



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 05:55 AM UTC

PDB ID : 1GRU / pdb_00001gru
EMDB ID : EMD-1046
Title : SOLUTION STRUCTURE OF GROES-ADP7-GROEL-ATP7 COMPLEX BY CRYO-EM
Authors : Ranson, N.A.; Farr, G.W.; Roseman, A.M.; Gowen, B.; Fenton, W.A.; Horwich, A.L.; Saibil, H.R.
Deposited on : 2001-12-16
Resolution : 12.50 Å(reported)
Based on initial model : 1GRU

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
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

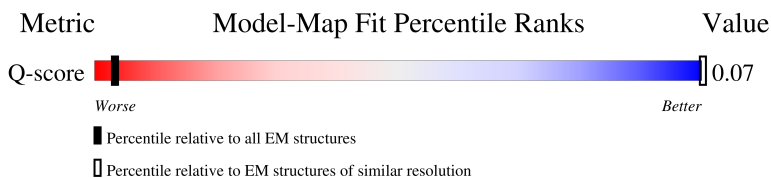
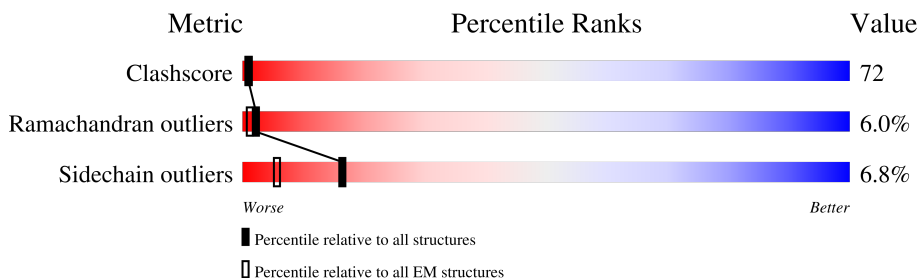
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 12.50 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.



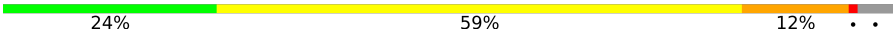
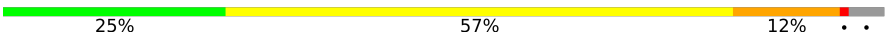
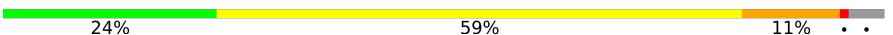
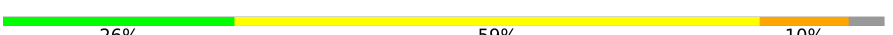
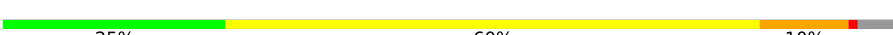
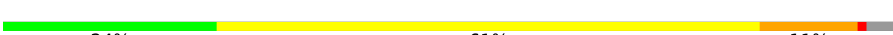
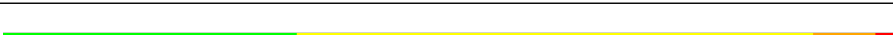
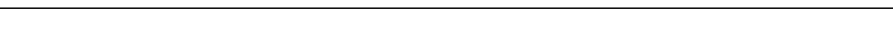
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	22 (23.00 - 24.00)

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	547	
1	B	547	
1	C	547	
1	D	547	

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Mol	Chain	Length	Quality of chain
1	E	547	 24% 59% 12% . .
1	F	547	 25% 57% 12% . .
1	G	547	 24% 59% 11% . .
1	H	547	 26% 59% 10% . .
1	I	547	 24% 61% 10% . .
1	J	547	 26% 59% 10% .
1	K	547	 25% 60% 10% . .
1	L	547	 24% 61% 11% . .
1	M	547	 24% 61% 10% . .
1	N	547	 25% 61% 10% . .
2	O	97	 30% 63% 6% .
2	P	97	 33% 58% 7% .
2	Q	97	 27% 62% 9% .
2	R	97	 26% 64% 10%
2	S	97	 28% 63% 8% .
2	T	97	 29% 59% 11% .
2	U	97	 28% 61% 10% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 58688 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 GROEL.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	B	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	C	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	D	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	E	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	F	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	G	525	Total	C	N	O	S	0	1
			3809	2368	654	767	20		
1	H	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	I	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	J	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	K	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	L	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	M	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		
1	N	525	Total	C	N	O	S	0	1
			3850	2394	663	773	20		

- Molecule 2 is a protein called GROES.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	97	Total	C	N	O	S	0	0
			725	452	127	145	1		

