



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 06:26 PM UTC

PDB ID : 1O1A / pdb_00001o1a
EMDB ID : EMD-1001
Title : MOLECULAR MODELS OF AVERAGED RIGOR CROSSBRIDGES FROM
TOMOGRAMS OF INSECT FLIGHT MUSCLE
Authors : Chen, L.F.; Winkler, H.; Reedy, M.K.; Reedy, M.C.; Taylor, K.A.
Deposited on : 2002-11-18
Resolution : 70.00 Å (reported)
Based on initial models : 1ATN, 2MYS

This is a wwPDB EM Validation Summary 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

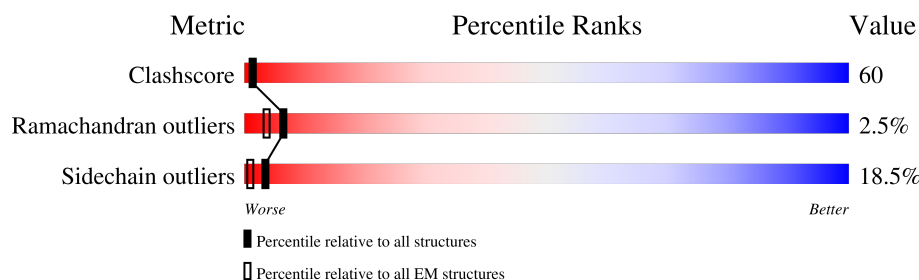
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 70.00 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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 $\leq 5\%$. 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	840	100% 25% 49% 22% .
1	D	840	100% 26% 48% 22% .
1	G	840	100% 24% 49% 22% 5%
1	J	840	100% 24% 50% 22% .
1	M	840	100% 25% 49% 22% .
1	P	840	100% 25% 49% 22% .
2	B	145	100% 67% 23% 6% .
2	E	145	100% 64% 26% 8% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	145	100% 61% 30% 6% .
2	K	145	100% 63% 26% 7% .
2	N	145	100% 64% 27% 6% .
2	Q	145	100% 63% 27% 6% .
3	C	147	100% 61% 36% .
3	F	147	100% 63% 33% .
3	I	147	93% 63% 34% .
3	L	147	100% 63% 33% .
3	O	147	100% 63% 33% .
3	R	147	100% 61% 35% .
4	1	375	99% 50% 36% 11% ..
4	2	375	99% 54% 35% 9% ..
4	3	375	99% 53% 36% 9% ..
4	4	375	99% 54% 34% 9% ..
4	5	375	99% 55% 34% 9% ..
4	6	375	99% 55% 33% 9% ..
4	7	375	99% 57% 32% 9% ..
4	8	375	99% 52% 33% 12% ..
4	9	375	99% 51% 35% 12% ..
4	V	375	99% 49% 35% 13% ..
4	W	375	99% 50% 35% 13% ..
4	X	375	99% 54% 33% 10% ..
4	Y	375	94% 54% 34% 9% ..
4	Z	375	99% 50% 35% 11% ..

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	MLY	A	505	-	-	X	-
1	MLY	A	553	-	-	X	-
1	MLY	A	764	-	-	X	-
1	MLY	A	837	-	-	X	-
1	MLY	A	839	-	-	X	-
1	MLY	D	553	-	-	X	-
1	MLY	D	764	-	-	X	-
1	MLY	D	782	-	-	X	-
1	MLY	G	505	-	-	X	-
1	MLY	G	553	-	-	X	-
1	MLY	G	764	-	-	X	-
1	MLY	G	84	-	-	X	-
1	MLY	J	505	-	-	X	-
1	MLY	J	553	-	-	X	-
1	MLY	J	839	-	-	X	-
1	MLY	J	84	-	-	X	-
1	MLY	M	839	-	-	X	-
1	MLY	P	839	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 94966 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 SKELETAL MUSCLE MYOSIN II.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	D	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	G	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	J	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	M	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		
1	P	840	Total	C	N	O	S	0	0
			6797	4382	1135	1243	37		

- Molecule 2 is a protein called SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	E	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	H	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	K	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	N	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		
2	Q	145	Total	C	N	O	S	0	0
			1127	717	177	227	6		

- Molecule 3 is a protein called SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	F	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	I	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	L	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	O	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		
3	R	147	Total	C	N	O	S	0	0
			1123	698	188	230	7		

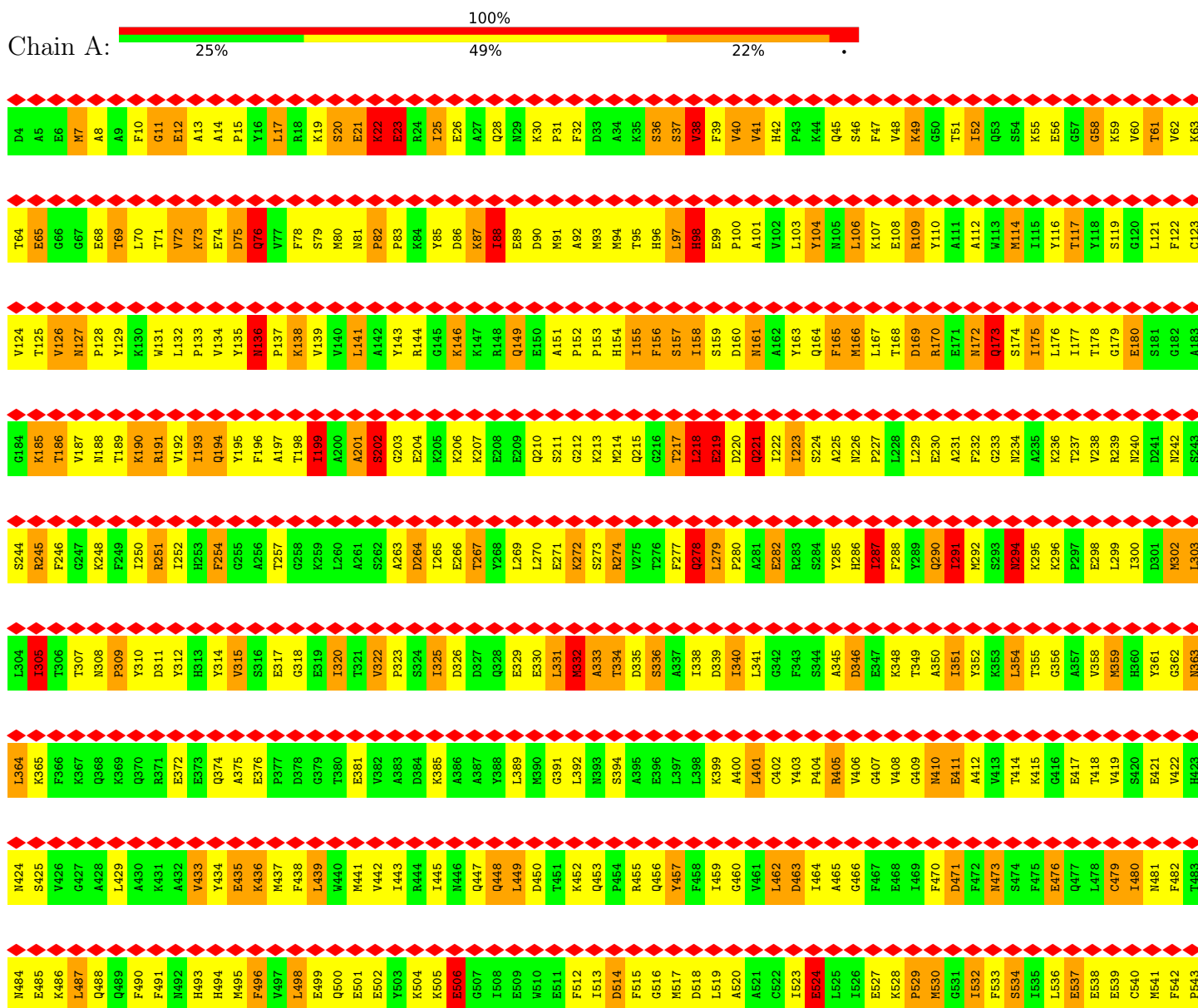
- Molecule 4 is a protein called SKELETAL MUSCLE ACTIN.

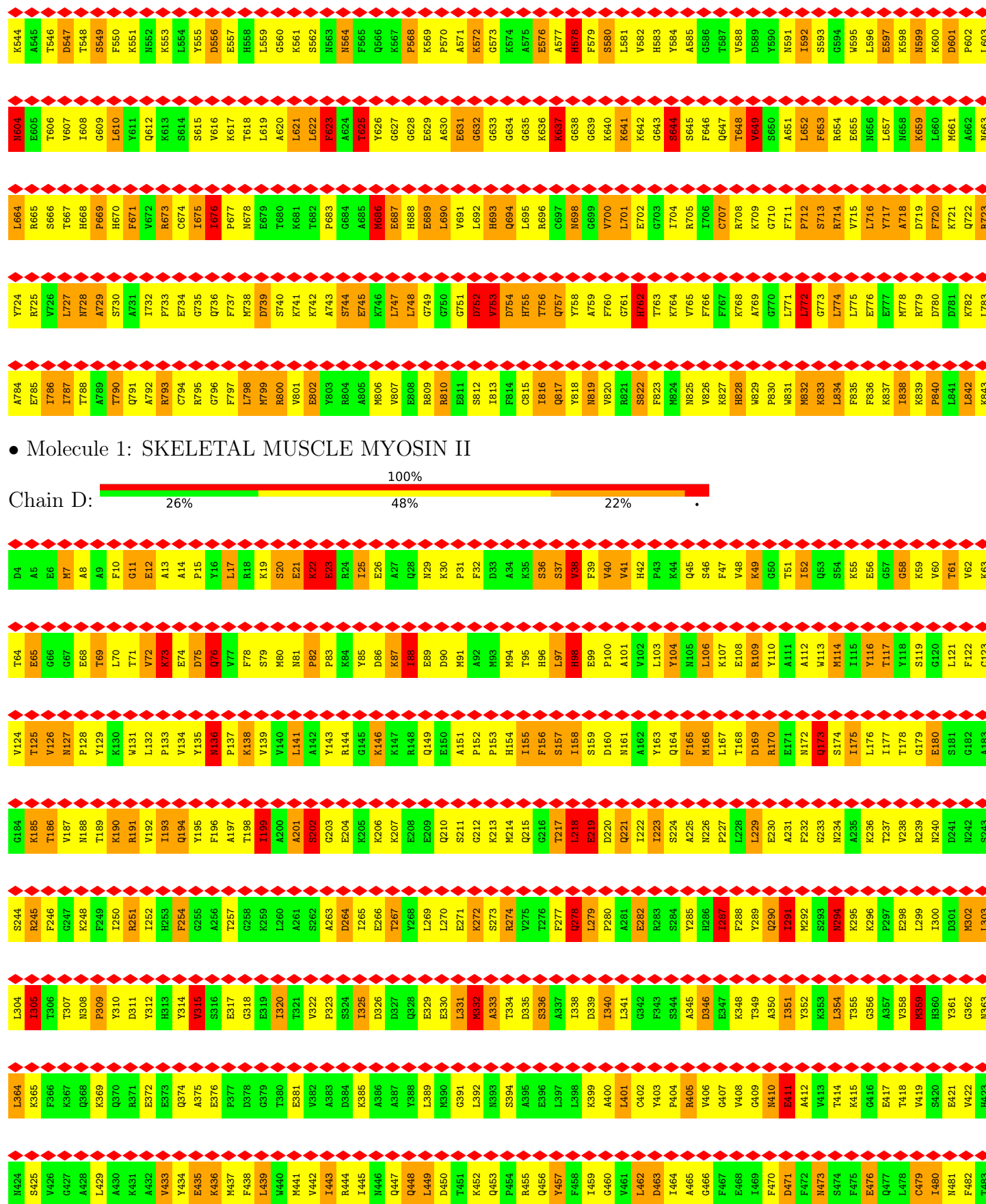
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	2	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	3	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	4	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	5	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	6	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	7	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	8	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	9	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	V	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	W	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	X	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Y	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		
4	Z	372	Total	C	N	O	S	0	0
			2906	1836	489	561	20		

3 Residue-property plots

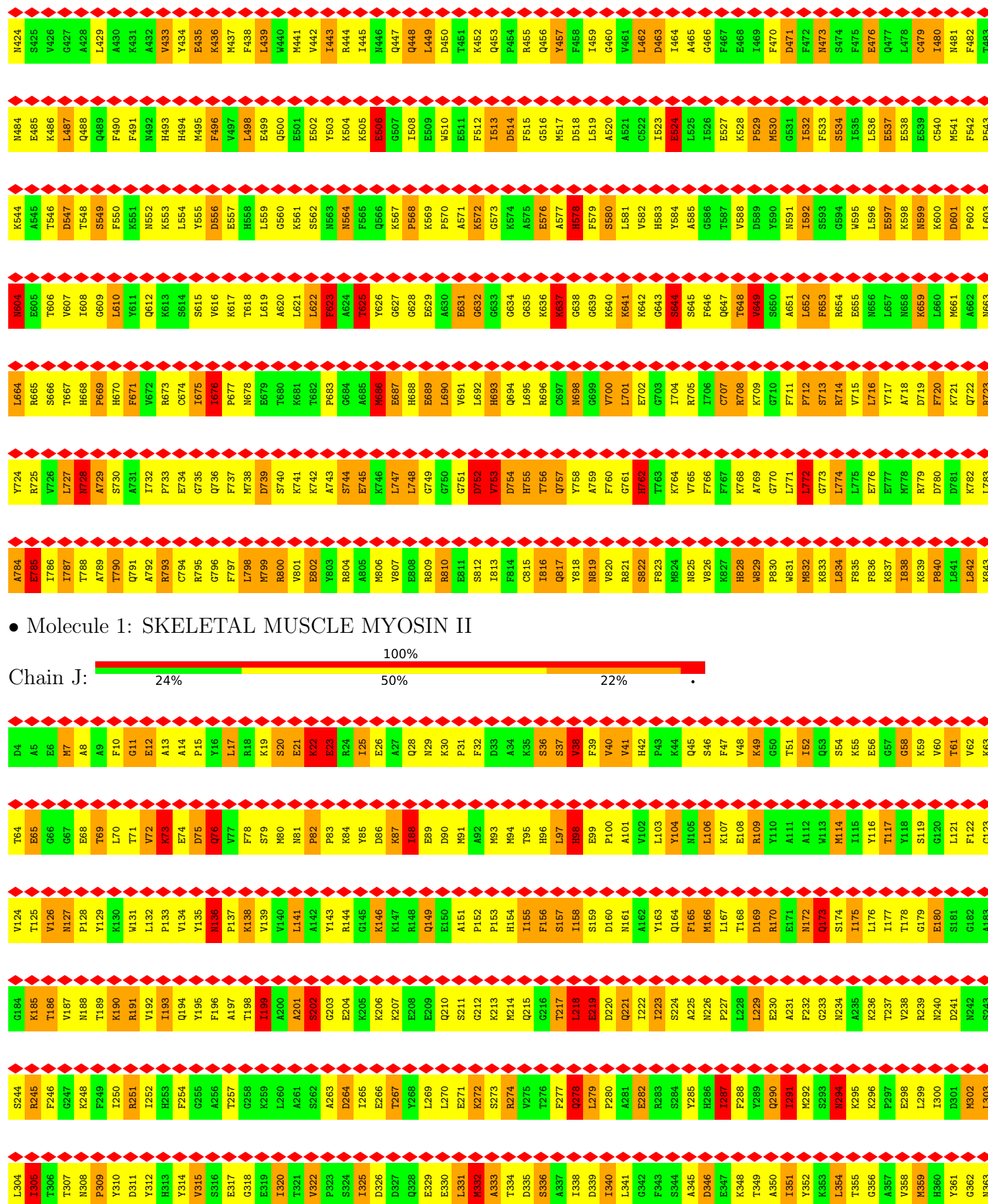
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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









A784	L784	Y724	L664	M604	K544	N484	N424	L364
R785	K365	R725	R665	E505	A545	E485	S425	K365
I786	F366	V726	T666	T606	T546	K486	V426	F366
T787	G667	L727	T667	V607	D547	L487	G427	K367
T788	H668	M728	H668	I608	T548	Q488	A428	Q368
A789	P669	A729	P669	G609	S549	Q489	L429	K369
T790	H670	S730	H670	L610	F550	F490	L429	Q370
Q791	F671	A731	F671	V611	K551	F491	K431	R371
A792	V672	I732	V672	Q612	N552	N492	A432	E372
R793	R673	P733	R673	K613	K553	H493	V433	E373
C794	E734	E734	C674	S614	L554	H494	Y434	Q374
R795	I675	G735	I675	S615	T555	M495	E435	A375
G796	T676	Q736	T676	V616	D556	F496	K436	E376
F797	P677	F737	P677	K617	E557	V497	M437	P377
L798	N678	M738	N678	T618	H558	L498	F438	D378
M799	E679	D739	E679	L619	L559	E499	L439	G379
R800	T680	S740	T680	A620	G560	Q500	L439	D379
V801	K681	K741	K681	L621	K561	E501	M441	T380
E802	T682	K742	T682	L622	S562	E502	V442	E381
Y803	P683	A743	P683	F623	N563	T503	I443	V382
R804	S744	S744	G684	A624	N564	K504	R444	A383
A805	A685	E745	A685	T625	F565	K505	I445	K385
M806	K746	K746	M686	V626	Q566	E506	M446	A386
V807	L747	L747	E687	G627	K567	G507	Q447	A387
E808	L748	H688	L748	P628	P568	I508	Q448	Y388
R809	E689	G749	E689	E629	K569	E509	L449	L389
R810	L690	G750	R810	A630	P570	W510	D450	M390
E811	V691	G751	V691	E631	A571	E511	T451	G391
S812	D752	D752	L692	G632	K572	F512	K452	L392
I813	H693	V753	H693	G633	G573	T513	Q453	N393
F814	D754	D754	Q694	G634	K574	D514	P454	S394
C815	H755	H755	L695	G635	A575	F515	R455	A395
L816	T756	T756	R696	K636	E576	G516	Q456	E396
Q817	G697	Q757	G697	K637	A577	M517	Y457	L397
Y818	N698	Y758	N698	G638	H578	D518	F458	L398
M819	A759	A759	G699	G639	F579	L519	I459	K399
V820	F760	F760	W700	K640	S580	A520	G460	A400
R821	L701	G761	L701	K641	L581	A521	V461	L401
S822	E702	H762	E702	K642	V582	C522	L462	C402
F823	G703	T763	G703	G643	H583	I523	D463	Y403
M824	K764	K764	T704	S644	Y584	E524	I464	P404
N825	V765	V765	R705	S645	A585	L525	A465	R405
V826	F766	F766	I706	F646	G586	I526	G466	V406
K827	C707	F767	C707	Q647	T587	E527	F467	G407
H828	K768	K768	R708	T648	V588	K528	E468	V408
W829	A769	A769	K709	V649	D589	P529	I469	G409
P830	G770	G770	G710	S650	Y590	M530	G470	N410
W831	F711	L771	F711	A651	N591	G531	D471	E411
M832	L772	L772	P712	L652	I592	I532	F472	A412
K833	G773	G773	S713	F653	S593	F533	M473	V413
L834	L774	L774	R714	R654	G594	S534	S474	T414
F835	L775	L775	V715	E655	N595	I535	F475	K415
F836	E776	E776	L716	M656	L596	L536	E476	G416
K837	E777	E777	Y717	L657	E597	E537	Q477	E417
I838	M778	M778	A718	M658	K598	E538	L478	T418
K839	R779	R779	D719	K659	N599	E539	C479	V419
P840	F720	D780	F720	L660	K600	C540	I480	S420
L841	K721	L781	K721	M661	D601	M541	M481	E421
L842	Q722	K782	Q722	A662	P602	F542	F482	V422
R843	R723	L783	R723	N663	L603	P543	T483	H423

• Molecule 1: SKELETAL MUSCLE MYOSIN II



S244	R245	F246	G247	K248	F249	L250	R251	L252	H253	F254	G255	A256	T257	G258	K259	L260	A261	S262	A263	D264	L265	E266	T267	Y268	L269	L270	E271	K272	S273	R274	V275	T276	F277	Q278	L279	P280	A281	E282	R283	S284	Y285	H286	F287	F288	Y289	Q290	I291	M292	S293	N294	K295	K296	P297	E298	L299	I300	D301	M302	L303
G184	K185	T186	V187	N188	T189	K190	R191	V192	I193	Q194	Y195	F196	A197	T198	I199	A200	A201	S202	G203	E204	K205	K206	K207	E208	E209	Q210	S211	G212	K213	M214	Q215	G216	T217	L218	E219	D220	Q221	I222	I223	S224	A225	N226	P227	L228	L229	E230	A231	F232	G233	N234	A235	K236	T237	V238	R239	N240	D241	K242	L243
V124	T125	V126	N127	N128	Y129	K130	V131	L132	P133	V134	Y135	N136	P137	K138	V139	Y140	L141	A142	Y143	R144	G145	K146	K147	R148	Q149	E150	A151	P152	P153	H154	I155	F156	S157	I158	S159	D160	N161	A162	Y163	Q164	F165	M166	L167	T168	D169	R170	E171	N172	Q173	S174	T175	L176	I177	T178	G179	E180	S181	G182	A183
T64	E65	G66	G67	E68	T69	L70	T71	V72	K73	E74	D75	Q76	V77	F78	S79	M80	N81	P82	P83	K84	Y85	D86	K87	E88	E89	D90	N91	A92	M93	M94	T95	H96	L97	H98	E99	P100	A101	V102	L103	Y104	N105	L106	K107	E108	R109	Y110	A111	A112	V113	M114	I115	Y116	T117	Y118	S119	G120	L121	F122	C123
D4	A5	E6	M7	A8	A9	F10	G11	E12	A13	A14	P15	Y16	L17	R18	K19	S20	E21	K22	E23	K24	I25	E26	Q27	K28	N29	K30	P31	F32	D33	A34	K35	S36	S37	V38	F39	V40	V41	H42	P43	K44	Q45	S46	F47	V48	G49	T50	T51	I52	Q53	S54	K55	E56	G57	G58	K59	V60	T61	V62	K63

● Molecule 1: SKELETAL MUSCLE MYOSIN II



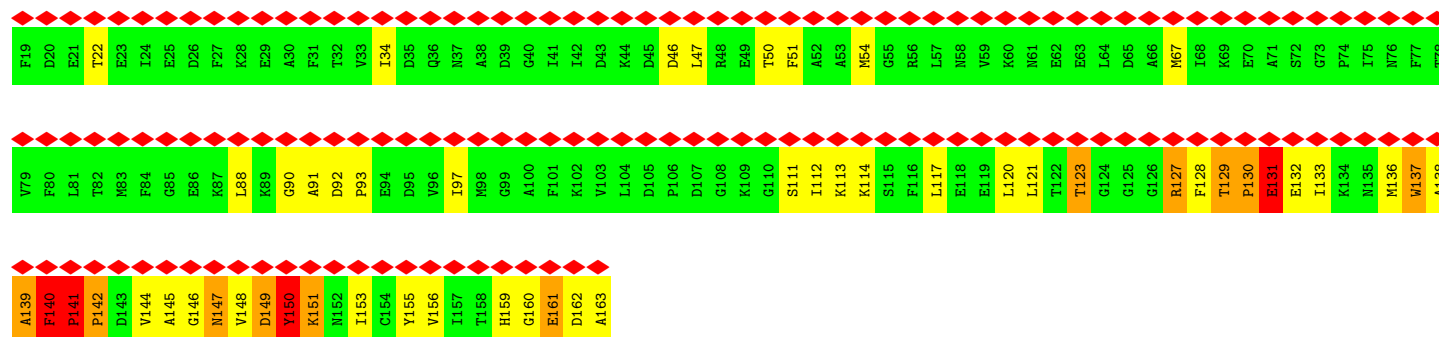
- Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

