q	A	2601	-	-	33/54/54/54	-

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2601	L9Q	O3-C11	4.30	1.45	1.33
2	A	2601	L9Q	O3-C11	4.29	1.45	1.33
2	A	2603	L9Q	O3-C11	4.29	1.45	1.33
2	A	2602	L9Q	O2-C31	4.02	1.45	1.34
2	B	2602	L9Q	O2-C31	4.00	1.45	1.34
2	C	2601	L9Q	O2-C31	4.00	1.45	1.34
2	B	2601	L9Q	O2-C31	3.99	1.45	1.34
2	A	2603	L9Q	O2-C31	3.98	1.45	1.34
2	A	2601	L9Q	O2-C31	3.98	1.45	1.34
2	B	2602	L9Q	O3-C11	3.95	1.44	1.33
2	A	2602	L9Q	O3-C11	3.94	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2601	L9Q	O3-C11	3.94	1.44	1.33
2	A	2601	L9Q	C40-C39	3.64	1.52	1.31
2	B	2601	L9Q	C40-C39	3.63	1.52	1.31
2	A	2603	L9Q	C40-C39	3.62	1.52	1.31
2	C	2601	L9Q	C40-C39	3.60	1.52	1.31
2	B	2602	L9Q	C40-C39	3.60	1.52	1.31
2	A	2602	L9Q	C40-C39	3.59	1.52	1.31

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2601	L9Q	O2-C31-C32	4.26	120.68	111.50
2	A	2602	L9Q	O2-C31-C32	4.25	120.66	111.50
2	B	2602	L9Q	O2-C31-C32	4.25	120.66	111.50
2	B	2601	L9Q	O2-C31-C32	3.94	120.00	111.50
2	A	2603	L9Q	O2-C31-C32	3.94	120.00	111.50
2	A	2601	L9Q	O2-C31-C32	3.94	119.99	111.50
2	A	2603	L9Q	C2-O2-C31	-3.08	110.21	117.79
2	B	2601	L9Q	C2-O2-C31	-3.08	110.22	117.79
2	A	2601	L9Q	C2-O2-C31	-3.07	110.22	117.79
2	A	2602	L9Q	C2-O2-C31	-2.73	111.08	117.79
2	C	2601	L9Q	C2-O2-C31	-2.72	111.08	117.79
2	B	2602	L9Q	C2-O2-C31	-2.71	111.12	117.79
2	C	2601	L9Q	O3-C11-C12	2.54	119.87	111.91
2	B	2602	L9Q	O3-C11-C12	2.53	119.86	111.91
2	A	2602	L9Q	O3-C11-C12	2.53	119.85	111.91
2	A	2601	L9Q	O3-C11-C12	2.35	119.28	111.91
2	A	2603	L9Q	O3-C11-C12	2.35	119.27	111.91
2	B	2601	L9Q	O3-C11-C12	2.34	119.26	111.91
2	A	2602	L9Q	C3-C2-C1	-2.15	106.70	111.79
2	C	2601	L9Q	C3-C2-C1	-2.14	106.72	111.79
2	B	2602	L9Q	C3-C2-C1	-2.14	106.72	111.79

There are no chirality outliers.

All (210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	L9Q	C4-O4P-P-O1P
2	A	2601	L9Q	O4P-C4-C5-N
2	A	2602	L9Q	C4-O4P-P-O1P
2	A	2602	L9Q	C4-O4P-P-O2P
2	A	2602	L9Q	C4-O4P-P-O3P

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Mol	Chain	Res	Type	Atoms
2	A	2602	L9Q	O31-C31-O2-C2
2	A	2602	L9Q	C32-C31-O2-C2
2	A	2603	L9Q	C4-O4P-P-O1P
2	A	2603	L9Q	O4P-C4-C5-N
2	B	2601	L9Q	C4-O4P-P-O1P
2	B	2601	L9Q	O4P-C4-C5-N
2	B	2602	L9Q	C4-O4P-P-O1P
2	B	2602	L9Q	C4-O4P-P-O2P
2	B	2602	L9Q	C4-O4P-P-O3P
2	B	2602	L9Q	O31-C31-O2-C2
2	B	2602	L9Q	C32-C31-O2-C2
2	C	2601	L9Q	C4-O4P-P-O1P
2	C	2601	L9Q	C4-O4P-P-O2P
2	C	2601	L9Q	C4-O4P-P-O3P
2	C	2601	L9Q	O31-C31-O2-C2
2	C	2601	L9Q	C32-C31-O2-C2
2	A	2601	L9Q	C17-C18-C19-C20
2	A	2603	L9Q	C17-C18-C19-C20
2	B	2601	L9Q	C17-C18-C19-C20
2	A	2602	L9Q	C21-C22-C23-C24
2	A	2602	L9Q	C23-C24-C25-C26
2	B	2602	L9Q	C21-C22-C23-C24
2	B	2602	L9Q	C23-C24-C25-C26
2	C	2601	L9Q	C21-C22-C23-C24
2	C	2601	L9Q	C23-C24-C25-C26
2	A	2601	L9Q	C15-C16-C17-C18
2	A	2603	L9Q	C15-C16-C17-C18
2	B	2601	L9Q	C15-C16-C17-C18
2	A	2601	L9Q	C2-C1-O3P-P
2	A	2603	L9Q	C2-C1-O3P-P
2	B	2601	L9Q	C2-C1-O3P-P
2	A	2601	L9Q	C21-C22-C23-C24
2	A	2603	L9Q	C21-C22-C23-C24
2	B	2601	L9Q	C21-C22-C23-C24
2	A	2602	L9Q	C12-C11-O3-C3
2	B	2602	L9Q	C12-C11-O3-C3
2	C	2601	L9Q	C12-C11-O3-C3
2	A	2602	L9Q	O11-C11-O3-C3
2	B	2602	L9Q	O11-C11-O3-C3
2	C	2601	L9Q	O11-C11-O3-C3
2	A	2601	L9Q	C31-C32-C33-C34
2	A	2603	L9Q	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
2	B	2601	L9Q	C31-C32-C33-C34
2	A	2602	L9Q	C18-C19-C20-C21
2	B	2602	L9Q	C18-C19-C20-C21
2	C	2601	L9Q	C18-C19-C20-C21
2	A	2601	L9Q	C11-C12-C13-C14
2	A	2603	L9Q	C11-C12-C13-C14
2	B	2601	L9Q	C11-C12-C13-C14
2	A	2601	L9Q	C24-C25-C26-C27
2	A	2603	L9Q	C24-C25-C26-C27
2	B	2601	L9Q	C24-C25-C26-C27
2	A	2601	L9Q	C1-O3P-P-O4P
2	A	2603	L9Q	C1-O3P-P-O4P
2	B	2601	L9Q	C1-O3P-P-O4P
2	A	2601	L9Q	C32-C31-O2-C2
2	A	2603	L9Q	C32-C31-O2-C2
2	B	2601	L9Q	C32-C31-O2-C2
2	A	2602	L9Q	C42-C43-C44-C45
2	B	2602	L9Q	C42-C43-C44-C45
2	C	2601	L9Q	C42-C43-C44-C45
2	A	2601	L9Q	C43-C44-C45-C46
2	A	2603	L9Q	C43-C44-C45-C46
2	A	2603	L9Q	C44-C45-C46-C47
2	B	2601	L9Q	C44-C45-C46-C47
2	A	2601	L9Q	C44-C45-C46-C47
2	B	2601	L9Q	C43-C44-C45-C46
2	A	2601	L9Q	O31-C31-O2-C2
2	A	2603	L9Q	O31-C31-O2-C2
2	B	2601	L9Q	O31-C31-O2-C2
2	A	2601	L9Q	C33-C34-C35-C36
2	A	2602	L9Q	C35-C36-C37-C38
2	A	2603	L9Q	C33-C34-C35-C36
2	B	2601	L9Q	C33-C34-C35-C36
2	C	2601	L9Q	C35-C36-C37-C38
2	B	2602	L9Q	C35-C36-C37-C38
2	C	2601	L9Q	C41-C42-C43-C44
2	A	2602	L9Q	C16-C17-C18-C19
2	A	2602	L9Q	C41-C42-C43-C44
2	B	2602	L9Q	C16-C17-C18-C19
2	B	2602	L9Q	C41-C42-C43-C44
2	C	2601	L9Q	C16-C17-C18-C19
2	A	2602	L9Q	O4P-C4-C5-N
2	B	2602	L9Q	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
2	C	2601	L9Q	O4P-C4-C5-N
2	A	2602	L9Q	C11-C12-C13-C14
2	B	2602	L9Q	C11-C12-C13-C14
2	C	2601	L9Q	C11-C12-C13-C14
2	A	2601	L9Q	C41-C42-C43-C44
2	A	2602	L9Q	C44-C45-C46-C47
2	A	2603	L9Q	C41-C42-C43-C44
2	B	2601	L9Q	C41-C42-C43-C44
2	B	2602	L9Q	C44-C45-C46-C47
2	C	2601	L9Q	C44-C45-C46-C47
2	A	2603	L9Q	C18-C19-C20-C21
2	A	2601	L9Q	C18-C19-C20-C21
2	B	2601	L9Q	C18-C19-C20-C21
2	A	2602	L9Q	C25-C26-C27-C28
2	C	2601	L9Q	C25-C26-C27-C28
2	B	2602	L9Q	C25-C26-C27-C28
2	B	2601	L9Q	C35-C36-C37-C38
2	A	2601	L9Q	C35-C36-C37-C38
2	A	2603	L9Q	C35-C36-C37-C38
2	C	2601	L9Q	C13-C14-C15-C16
2	A	2602	L9Q	C13-C14-C15-C16
2	B	2602	L9Q	C13-C14-C15-C16
2	B	2601	L9Q	C19-C20-C21-C22
2	A	2601	L9Q	C19-C20-C21-C22
2	A	2603	L9Q	C19-C20-C21-C22
2	A	2602	L9Q	C40-C41-C42-C43
2	B	2602	L9Q	C40-C41-C42-C43
2	C	2601	L9Q	C40-C41-C42-C43
2	A	2601	L9Q	C1-C2-C3-O3
2	A	2602	L9Q	C1-C2-C3-O3
2	A	2603	L9Q	C1-C2-C3-O3
2	B	2601	L9Q	C1-C2-C3-O3
2	B	2602	L9Q	C1-C2-C3-O3
2	C	2601	L9Q	C1-C2-C3-O3
2	A	2602	L9Q	C45-C46-C47-C48
2	B	2602	L9Q	C45-C46-C47-C48
2	C	2601	L9Q	C45-C46-C47-C48
2	A	2601	L9Q	C39-C40-C41-C42
2	A	2603	L9Q	C39-C40-C41-C42
2	B	2601	L9Q	C39-C40-C41-C42
2	A	2602	L9Q	C20-C21-C22-C23
2	B	2602	L9Q	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	C	2601	L9Q	C20-C21-C22-C23
2	A	2601	L9Q	O2-C2-C3-O3
2	A	2603	L9Q	O2-C2-C3-O3
2	B	2601	L9Q	O2-C2-C3-O3
2	A	2601	L9Q	C45-C46-C47-C48
2	A	2603	L9Q	C45-C46-C47-C48
2	B	2601	L9Q	C45-C46-C47-C48
2	A	2602	L9Q	C32-C33-C34-C35
2	B	2602	L9Q	C32-C33-C34-C35
2	C	2601	L9Q	C32-C33-C34-C35
2	A	2602	L9Q	C22-C23-C24-C25
2	B	2602	L9Q	C22-C23-C24-C25
2	C	2601	L9Q	C22-C23-C24-C25
2	A	2602	L9Q	C43-C44-C45-C46
2	B	2602	L9Q	C43-C44-C45-C46
2	C	2601	L9Q	C43-C44-C45-C46
2	A	2602	L9Q	O2-C2-C3-O3
2	B	2602	L9Q	O2-C2-C3-O3
2	C	2601	L9Q	O2-C2-C3-O3
2	A	2602	L9Q	C39-C40-C41-C42
2	B	2602	L9Q	C39-C40-C41-C42
2	C	2601	L9Q	C39-C40-C41-C42
2	A	2601	L9Q	O3P-C1-C2-C3
2	A	2603	L9Q	O3P-C1-C2-C3
2	B	2601	L9Q	O3P-C1-C2-C3
2	A	2601	L9Q	C42-C43-C44-C45
2	A	2603	L9Q	C42-C43-C44-C45
2	B	2601	L9Q	C42-C43-C44-C45
2	A	2601	L9Q	C1-O3P-P-O1P
2	A	2603	L9Q	C1-O3P-P-O1P
2	B	2601	L9Q	C1-O3P-P-O1P
2	A	2602	L9Q	C38-C39-C40-C41
2	B	2602	L9Q	C38-C39-C40-C41
2	C	2601	L9Q	C38-C39-C40-C41
2	B	2601	L9Q	C32-C33-C34-C35
2	A	2603	L9Q	C16-C17-C18-C19
2	A	2601	L9Q	C16-C17-C18-C19
2	A	2601	L9Q	C32-C33-C34-C35
2	A	2603	L9Q	C32-C33-C34-C35
2	B	2601	L9Q	C16-C17-C18-C19
2	B	2602	L9Q	C14-C15-C16-C17
2	A	2602	L9Q	C14-C15-C16-C17