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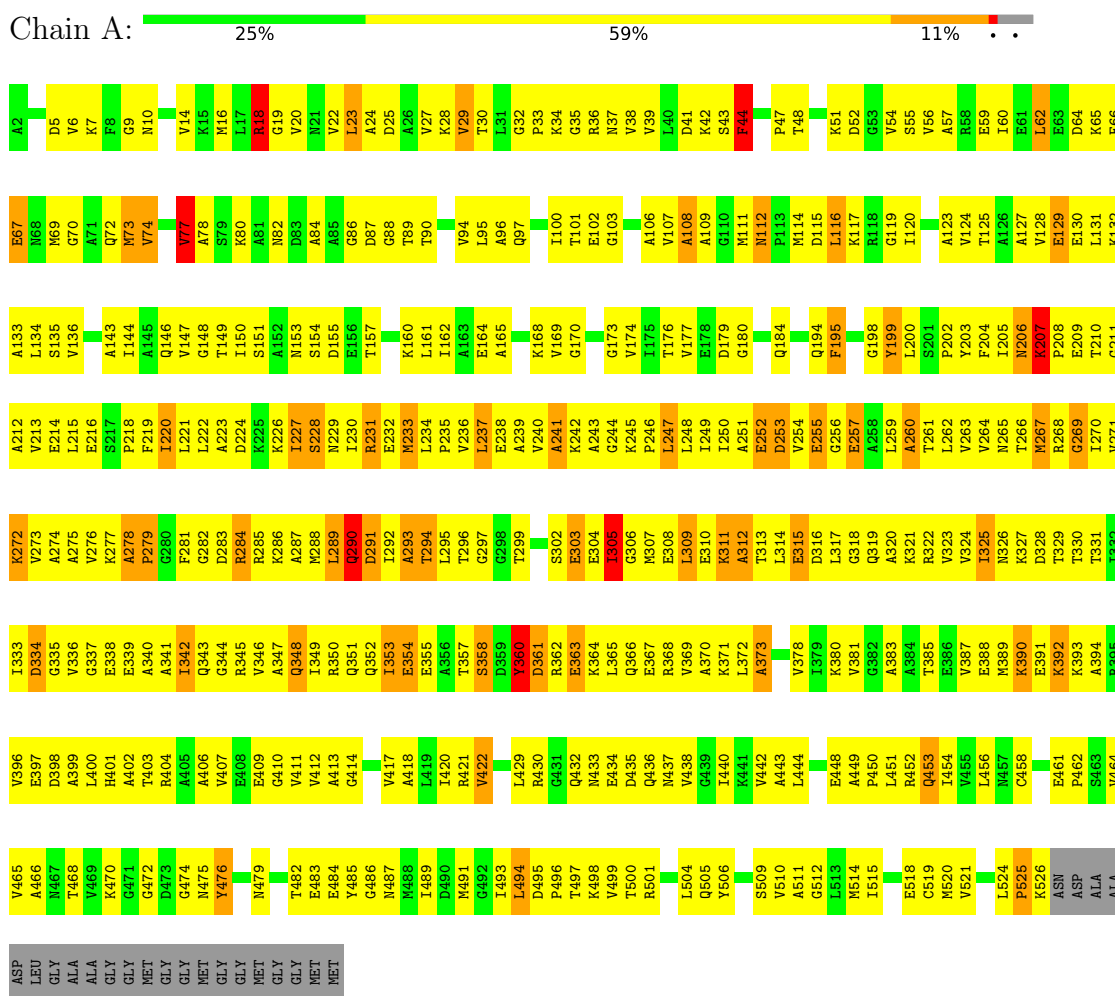
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Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	97	Total 725	C 452	N 127	O 145	S 1	0	0
2	Q	97	Total 725	C 452	N 127	O 145	S 1	0	0
2	R	97	Total 725	C 452	N 127	O 145	S 1	0	0
2	S	97	Total 725	C 452	N 127	O 145	S 1	0	0
2	T	97	Total 725	C 452	N 127	O 145	S 1	0	0
2	U	97	Total 725	C 452	N 127	O 145	S 1	0	0

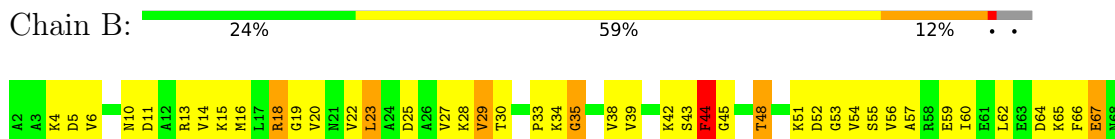
3 Residue-property plots

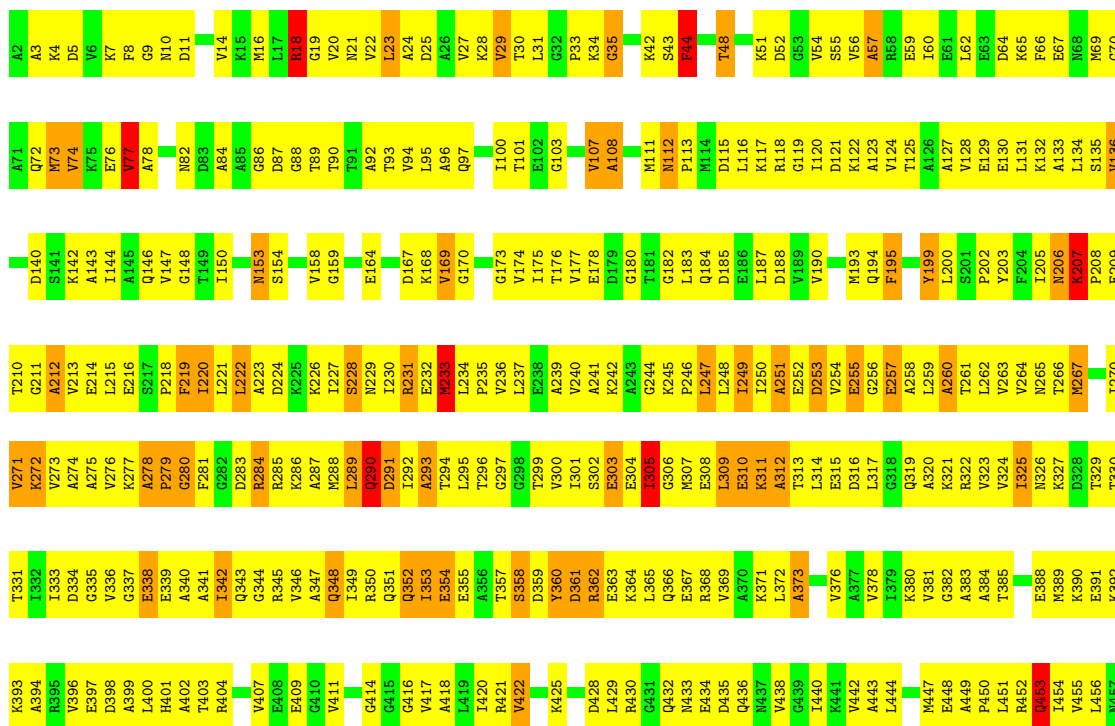
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