Device Type	Percentage
Smartphones	100%
Tablets	67%
Smart TVs	23%
Other devices	6%

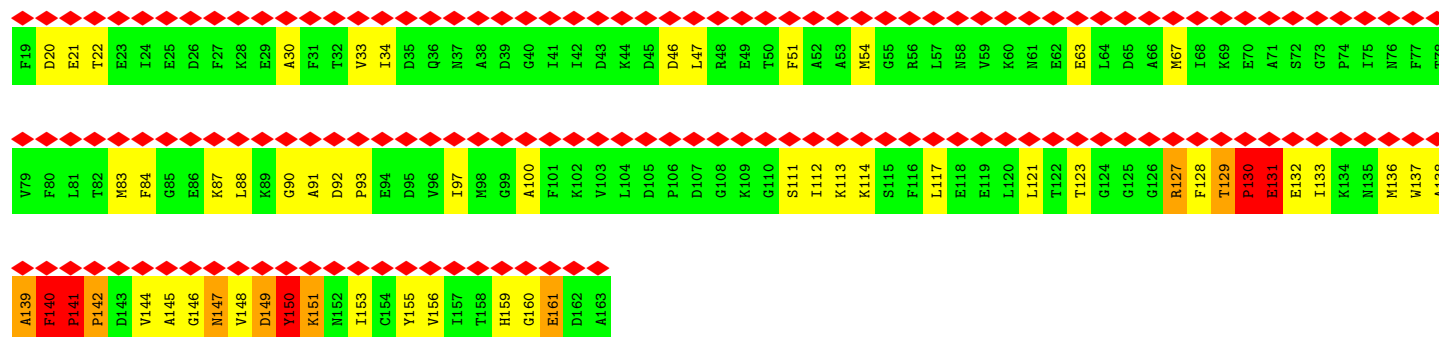


WORLDWIDE
PDB
PROTEIN DATA BANK

• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

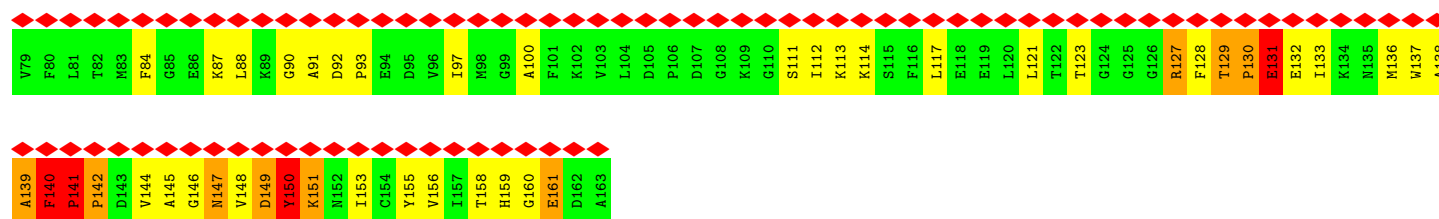


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

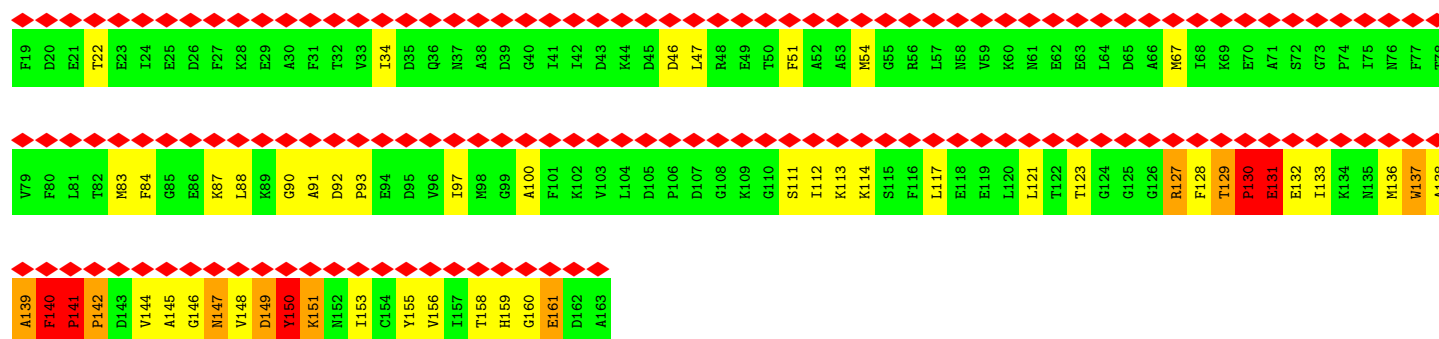


• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN

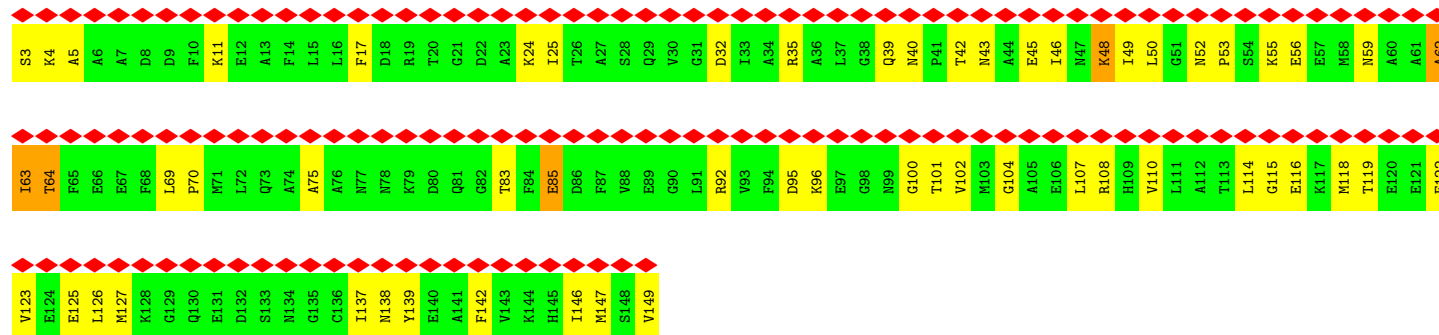




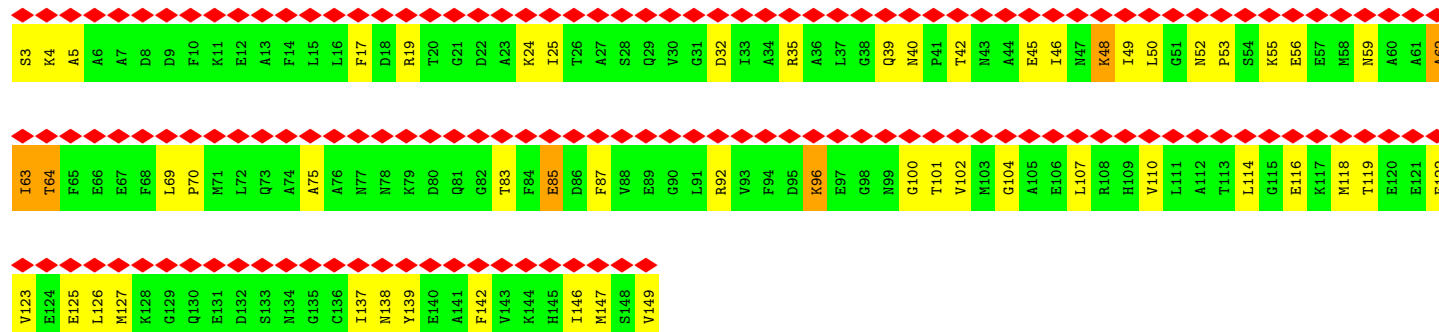
• Molecule 2: SKELETAL MUSCLE MYOSIN II REGULATORY LIGHT CHAIN



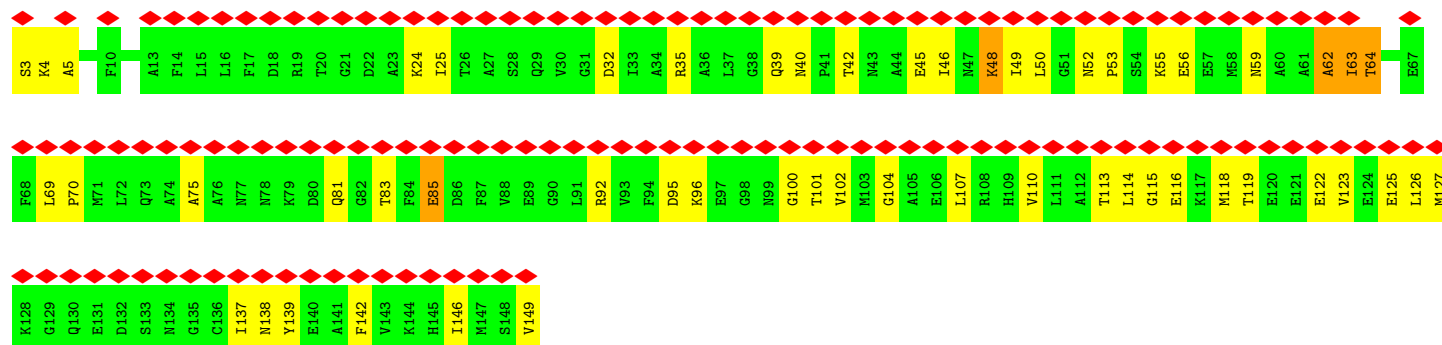
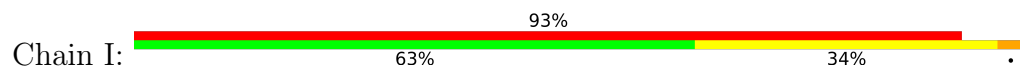
• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



• Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



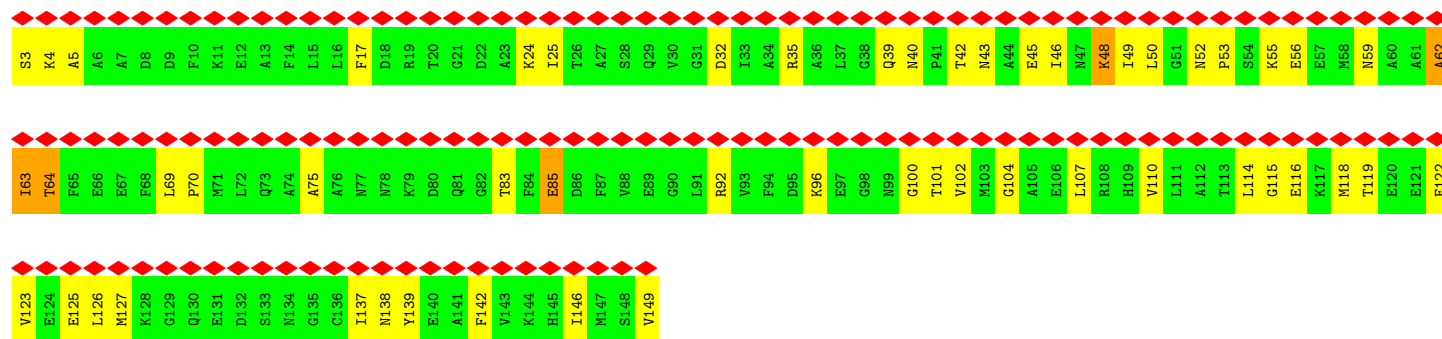
- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN



- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

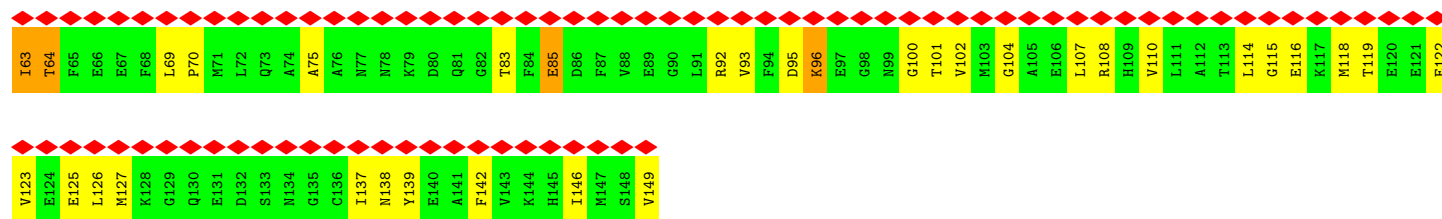


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

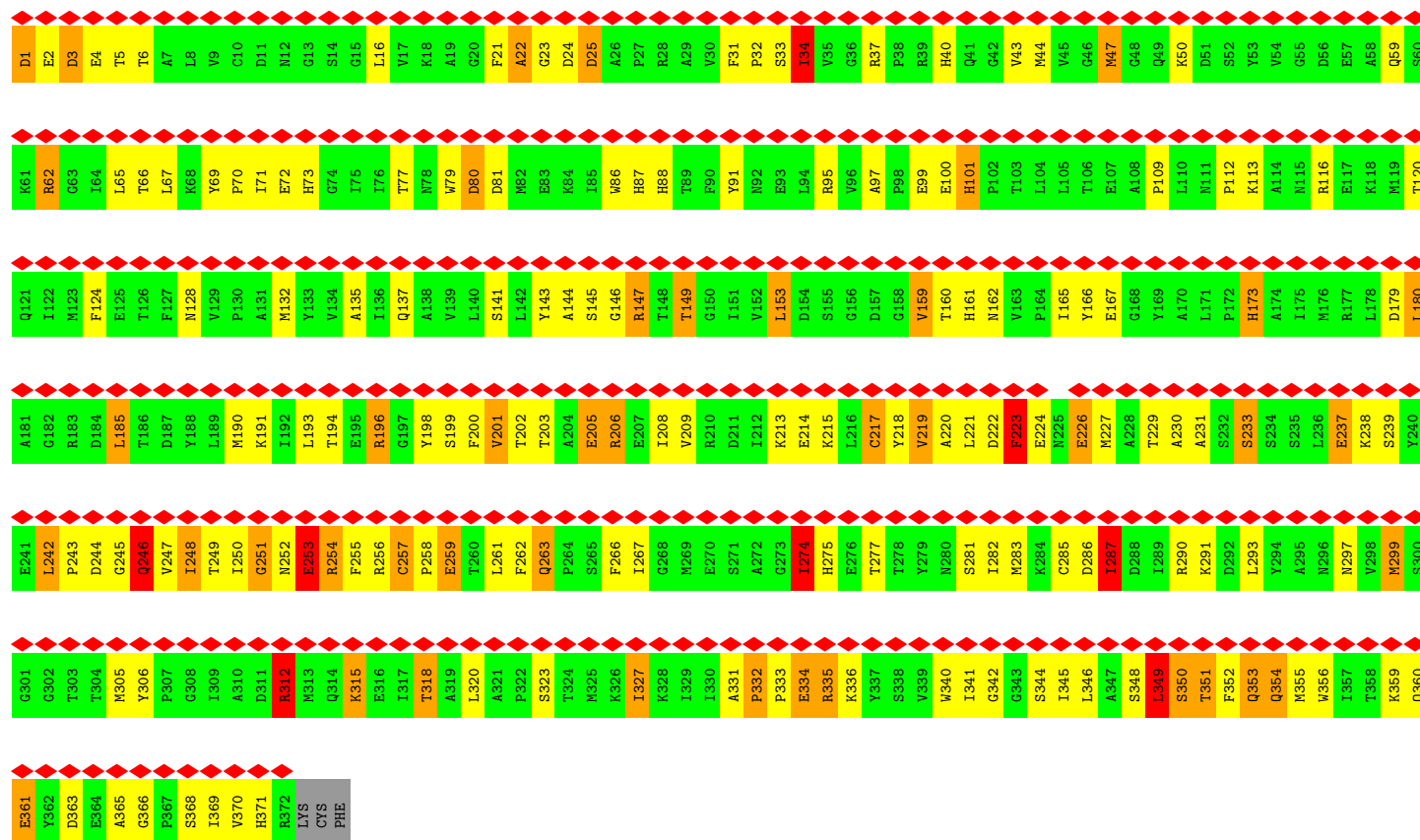


- Molecule 3: SKELETAL MUSCLE MYOSIN II ESSENTIAL LIGHT CHAIN

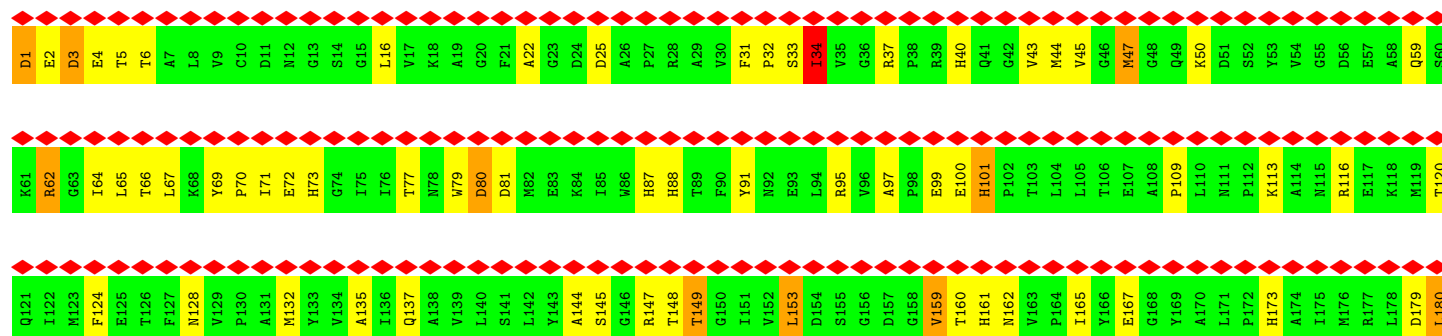


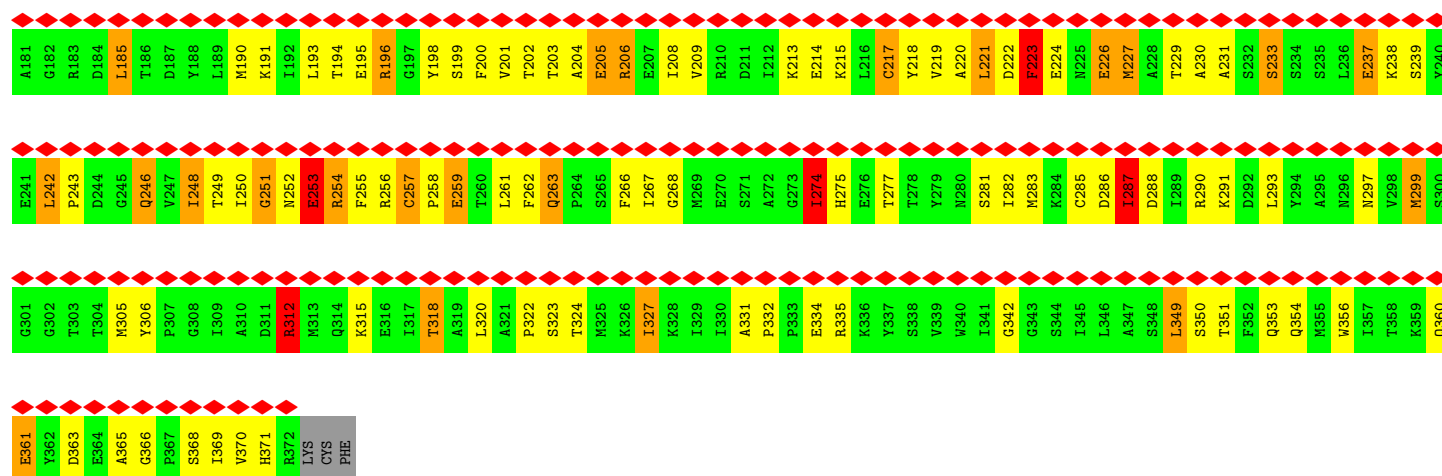


• Molecule 4: SKELETAL MUSCLE ACTIN

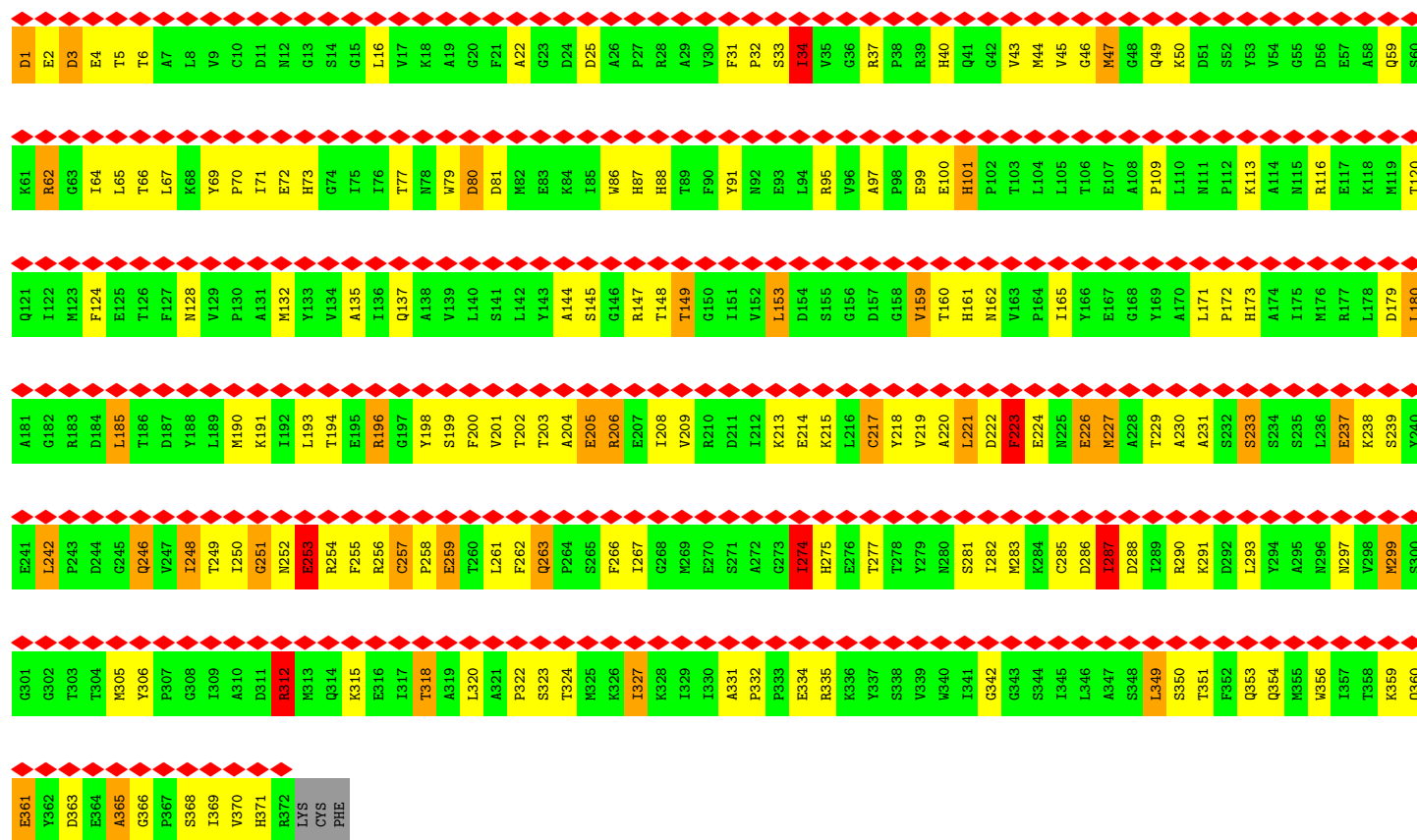


• Molecule 4: SKELETAL MUSCLE ACTIN

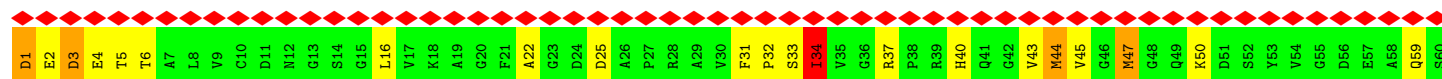


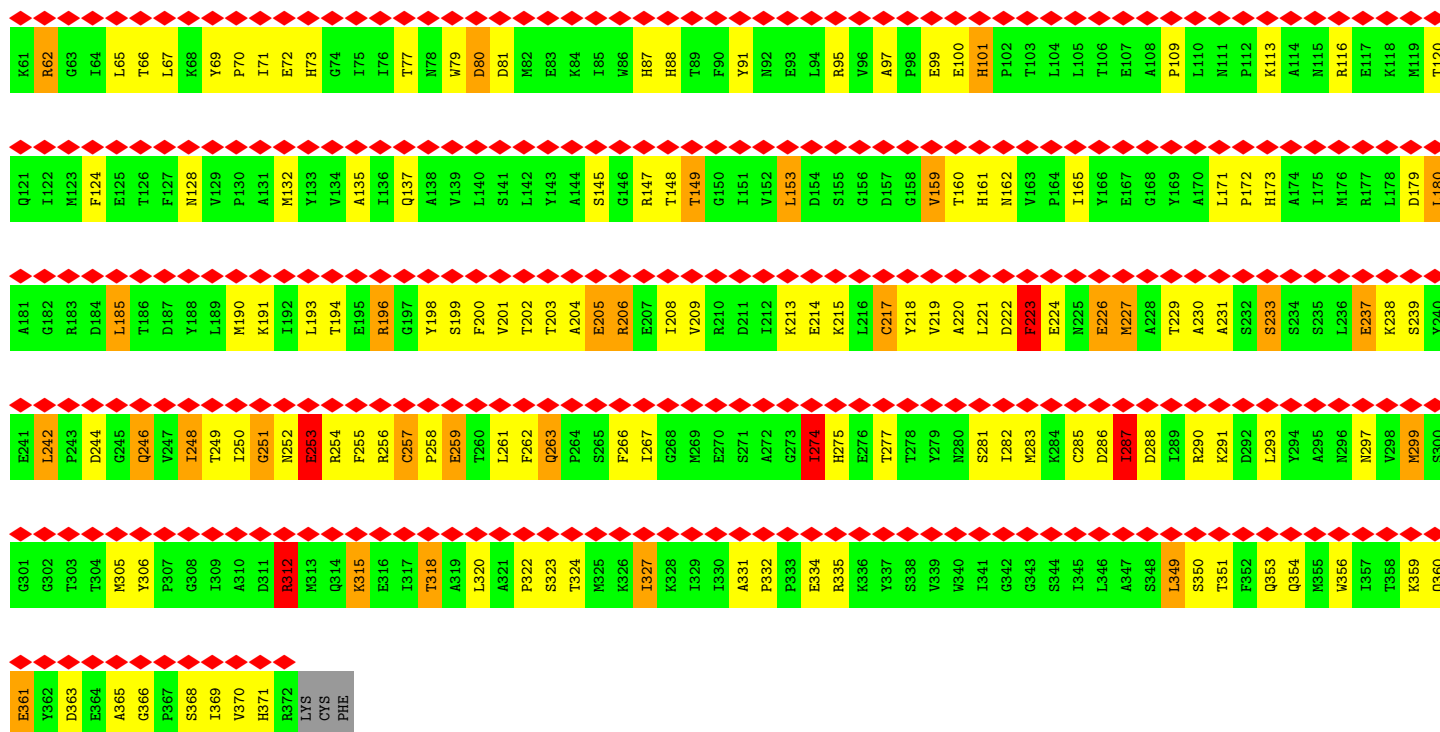


• Molecule 4: SKELETAL MUSCLE ACTIN

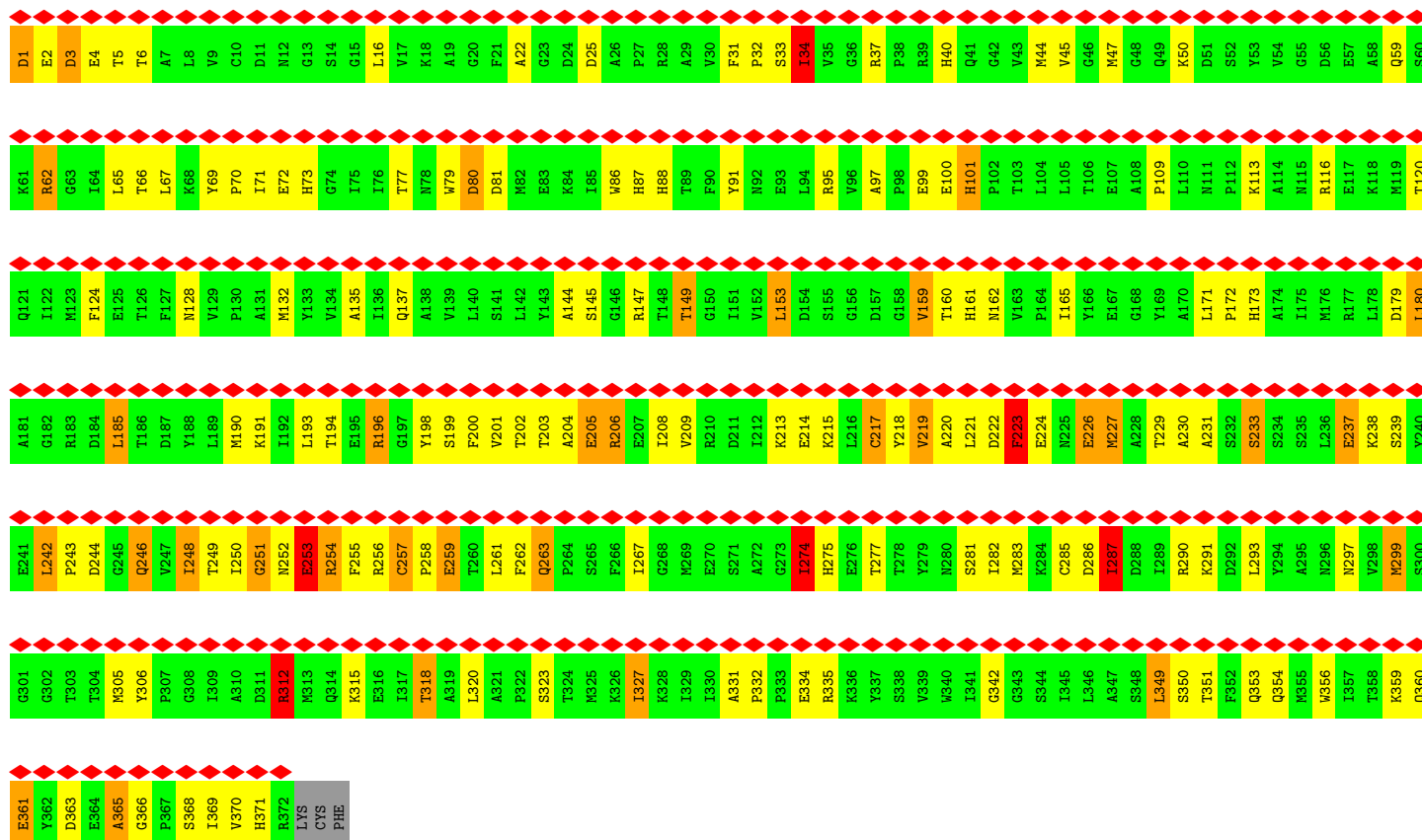


• Molecule 4: SKELETAL MUSCLE ACTIN

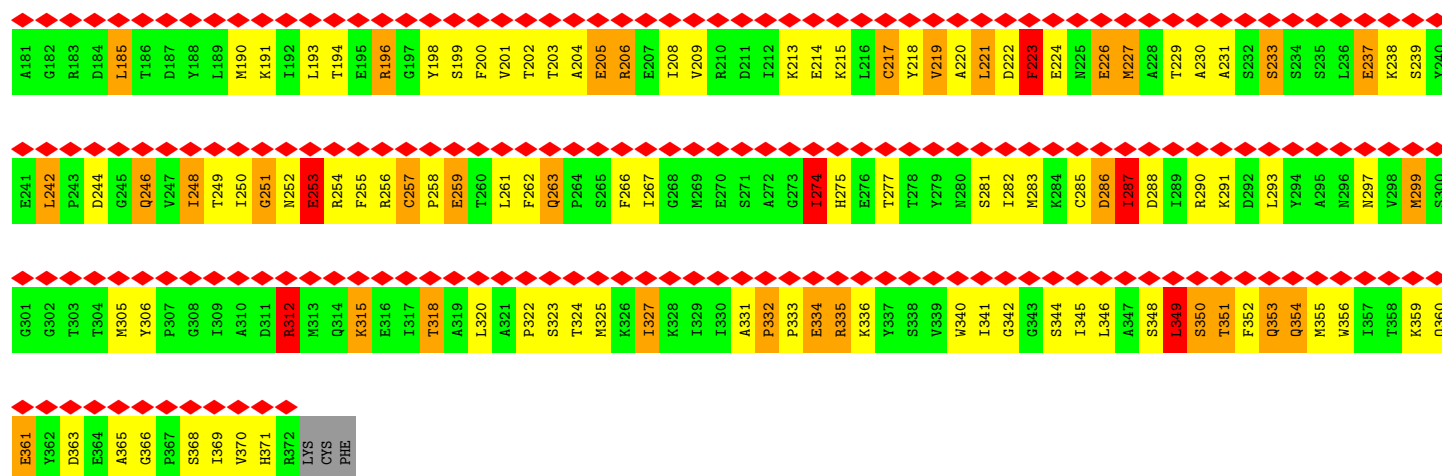




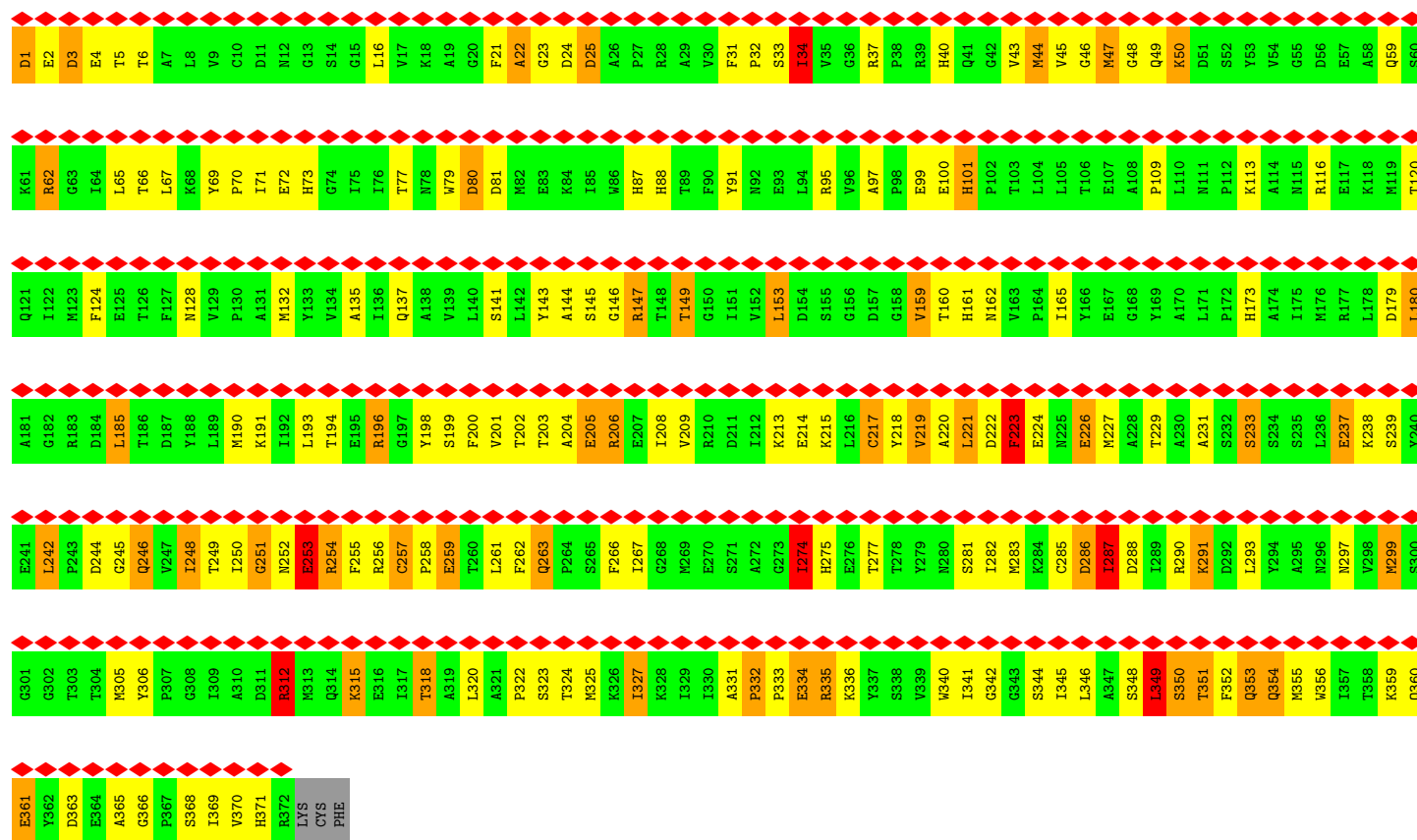
● Molecule 4: SKELETAL MUSCLE ACTIN



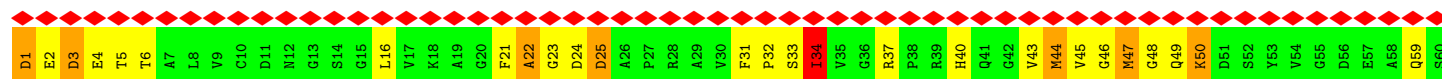




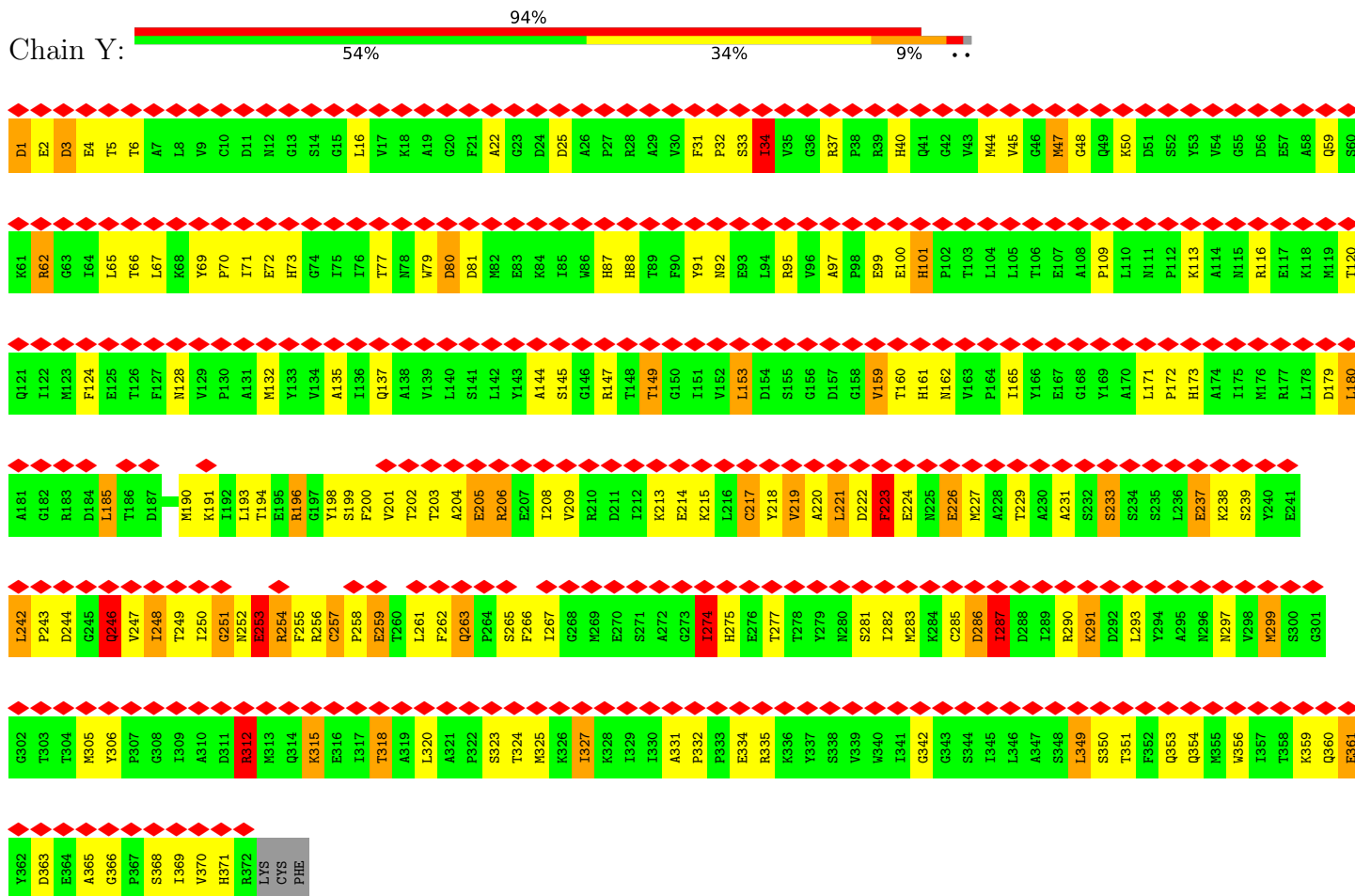
• Molecule 4: SKELETAL MUSCLE ACTIN



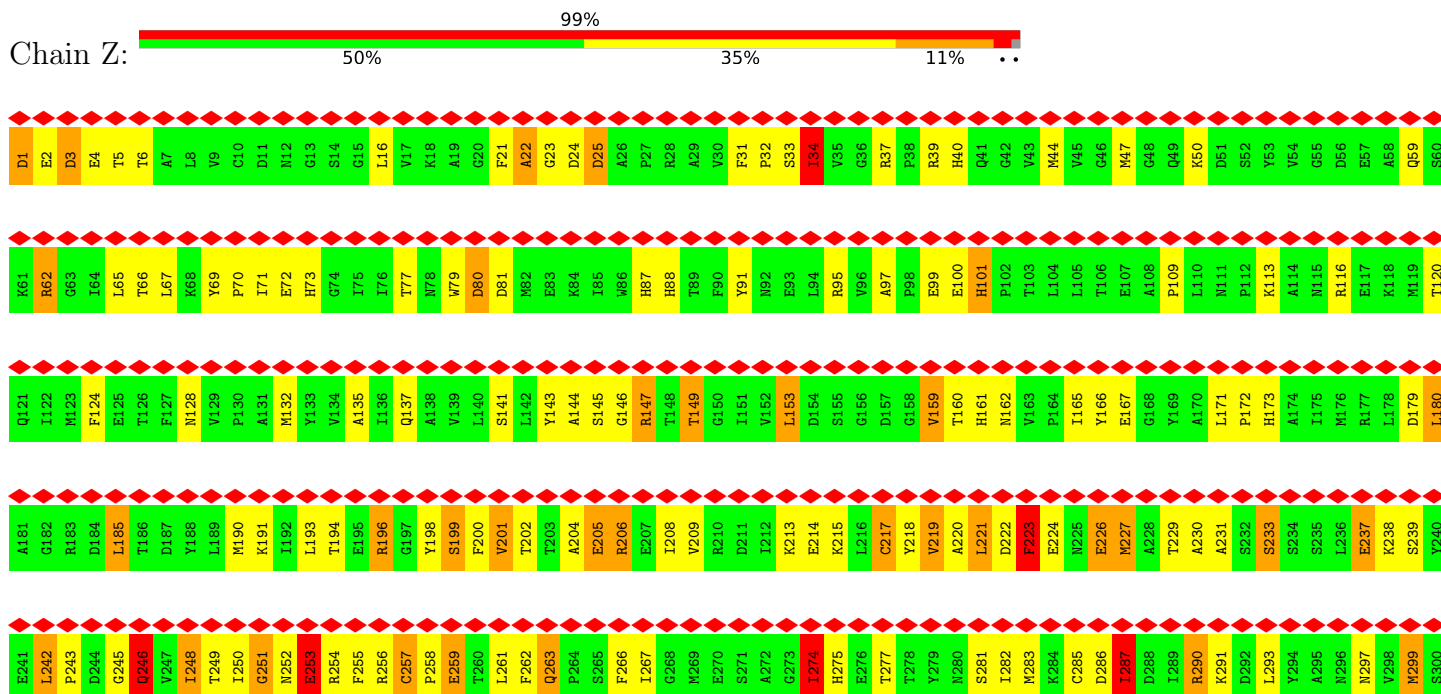
• Molecule 4: SKELETAL MUSCLE ACTIN



Chain Y:



Chain Z:



E361	G301
Y362	G302
D363	T303
E364	T304
A365	M305
G366	Y306
P367	P307
S368	G308
T369	T309
V370	A310
H371	D311
R372	B312
LYS	M313
CYS	Q314
PHE	K315
	E316
	I317
	T318
	A319
	L320
	A321
	P322
	S323
	T324
	M325
	K326
	I327
	K328
	I329
	T330
	A331
	P332
	P333
	E334
	R335
	K336
	Y337
	S338
	V339
	V340
	I341
	G342
	G343
	S344
	I345
	L346
	A347
	S348
	L349
	S350
	T351
	F352
	Q353
	Q354
	M355
	V356
	I357
	T358
	K359
	Q360