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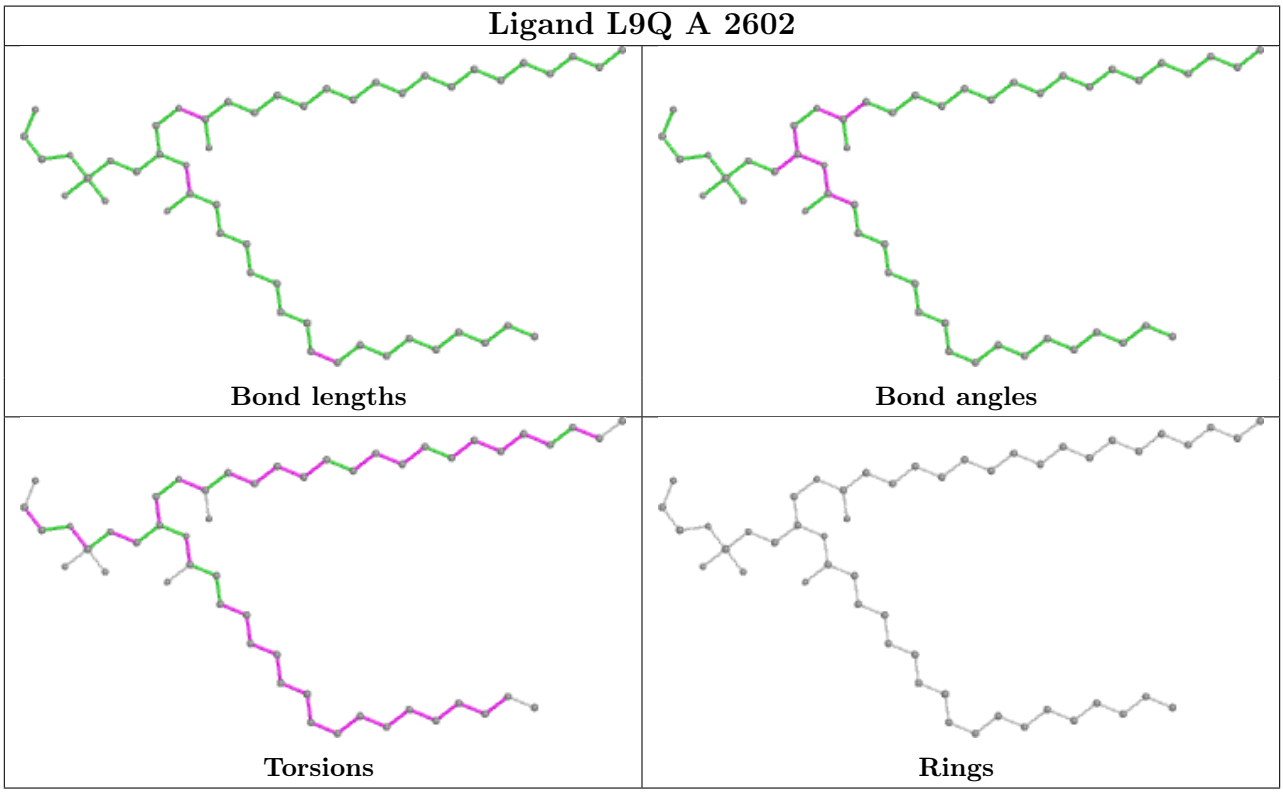
Mol	Chain	Res	Type	Atoms
2	C	2601	L9Q	C14-C15-C16-C17
2	A	2602	L9Q	C2-C1-O3P-P
2	A	2602	L9Q	C37-C38-C39-C40
2	B	2602	L9Q	C37-C38-C39-C40
2	C	2601	L9Q	C37-C38-C39-C40
2	A	2601	L9Q	C4-O4P-P-O3P
2	A	2603	L9Q	C4-O4P-P-O3P
2	B	2601	L9Q	C4-O4P-P-O3P
2	A	2602	L9Q	C34-C35-C36-C37
2	B	2602	L9Q	C34-C35-C36-C37
2	C	2601	L9Q	C34-C35-C36-C37
2	B	2602	L9Q	C2-C1-O3P-P
2	C	2601	L9Q	C2-C1-O3P-P
2	A	2602	L9Q	C36-C37-C38-C39
2	B	2602	L9Q	C36-C37-C38-C39
2	C	2601	L9Q	C36-C37-C38-C39
2	B	2602	L9Q	C33-C34-C35-C36
2	C	2601	L9Q	C33-C34-C35-C36
2	A	2602	L9Q	C33-C34-C35-C36
2	A	2602	L9Q	C12-C13-C14-C15
2	B	2602	L9Q	C12-C13-C14-C15
2	C	2601	L9Q	C12-C13-C14-C15
2	A	2601	L9Q	C14-C15-C16-C17
2	A	2603	L9Q	C14-C15-C16-C17
2	B	2601	L9Q	C14-C15-C16-C17
2	A	2601	L9Q	C38-C39-C40-C41
2	A	2603	L9Q	C38-C39-C40-C41
2	B	2601	L9Q	C38-C39-C40-C41
2	B	2602	L9Q	C17-C18-C19-C20
2	C	2601	L9Q	C17-C18-C19-C20
2	A	2602	L9Q	C17-C18-C19-C20
2	A	2601	L9Q	O2-C31-C32-C33
2	A	2603	L9Q	O2-C31-C32-C33
2	B	2601	L9Q	O2-C31-C32-C33
2	A	2601	L9Q	O3P-C1-C2-O2
2	A	2603	L9Q	O3P-C1-C2-O2
2	B	2601	L9Q	O3P-C1-C2-O2

There are no ring outliers.