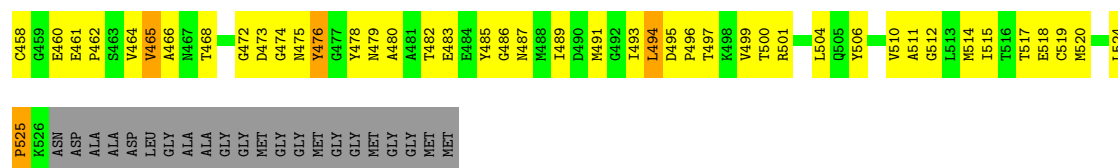
• Molecule 1: GROEL



• Molecule 1: GROEL

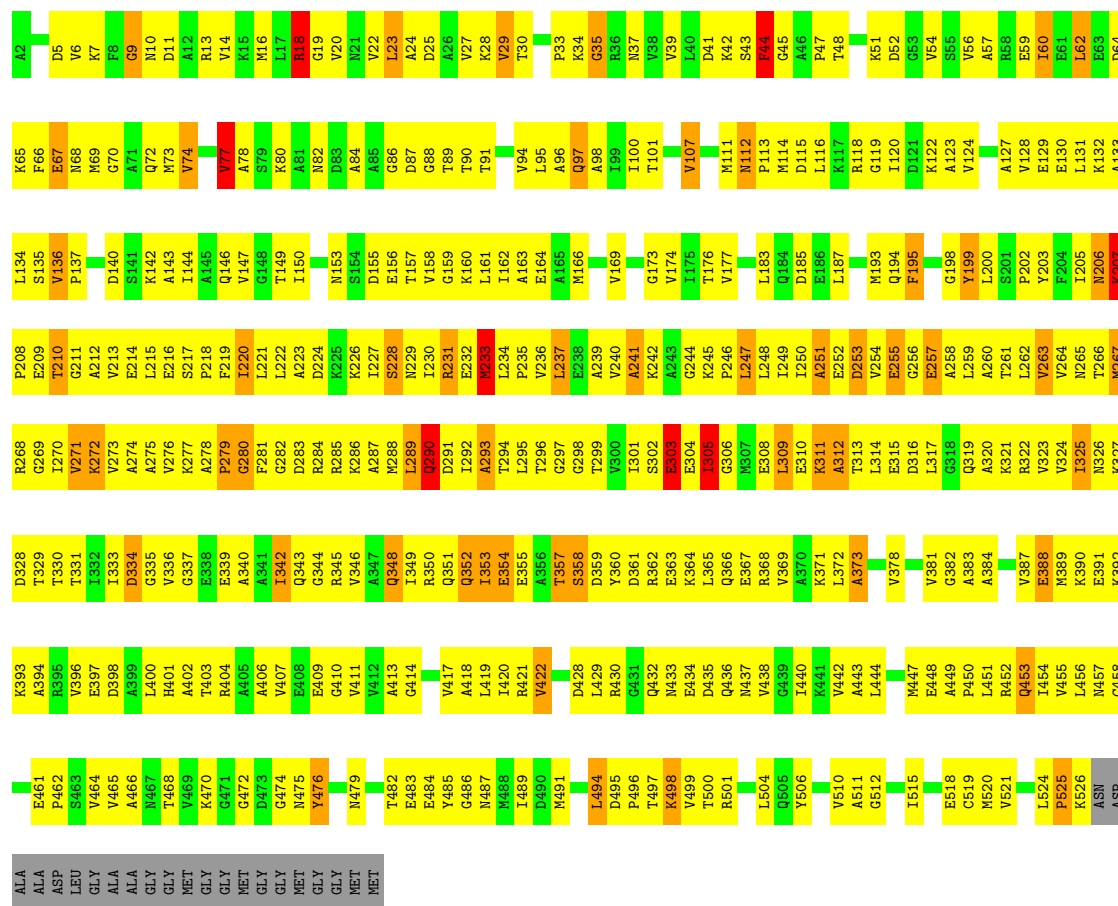






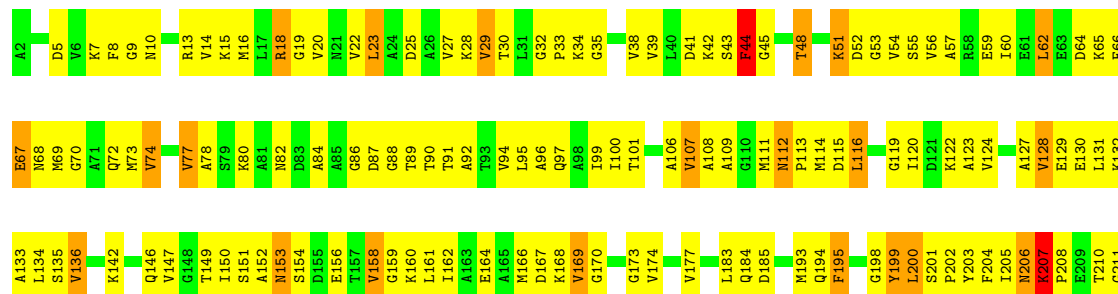
• Molecule 1: GROEL

Chain D: 25% 59% 10% . .