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI/PHILIPS EM400	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	17000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum voxel value	366.680	Depositor
Minimum voxel value	-417.992	Depositor
Average voxel value	1.860	Depositor
Voxel value standard deviation	47.792	Depositor
Recommended contour level	81.2	Depositor
Tomogram size ($\text{\AA}$)	9280, 9280, 464	wwPDB
Tomogram dimensions	600, 600, 30	wwPDB
Tomogram angles ($^\circ$)	90, 90, 90	wwPDB
Grid spacing ($\text{\AA}$)	15.4667, 15.4667, 15.4667	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.84	40/6448 (0.6%)	2.13	152/8729 (1.7%)
1	D	1.84	41/6448 (0.6%)	2.13	152/8729 (1.7%)
1	G	1.84	42/6449 (0.7%)	2.13	160/8732 (1.8%)
1	J	1.85	40/6449 (0.6%)	2.19	147/8732 (1.7%)
1	M	2.05	43/6447 (0.7%)	2.16	157/8726 (1.8%)
1	P	1.89	41/6447 (0.6%)	2.20	154/8726 (1.8%)
2	B	1.36	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	E	1.35	15/1148 (1.3%)	1.46	21/1548 (1.4%)
2	H	1.37	15/1148 (1.3%)	1.47	21/1548 (1.4%)
2	K	1.38	16/1148 (1.4%)	1.47	21/1548 (1.4%)
2	N	1.37	14/1148 (1.2%)	1.47	21/1548 (1.4%)
2	Q	1.38	16/1148 (1.4%)	1.47	21/1548 (1.4%)
3	C	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	F	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	I	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	L	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
3	O	0.88	4/1136 (0.4%)	1.18	5/1525 (0.3%)
3	R	0.88	4/1136 (0.4%)	1.18	6/1525 (0.4%)
4	1	1.16	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	2	1.17	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	3	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	4	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	5	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	6	1.17	13/2968 (0.4%)	2.00	101/4023 (2.5%)
4	7	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	8	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	9	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	V	1.17	13/2968 (0.4%)	2.00	98/4023 (2.4%)
4	W	1.17	13/2968 (0.4%)	2.00	100/4023 (2.5%)
4	X	1.17	13/2968 (0.4%)	2.00	99/4023 (2.5%)
4	Y	1.16	13/2968 (0.4%)	2.00	97/4023 (2.4%)
4	Z	1.17	13/2968 (0.4%)	2.00	102/4023 (2.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.50	545/93944 (0.6%)	1.99	2471/127134 (1.9%)

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	1	4
1	D	1	4
1	G	1	4
1	J	1	6
1	M	1	4
1	P	1	6
2	B	0	3
2	E	0	3
2	H	0	3
2	K	0	3
2	N	0	3
2	Q	0	3
3	C	0	2
3	F	0	2
3	I	0	2
3	L	0	2
3	O	0	2
3	R	0	2
4	1	0	1
4	2	0	1
4	3	0	1
4	4	0	1
4	5	0	1
4	6	0	1
4	7	0	1
4	8	0	1
4	9	0	1
4	V	0	1
4	W	0	1
4	X	0	1
4	Y	0	1
4	Z	0	1
All	All	6	72

The worst 5 of 545 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	806	MET	C-N	56.30	1.99	1.33
1	M	709	LYS	C-N	45.45	1.99	1.33
1	D	648	THR	CB-OG1	42.73	2.12	1.43
1	J	648	THR	CB-OG1	42.72	2.12	1.43
1	P	648	THR	CB-OG1	42.69	2.12	1.43

The worst 5 of 2471 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	637	LYS	O-C-N	-74.34	23.72	122.59
1	M	637	LYS	O-C-N	-74.28	23.80	122.59
1	D	637	LYS	O-C-N	-74.27	23.81	122.59
1	P	637	LYS	O-C-N	-74.27	23.81	122.59
1	A	637	LYS	O-C-N	-74.27	23.81	122.59

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	648	THR	CB
1	D	648	THR	CB
1	G	648	THR	CB
1	J	648	THR	CB
1	M	648	THR	CB

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	623	PHE	Sidechain
1	A	637	LYS	Mainchain
1	A	649	VAL	Mainchain
1	A	98	HIS	Mainchain
2	B	22	THR	Mainchain

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	6797	0	6764	1545	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	6797	0	6764	1441	0
1	G	6797	0	6772	1589	0
1	J	6797	0	6763	1456	0
1	M	6797	0	6777	1395	0
1	P	6797	0	6775	1458	0
2	B	1127	0	1085	249	0
2	E	1127	0	1086	265	0
2	H	1127	0	1088	297	0
2	K	1127	0	1088	277	0
2	N	1127	0	1088	251	0
2	Q	1127	0	1088	255	0
3	C	1123	0	1083	198	0
3	F	1123	0	1083	172	0
3	I	1123	0	1083	189	0
3	L	1123	0	1083	162	0
3	O	1123	0	1084	184	0
3	R	1123	0	1084	192	0
4	1	2906	0	2856	426	0
4	2	2906	0	2860	209	0
4	3	2906	0	2863	173	0
4	4	2906	0	2863	182	0
4	5	2906	0	2865	98	0
4	6	2906	0	2865	103	0
4	7	2906	0	2866	80	0
4	8	2906	0	2857	318	0
4	9	2906	0	2855	352	0
4	V	2906	0	2851	385	0
4	W	2906	0	2851	400	0
4	X	2906	0	2863	183	0
4	Y	2906	0	2863	200	0
4	Z	2906	0	2855	386	0
All	All	94966	0	93671	11334	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 60.

The worst 5 of 11334 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)
2:N:144:VAL:HG13	2:N:153:ILE:CD1	1.22	1.68
1:J:797:PHE:CE1	3:L:146:ILE:HG23	1.24	1.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:TRP:CZ3	2:B:50:THR:HG21	1.27	1.67
1:A:753:VAL:HG12	1:A:775:LEU:CG	1.22	1.66
4:2:287:ILE:CG2	4:4:202:THR:HB	1.23	1.66

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	789/840 (94%)	652 (83%)	111 (14%)	26 (3%)	3	21
1	D	789/840 (94%)	651 (82%)	112 (14%)	26 (3%)	3	21
1	G	791/840 (94%)	650 (82%)	114 (14%)	27 (3%)	3	21
1	J	791/840 (94%)	652 (82%)	112 (14%)	27 (3%)	3	21
1	M	788/840 (94%)	651 (83%)	110 (14%)	27 (3%)	3	21
1	P	787/840 (94%)	651 (83%)	109 (14%)	27 (3%)	3	21
2	B	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	E	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	H	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	K	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	N	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
2	Q	143/145 (99%)	126 (88%)	9 (6%)	8 (6%)	1	14
3	C	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	F	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	I	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	L	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
3	O	143/147 (97%)	133 (93%)	10 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	143/147 (97%)	133 (93%)	10 (7%)	0	100	100
4	1	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	2	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	3	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	4	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	5	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	6	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	7	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	8	370/375 (99%)	333 (90%)	31 (8%)	6 (2%)	7	38
4	9	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	V	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	W	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	X	370/375 (99%)	335 (90%)	29 (8%)	6 (2%)	7	38
4	Y	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
4	Z	370/375 (99%)	334 (90%)	30 (8%)	6 (2%)	7	38
All	All	11631/12042 (97%)	10138 (87%)	1201 (10%)	292 (2%)	6	26

5 of 292 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	202	SER
1	A	572	LYS
1	A	712	PRO
1	A	729	ALA

5.3.2 Protein sidechains ⓘ

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	672/672 (100%)	491 (73%)	181 (27%)	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	G	672/672 (100%)	492 (73%)	180 (27%)	0	3
1	J	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	M	672/672 (100%)	491 (73%)	181 (27%)	0	3
1	P	672/672 (100%)	490 (73%)	182 (27%)	0	3
2	B	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	E	120/120 (100%)	120 (100%)	0	100	100
2	H	120/120 (100%)	120 (100%)	0	100	100
2	K	120/120 (100%)	119 (99%)	1 (1%)	73	80
2	N	120/120 (100%)	120 (100%)	0	100	100
2	Q	120/120 (100%)	120 (100%)	0	100	100
3	C	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	F	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	I	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	L	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	O	117/117 (100%)	113 (97%)	4 (3%)	32	54
3	R	117/117 (100%)	113 (97%)	4 (3%)	32	54
4	1	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	2	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	3	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	4	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	5	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	6	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	7	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	8	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	9	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	V	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	W	315/318 (99%)	265 (84%)	50 (16%)	2	11
4	X	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Y	315/318 (99%)	264 (84%)	51 (16%)	2	11
4	Z	315/318 (99%)	264 (84%)	51 (16%)	2	11

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	9864/9906 (100%)	8040 (82%)	1824 (18%)	3 8

5 of 1824 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	7	MET
4	Z	16	LEU
4	1	293	LEU
4	Y	287	ILE
4	V	274	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 285 such sidechains are listed below:

Mol	Chain	Res	Type
4	7	40	HIS
4	7	360	GLN
4	W	252	ASN
1	J	164	GLN
1	J	29	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

270 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MLY	G	839	1	9,10,11	0.65	0	6,11,13	0.81	0
1	MLY	J	59	1	9,10,11	0.86	0	6,11,13	0.48	0
1	MLY	J	63	1	9,10,11	0.84	0	6,11,13	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	M	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	A	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.44	0
1	MLY	D	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	G	782	1	9,10,11	0.80	0	6,11,13	0.35	0
1	MLY	G	486	1	9,10,11	0.67	0	6,11,13	0.40	0
1	MLY	J	130	1	9,10,11	0.75	0	6,11,13	0.73	0
1	MLY	G	30	1	9,10,11	0.90	0	6,11,13	0.31	0
1	MLY	M	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	G	107	1	9,10,11	0.50	0	6,11,13	0.34	0
1	MLY	P	782	1	9,10,11	0.80	0	6,11,13	0.37	0
1	MLY	A	436	1	9,10,11	0.93	1 (11%)	6,11,13	0.46	0
1	MLY	D	353	1	9,10,11	0.87	0	6,11,13	0.80	0
1	MLY	J	272	1	9,10,11	0.91	1 (11%)	6,11,13	0.54	0
1	MLY	P	600	1	9,10,11	0.53	0	6,11,13	0.38	0
1	MLY	J	19	1	9,10,11	1.09	1 (11%)	6,11,13	0.58	0
1	MLY	J	681	1	9,10,11	0.57	0	6,11,13	0.46	0
1	MLY	P	138	1	9,10,11	1.18	1 (11%)	6,11,13	0.80	0
1	MLY	G	272	1	9,10,11	0.87	1 (11%)	6,11,13	0.55	0
1	MLY	M	248	1	9,10,11	0.81	0	6,11,13	0.66	0
1	MLY	M	553	1	9,10,11	0.64	0	6,11,13	0.55	0
1	MLY	A	833	1	9,10,11	1.12	2 (22%)	6,11,13	0.31	0
1	MLY	G	837	1	9,10,11	0.59	0	6,11,13	0.55	0
1	MLY	A	551	1	9,10,11	0.53	0	6,11,13	0.18	0
1	MLY	M	598	1	9,10,11	0.82	0	6,11,13	0.42	0
1	MLY	M	659	1	9,10,11	0.83	0	6,11,13	0.57	0
1	MLY	P	59	1	9,10,11	0.84	0	6,11,13	0.48	0
1	MLY	G	764	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	M	272	1	9,10,11	0.92	1 (11%)	6,11,13	0.56	0
1	MLY	M	827	1	9,10,11	0.70	0	6,11,13	0.47	0
1	MLY	M	431	1	9,10,11	0.50	0	6,11,13	0.44	0
1	MLY	M	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	G	138	1	9,10,11	1.23	1 (11%)	6,11,13	0.83	0
1	MLY	M	617	1	9,10,11	0.89	0	6,11,13	0.34	0
1	MLY	A	248	1	9,10,11	0.80	0	6,11,13	0.64	0
1	MLY	P	681	1	9,10,11	0.58	0	6,11,13	0.46	0
1	MLY	G	613	1	9,10,11	0.60	0	6,11,13	0.61	0
1	MLY	D	782	1	9,10,11	0.81	0	6,11,13	0.35	0
1	MLY	J	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.75	0
1	MLY	D	598	1	9,10,11	0.82	0	6,11,13	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	M	236	1	9,10,11	0.85	1 (11%)	6,11,13	0.48	0
1	MLY	G	296	1	9,10,11	0.62	0	6,11,13	0.37	0
1	MLY	D	138	1	9,10,11	1.23	1 (11%)	6,11,13	0.82	0
1	MLY	G	617	1	9,10,11	0.89	0	6,11,13	0.36	0
1	MLY	M	367	1	9,10,11	0.58	0	6,11,13	0.37	0
1	MLY	J	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	D	107	1	9,10,11	0.52	0	6,11,13	0.33	0
1	MLY	D	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	G	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.43	0
1	MLY	M	87	1	9,10,11	1.12	1 (11%)	6,11,13	0.44	0
1	MLY	M	504	1	9,10,11	0.85	0	6,11,13	0.24	0
1	MLY	D	248	1	9,10,11	0.81	0	6,11,13	0.66	0
1	MLY	J	782	1	9,10,11	0.82	0	6,11,13	0.37	0
1	MLY	M	528	1	9,10,11	0.90	0	6,11,13	0.65	0
1	MLY	D	130	1	9,10,11	0.79	0	6,11,13	0.72	0
1	MLY	D	837	1	9,10,11	0.60	0	6,11,13	0.58	0
1	MLY	M	63	1	9,10,11	0.87	0	6,11,13	0.43	0
1	MLY	D	295	1	9,10,11	0.74	0	6,11,13	0.36	0
1	MLY	D	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.59	0
1	MLY	P	190	1	9,10,11	1.20	2 (22%)	6,11,13	0.53	0
1	MLY	J	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	A	19	1	9,10,11	1.00	1 (11%)	6,11,13	0.58	0
1	MLY	J	107	1	9,10,11	0.48	0	6,11,13	0.33	0
1	MLY	J	369	1	9,10,11	0.71	0	6,11,13	0.46	0
1	MLY	G	505	1	9,10,11	0.77	0	6,11,13	0.35	0
1	MLY	D	30	1	9,10,11	0.94	0	6,11,13	0.32	0
1	MLY	G	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	J	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	P	55	1	9,10,11	0.73	0	6,11,13	0.80	0
1	MLY	P	764	1	9,10,11	0.81	0	6,11,13	0.39	0
1	MLY	P	385	1	9,10,11	0.92	1 (11%)	6,11,13	0.45	0
1	MLY	A	553	1,4	9,10,11	0.65	0	6,11,13	0.55	0
1	MLY	J	248	1	9,10,11	0.82	0	6,11,13	0.66	0
1	MLY	J	504	1	9,10,11	0.84	0	6,11,13	0.22	0
1	MLY	P	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.58	0
1	MLY	A	598	1	9,10,11	0.83	0	6,11,13	0.43	0
1	MLY	M	436	1	9,10,11	0.96	1 (11%)	6,11,13	0.47	0
1	MLY	J	659	1	9,10,11	0.84	1 (11%)	6,11,13	0.58	0
1	MLY	A	486	1	9,10,11	0.68	0	6,11,13	0.39	0
1	MLY	G	248	1	9,10,11	0.77	0	6,11,13	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	M	833	1	9,10,11	1.16	2 (22%)	6,11,13	0.30	0
1	MLY	M	296	1	9,10,11	0.64	0	6,11,13	0.35	0
1	MLY	G	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.58	0
1	MLY	G	768	1	9,10,11	0.75	0	6,11,13	0.42	0
1	MLY	G	369	1	9,10,11	0.72	0	6,11,13	0.46	0
1	MLY	M	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	D	35	1	9,10,11	0.73	0	6,11,13	0.37	0
1	MLY	D	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	P	367	1	9,10,11	0.58	0	6,11,13	0.37	0
1	MLY	P	617	1	9,10,11	0.93	1 (11%)	6,11,13	0.33	0
1	MLY	D	505	1	9,10,11	0.78	0	6,11,13	0.35	0
1	MLY	G	431	1	9,10,11	0.49	0	6,11,13	0.45	0
1	MLY	M	138	1	9,10,11	1.22	1 (11%)	6,11,13	0.82	0
1	MLY	P	248	1	9,10,11	0.82	0	6,11,13	0.64	0
1	MLY	P	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	M	19	1	9,10,11	1.05	1 (11%)	6,11,13	0.59	0
1	MLY	J	348	1	9,10,11	0.76	0	6,11,13	0.46	0
1	MLY	A	681	1	9,10,11	0.55	0	6,11,13	0.45	0
1	MLY	P	415	1	9,10,11	0.73	0	6,11,13	0.19	0
1	MLY	A	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	A	764	1	9,10,11	0.84	0	6,11,13	0.35	0
1	MLY	D	827	1	9,10,11	0.66	0	6,11,13	0.47	0
1	MLY	M	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	P	272	1	9,10,11	0.86	1 (11%)	6,11,13	0.55	0
1	MLY	D	431	1	9,10,11	0.53	0	6,11,13	0.45	0
1	MLY	P	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.76	0
1	MLY	J	35	1	9,10,11	0.72	0	6,11,13	0.38	0
1	MLY	M	353	1	9,10,11	0.88	0	6,11,13	0.80	0
1	MLY	G	598	1	9,10,11	0.81	0	6,11,13	0.42	0
1	MLY	A	138	1	9,10,11	1.21	1 (11%)	6,11,13	0.83	0
1	MLY	G	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	J	505	1	9,10,11	0.85	1 (11%)	6,11,13	0.35	0
1	MLY	J	553	1	9,10,11	0.64	0	6,11,13	0.54	0
1	MLY	A	84	1	9,10,11	0.50	0	6,11,13	0.79	0
1	MLY	M	369	1	9,10,11	0.72	0	6,11,13	0.47	0
1	MLY	A	59	1	9,10,11	0.85	0	6,11,13	0.47	0
1	MLY	D	367	1	9,10,11	0.58	0	6,11,13	0.39	0
1	MLY	D	600	1	9,10,11	0.52	0	6,11,13	0.38	0
1	MLY	A	827	1	9,10,11	0.69	0	6,11,13	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	G	367	1	9,10,11	0.61	0	6,11,13	0.38	0
1	MLY	G	553	1,4	9,10,11	0.64	0	6,11,13	0.54	0
1	MLY	A	107	1	9,10,11	0.48	0	6,11,13	0.34	0
1	MLY	A	613	1	9,10,11	0.58	0	6,11,13	0.61	0
1	MLY	J	827	1	9,10,11	0.73	0	6,11,13	0.48	0
1	MLY	M	768	1	9,10,11	0.77	0	6,11,13	0.43	0
1	MLY	A	130	1	9,10,11	0.79	0	6,11,13	0.73	0
1	MLY	G	551	1	9,10,11	0.54	0	6,11,13	0.20	0
1	MLY	A	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.48	0
1	MLY	G	528	1	9,10,11	0.91	0	6,11,13	0.66	0
1	MLY	G	49	1	9,10,11	0.98	1 (11%)	6,11,13	0.74	0
1	MLY	G	63	1	9,10,11	0.85	0	6,11,13	0.43	0
1	MLY	P	839	1	9,10,11	0.65	0	6,11,13	0.76	0
1	MLY	G	55	1	9,10,11	0.75	0	6,11,13	0.80	0
1	MLY	J	367	1	9,10,11	0.58	0	6,11,13	0.37	0
1	MLY	J	600	1	9,10,11	0.53	0	6,11,13	0.37	0
1	MLY	J	764	1	9,10,11	0.79	0	6,11,13	0.36	0
1	MLY	P	505	1	9,10,11	0.85	0	6,11,13	0.33	0
1	MLY	P	553	1	9,10,11	0.65	0	6,11,13	0.53	0
1	MLY	A	415	1	9,10,11	0.73	0	6,11,13	0.19	0
1	MLY	P	107	1	9,10,11	0.49	0	6,11,13	0.33	0
1	MLY	J	138	1	9,10,11	1.19	1 (11%)	6,11,13	0.81	0
1	MLY	P	598	1	9,10,11	0.82	0	6,11,13	0.41	0
1	MLY	A	528	1	9,10,11	0.88	0	6,11,13	0.67	0
1	MLY	M	764	1	9,10,11	0.81	0	6,11,13	0.37	0
1	MLY	D	49	1	9,10,11	1.00	1 (11%)	6,11,13	0.75	0
1	MLY	A	839	1	9,10,11	0.65	0	6,11,13	0.82	0
1	MLY	A	30	1	9,10,11	0.92	0	6,11,13	0.32	0
1	MLY	A	190	1	9,10,11	1.21	2 (22%)	6,11,13	0.51	0
1	MLY	D	190	1	9,10,11	1.17	2 (22%)	6,11,13	0.55	0
1	MLY	M	190	1	9,10,11	1.19	2 (22%)	6,11,13	0.52	0
1	MLY	P	35	1	9,10,11	0.73	0	6,11,13	0.38	0
1	MLY	G	436	1	9,10,11	0.93	1 (11%)	6,11,13	0.46	0
1	MLY	P	528	1	9,10,11	0.89	0	6,11,13	0.65	0
1	MLY	J	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	J	295	1	9,10,11	0.75	0	6,11,13	0.37	0
1	MLY	A	617	1	9,10,11	0.88	0	6,11,13	0.35	0
1	MLY	A	272	1	9,10,11	0.89	1 (11%)	6,11,13	0.56	0
1	MLY	D	553	1,4	9,10,11	0.66	0	6,11,13	0.55	0
1	MLY	J	431	1	9,10,11	0.52	0	6,11,13	0.45	0
1	MLY	D	236	1	9,10,11	0.83	1 (11%)	6,11,13	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	P	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	P	295	1	9,10,11	0.78	0	6,11,13	0.37	0
1	MLY	G	59	1	9,10,11	0.82	0	6,11,13	0.49	0
1	MLY	P	431	1	9,10,11	0.53	0	6,11,13	0.44	0
1	MLY	D	272	1	9,10,11	0.85	1 (11%)	6,11,13	0.57	0
1	MLY	G	348	1	9,10,11	0.79	0	6,11,13	0.47	0
1	MLY	D	385	1	9,10,11	0.91	1 (11%)	6,11,13	0.46	0
1	MLY	J	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.46	0
1	MLY	D	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	G	84	1	9,10,11	0.50	0	6,11,13	0.80	0
1	MLY	M	782	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	A	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.43	0
1	MLY	A	768	1	9,10,11	0.77	0	6,11,13	0.41	0
1	MLY	D	87	1	9,10,11	1.09	1 (11%)	6,11,13	0.43	0
1	MLY	D	768	1	9,10,11	0.76	0	6,11,13	0.40	0
1	MLY	D	839	1	9,10,11	0.67	0	6,11,13	0.79	0
1	MLY	P	130	1	9,10,11	0.75	0	6,11,13	0.72	0
1	MLY	D	63	1	9,10,11	0.87	0	6,11,13	0.45	0
1	MLY	P	833	1	9,10,11	1.12	2 (22%)	6,11,13	0.31	0
1	MLY	J	236	1	9,10,11	0.84	1 (11%)	6,11,13	0.47	0
1	MLY	M	486	1	9,10,11	0.66	0	6,11,13	0.40	0
1	MLY	P	296	1	9,10,11	0.62	0	6,11,13	0.35	0
1	MLY	A	431	1	9,10,11	0.50	0	6,11,13	0.44	0
1	MLY	M	30	1	9,10,11	0.91	0	6,11,13	0.32	0
1	MLY	P	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	M	130	1	9,10,11	0.76	0	6,11,13	0.73	0
1	MLY	D	486	1	9,10,11	0.67	0	6,11,13	0.41	0
1	MLY	A	600	1	9,10,11	0.52	0	6,11,13	0.40	0
1	MLY	A	782	1	9,10,11	0.83	0	6,11,13	0.36	0
1	MLY	G	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	J	551	1	9,10,11	0.54	0	6,11,13	0.19	0
1	MLY	D	617	1	9,10,11	0.91	0	6,11,13	0.34	0
1	MLY	M	415	1	9,10,11	0.76	0	6,11,13	0.19	0
1	MLY	J	87	1	9,10,11	1.11	1 (11%)	6,11,13	0.42	0
1	MLY	P	348	1	9,10,11	0.76	0	6,11,13	0.47	0
1	MLY	J	839	1	9,10,11	0.66	0	6,11,13	0.76	0
1	MLY	M	49	1	9,10,11	0.97	1 (11%)	6,11,13	0.74	0
1	MLY	A	348	1	9,10,11	0.79	0	6,11,13	0.48	0
1	MLY	M	613	1	9,10,11	0.58	0	6,11,13	0.62	0
1	MLY	P	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.49	0
1	MLY	J	486	1	9,10,11	0.65	0	6,11,13	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	296	1	9,10,11	0.62	0	6,11,13	0.36	0
1	MLY	J	617	1	9,10,11	0.92	1 (11%)	6,11,13	0.33	0
1	MLY	A	49	1	9,10,11	0.95	1 (11%)	6,11,13	0.74	0
1	MLY	G	19	1	9,10,11	1.03	1 (11%)	6,11,13	0.60	0
1	MLY	A	504	1	9,10,11	0.88	0	6,11,13	0.25	0
1	MLY	G	681	1	9,10,11	0.60	0	6,11,13	0.46	0
1	MLY	P	551	1	9,10,11	0.53	0	6,11,13	0.20	0
1	MLY	D	764	1	9,10,11	0.82	0	6,11,13	0.36	0
1	MLY	G	827	1	9,10,11	0.67	0	6,11,13	0.48	0
1	MLY	P	768	1	9,10,11	0.75	0	6,11,13	0.41	0
1	MLY	M	839	1	9,10,11	0.67	0	6,11,13	0.77	0
1	MLY	M	84	1	9,10,11	0.51	0	6,11,13	0.80	0
1	MLY	D	84	1	9,10,11	0.50	0	6,11,13	0.81	0
1	MLY	G	190	1	9,10,11	1.18	2 (22%)	6,11,13	0.52	0
1	MLY	G	353	1	9,10,11	0.88	0	6,11,13	0.81	0
1	MLY	J	598	1	9,10,11	0.81	0	6,11,13	0.41	0
1	MLY	G	833	1	9,10,11	1.13	2 (22%)	6,11,13	0.31	0
1	MLY	J	55	1	9,10,11	0.72	0	6,11,13	0.80	0
1	MLY	M	107	1	9,10,11	0.50	0	6,11,13	0.34	0
1	MLY	D	436	1	9,10,11	0.98	1 (11%)	6,11,13	0.49	0
1	MLY	P	19	1	9,10,11	1.09	1 (11%)	6,11,13	0.56	0
1	MLY	P	63	1	9,10,11	0.84	0	6,11,13	0.43	0
1	MLY	P	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	J	768	1	9,10,11	0.77	0	6,11,13	0.42	0
1	MLY	P	486	1	9,10,11	0.65	0	6,11,13	0.40	0
1	MLY	P	827	1	9,10,11	0.71	0	6,11,13	0.47	0
1	MLY	D	833	1	9,10,11	1.12	1 (11%)	6,11,13	0.31	0
1	MLY	M	837	1	9,10,11	0.57	0	6,11,13	0.56	0
1	MLY	P	353	1	9,10,11	0.86	0	6,11,13	0.80	0
1	MLY	G	385	1	9,10,11	0.93	1 (11%)	6,11,13	0.45	0
1	MLY	G	35	1	9,10,11	0.73	0	6,11,13	0.39	0
1	MLY	M	35	1	9,10,11	0.74	0	6,11,13	0.38	0
1	MLY	J	84	1	9,10,11	0.50	0	6,11,13	0.82	0
1	MLY	D	504	1	9,10,11	0.87	0	6,11,13	0.20	0
1	MLY	P	369	1	9,10,11	0.70	0	6,11,13	0.45	0
1	MLY	A	369	1	9,10,11	0.73	0	6,11,13	0.46	0
1	MLY	D	296	1	9,10,11	0.63	0	6,11,13	0.36	0
1	MLY	G	504	1	9,10,11	0.89	0	6,11,13	0.23	0
1	MLY	D	528	1	9,10,11	0.93	0	6,11,13	0.63	0
1	MLY	M	385	1	9,10,11	0.95	1 (11%)	6,11,13	0.45	0
1	MLY	P	84	1	9,10,11	0.51	0	6,11,13	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	A	55	1	9,10,11	0.73	0	6,11,13	0.79	0
1	MLY	J	436	1	9,10,11	0.95	1 (11%)	6,11,13	0.48	0
1	MLY	G	295	1	9,10,11	0.75	0	6,11,13	0.36	0
1	MLY	J	30	1	9,10,11	0.91	0	6,11,13	0.31	0
1	MLY	D	19	1	9,10,11	1.09	1 (11%)	6,11,13	0.57	0
1	MLY	A	837	1	9,10,11	0.58	0	6,11,13	0.55	0
1	MLY	J	190	1	9,10,11	1.22	2 (22%)	6,11,13	0.53	0
1	MLY	J	353	1	9,10,11	0.87	0	6,11,13	0.81	0
1	MLY	A	295	1	9,10,11	0.76	0	6,11,13	0.35	0
1	MLY	A	63	1	9,10,11	0.87	0	6,11,13	0.42	0
1	MLY	A	659	1	9,10,11	0.85	1 (11%)	6,11,13	0.59	0
1	MLY	J	833	1	9,10,11	1.12	2 (22%)	6,11,13	0.30	0
1	MLY	M	295	1	9,10,11	0.75	0	6,11,13	0.37	0
1	MLY	P	504	1	9,10,11	0.84	0	6,11,13	0.23	0
1	MLY	J	296	1	9,10,11	0.66	0	6,11,13	0.35	0
1	MLY	G	130	1	9,10,11	0.76	0	6,11,13	0.74	0
1	MLY	D	369	1	9,10,11	0.70	0	6,11,13	0.46	0
1	MLY	D	59	1	9,10,11	0.85	0	6,11,13	0.48	0
1	MLY	D	415	1	9,10,11	0.75	0	6,11,13	0.19	0
1	MLY	P	87	1	9,10,11	1.10	1 (11%)	6,11,13	0.42	0
1	MLY	A	505	1	9,10,11	0.81	0	6,11,13	0.33	0
1	MLY	A	353	1	9,10,11	0.88	0	6,11,13	0.80	0
1	MLY	A	367	1	9,10,11	0.60	0	6,11,13	0.36	0
1	MLY	M	505	1	9,10,11	0.85	0	6,11,13	0.34	0