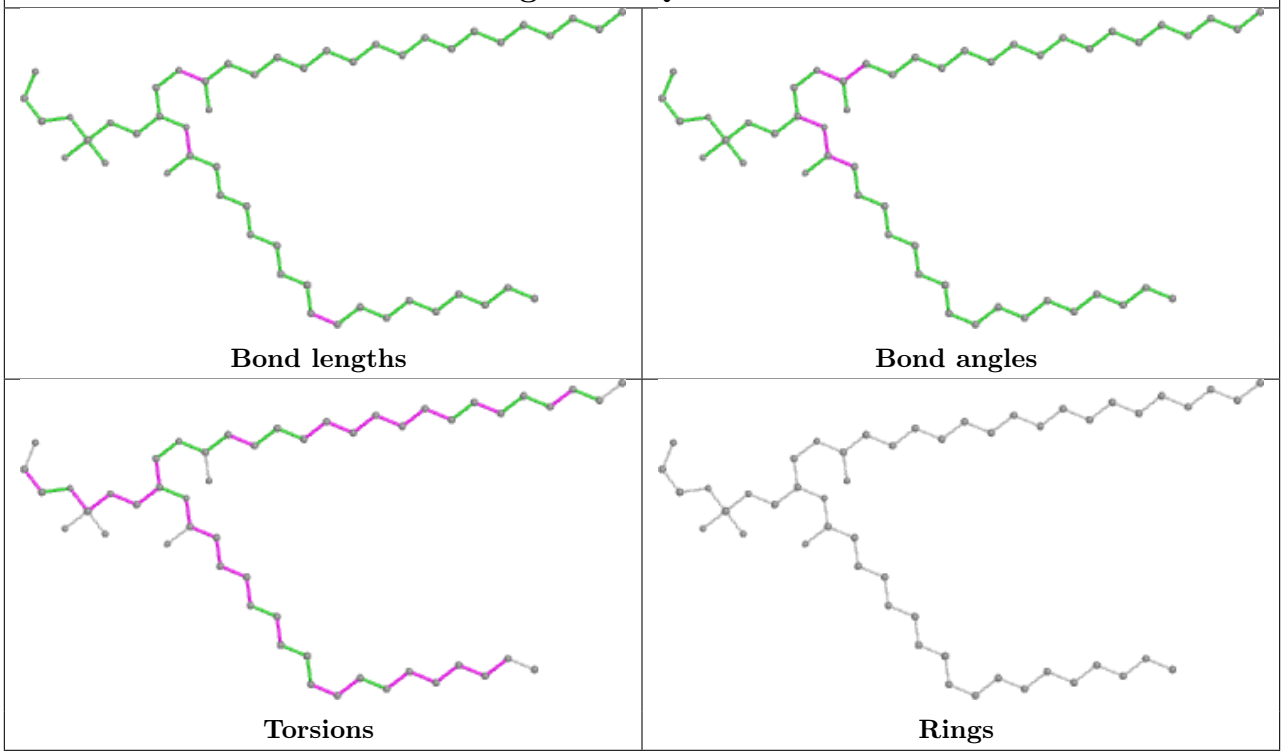
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2602	L9Q	4	0
2	A	2603	L9Q	2	0
2	C	2601	L9Q	1	0
2	B	2601	L9Q	3	0
2	B	2602	L9Q	3	0
2	A	2601	L9Q	3	0

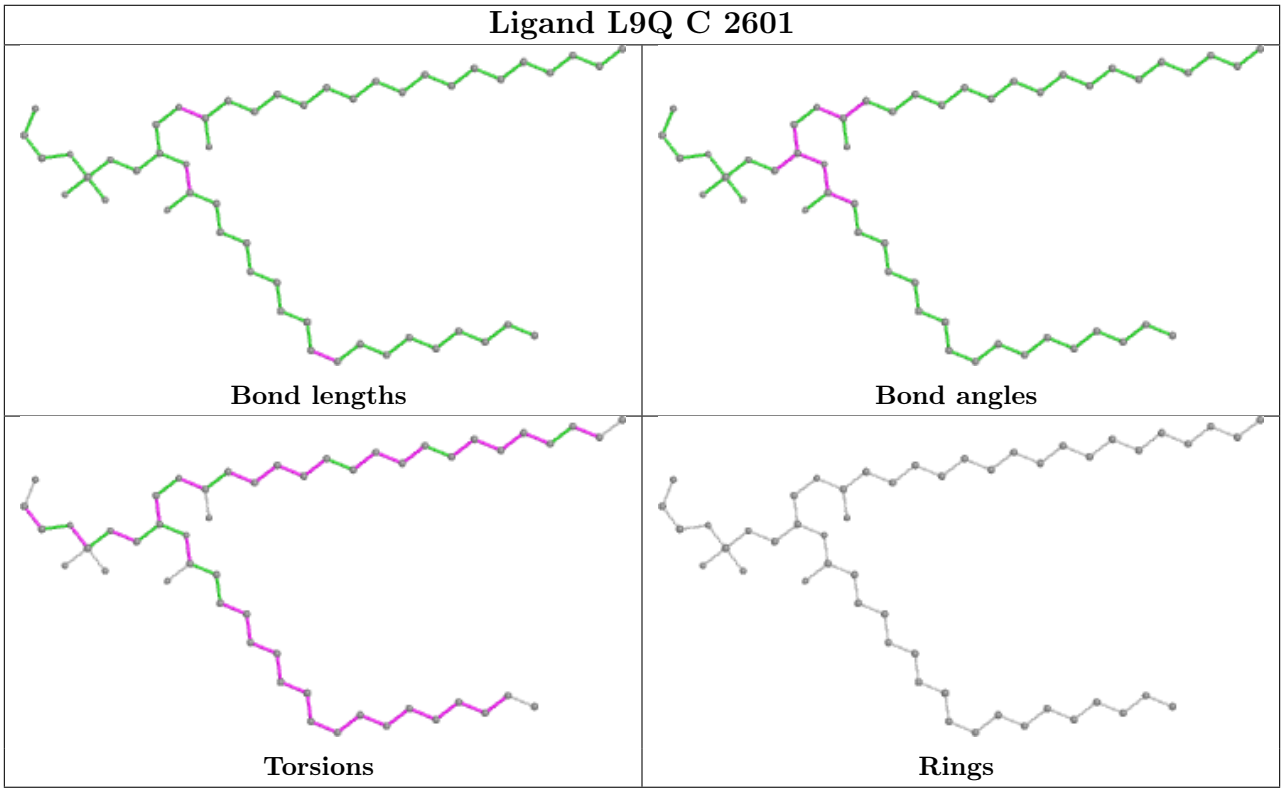
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