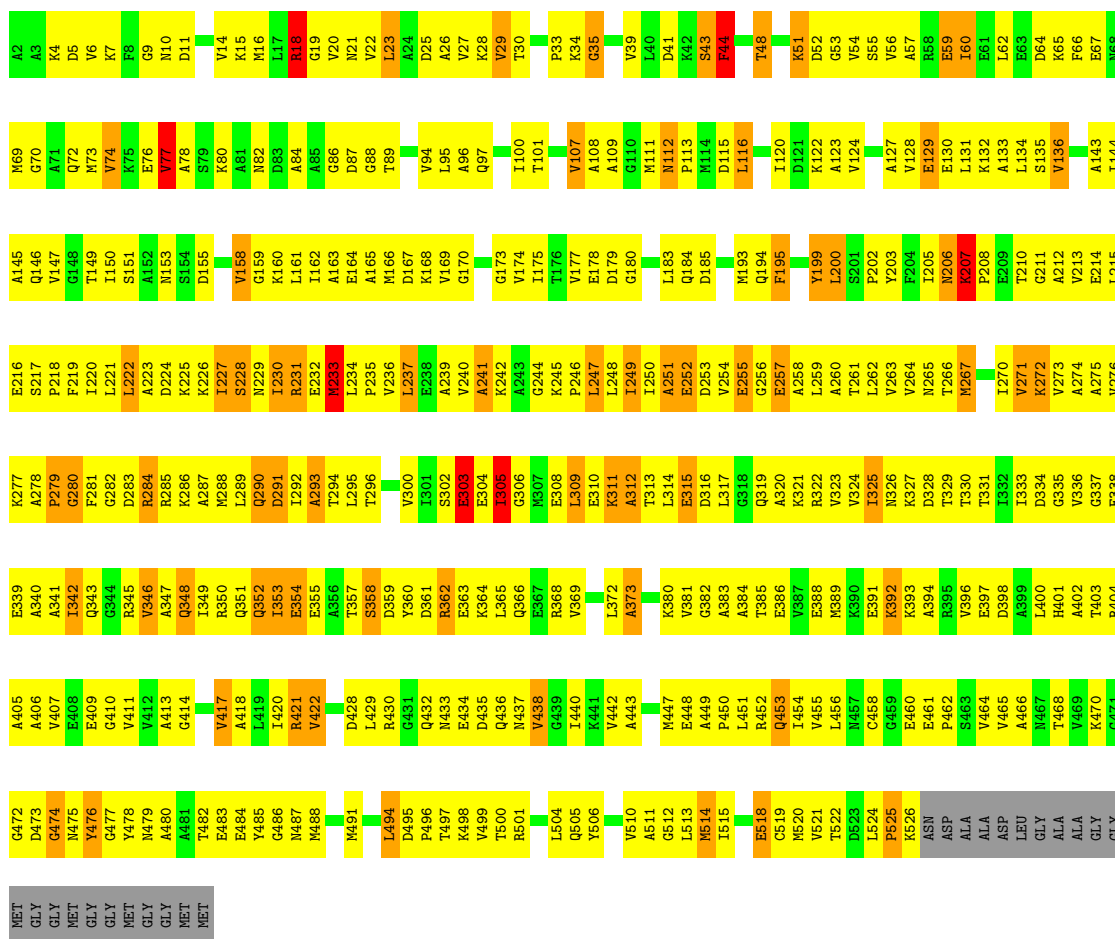


• Molecule 1: GROEL

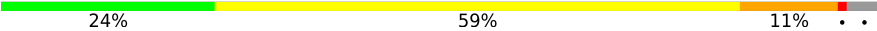
Chain E: 24% 59% 12% . .