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
1	MLY	G	839	1	-	3/8/9/11	-
1	MLY	J	59	1	-	3/8/9/11	-
1	MLY	J	63	1	-	4/8/9/11	-
1	MLY	M	348	1	-	5/8/9/11	-
1	MLY	M	681	1	-	4/8/9/11	-
1	MLY	A	385	1	-	2/8/9/11	-
1	MLY	D	681	1	-	4/8/9/11	-
1	MLY	G	782	1	-	6/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	G	486	1	-	2/8/9/11	-
1	MLY	J	130	1	-	5/8/9/11	-
1	MLY	G	30	1	-	3/8/9/11	-
1	MLY	M	600	1	-	3/8/9/11	-
1	MLY	G	107	1	-	2/8/9/11	-
1	MLY	P	782	1	-	6/8/9/11	-
1	MLY	A	436	1	-	4/8/9/11	-
1	MLY	D	353	1	-	4/8/9/11	-
1	MLY	J	272	1	-	3/8/9/11	-
1	MLY	P	600	1	-	3/8/9/11	-
1	MLY	J	19	1	-	4/8/9/11	-
1	MLY	J	681	1	-	4/8/9/11	-
1	MLY	P	138	1	-	4/8/9/11	-
1	MLY	G	272	1	-	3/8/9/11	-
1	MLY	M	248	1	-	6/8/9/11	-
1	MLY	M	553	1	-	4/8/9/11	-
1	MLY	A	833	1	-	6/8/9/11	-
1	MLY	G	837	1	-	6/8/9/11	-
1	MLY	A	551	1	-	3/8/9/11	-
1	MLY	M	598	1	-	5/8/9/11	-
1	MLY	M	659	1	-	3/8/9/11	-
1	MLY	P	59	1	-	3/8/9/11	-
1	MLY	G	764	1	-	2/8/9/11	-
1	MLY	M	272	1	-	3/8/9/11	-
1	MLY	M	827	1	-	1/8/9/11	-
1	MLY	M	431	1	-	4/8/9/11	-
1	MLY	M	55	1	-	6/8/9/11	-
1	MLY	G	138	1	-	4/8/9/11	-
1	MLY	M	617	1	-	2/8/9/11	-
1	MLY	A	248	1	-	6/8/9/11	-
1	MLY	P	681	1	-	4/8/9/11	-
1	MLY	G	613	1	-	3/8/9/11	-
1	MLY	D	782	1	-	6/8/9/11	-
1	MLY	J	49	1	-	3/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	598	1	-	5/8/9/11	-
1	MLY	M	236	1	-	3/8/9/11	-
1	MLY	G	296	1	-	4/8/9/11	-
1	MLY	D	138	1	-	4/8/9/11	-
1	MLY	G	617	1	-	2/8/9/11	-
1	MLY	M	367	1	-	2/8/9/11	-
1	MLY	J	528	1	-	4/8/9/11	-
1	MLY	D	107	1	-	2/8/9/11	-
1	MLY	D	613	1	-	3/8/9/11	-
1	MLY	G	87	1	-	2/8/9/11	-
1	MLY	M	87	1	-	2/8/9/11	-
1	MLY	M	504	1	-	4/8/9/11	-
1	MLY	D	248	1	-	6/8/9/11	-
1	MLY	J	782	1	-	6/8/9/11	-
1	MLY	M	528	1	-	4/8/9/11	-
1	MLY	D	130	1	-	5/8/9/11	-
1	MLY	D	837	1	-	6/8/9/11	-
1	MLY	M	63	1	-	4/8/9/11	-
1	MLY	D	295	1	-	2/8/9/11	-
1	MLY	D	659	1	-	3/8/9/11	-
1	MLY	P	190	1	-	4/8/9/11	-
1	MLY	J	415	1	-	3/8/9/11	-
1	MLY	A	19	1	-	4/8/9/11	-
1	MLY	J	107	1	-	2/8/9/11	-
1	MLY	J	369	1	-	2/8/9/11	-
1	MLY	G	505	1	-	5/8/9/11	-
1	MLY	D	30	1	-	3/8/9/11	-
1	MLY	G	600	1	-	3/8/9/11	-
1	MLY	J	613	1	-	3/8/9/11	-
1	MLY	P	55	1	-	6/8/9/11	-
1	MLY	P	764	1	-	2/8/9/11	-
1	MLY	P	385	1	-	2/8/9/11	-
1	MLY	A	553	1,4	-	4/8/9/11	-
1	MLY	J	248	1	-	6/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	504	1	-	4/8/9/11	-
1	MLY	P	659	1	-	3/8/9/11	-
1	MLY	A	598	1	-	5/8/9/11	-
1	MLY	M	436	1	-	4/8/9/11	-
1	MLY	J	659	1	-	3/8/9/11	-
1	MLY	A	486	1	-	2/8/9/11	-
1	MLY	G	248	1	-	6/8/9/11	-
1	MLY	D	348	1	-	5/8/9/11	-
1	MLY	M	833	1	-	6/8/9/11	-
1	MLY	M	296	1	-	4/8/9/11	-
1	MLY	G	659	1	-	3/8/9/11	-
1	MLY	G	768	1	-	4/8/9/11	-
1	MLY	G	369	1	-	2/8/9/11	-
1	MLY	M	551	1	-	3/8/9/11	-
1	MLY	D	35	1	-	3/8/9/11	-
1	MLY	D	55	1	-	6/8/9/11	-
1	MLY	P	367	1	-	2/8/9/11	-
1	MLY	P	617	1	-	2/8/9/11	-
1	MLY	D	505	1	-	5/8/9/11	-
1	MLY	G	431	1	-	4/8/9/11	-
1	MLY	M	138	1	-	4/8/9/11	-
1	MLY	P	248	1	-	6/8/9/11	-
1	MLY	P	236	1	-	3/8/9/11	-
1	MLY	M	19	1	-	4/8/9/11	-
1	MLY	J	348	1	-	5/8/9/11	-
1	MLY	A	681	1	-	4/8/9/11	-
1	MLY	P	415	1	-	3/8/9/11	-
1	MLY	A	35	1	-	3/8/9/11	-
1	MLY	A	764	1	-	2/8/9/11	-
1	MLY	D	827	1	-	1/8/9/11	-
1	MLY	M	59	1	-	3/8/9/11	-
1	MLY	P	272	1	-	3/8/9/11	-
1	MLY	D	431	1	-	4/8/9/11	-
1	MLY	P	49	1	-	3/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	35	1	-	3/8/9/11	-
1	MLY	M	353	1	-	4/8/9/11	-
1	MLY	G	598	1	-	5/8/9/11	-
1	MLY	A	138	1	-	4/8/9/11	-
1	MLY	G	236	1	-	3/8/9/11	-
1	MLY	J	505	1	-	5/8/9/11	-
1	MLY	J	553	1	-	4/8/9/11	-
1	MLY	A	84	1	-	4/8/9/11	-
1	MLY	M	369	1	-	2/8/9/11	-
1	MLY	A	59	1	-	3/8/9/11	-
1	MLY	D	367	1	-	2/8/9/11	-
1	MLY	D	600	1	-	3/8/9/11	-
1	MLY	A	827	1	-	1/8/9/11	-
1	MLY	G	367	1	-	2/8/9/11	-
1	MLY	G	553	1,4	-	4/8/9/11	-
1	MLY	A	107	1	-	2/8/9/11	-
1	MLY	A	613	1	-	3/8/9/11	-
1	MLY	J	827	1	-	1/8/9/11	-
1	MLY	M	768	1	-	4/8/9/11	-
1	MLY	A	130	1	-	5/8/9/11	-
1	MLY	G	551	1	-	3/8/9/11	-
1	MLY	A	236	1	-	3/8/9/11	-
1	MLY	G	528	1	-	4/8/9/11	-
1	MLY	G	49	1	-	3/8/9/11	-
1	MLY	G	63	1	-	4/8/9/11	-
1	MLY	P	839	1	-	3/8/9/11	-
1	MLY	G	55	1	-	6/8/9/11	-
1	MLY	J	367	1	-	2/8/9/11	-
1	MLY	J	600	1	-	3/8/9/11	-
1	MLY	J	764	1	-	2/8/9/11	-
1	MLY	P	505	1	-	5/8/9/11	-
1	MLY	P	553	1	-	4/8/9/11	-
1	MLY	A	415	1	-	3/8/9/11	-
1	MLY	P	107	1	-	2/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	J	138	1	-	4/8/9/11	-
1	MLY	P	598	1	-	5/8/9/11	-
1	MLY	A	528	1	-	4/8/9/11	-
1	MLY	M	764	1	-	2/8/9/11	-
1	MLY	D	49	1	-	3/8/9/11	-
1	MLY	A	839	1	-	3/8/9/11	-
1	MLY	A	30	1	-	3/8/9/11	-
1	MLY	A	190	1	-	4/8/9/11	-
1	MLY	D	190	1	-	4/8/9/11	-
1	MLY	M	190	1	-	4/8/9/11	-
1	MLY	P	35	1	-	3/8/9/11	-
1	MLY	G	436	1	-	4/8/9/11	-
1	MLY	P	528	1	-	4/8/9/11	-
1	MLY	J	837	1	-	6/8/9/11	-
1	MLY	J	295	1	-	2/8/9/11	-
1	MLY	A	617	1	-	2/8/9/11	-
1	MLY	A	272	1	-	3/8/9/11	-
1	MLY	D	553	1,4	-	5/8/9/11	-
1	MLY	J	431	1	-	4/8/9/11	-
1	MLY	D	236	1	-	3/8/9/11	-
1	MLY	P	837	1	-	6/8/9/11	-
1	MLY	P	295	1	-	2/8/9/11	-
1	MLY	G	59	1	-	3/8/9/11	-
1	MLY	P	431	1	-	4/8/9/11	-
1	MLY	D	272	1	-	3/8/9/11	-
1	MLY	G	348	1	-	5/8/9/11	-
1	MLY	D	385	1	-	2/8/9/11	-
1	MLY	J	385	1	-	2/8/9/11	-
1	MLY	D	551	1	-	3/8/9/11	-
1	MLY	G	84	1	-	4/8/9/11	-
1	MLY	M	782	1	-	6/8/9/11	-
1	MLY	A	87	1	-	2/8/9/11	-
1	MLY	A	768	1	-	4/8/9/11	-
1	MLY	D	87	1	-	2/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	768	1	-	4/8/9/11	-
1	MLY	D	839	1	-	3/8/9/11	-
1	MLY	P	130	1	-	5/8/9/11	-
1	MLY	D	63	1	-	4/8/9/11	-
1	MLY	P	833	1	-	6/8/9/11	-
1	MLY	J	236	1	-	3/8/9/11	-
1	MLY	M	486	1	-	2/8/9/11	-
1	MLY	P	296	1	-	4/8/9/11	-
1	MLY	A	431	1	-	4/8/9/11	-
1	MLY	M	30	1	-	3/8/9/11	-
1	MLY	P	613	1	-	3/8/9/11	-
1	MLY	M	130	1	-	5/8/9/11	-
1	MLY	D	486	1	-	2/8/9/11	-
1	MLY	A	600	1	-	3/8/9/11	-
1	MLY	A	782	1	-	6/8/9/11	-
1	MLY	G	415	1	-	3/8/9/11	-
1	MLY	J	551	1	-	3/8/9/11	-
1	MLY	D	617	1	-	2/8/9/11	-
1	MLY	M	415	1	-	3/8/9/11	-
1	MLY	J	87	1	-	2/8/9/11	-
1	MLY	P	348	1	-	5/8/9/11	-
1	MLY	J	839	1	-	3/8/9/11	-
1	MLY	M	49	1	-	3/8/9/11	-
1	MLY	A	348	1	-	5/8/9/11	-
1	MLY	M	613	1	-	3/8/9/11	-
1	MLY	P	436	1	-	4/8/9/11	-
1	MLY	J	486	1	-	2/8/9/11	-
1	MLY	A	296	1	-	4/8/9/11	-
1	MLY	J	617	1	-	2/8/9/11	-
1	MLY	A	49	1	-	3/8/9/11	-
1	MLY	G	19	1	-	4/8/9/11	-
1	MLY	A	504	1	-	4/8/9/11	-
1	MLY	G	681	1	-	4/8/9/11	-
1	MLY	P	551	1	-	3/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	D	764	1	-	2/8/9/11	-
1	MLY	G	827	1	-	1/8/9/11	-
1	MLY	P	768	1	-	4/8/9/11	-
1	MLY	M	839	1	-	3/8/9/11	-
1	MLY	M	84	1	-	4/8/9/11	-
1	MLY	D	84	1	-	4/8/9/11	-
1	MLY	G	190	1	-	4/8/9/11	-
1	MLY	G	353	1	-	4/8/9/11	-
1	MLY	J	598	1	-	5/8/9/11	-
1	MLY	G	833	1	-	6/8/9/11	-
1	MLY	J	55	1	-	6/8/9/11	-
1	MLY	M	107	1	-	2/8/9/11	-
1	MLY	D	436	1	-	4/8/9/11	-
1	MLY	P	19	1	-	4/8/9/11	-
1	MLY	P	63	1	-	4/8/9/11	-
1	MLY	P	30	1	-	3/8/9/11	-
1	MLY	J	768	1	-	4/8/9/11	-
1	MLY	P	486	1	-	2/8/9/11	-
1	MLY	P	827	1	-	1/8/9/11	-
1	MLY	D	833	1	-	6/8/9/11	-
1	MLY	M	837	1	-	6/8/9/11	-
1	MLY	P	353	1	-	4/8/9/11	-
1	MLY	G	385	1	-	2/8/9/11	-
1	MLY	G	35	1	-	3/8/9/11	-
1	MLY	M	35	1	-	3/8/9/11	-
1	MLY	J	84	1	-	4/8/9/11	-
1	MLY	D	504	1	-	4/8/9/11	-
1	MLY	P	369	1	-	2/8/9/11	-
1	MLY	A	369	1	-	2/8/9/11	-
1	MLY	D	296	1	-	4/8/9/11	-
1	MLY	G	504	1	-	4/8/9/11	-
1	MLY	D	528	1	-	4/8/9/11	-
1	MLY	M	385	1	-	2/8/9/11	-
1	MLY	P	84	1	-	4/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	55	1	-	6/8/9/11	-
1	MLY	J	436	1	-	4/8/9/11	-
1	MLY	G	295	1	-	2/8/9/11	-
1	MLY	J	30	1	-	3/8/9/11	-
1	MLY	D	19	1	-	4/8/9/11	-
1	MLY	A	837	1	-	6/8/9/11	-
1	MLY	J	190	1	-	4/8/9/11	-
1	MLY	J	353	1	-	4/8/9/11	-
1	MLY	A	295	1	-	2/8/9/11	-
1	MLY	A	63	1	-	4/8/9/11	-
1	MLY	A	659	1	-	3/8/9/11	-
1	MLY	J	833	1	-	6/8/9/11	-
1	MLY	M	295	1	-	2/8/9/11	-
1	MLY	P	504	1	-	4/8/9/11	-
1	MLY	J	296	1	-	4/8/9/11	-
1	MLY	G	130	1	-	5/8/9/11	-
1	MLY	D	369	1	-	2/8/9/11	-
1	MLY	D	59	1	-	3/8/9/11	-
1	MLY	D	415	1	-	3/8/9/11	-
1	MLY	P	87	1	-	2/8/9/11	-
1	MLY	A	505	1	-	5/8/9/11	-
1	MLY	A	353	1	-	4/8/9/11	-
1	MLY	A	367	1	-	2/8/9/11	-
1	MLY	M	505	1	-	5/8/9/11	-

The worst 5 of 79 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	138	MLY	CB-CA	-3.29	1.48	1.53
1	D	138	MLY	CB-CA	-3.25	1.48	1.53
1	M	138	MLY	CB-CA	-3.21	1.48	1.53
1	A	138	MLY	CB-CA	-3.19	1.48	1.53
1	J	138	MLY	CB-CA	-3.15	1.48	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 967 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	19	MLY	C-CA-CB-CG
1	A	49	MLY	N-CA-CB-CG
1	A	49	MLY	C-CA-CB-CG
1	A	55	MLY	N-CA-CB-CG
1	A	55	MLY	C-CA-CB-CG

There are no ring outliers.