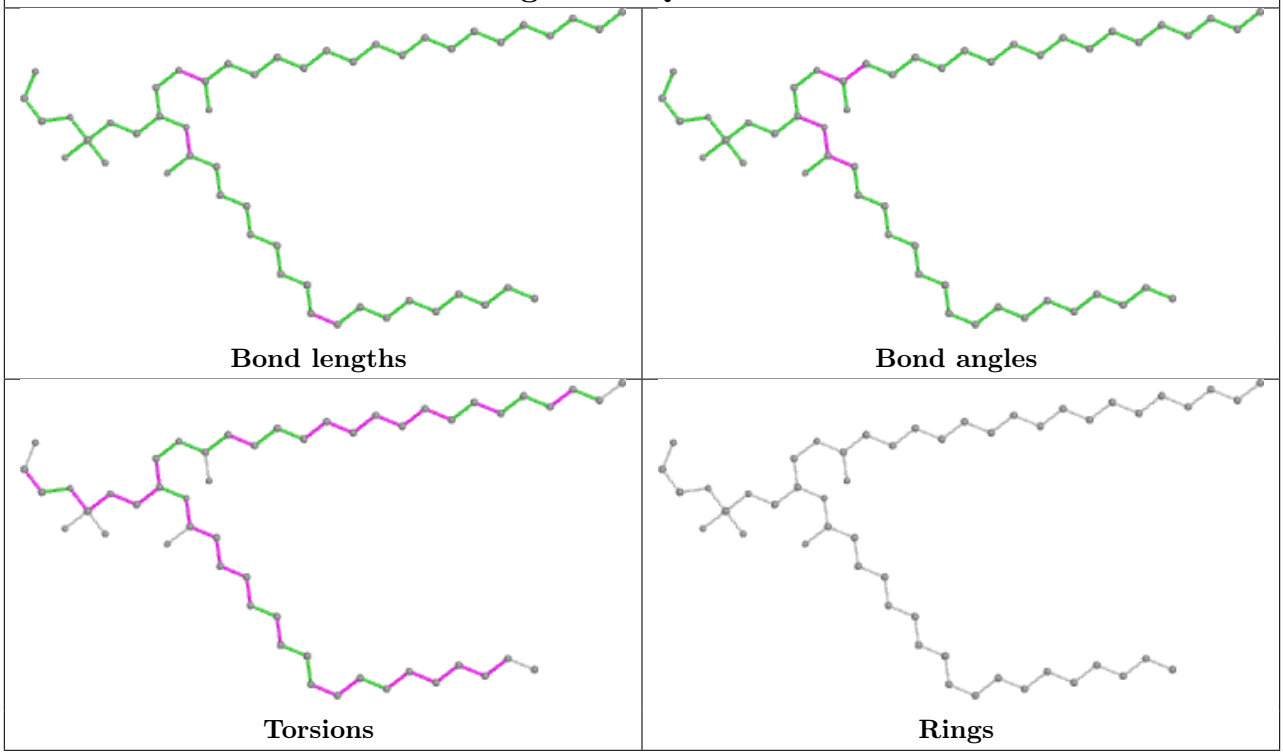
Ligand L9Q A 2603



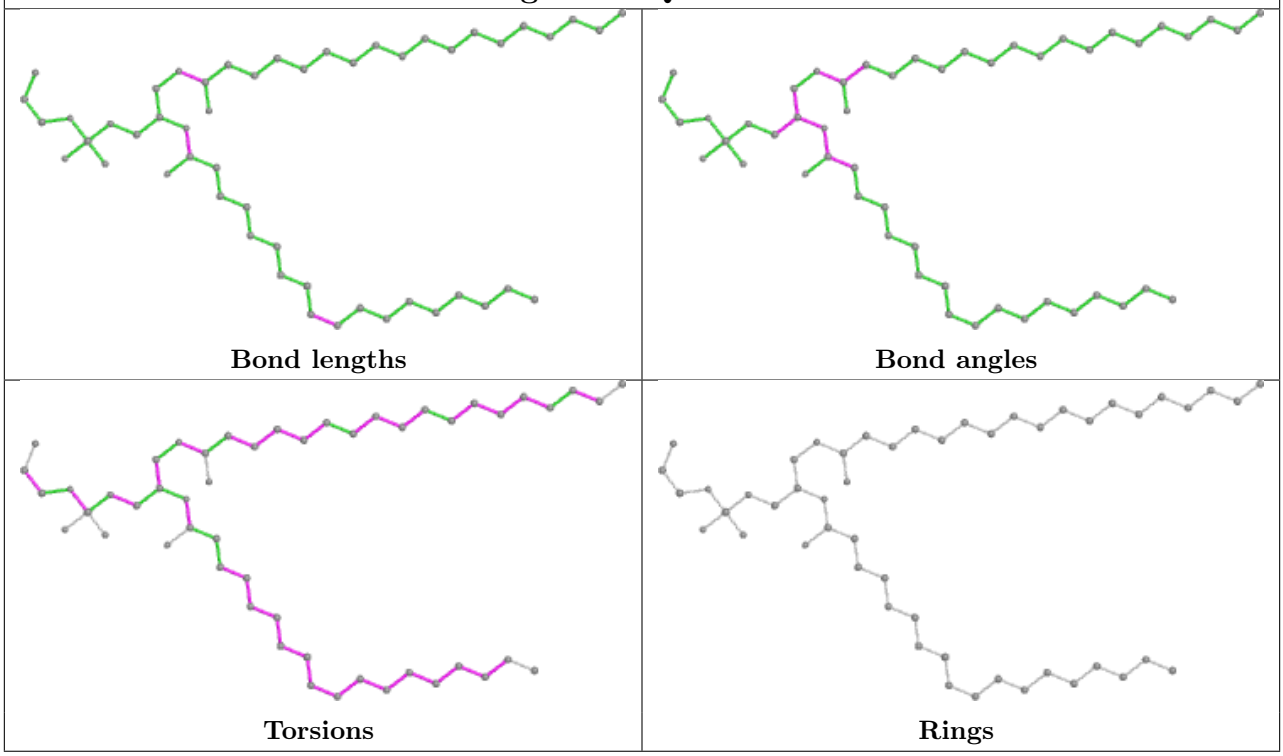
Ligand L9Q C 2601

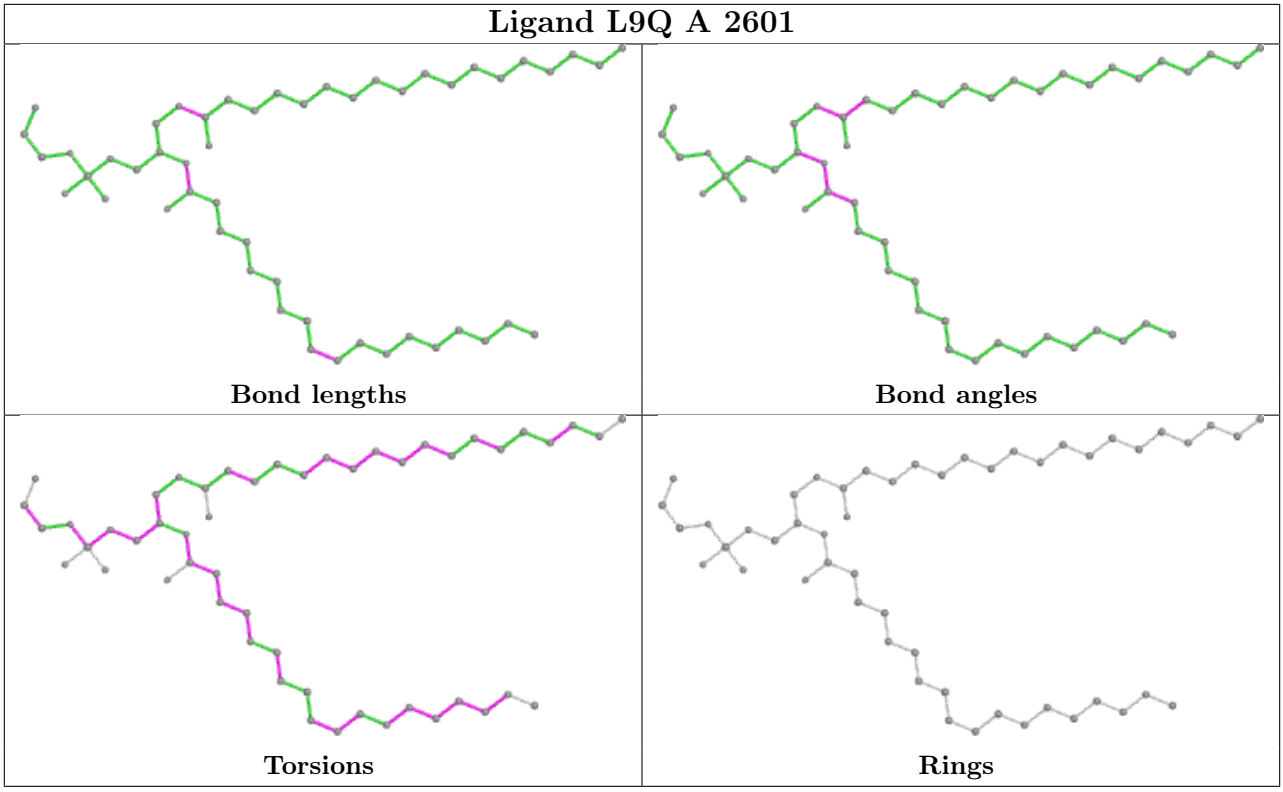


Ligand L9Q B 2601



Ligand L9Q B 2602





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

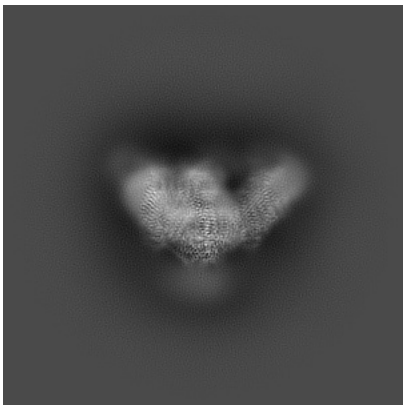
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-39205. These allow visual inspection of the internal detail of the map and identification of artifacts.