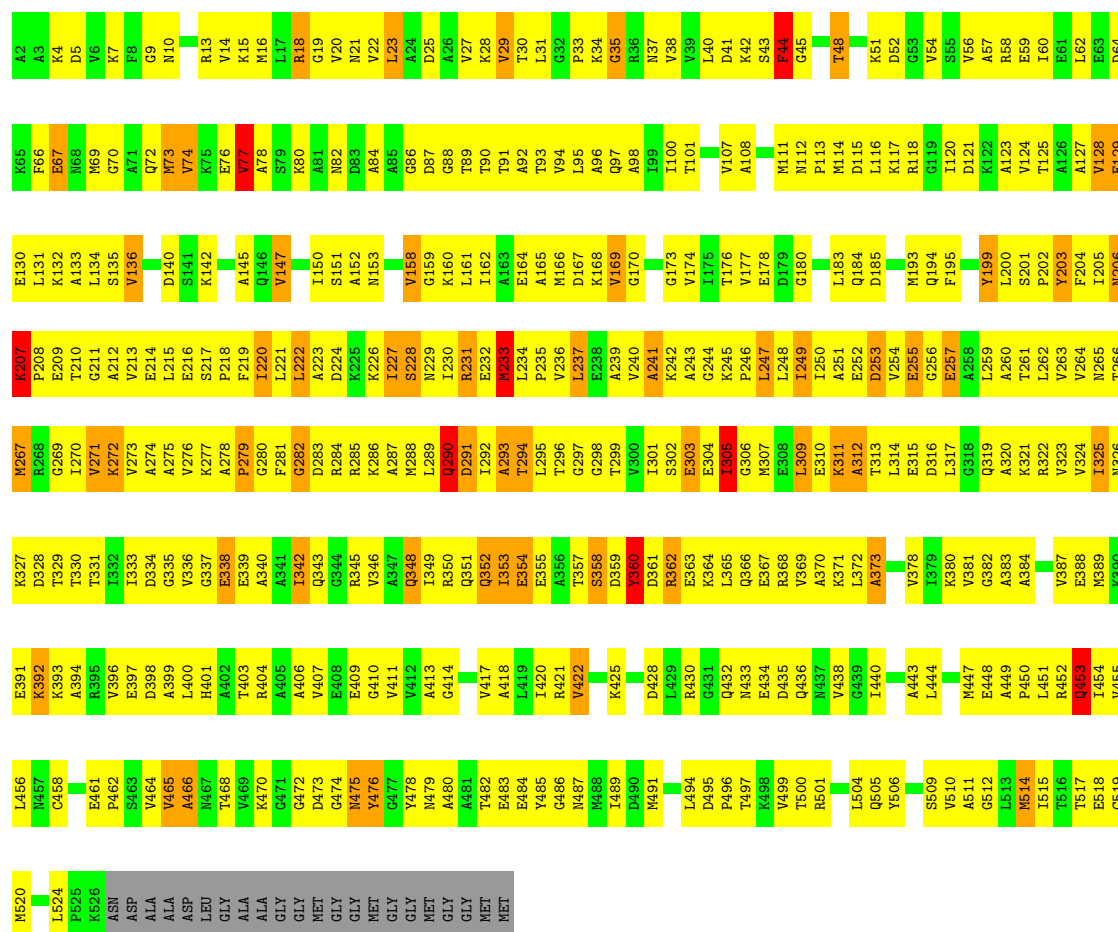


- Molecule 1: GROEL



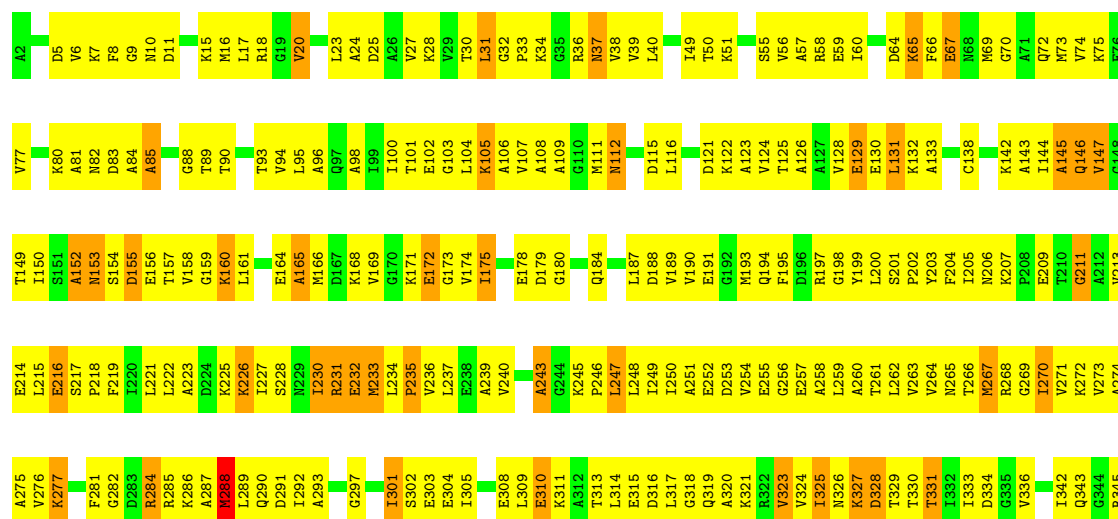
- Molecule 1: GROEL

Chain G:  24% 59% 11% . .



• Molecule 1: GROEL

Chain H:  26% 59% 10% . .



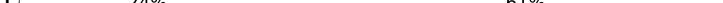
Q72	M73	K141	S141	E209	L270	G385	E387	P462	GLY
M73	K142	T210	K142	T210	V271	V336	D388	S463	ALA
V74	I143	G211	I143	G211	K272	E339	A399	V465	ALA
K75	I144	A212	I144	A212	V273	L400	L400	V466	GLY
E76	A145	V213	A145	V213	A274	H401	H401	A466	GLY
V77	Q146	E214	Q146	E214	A275	A402	A402	V469	MET
N82	V147	L215	V147	L215	V276	T403	T403	V469	GLY
A85	G148	E216	G148	E216	K277	R404	R404	G474	GLY
G88	T149	S217	T149	S217	F281	A405	A405	G474	MET
T89	I150	F218	I150	F218	G282	A406	A406	N475	GLY
T90	S151	F219	S151	F219	D283	V407	V407	N476	GLY
T93	A152	G220	A152	G220	R284	E408	E408	G477	MET
V94	N153	L221	V94	N153	R285	I349	I349	N478	GLY
L95	S154	L222	L95	S154	R286	G410	G410	E483	GLY
A96	D155	A223	A96	D155	K286	V411	V411	E483	MET
Q97	E156	D224	Q97	E156	A287	G413	G413	E484	MET
A98	T157	K225	A98	T157	M288	G414	G414	Y485	ALA
I100	V158	K226	I100	V158	Q289	G415	G415	G486	ALA
T101	A159	L227	T101	A159	D291	G416	G416	N487	ALA
E102	K160	S228	E102	K160	L292	G417	G417	N488	ALA
G163	L161	M229	G163	L161	L293	E489	E489	D490	ALA
L104	E164	R230	L104	E164	A293	A418	A418	L493	ALA
K105	A165	E232	K105	A165	T294	L419	L419	L494	ALA
A106	G170	M233	A106	G170	T295	G359	G359	D495	ALA
V107	D167	L234	V107	D167	G297	D361	D361	P496	ALA
A108	K168	P235	A108	K168	I301	E363	E363	T497	ALA
A109	V169	V236	A109	V169	S302	K364	K364	K498	ALA
G110	G171	L237	G110	G171	E303	L365	L365	N499	ALA
M111	K171	E238	M111	K171	E304	Q366	Q366	T500	ALA
P113	A172	A239	P113	A172	I305	E367	E367	S501	ALA
M114	G173	V240	M114	G173	E308	R368	R368	S502	ALA
D115	V174	G180	D115	V174	L309	Q432	Q432	A503	ALA
L116	I175	G180	L116	I175	E310	L504	L504	Q505	ALA
K117	G186	G180	K117	G186	K311	K371	K371	Y506	ALA
I120	L187	G186	I120	L187	E312	L372	L372	S509	ALA
D121	D188	L247	D121	D188	T313	G374	G374	V510	ALA
K122	V189	L248	K122	V189	L314	V376	V376	G512	ALA
A123	V190	L249	A123	V190	E315	V438	V438	T515	ALA
T125	E191	A251	T125	E191	D316	Q439	Q439	T516	ALA
V128	G192	D253	V128	G192	L317	L440	L440	C519	ALA
E129	M193	V254	E129	M193	Q318	K380	K380	V520	ALA
E130	Q194	E255	E130	Q194	G319	V381	V381	V521	ALA
L131	F195	G256	L131	F195	A320	G382	G382	T522	ALA
K132	D196	E257	K132	D196	K321	A384	A384	D523	ALA
S135	R197	A258	S135	R197	V323	T385	T385	P525	ALA
V136	G198	L259	V136	G198	V324	E386	E386	K526	ALA
P137	Y199	A260	P137	Y199	I325	V387	V387	ASP	ALA
C138	L200	L261	C138	L200	K326	E388	E388	ASP	ALA
S139	S201	T261	S139	S201	D328	K390	K390	ASP	ALA
P139	P202	V263	P139	P202	T329	E391	E391	ASP	ALA
C139	Y203	V264	C139	Y203	T330	N457	N457	ASP	ALA
N206	F204	V265	N206	F204	T331	C458	C458	ASP	ALA
K207	I205	T266	K207	I205	I332	G459	G459	ASP	ALA
S139	N206	M267	S139	N206	D334	E461	E461	LEU	ALA
D140	P208	G269	D140	P208					