185 monomers are involved in 666 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	839	MLY	4	0
1	J	59	MLY	3	0
1	J	63	MLY	4	0
1	M	348	MLY	5	0
1	G	782	MLY	1	0
1	G	486	MLY	3	0
1	G	30	MLY	1	0
1	M	600	MLY	1	0
1	G	107	MLY	3	0
1	P	782	MLY	3	0
1	A	436	MLY	2	0
1	J	272	MLY	1	0
1	P	600	MLY	1	0
1	P	138	MLY	2	0
1	G	272	MLY	1	0
1	M	248	MLY	2	0
1	M	553	MLY	2	0
1	A	833	MLY	1	0
1	G	837	MLY	1	0
1	A	551	MLY	2	0
1	M	598	MLY	1	0
1	M	659	MLY	2	0
1	P	59	MLY	2	0
1	G	764	MLY	17	0
1	M	272	MLY	1	0
1	M	55	MLY	1	0
1	G	138	MLY	2	0
1	M	617	MLY	1	0
1	A	248	MLY	2	0
1	D	782	MLY	52	0
1	J	49	MLY	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	598	MLY	1	0
1	G	296	MLY	3	0
1	D	138	MLY	2	0
1	G	617	MLY	1	0
1	J	528	MLY	3	0
1	D	107	MLY	3	0
1	G	87	MLY	2	0
1	M	87	MLY	2	0
1	M	504	MLY	1	0
1	D	248	MLY	2	0
1	J	782	MLY	1	0
1	M	528	MLY	3	0
1	D	837	MLY	1	0
1	M	63	MLY	4	0
1	D	295	MLY	6	0
1	D	659	MLY	2	0
1	P	190	MLY	2	0
1	J	415	MLY	1	0
1	J	107	MLY	3	0
1	J	369	MLY	1	0
1	G	505	MLY	19	0
1	D	30	MLY	1	0
1	G	600	MLY	1	0
1	P	55	MLY	1	0
1	P	764	MLY	3	0
1	A	553	MLY	18	0
1	J	248	MLY	2	0
1	J	504	MLY	1	0
1	P	659	MLY	2	0
1	A	598	MLY	1	0
1	M	436	MLY	2	0
1	J	659	MLY	2	0
1	A	486	MLY	3	0
1	G	248	MLY	2	0
1	D	348	MLY	6	0
1	M	296	MLY	3	0
1	G	659	MLY	2	0
1	G	768	MLY	2	0
1	D	55	MLY	1	0
1	P	617	MLY	1	0
1	M	138	MLY	2	0
1	P	248	MLY	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	J	348	MLY	6	0
1	P	415	MLY	1	0
1	A	764	MLY	10	0
1	M	59	MLY	2	0
1	P	272	MLY	1	0
1	P	49	MLY	3	0
1	G	598	MLY	1	0
1	A	138	MLY	2	0
1	J	505	MLY	9	0
1	J	553	MLY	12	0
1	A	59	MLY	3	0
1	D	600	MLY	1	0
1	A	827	MLY	1	0
1	G	553	MLY	26	0
1	A	107	MLY	3	0
1	M	768	MLY	2	0
1	G	528	MLY	2	0
1	G	49	MLY	3	0
1	G	63	MLY	3	0
1	P	839	MLY	8	0
1	G	55	MLY	1	0
1	J	600	MLY	1	0
1	J	764	MLY	3	0
1	P	505	MLY	2	0
1	P	553	MLY	2	0
1	A	415	MLY	1	0
1	P	107	MLY	3	0
1	J	138	MLY	2	0
1	P	598	MLY	1	0
1	A	528	MLY	3	0
1	M	764	MLY	1	0
1	D	49	MLY	3	0
1	A	839	MLY	8	0
1	A	30	MLY	1	0
1	A	190	MLY	2	0
1	D	190	MLY	2	0
1	M	190	MLY	2	0
1	P	35	MLY	1	0
1	G	436	MLY	2	0
1	P	528	MLY	3	0
1	J	837	MLY	1	0
1	J	295	MLY	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	617	MLY	1	0
1	A	272	MLY	1	0
1	D	553	MLY	16	0
1	P	837	MLY	1	0
1	P	295	MLY	6	0
1	G	59	MLY	2	0
1	D	272	MLY	1	0
1	G	348	MLY	5	0
1	D	551	MLY	2	0
1	G	84	MLY	28	0
1	M	782	MLY	4	0
1	A	87	MLY	3	0
1	A	768	MLY	6	0
1	D	87	MLY	2	0
1	D	839	MLY	4	0
1	D	63	MLY	4	0
1	M	486	MLY	3	0
1	P	296	MLY	2	0
1	M	30	MLY	1	0
1	D	486	MLY	3	0
1	A	600	MLY	1	0
1	A	782	MLY	6	0
1	G	415	MLY	1	0
1	D	617	MLY	1	0
1	M	415	MLY	1	0
1	J	87	MLY	3	0
1	P	348	MLY	4	0
1	J	839	MLY	9	0
1	M	49	MLY	4	0
1	A	348	MLY	6	0
1	P	436	MLY	2	0
1	J	486	MLY	3	0
1	A	296	MLY	3	0
1	J	617	MLY	1	0
1	A	49	MLY	4	0
1	A	504	MLY	1	0
1	D	764	MLY	8	0
1	M	839	MLY	7	0
1	G	190	MLY	2	0
1	J	598	MLY	1	0
1	J	55	MLY	1	0
1	M	107	MLY	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	436	MLY	2	0
1	P	63	MLY	4	0
1	P	30	MLY	1	0
1	J	768	MLY	1	0
1	P	486	MLY	3	0
1	M	837	MLY	1	0
1	M	35	MLY	3	0
1	J	84	MLY	18	0
1	D	296	MLY	3	0
1	G	504	MLY	1	0
1	D	528	MLY	3	0
1	A	55	MLY	1	0
1	J	436	MLY	2	0
1	G	295	MLY	6	0
1	J	30	MLY	1	0
1	A	837	MLY	11	0
1	J	190	MLY	2	0
1	A	295	MLY	6	0
1	A	63	MLY	3	0
1	A	659	MLY	2	0
1	M	295	MLY	6	0
1	P	504	MLY	1	0
1	J	296	MLY	3	0
1	D	369	MLY	1	0
1	D	59	MLY	3	0
1	D	415	MLY	1	0
1	P	87	MLY	3	0
1	A	505	MLY	20	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	7
1	P	6
1	D	4
1	A	4
1	J	3
1	G	3
3	C	1
3	F	1
3	I	1
3	L	1
3	O	1
3	R	1
2	H	1
2	B	1
2	E	1
2	K	1
2	N	1
2	Q	1

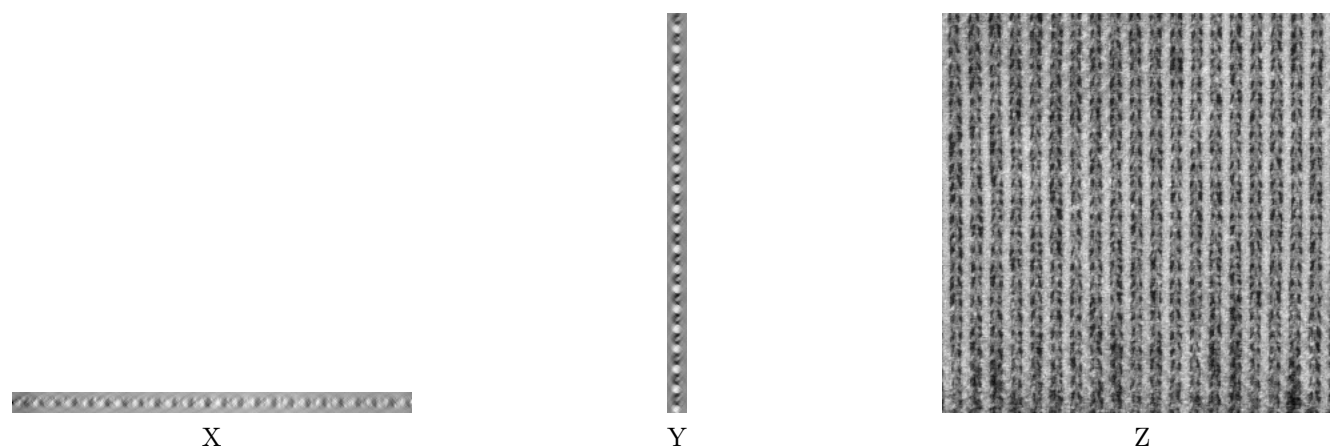
The worst 5 of 39 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	J	769:ALA	C	770:GLY	N	5.57
1	D	769:ALA	C	770:GLY	N	4.88
1	G	769:ALA	C	770:GLY	N	4.51
1	D	709:LYS	C	710:GLY	N	3.44
1	M	786:ILE	C	787:ILE	N	2.71

6 Tomogram visualisation [i](#)

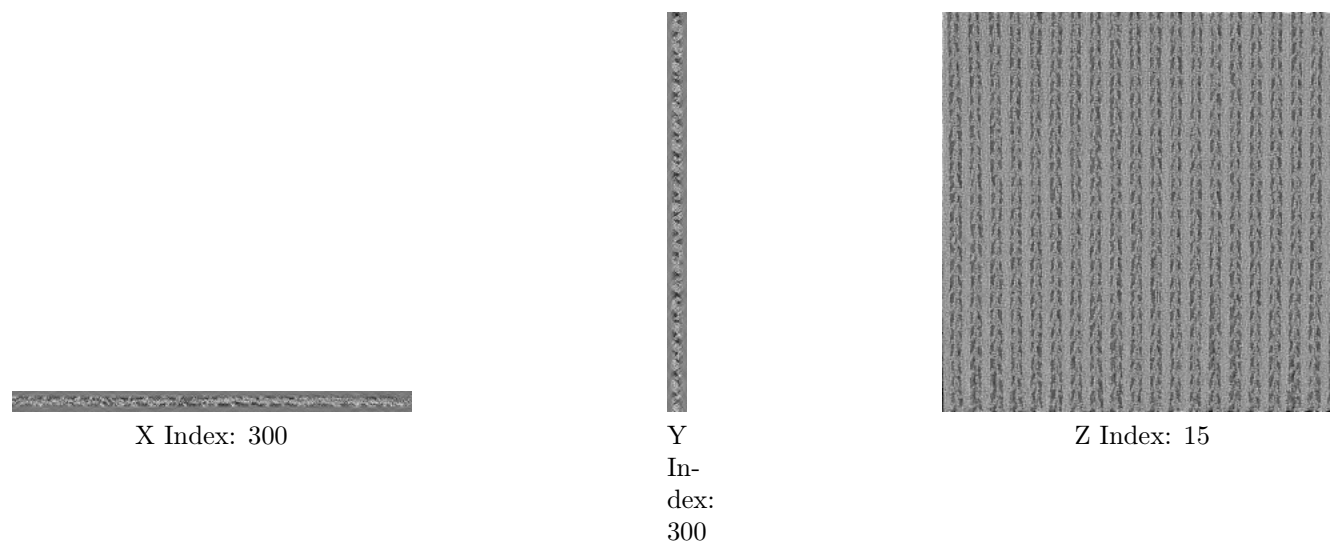
This section contains visualisations of the EMDB entry EMD-1001. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

6.1 Orthogonal projections [i](#)



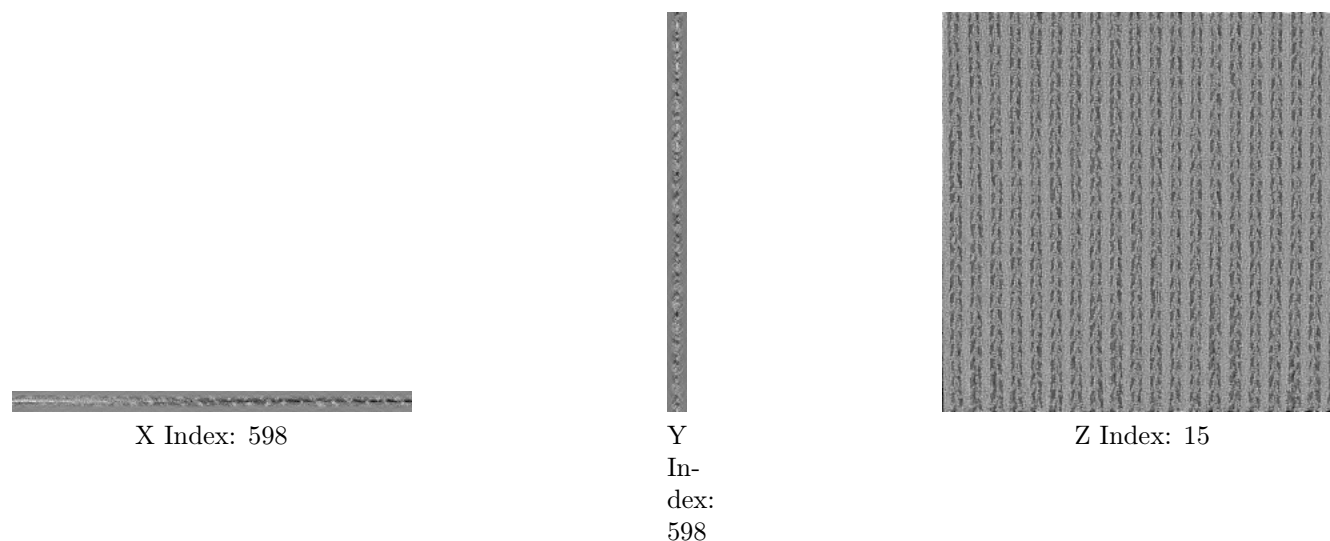
The images above show the tomogram projected in three orthogonal directions.

6.2 Central slices [i](#)



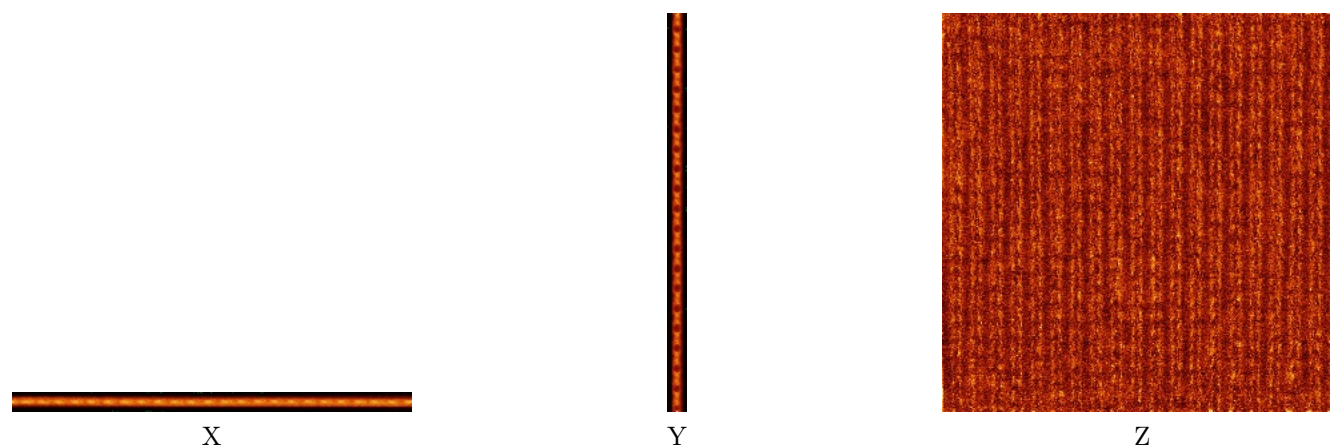
The images above show central slices of the tomogram in three orthogonal directions.

6.3 Largest variance slices [i](#)



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

6.4 Orthogonal standard-deviation projections (False-color) [i](#)



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

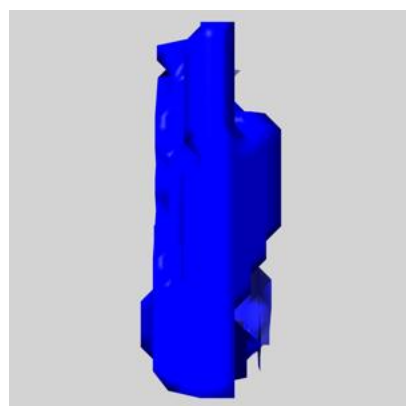
6.5 Mask visualisation [i](#)

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

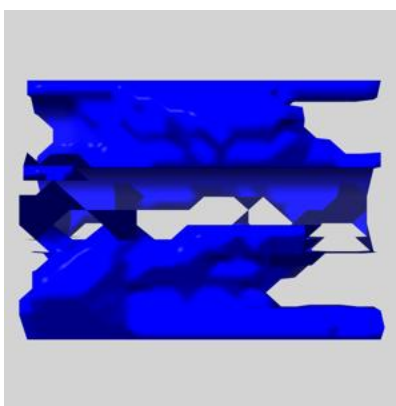
A mask typically either:

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

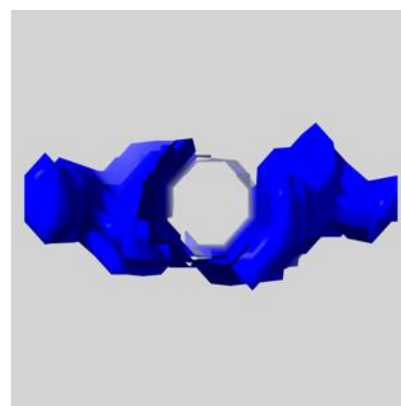
6.5.1 emd_1001_msk_25.map [i](#)



X

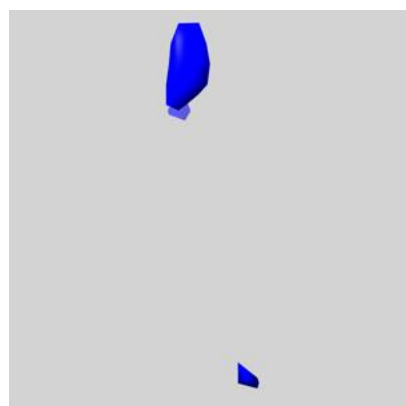


Y

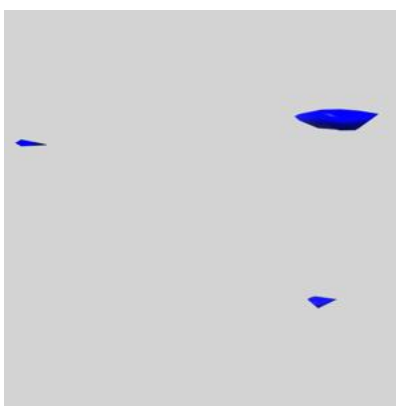


Z

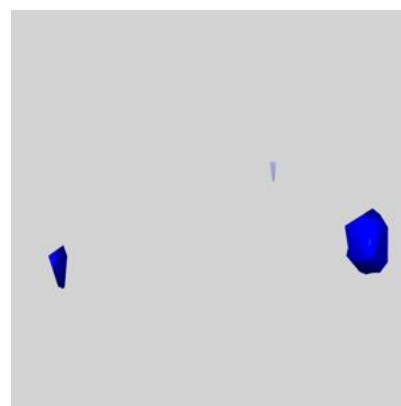
6.5.2 emd_1001_msk_24.map [i](#)



X

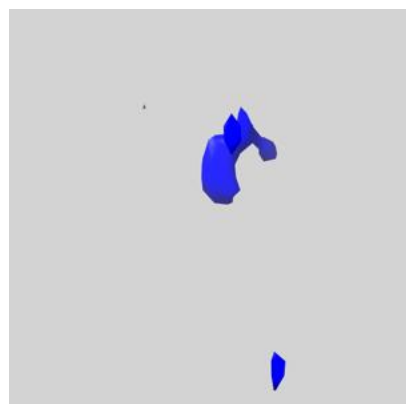


Y

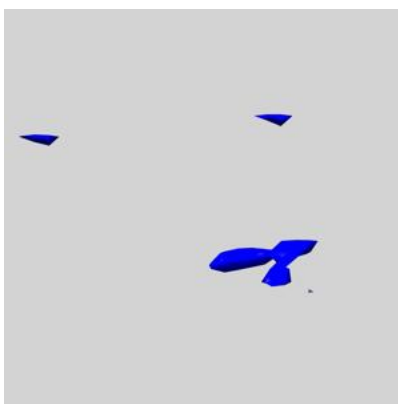


Z

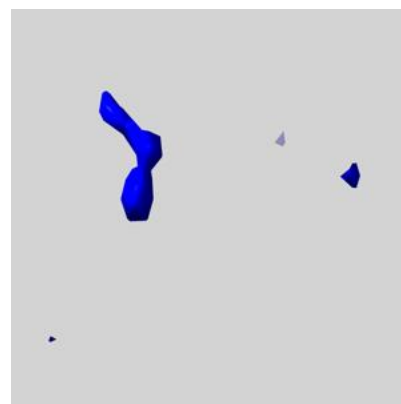
6.5.3 emd_1001_msk_23.map [i](#)



X

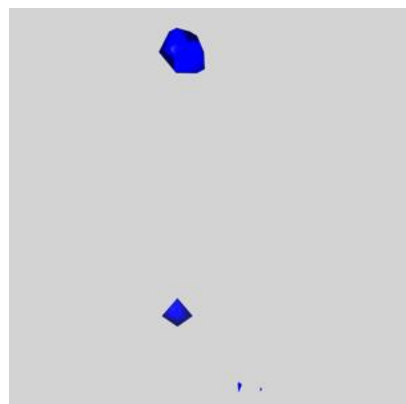


Y

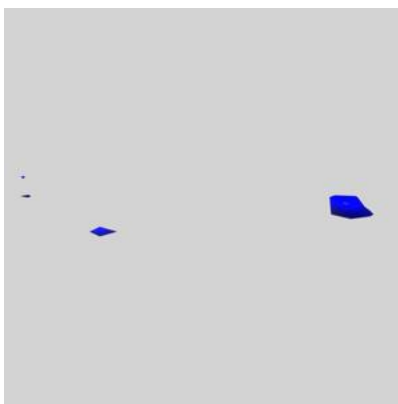


Z

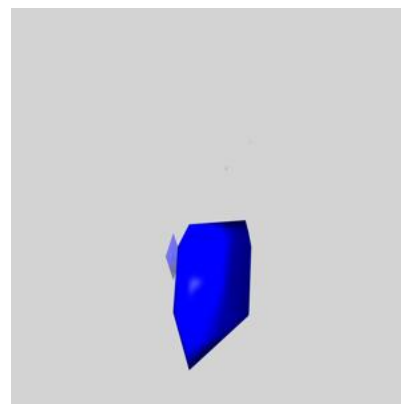
6.5.4 emd_1001_msk_22.map [i](#)



X

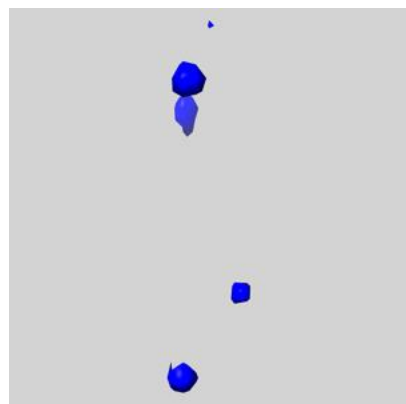


Y

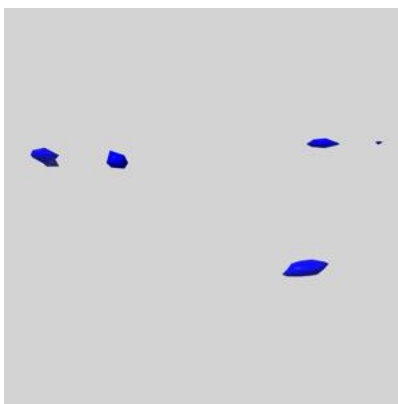


Z

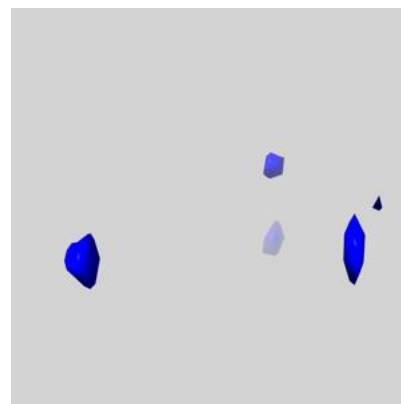
6.5.5 emd_1001_msk_21.map [i](#)