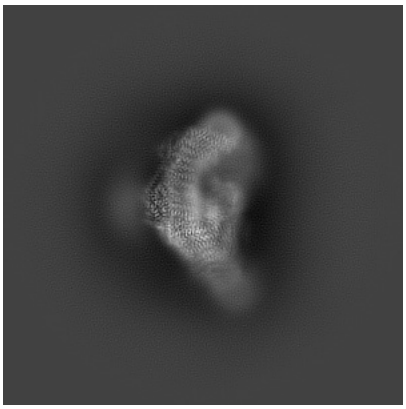
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

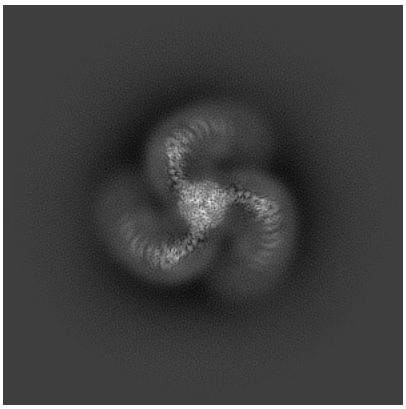
6.1.1 Primary map



X

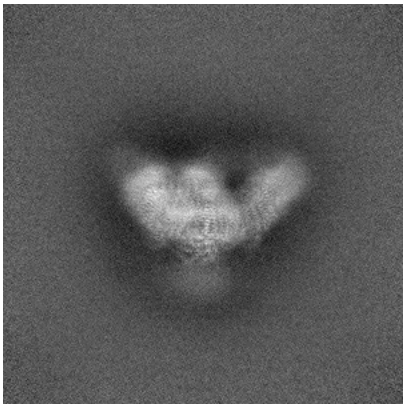


Y

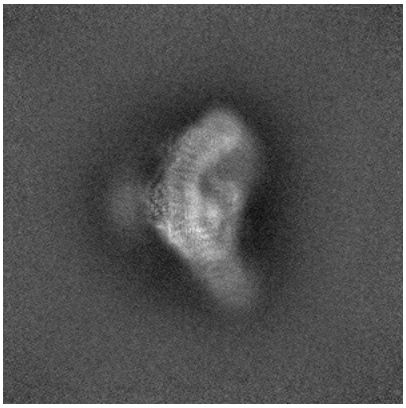


Z

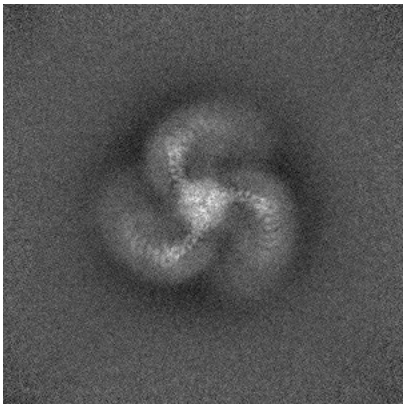
6.1.2 Raw map



X



Y

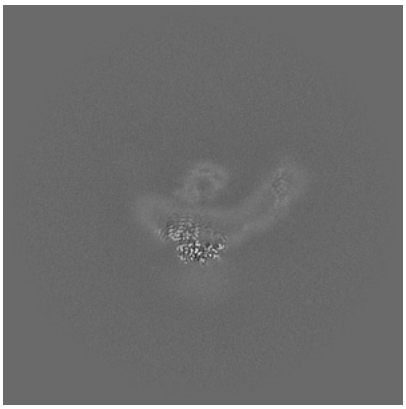


Z

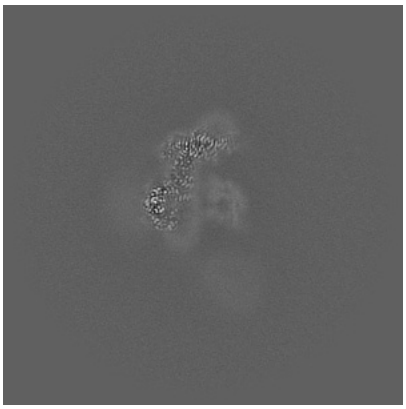
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

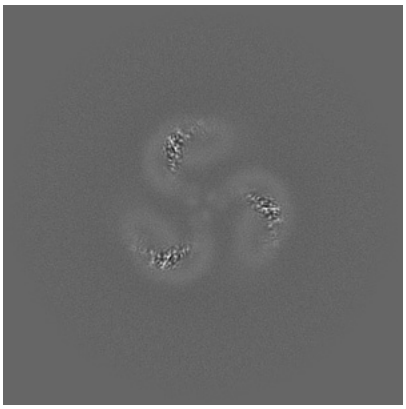
6.2.1 Primary map



X Index: 320

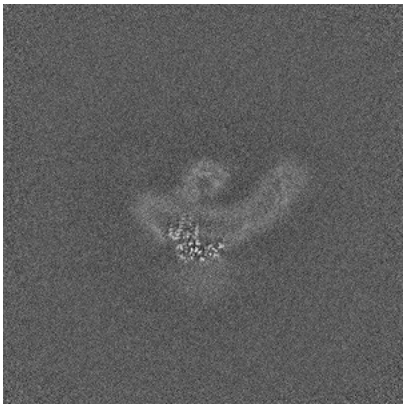


Y Index: 320

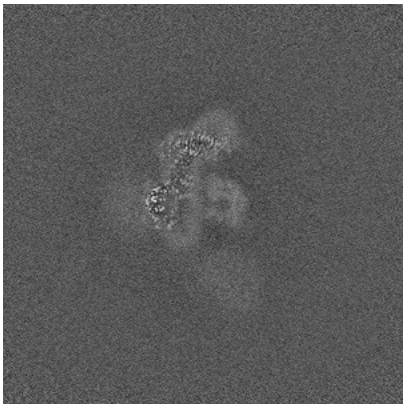


Z Index: 320

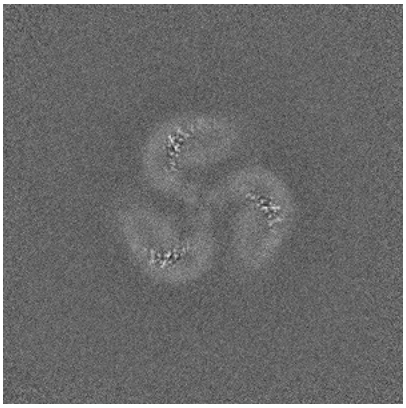
6.2.2 Raw map



X Index: 320



Y Index: 320

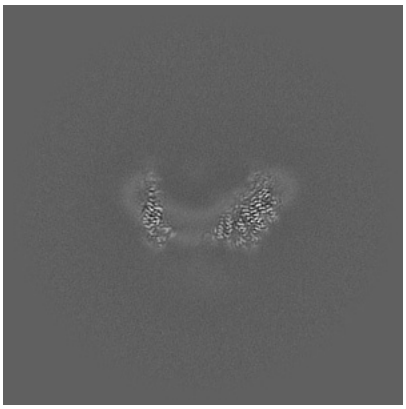


Z Index: 320

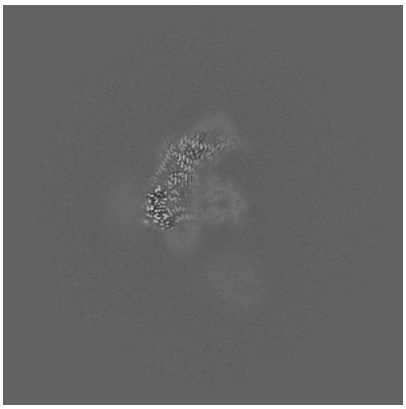
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

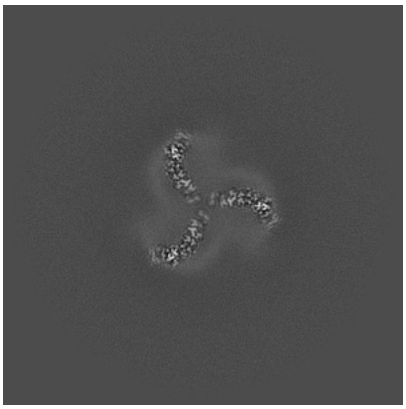
6.3.1 Primary map



X Index: 276

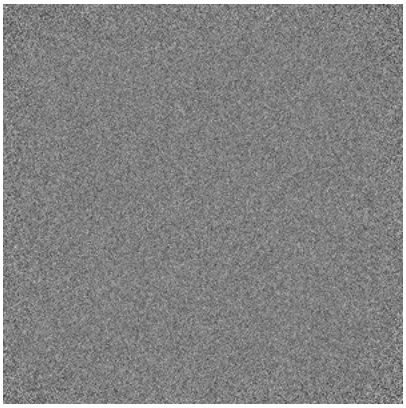


Y Index: 327

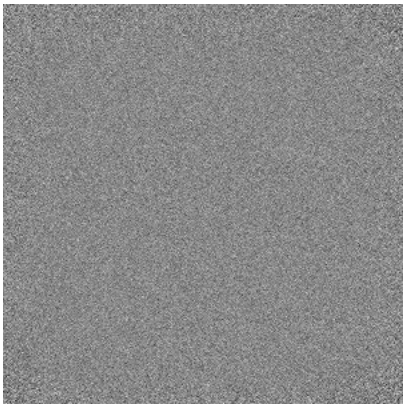


Z Index: 293

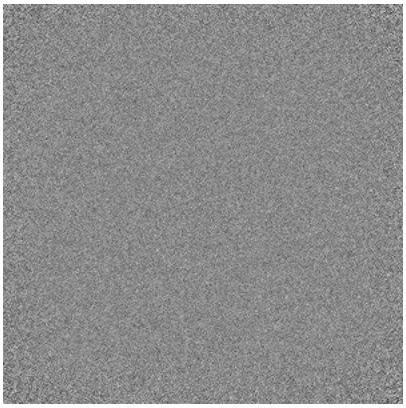
6.3.2 Raw map



X Index: 0



Y Index: 0



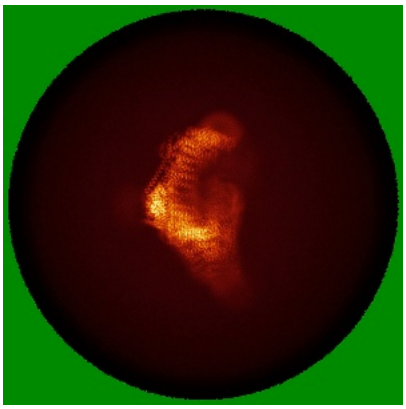
Z Index: 0

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

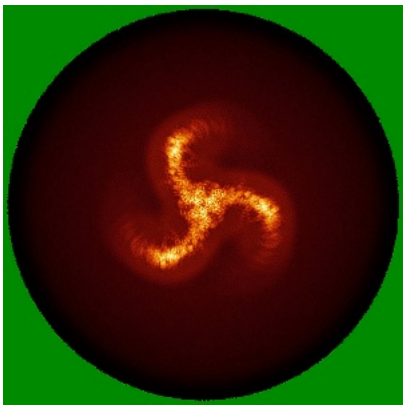
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