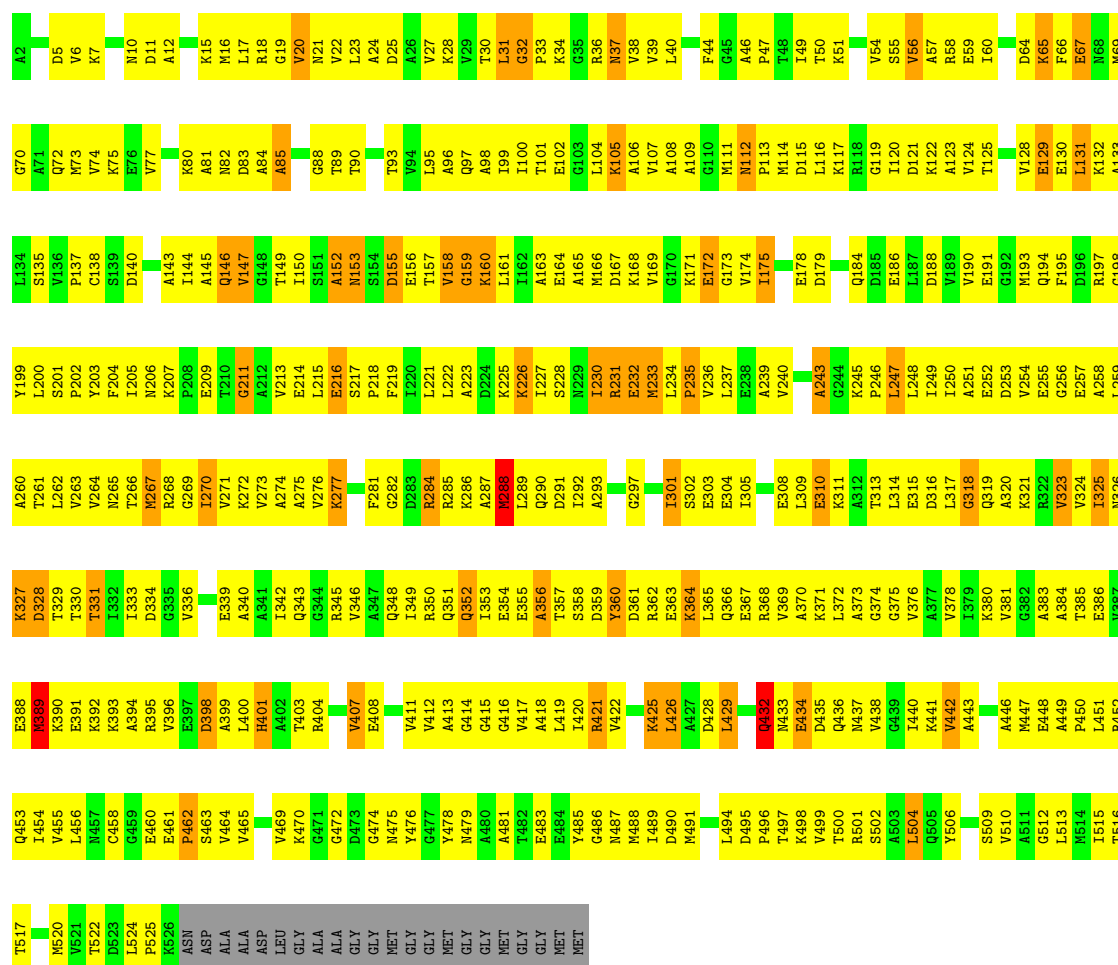
• Molecule 1: GROEL

Chain K:  25% 60% 10%

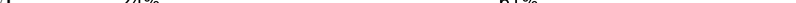
A2	D5	V77	A143	P208	G269	D334	V396
D5	V6	A81	I144	E209	I270	G335	E397
K7	N82	N82	Q145	G211	V271	V336	D398
F8	D83	D83	A146	A212	K272	E339	A399
N10	A84	A84	V147	E213	A274	A340	L400
G9	A85	A85	G148	E214	A275	A341	H401
D11	G88	G88	T149	L216	V276	I342	A402
K15	T89	T89	I150	E216	K277	Q343	A402
M16	T90	T90	M153	S217	F281	G344	R404
L17	T91	T91	S154	P218	G282	G345	A405
R18	A92	A92	D155	F219	D283	V346	A406
G19	T93	T93	E156	L220	R284	A347	V407
V20	Y94	Y94	T157	L221	R285	Q348	E408
N21	L95	L95	V158	L222	K286	I349	E409
G22	A96	A96	G160	A223	A287	Q351	G410
L23	A98	A98	L161	K225	M288	Q352	V411
L24	I99	I99	E164	K226	L289	L353	G414
D25	I100	I100	A165	L227	Q290	G415	G415
A26	T101	T101	M166	S228	D291	E355	G416
V27	E102	E102	D167	M229	I292	A356	V417
K34	A108	A108	G173	L230	A293	T357	A418
G35	A109	A109	V174	R231	T294	S358	L419
R36	G110	G110	I175	E232	L295	D359	I420
N37	M111	M111	E178	M233	T286	Y360	R421
V38	N112	N112	D179	V240	G297	D361	V422
L40	P113	P113	G180	A243	E308	R362	K425
T49	D115	D115	Q184	G244	L309	E363	L426
T50	L116	L116	D185	K245	E310	K364	A427
K51	K117	K117	E186	P246	K311	L372	D428
S55	R118	R118	L187	L247	A312	G374	L429
V56	G119	G119	D188	L248	T313	G375	G439
A57	D120	D120	V189	L249	L314	V376	I440
R68	D121	D121	E191	A251	E315	L317	K441
E59	K122	K122	G192	E252	D316	G318	V442
F67	A123	A123	M193	D253	Q319	V381	G443
N69	V124	V124	Q194	V254	A320	A383	M447
D64	T125	T125	F195	E255	K321	A384	E448
K65	V128	V128	D196	G256	V323	T385	A449
F66	E129	E129	R197	E257	V324	E386	P450
E67	L130	L130	G198	A258	I325	E388	L451
E67	K132	K132	V199	L259	K326	K389	Q452
N69	S135	S135	S201	T261	K327	Q453	I454
D72	C138	C138	P202	V263	D328	K390	V455
M73	S139	S139	F204	V264	T329	E391	C458
V74	D140	D140	I205	N265	T330	K392	G458
K75	S141	S141	N206	T266	T331	K393	E460
E76	K142	K142	K207	R268	I332	R395	