X

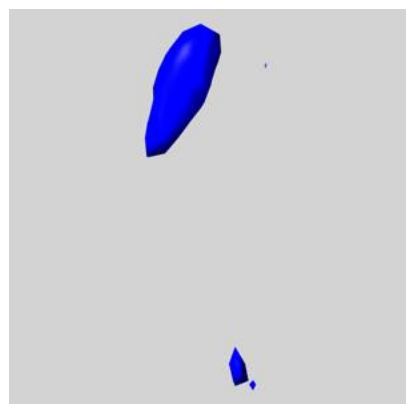


Y

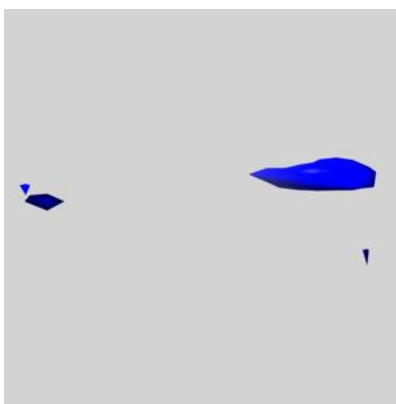


Z

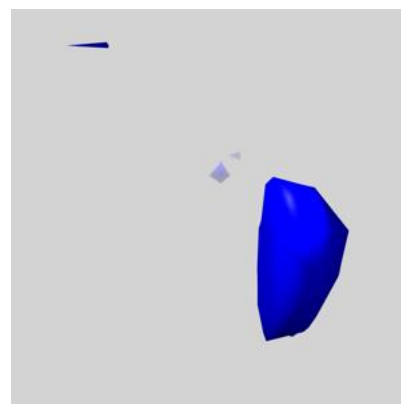
6.5.6 emd_1001_msk_20.map [i](#)



X

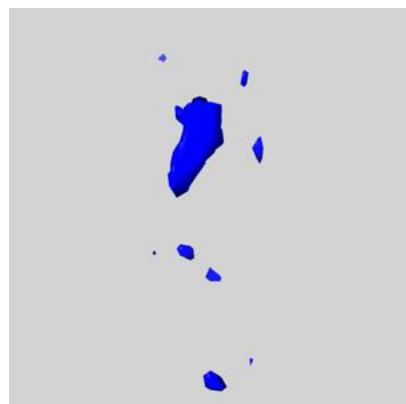


Y

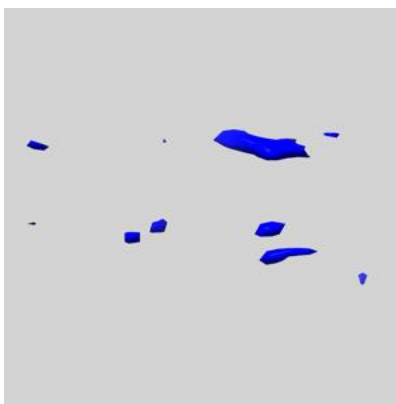


Z

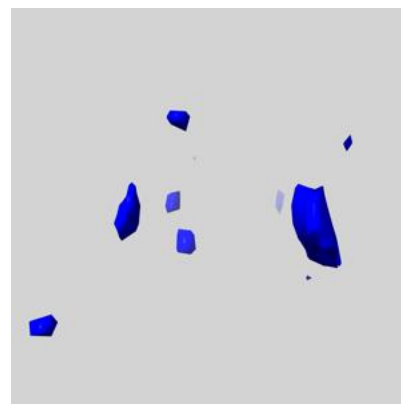
6.5.7 emd_1001_msk_19.map [i](#)



X

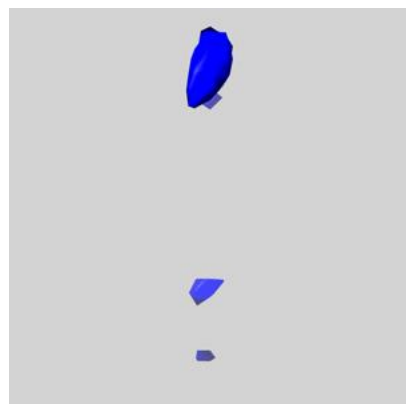


Y

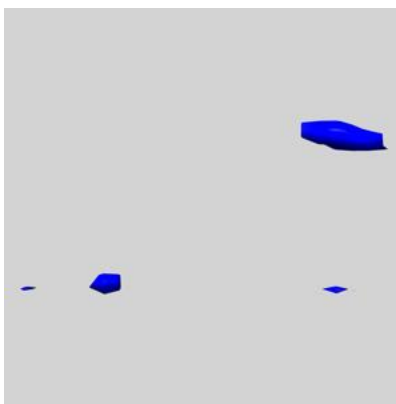


Z

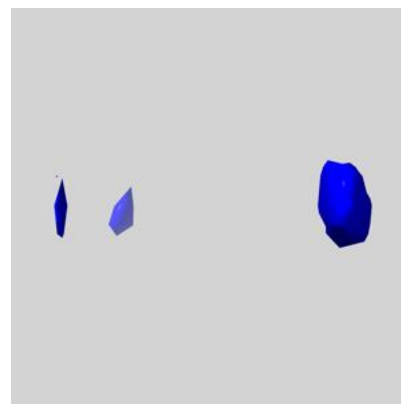
6.5.8 emd_1001_msk_18.map [i](#)



X

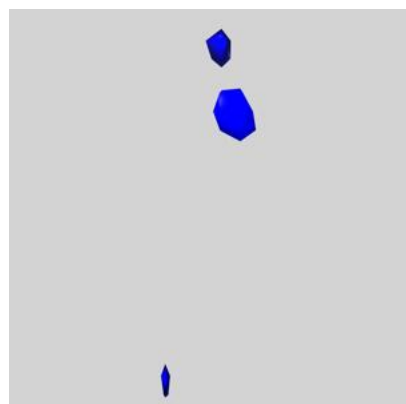


Y

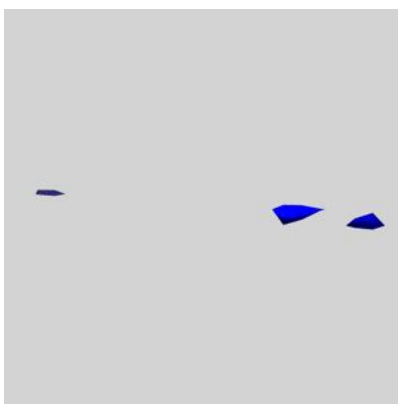


Z

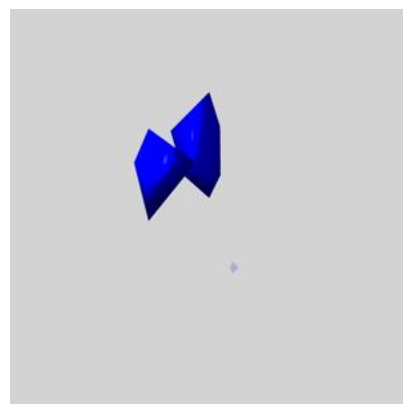
6.5.9 emd_1001_msk_17.map [i](#)



X

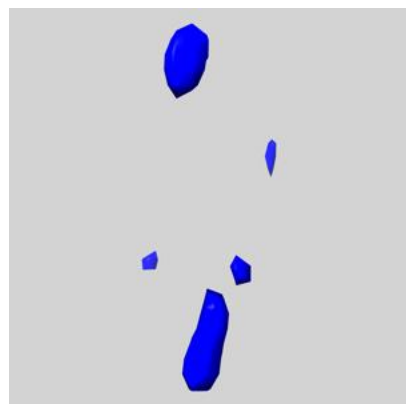


Y

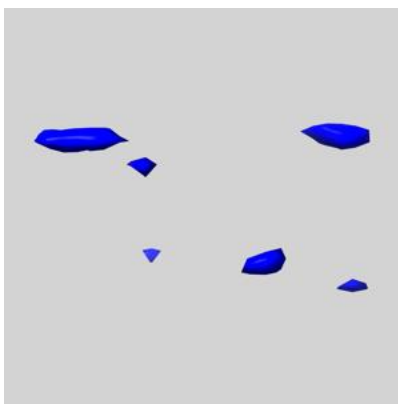


Z

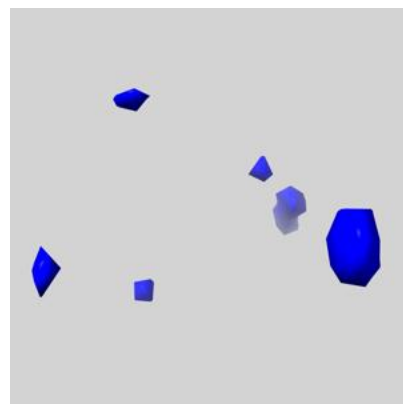
6.5.10 emd_1001_msk_16.map [i](#)



X

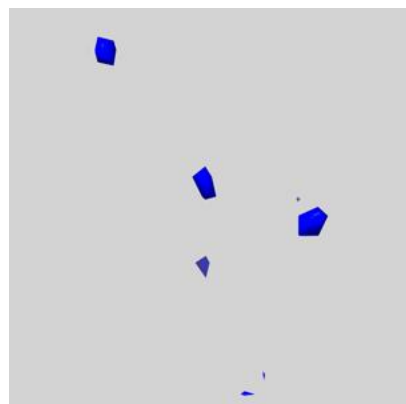


Y

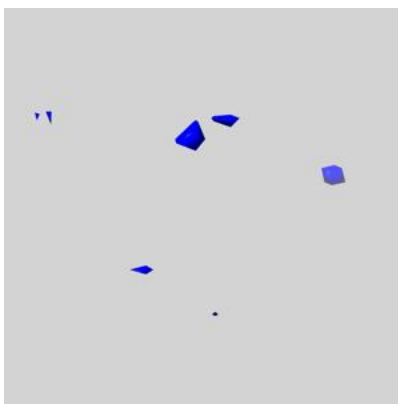


Z

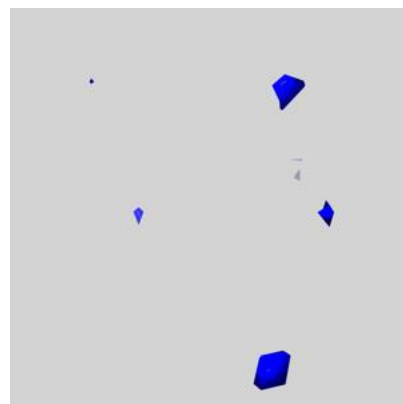
6.5.11 emd_1001_msk_15.map [i](#)



X

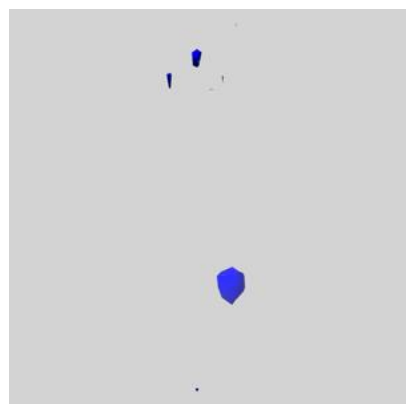


Y

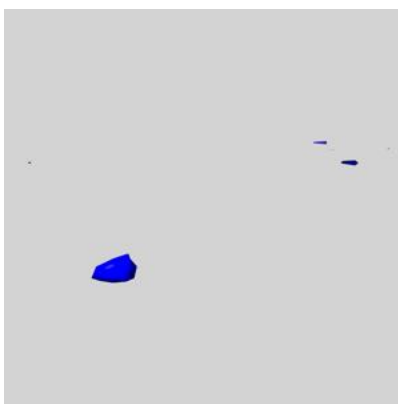


Z

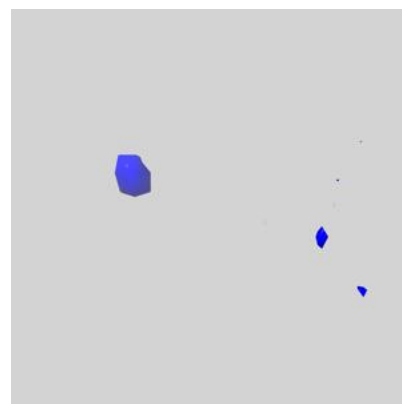
6.5.12 emd_1001_msk_14.map [i](#)



X

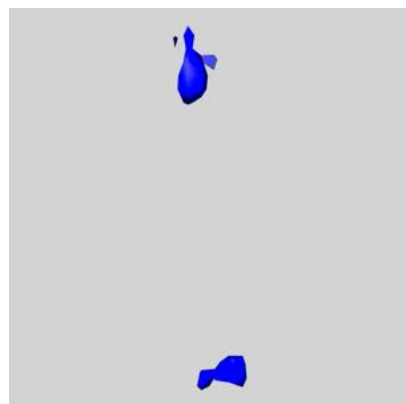


Y

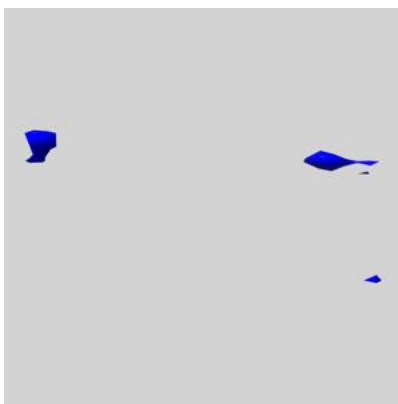


Z

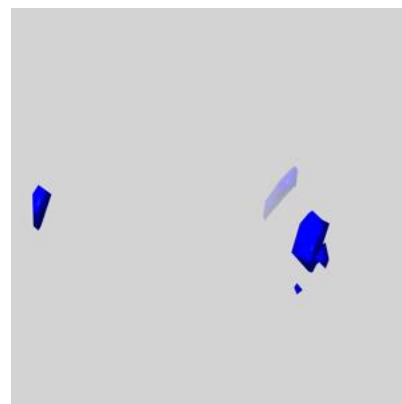
6.5.13 emd_1001_msk_13.map [i](#)



X

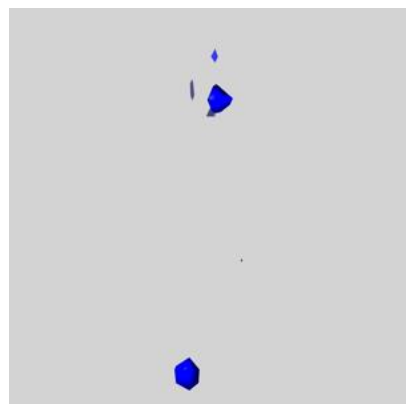


Y

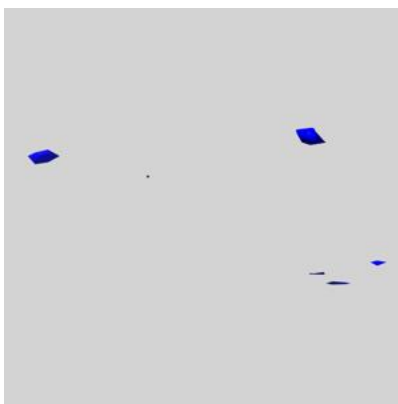


Z

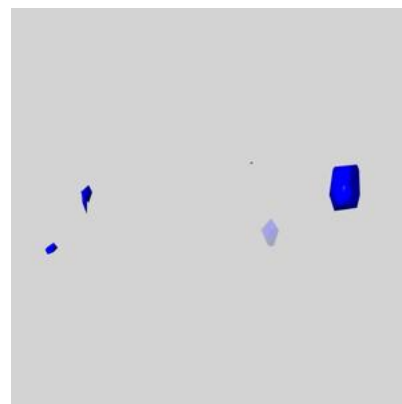
6.5.14 emd_1001_msk_12.map [i](#)



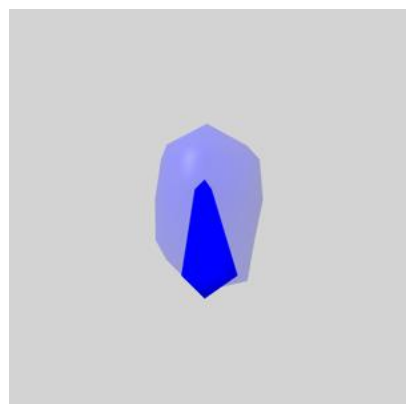
X



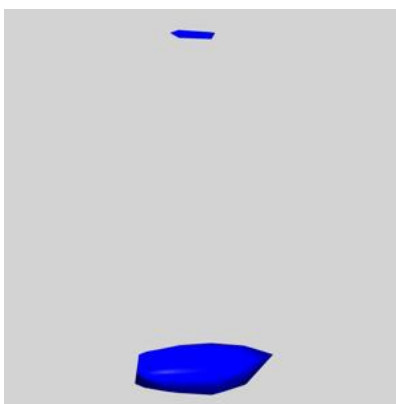
Y



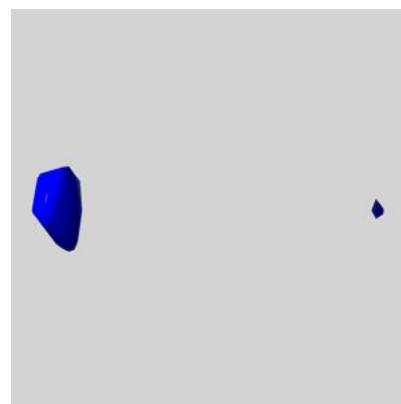
Z

6.5.15 emd_1001_msk_11.map [i](#)

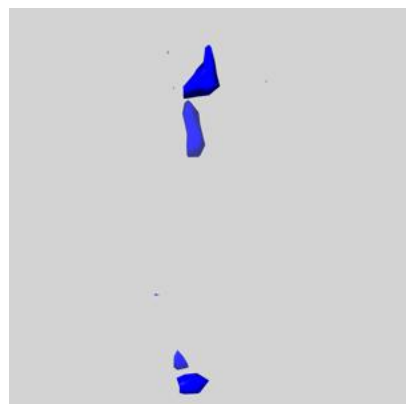
X



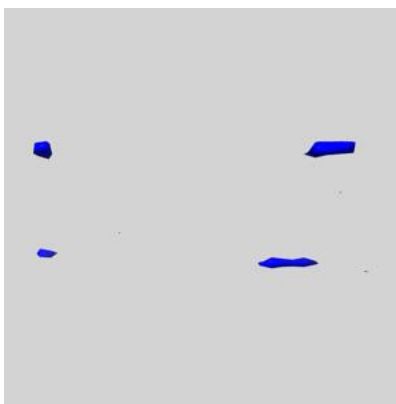
Y



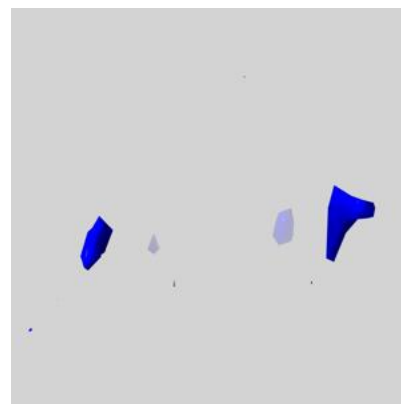
Z

6.5.16 emd_1001_msk_10.map [i](#)

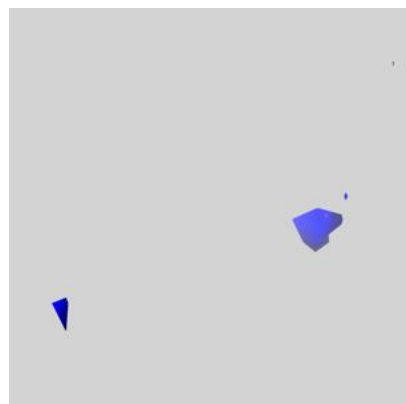
X



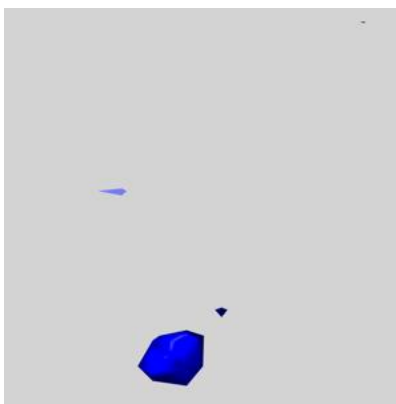
Y



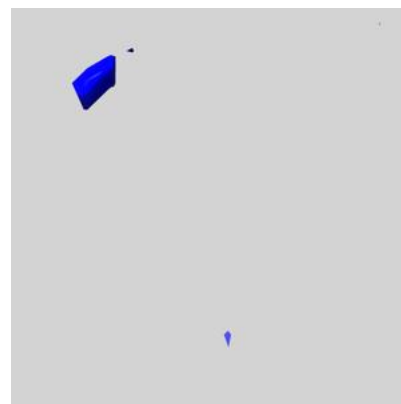
Z

6.5.17 emd_1001_msk_9.map [i](#)

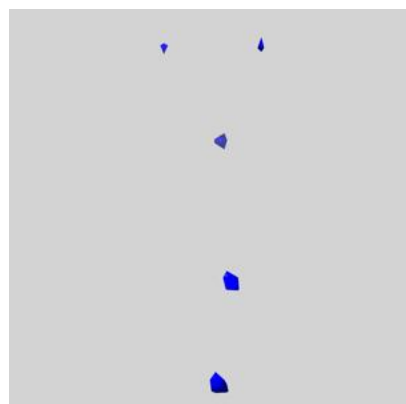
X



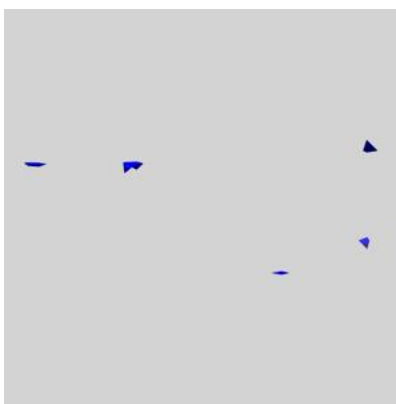
Y



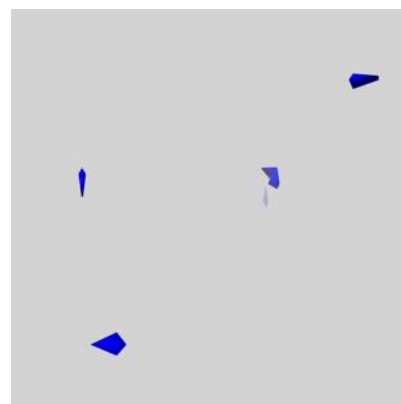
Z

6.5.18 emd_1001_msk_8.map [i](#)