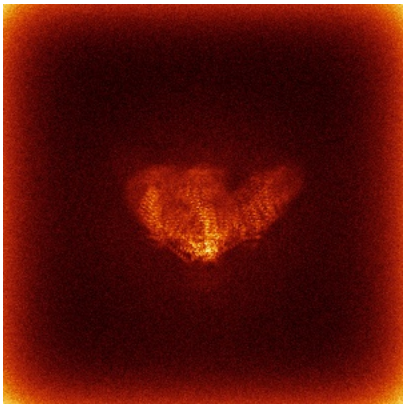


Y

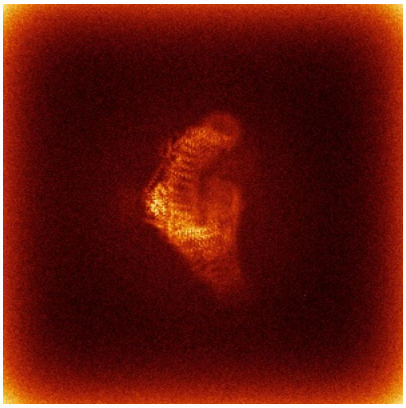


Z

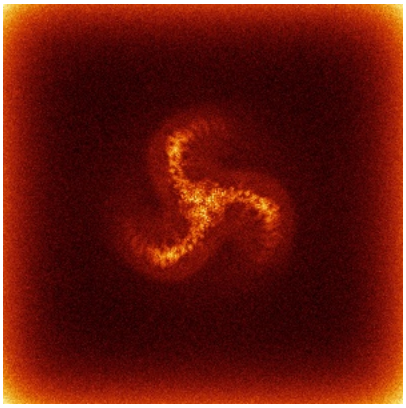
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

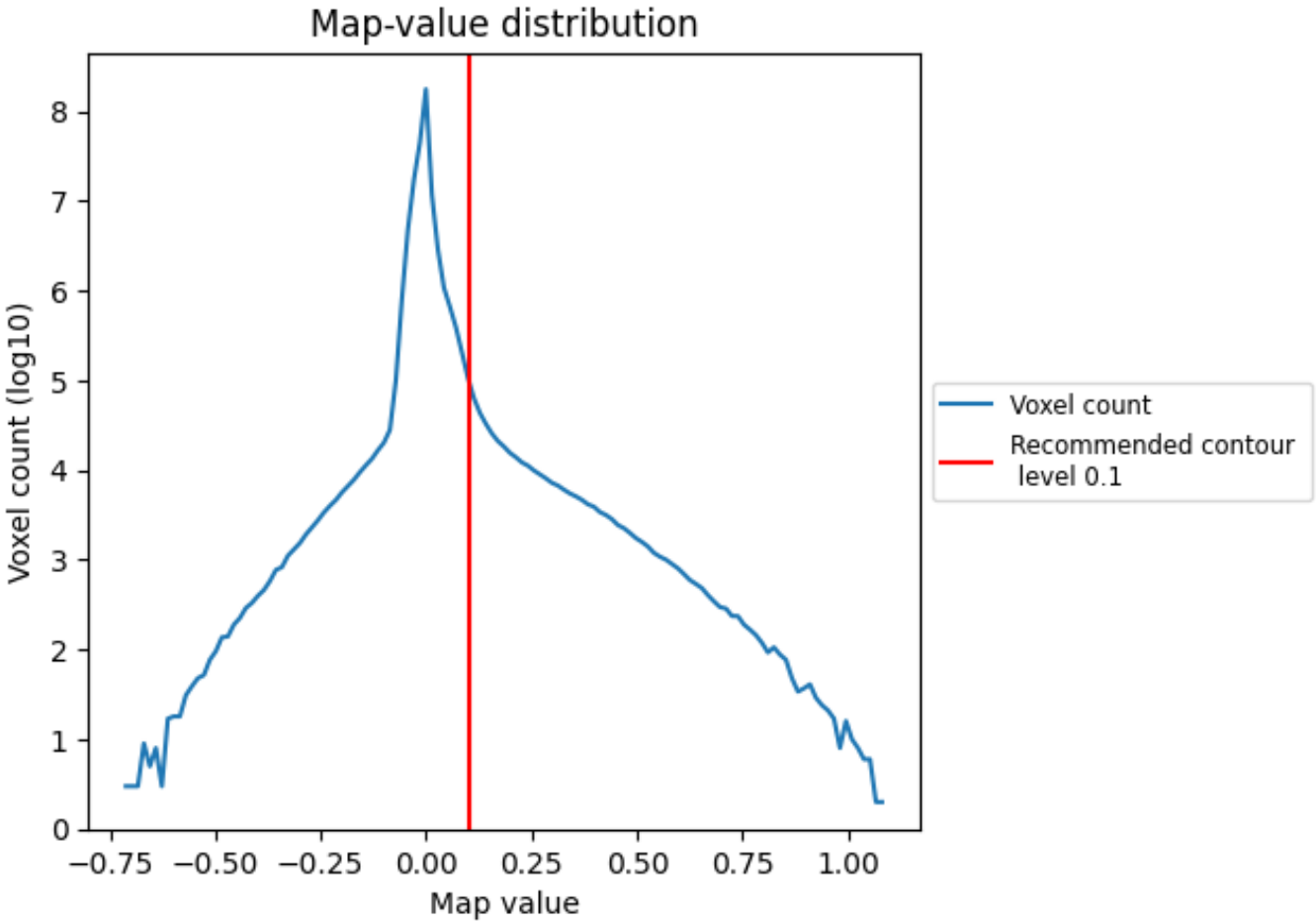
6.6 Mask visualisation (i)

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

7 Map analysis

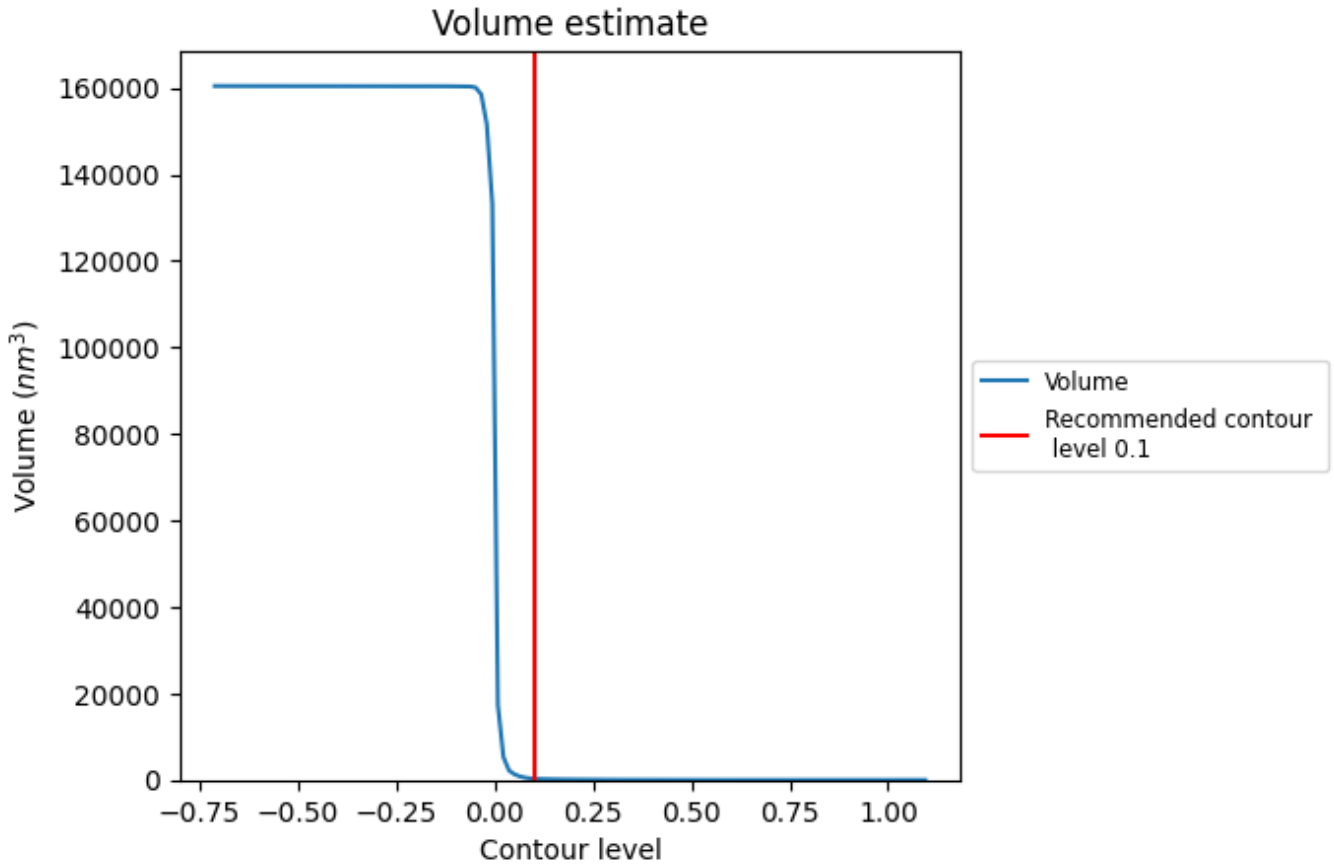
This section contains the results of statistical analysis of the map.