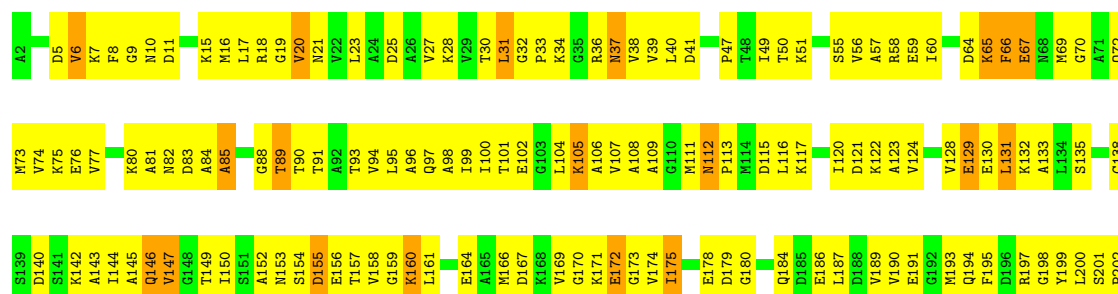
- Molecule 1: GROEL

Chain L:  24% 61% 11% ..



- Molecule 1: GROEL

Chain M:  24% 61% 10% ..



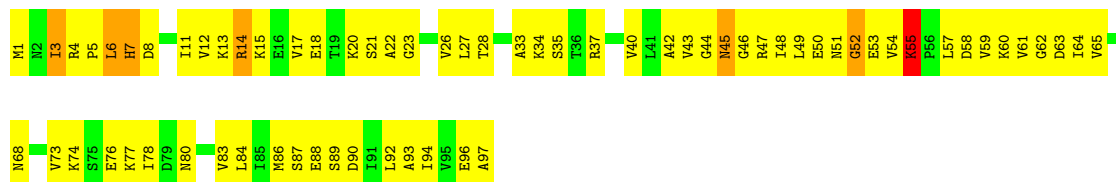
T522	P525	C458	K393	T331	V265	Y203
D523	K526	G459	A394	I332	N265	F204
L524	ASN	A526	R395	I333	T266	
P525	ASP	E461	V396	D334	M267	N206
K526	ALA	P462	E397	G335	R268	K207
ASN	ALA	S463	D398	V336	G269	P208
ASP	ASP	V464	A399	E339	I270	E209
ALA	LEU	V465	L400	A340	V271	T210
ALA	ALA		H401	A341	K272	G211
ASP	ALA	V469	A402	I342	V273	A212
LEU	ALA	T403	T403	I342	A274	V213
ALA	GLY	R404	R404	Q343	A275	E214
GLY	GLY	A405	A405	G344	V276	L215
ALA	MET	D475	A406	R345	K277	E216
ALA	GLY	M475	V407	V346		S217
ALA	GLY	M476	E408	A347		T217
ALA	MET	Y476	E409	Q348	F281	G282
ALA	MET	G477	G410	I349	D283	F219
ALA	MET	Y478	V411	R350	R284	L221
ALA	MET	M479	V412	Q351	R285	L222
ALA	MET		A413	Q352	K286	A223
ALA	MET	E483	G414	I353	K287	D224
ALA	MET	E484	G415	E354	M288	K225
ALA	MET	Y485	G416	E355	L289	K226
ALA	MET	G486	V417	A356	Q290	I227
ALA	MET	N487	A418	T357	Q291	S228
ALA	MET	M488	L419	S358	I292	I229
ALA	MET	D490	I420	D359	A293	I230
ALA	MET		R421	Y360	R231	E232
ALA	MET		V422	D361	E232	E232
ALA	MET		A423	R362	M233	M233
ALA	MET	I493	S424	E363	I301	L234
ALA	MET	D495	K425	K364	S302	P235
ALA	MET	P496	L426	L365	E303	V236
ALA	MET	T497	A427	Q366	E304	L237
ALA	MET	K498	D428	E367	I305	E238
ALA	MET	V499	L429	R368	I305	E238
ALA	MET	T500	R430	V369	E308	A239
ALA	MET	R501	G431	A370	L309	V240
ALA	MET	S502	Q432	K371	E310	
ALA	MET	A503	N433	L372	A243	A243
ALA	MET	L504	E434	A373	K311	G244
ALA	MET	Q505	D435	G374	A312	K245
ALA	MET	Y506	Q436	G375	T313	P246
ALA	MET	A507	N437	V376	L314	L247
ALA	MET	S509	V438		E315	L248
ALA	MET	V510	I440		D316	I249
ALA	MET	V510	E509		L317	I250
ALA	MET	L513	V510		Q319	E252
ALA	MET	M514	V442		A320	D253
ALA	MET	L515	E448		K321	V254
ALA	MET	T516	A449		R322	E255
ALA	MET	T517	P450		V323	G256
ALA	MET	M520	P450		V324	E257
ALA	MET	V521	L451		I325	E257
ALA	MET	T522	R451		N326	A258
ALA	MET	D523	R452		K327	L259
ALA	MET	L524	Q453		K389	A260
ALA	MET		I454		K390	T261
ALA	MET		V455		E391	L262
ALA	MET				K392	T329
ALA	MET				T330	T330