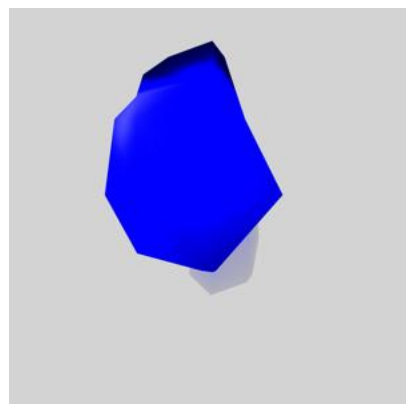
X



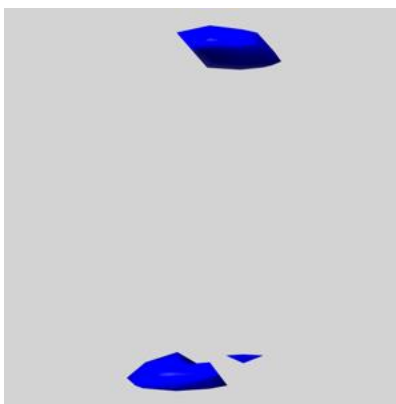
Y



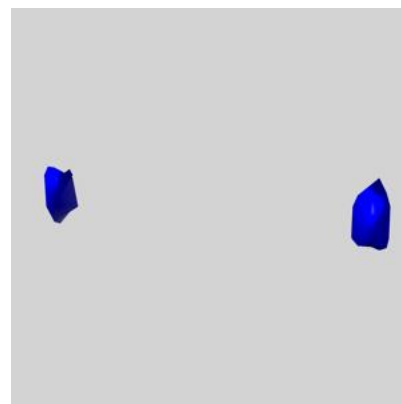
Z

6.5.19 emd_1001_msk_7.map [i](#)

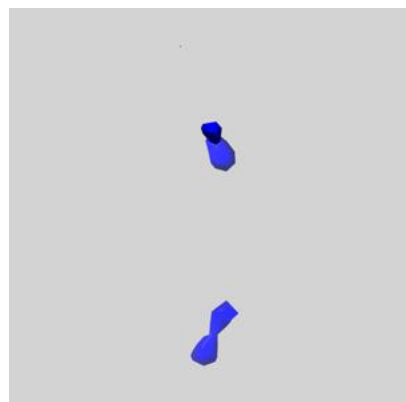
X



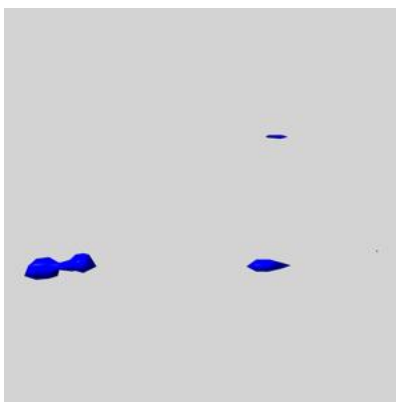
Y



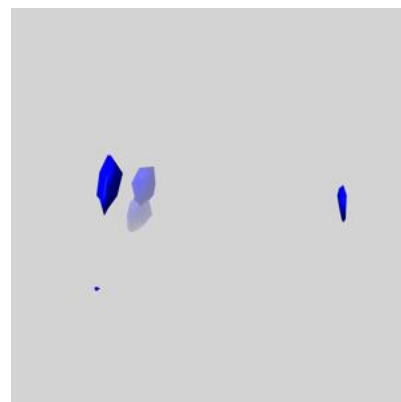
Z

6.5.20 emd_1001_msk_6.map [i](#)

X



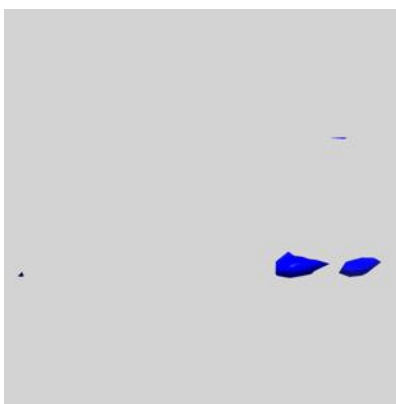
Y



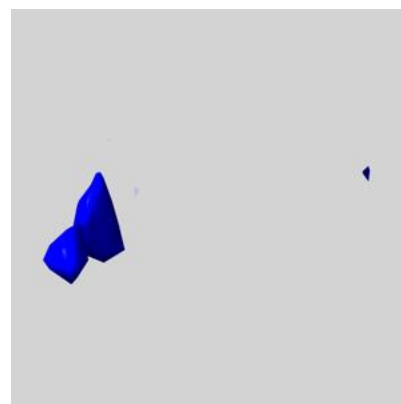
Z

6.5.21 emd_1001_msk_5.map [i](#)

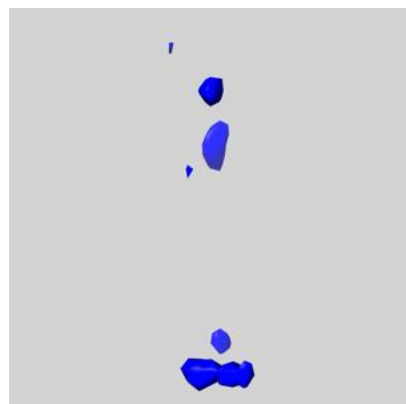
X



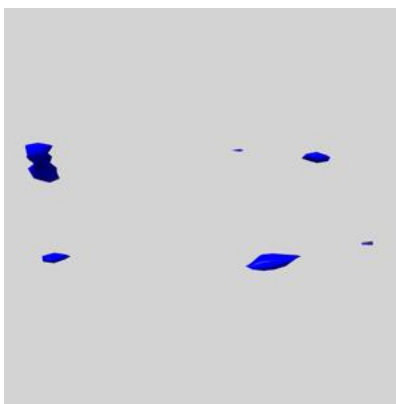
Y



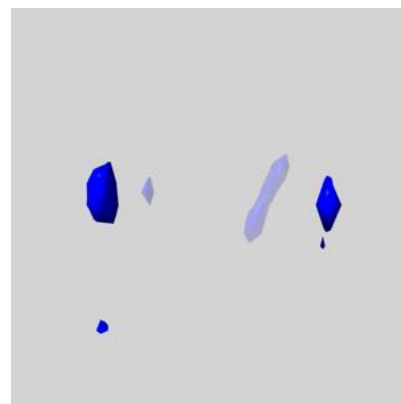
Z

6.5.22 emd_1001_msk_4.map [i](#)

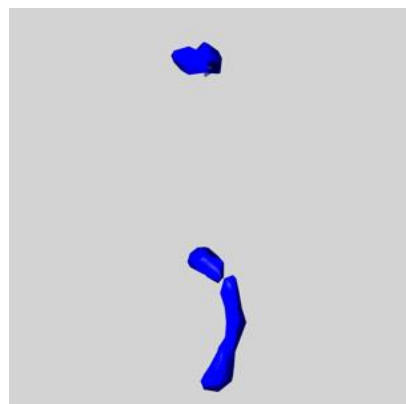
X



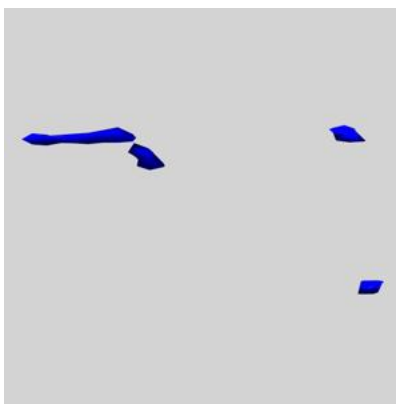
Y



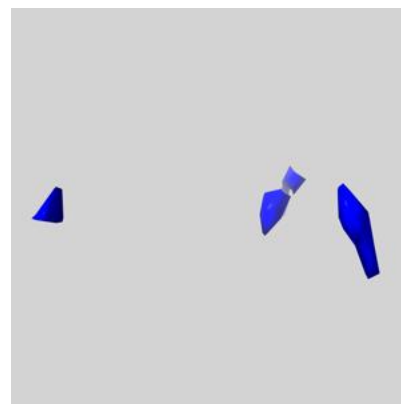
Z

6.5.23 emd_1001_msk_3.map [i](#)

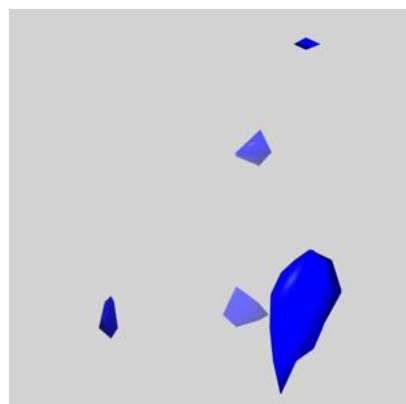
X



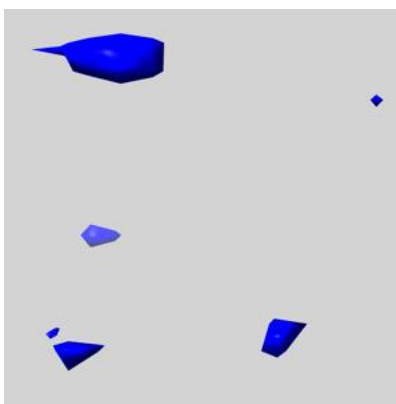
Y



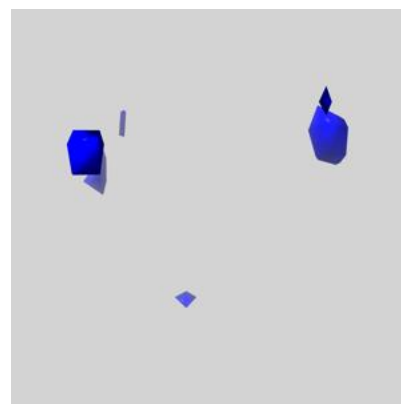
Z

6.5.24 emd_1001_msk_2.map [i](#)

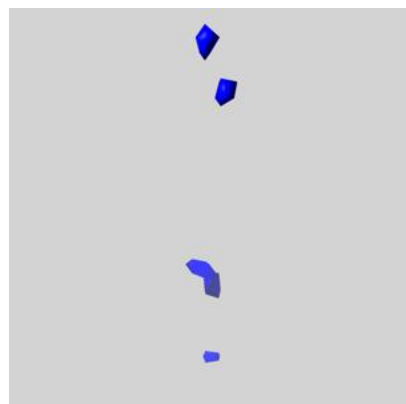
X



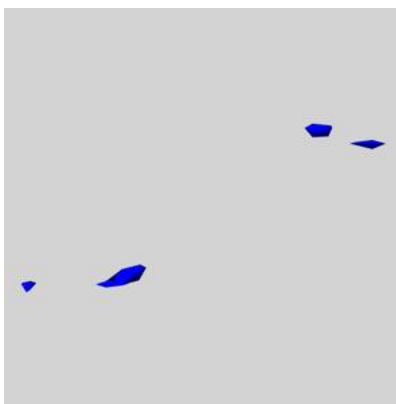
Y



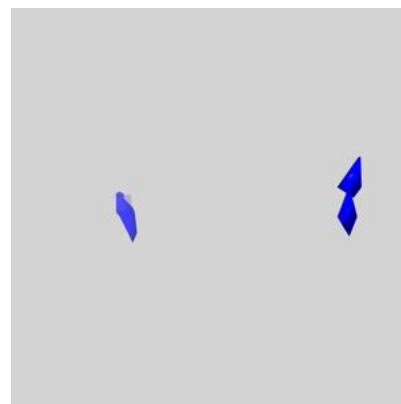
Z

6.5.25 emd_1001_msk_1.map [i](#)

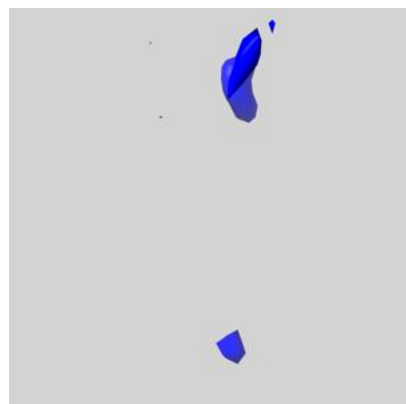
X



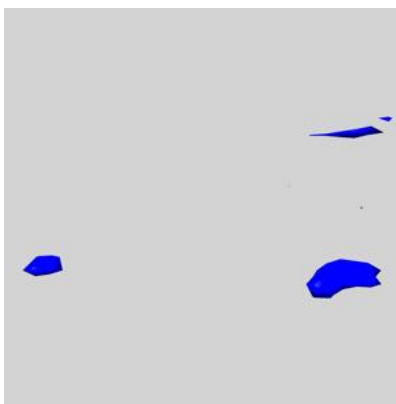
Y



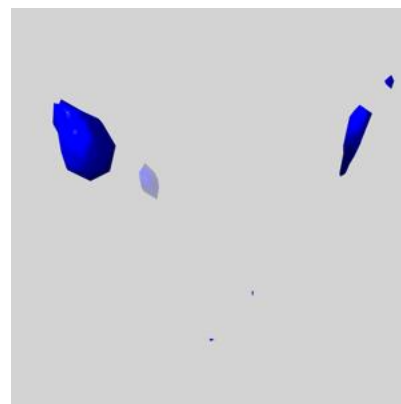
Z

6.5.26 emd_1001_msk_26.map [i](#)

X



Y

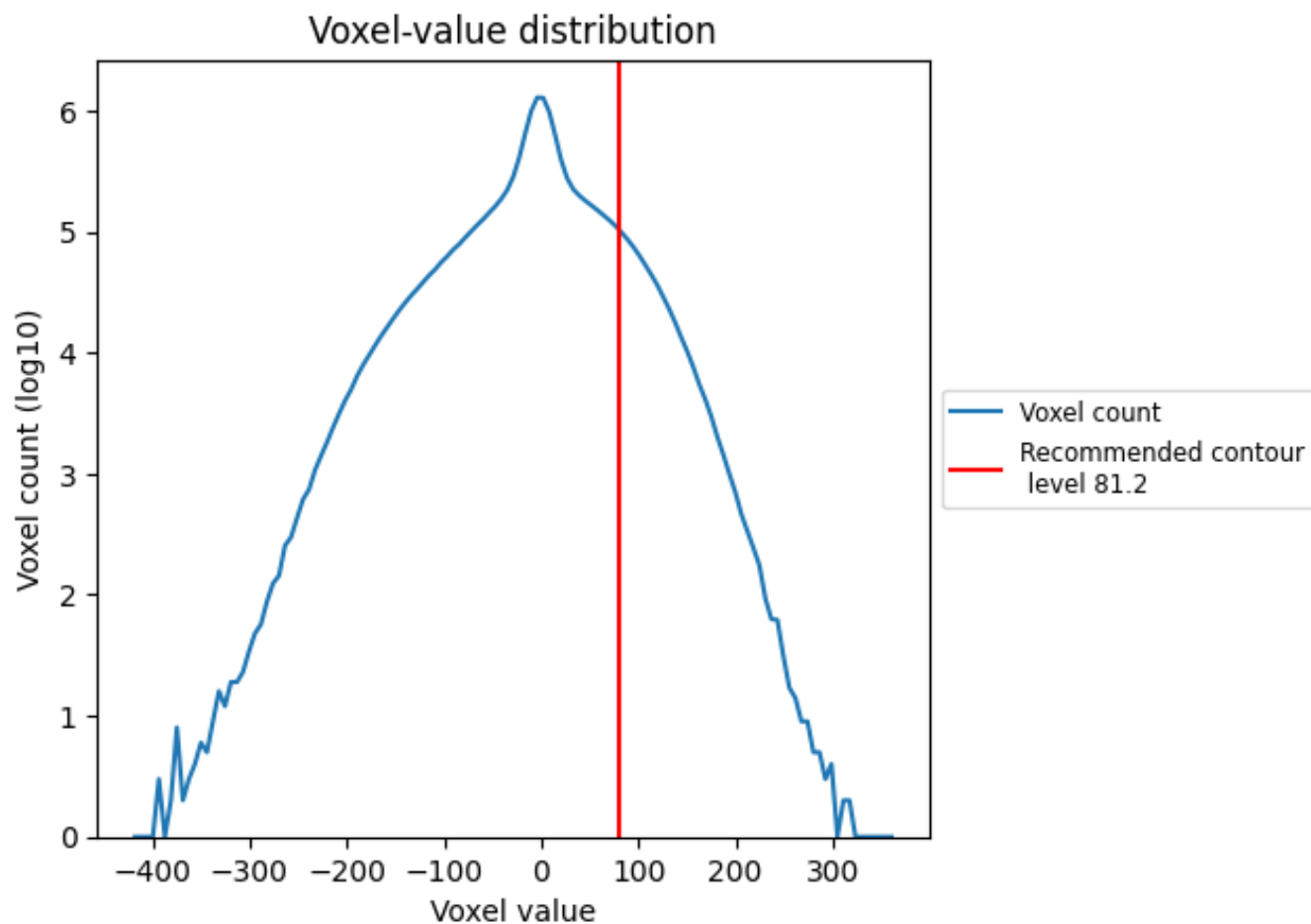


Z

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

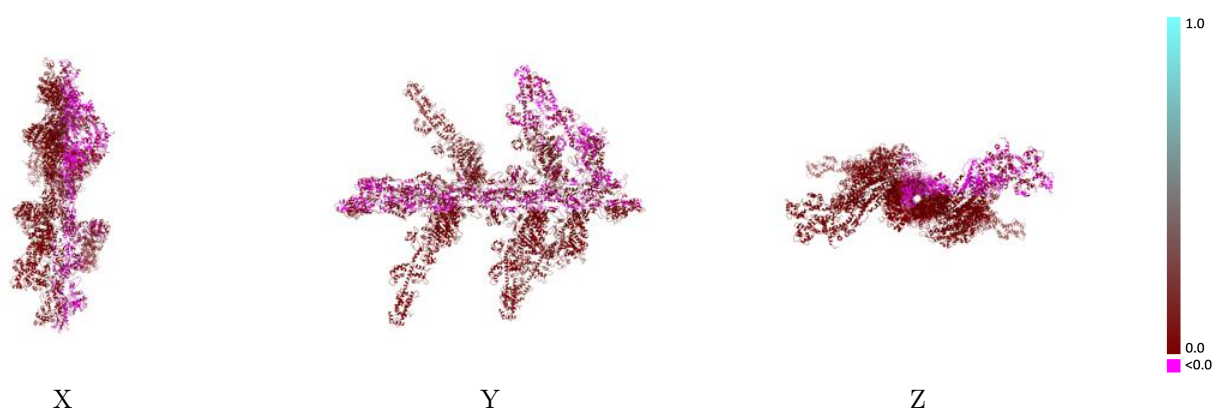
8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1001 and PDB model 1O1A. Per-residue inclusion information can be found in section 3 on page 7.

8.1 Map-model overlay [i](#)

This section was not generated.

8.2 Q-score mapped to coordinate model [i](#)

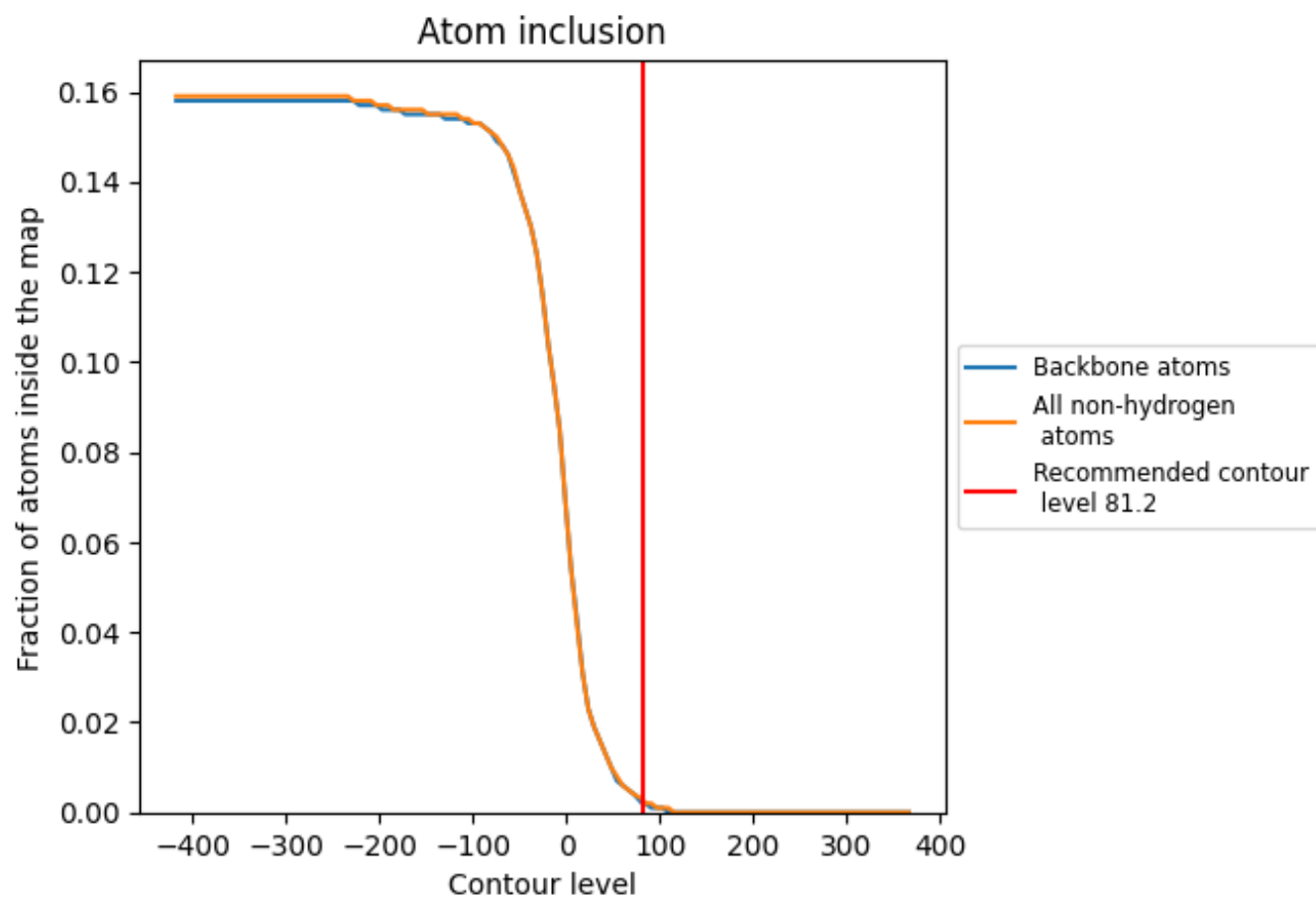


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (81.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0030	 -0.0010
1	 0.0010	 0.0110
2	 0.0000	 0.0000
3	 0.0000	 -0.0070
4	 0.0000	 -0.0060
5	 0.0000	 -0.0050
6	 0.0000	 -0.0070
7	 0.0000	 0.0140
8	 0.0000	 -0.0050
9	 0.0000	 0.0020
A	 0.0000	 -0.0140
B	 0.0000	 -0.0020
C	 0.0000	 0.0120
D	 0.0000	 0.0000
E	 0.0000	 0.0000
F	 0.0000	 0.0000
G	 0.0000	 0.0060
H	 0.0000	 -0.0090
I	 0.0700	 0.0020
J	 0.0000	 -0.0020
K	 0.0000	 0.0000
L	 0.0000	 0.0000
M	 0.0000	 0.0000
N	 0.0000	 0.0000
O	 0.0000	 0.0000
P	 0.0000	 0.0020
Q	 0.0000	 0.0000
R	 0.0000	 0.0000
V	 0.0000	 -0.0010
W	 0.0000	 -0.0080
X	 0.0000	 -0.0030
Y	 0.0550	 -0.0020
Z	 0.0000	 0.0040