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.

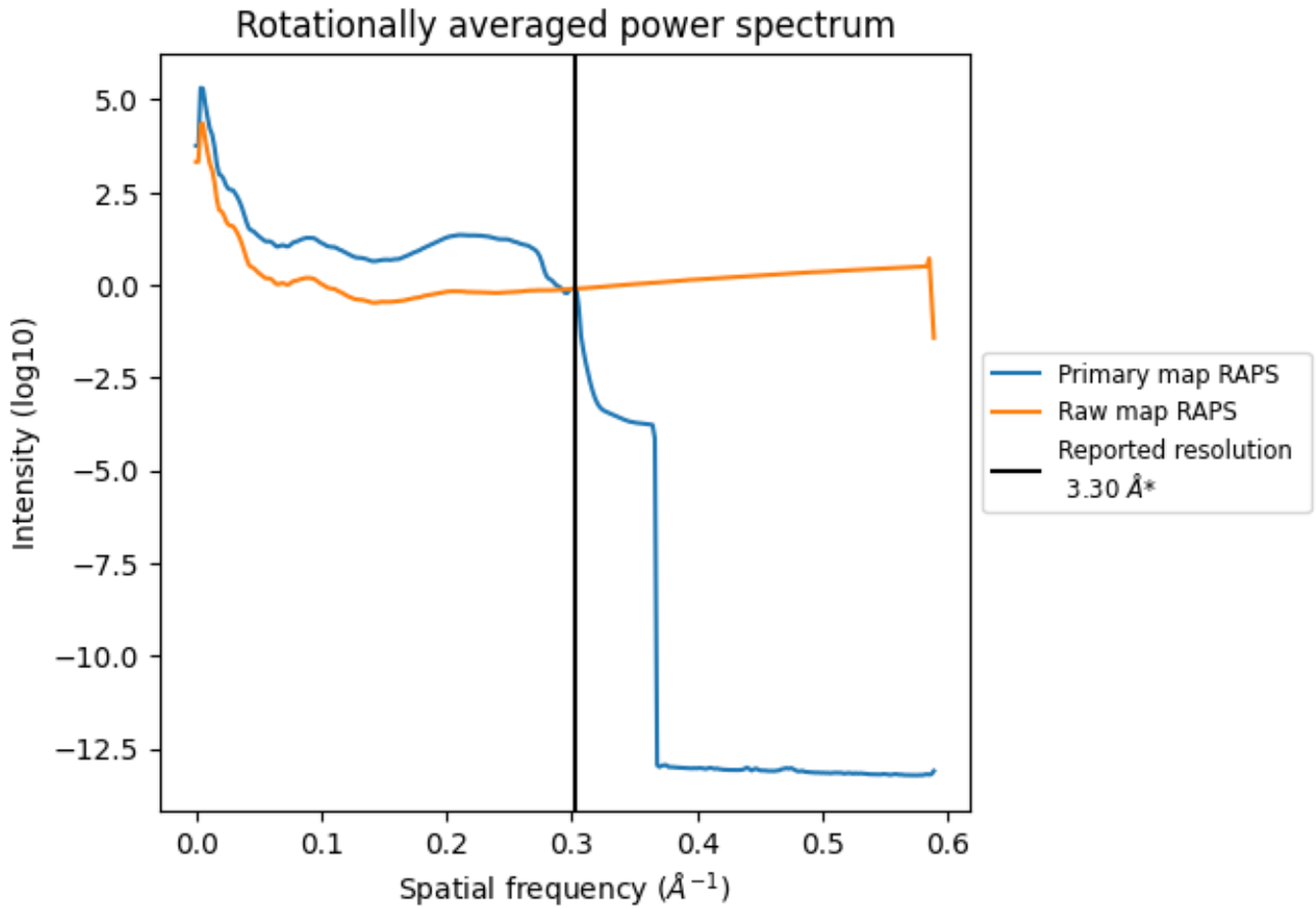
7.2 Volume estimate



The volume at the recommended contour level is 286 nm^3; this corresponds to an approximate mass of 258 kDa.

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

7.3 Rotationally averaged power spectrum (i)

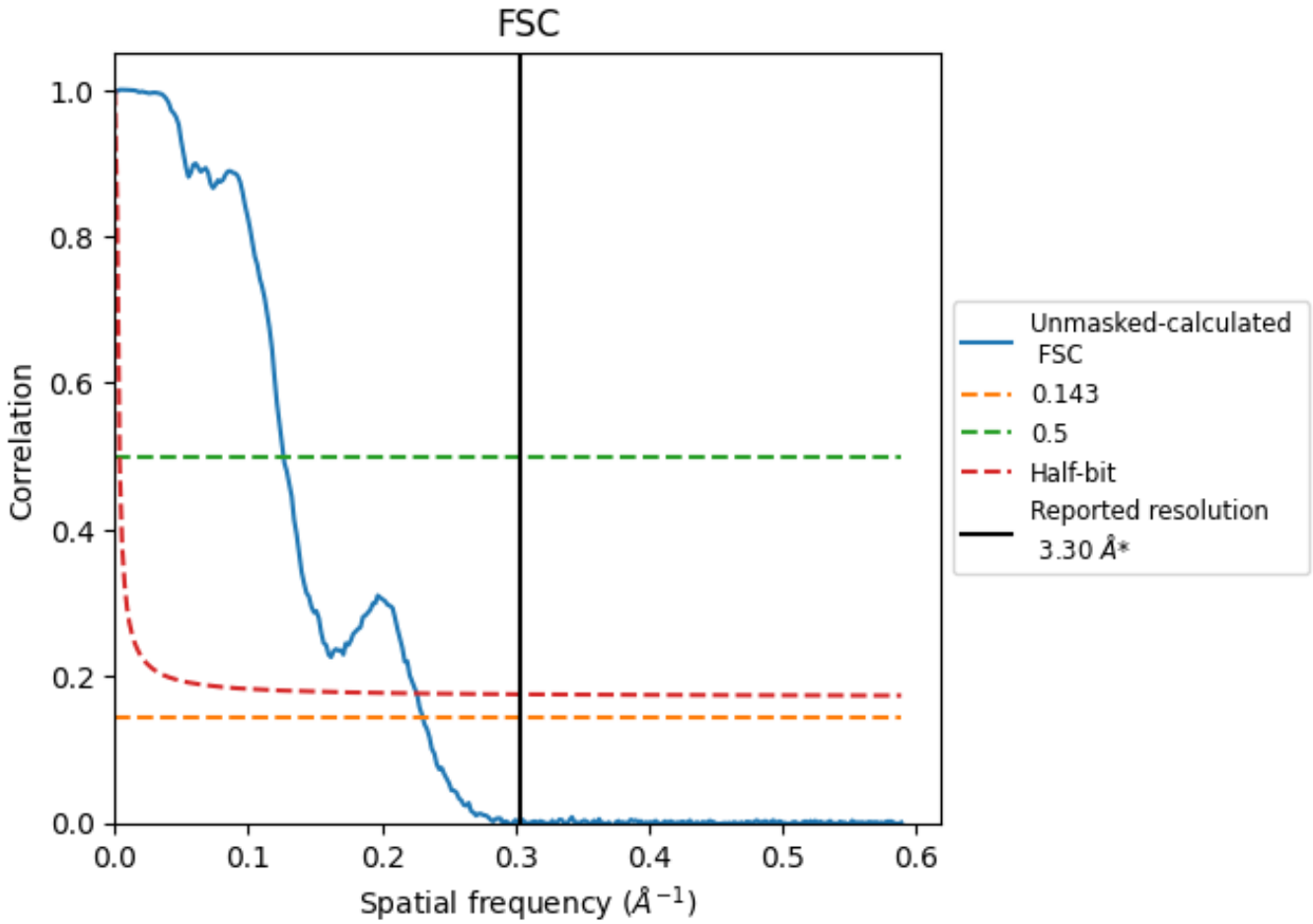


*Reported resolution corresponds to spatial frequency of 0.303 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

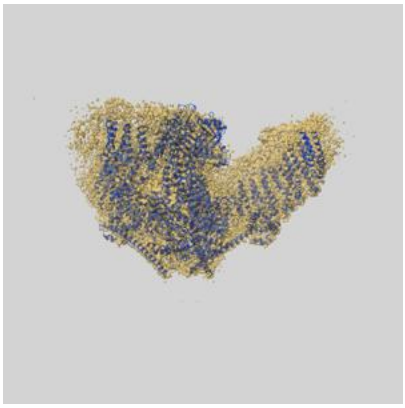
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.34	7.91	4.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.34 differs from the reported value 3.3 by more than 10 %

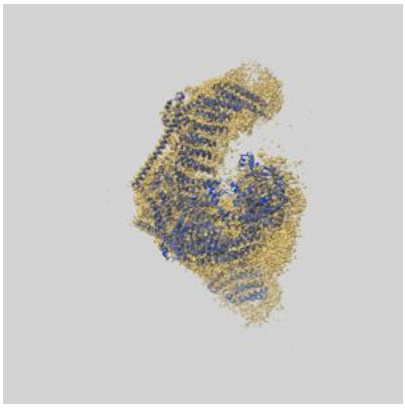
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-39205 and PDB model 8YEZ. Per-residue inclusion information can be found in section 3 on page 5.

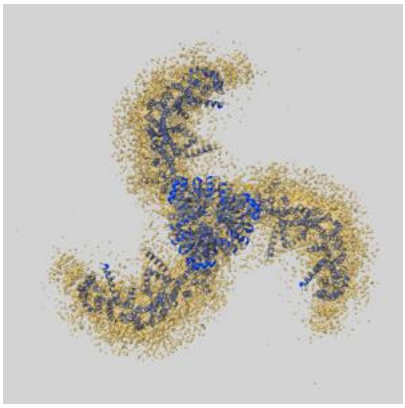
9.1 Map-model overlay



X



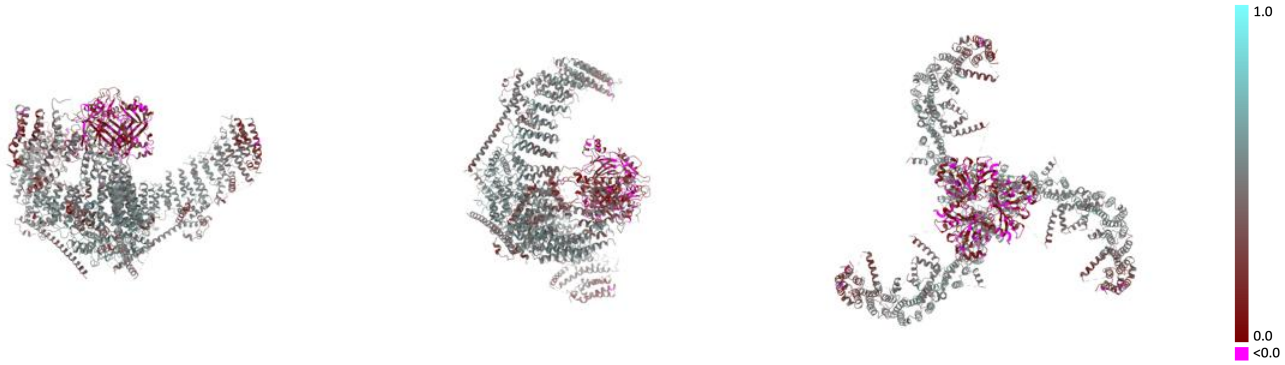
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

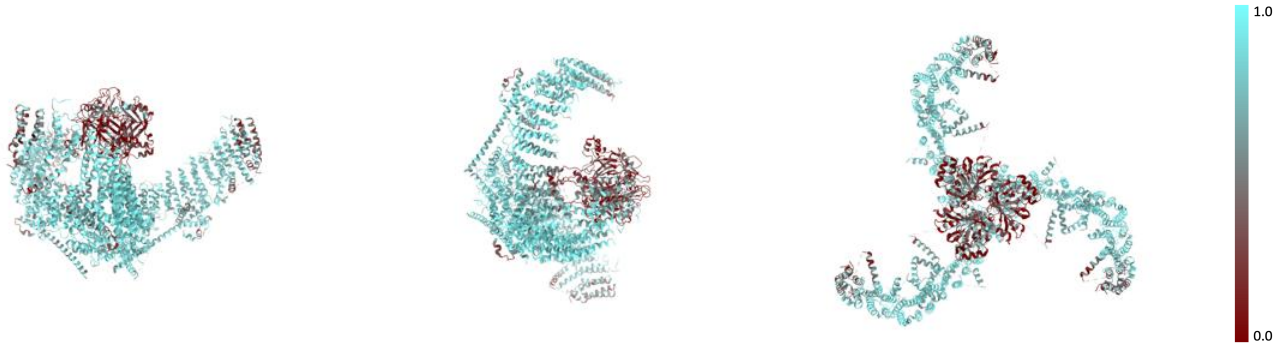
9.2 Q-score mapped to coordinate model (i)



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.

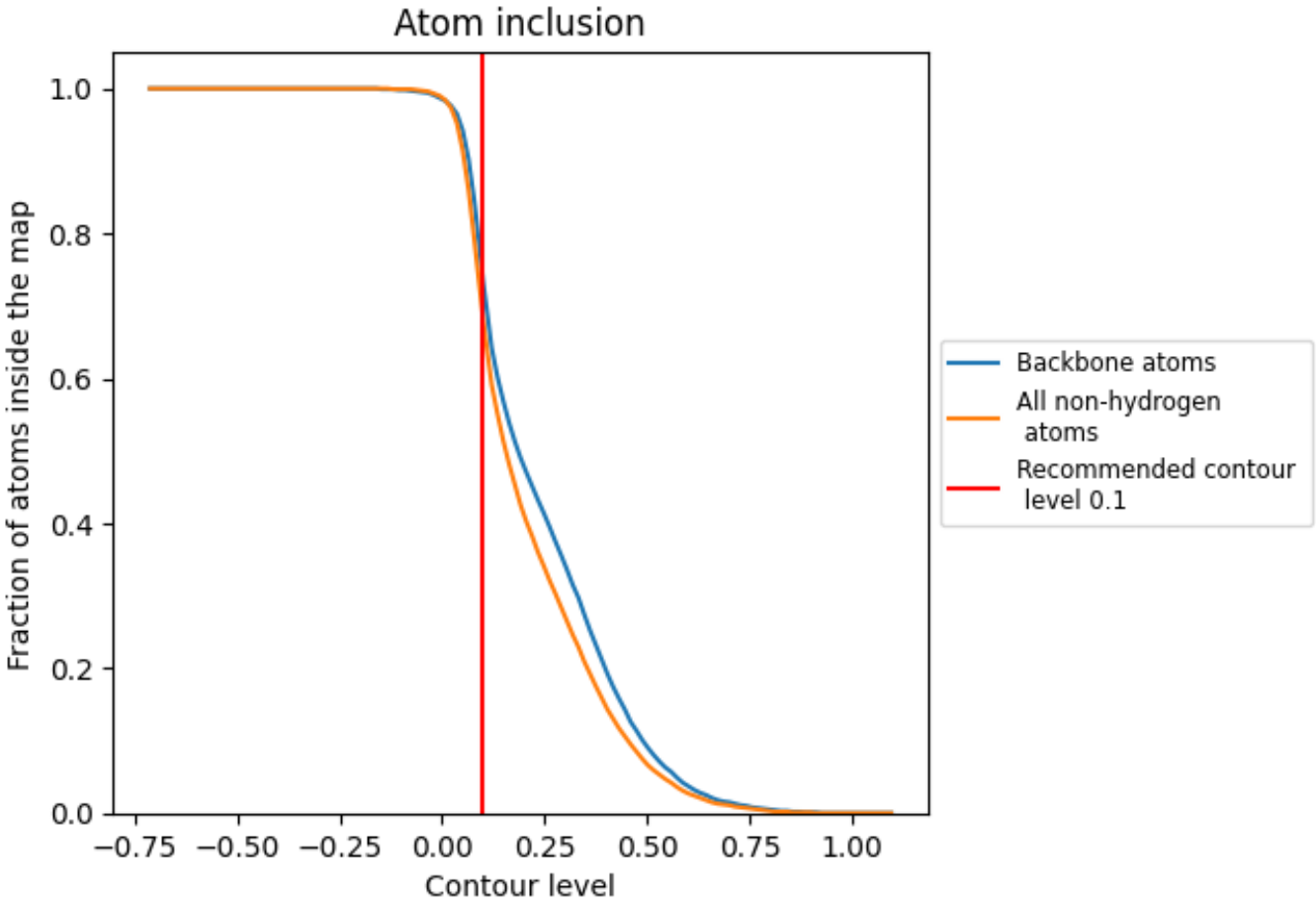
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 68% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6810	0.4010
A	0.6800	0.4000
B	0.6810	0.4010
C	0.6840	0.4010