• Molecule 1: GROEL

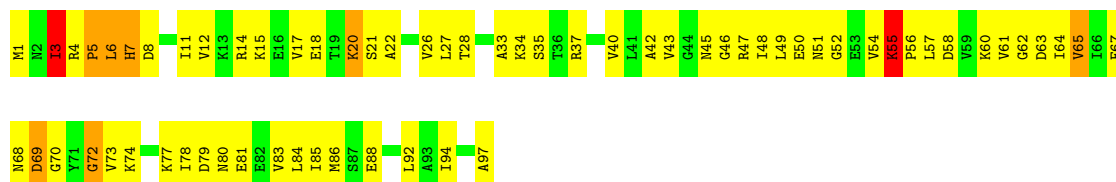
Chain N: 25% 61% 10% . .

A2	K75	D140	F204	N265	I392	A394	E481	T522
D5	E76	S141	I205	T266	I333	R395	P462	D523
V6	V77	K142	N206	M267	D334	V396	S463	L524
		A143	K207	R268	G335	E397	V465	P525
		I144	P208	G269	V336	D398	V465	K526
		A81	E209	I270	E339	A466	M467	ASN
		D11	G211	V271	A340	L400	M467	ASP
		K15	A212	K272	A341	H401	T468	ALA
		M16	E213	A274	I342	A402	V469	ALA
		L17	E214	A275	Q343	T403	K470	ASP
		R18	E215	V276	Q343	R404	G471	LEU
		G19	L216	K277	G344	A405	G471	GLY
		V20	E217		R345	A406	D472	ALA
			S217		V346	V407	G474	ALA
			F218		A347	E408	G474	ALA
			F219		Q348	E409	N475	GLY
			L220		I349	G410	Y476	GLY
			L221		R350	G411	G477	MET
			L222		Q351	V411	Y478	MET
			A223		Q352	V412	M479	GLY
			D224		I353	A413	A480	MET
			K225		E354	G414	A481	GLY
			K226		E355	G415	T482	GLY
			I227		A356	V417	E483	MET
			S228		T357	A418	Y485	GLY
			I229		S358	L419	G486	MET
			I230		D359	I420	N487	MET
			E232		Y360	R421	N488	MET
			M233		R362	V422	I489	MET
			L234		E363	K425	D490	MET
			P235		K364	A426	M491	MET
			V236		L365	L427	L484	MET
			E238		Q366	A427	D495	MET
			A239		E367	L429	P496	MET
			V240		R368	T497	T497	MET
					V369	G432	K498	MET
					A370	M433	V499	MET
					K371	E434	T500	MET
					L372	D435	R501	MET
					A373	Q436	S502	MET
					G374	M437	A503	MET
					G375	V438	L504	MET
					V376	G439	Q505	MET
						I440	Y506	MET
						V442	A507	MET
						V442	S509	MET
							V510	MET
							A511	MET
							G512	MET
							L513	MET
							M514	MET
							T515	MET
							L516	MET
							T517	MET
							E518	MET
							C519	MET
							G459	MET
							E460	MET

• Molecule 2: GROES

Chain O:  30% 63% 6%

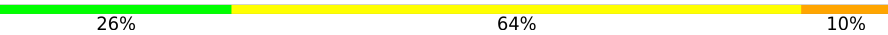
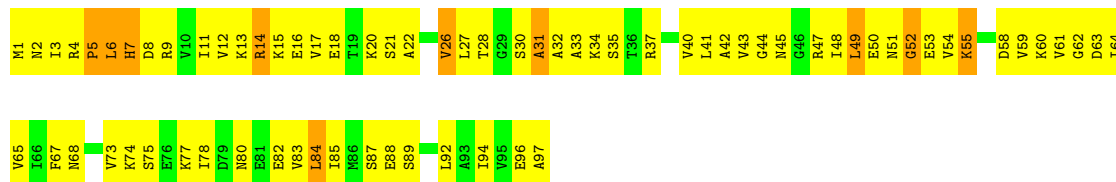
• Molecule 2: GROES

Chain P:  33% 58% 7%

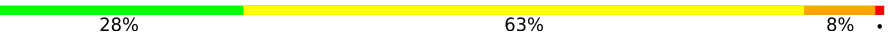
• Molecule 2: GROES

Chain Q:  27% 62% 9%

• Molecule 2: GROES

Chain R:  26% 64% 10%

• Molecule 2: GROES

Chain S:  28% 63% 8%

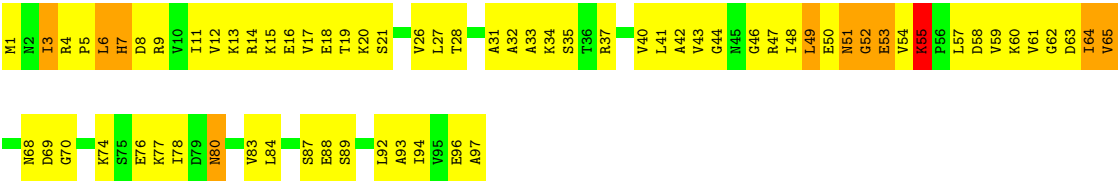
• Molecule 2: GROES

Chain T: 29% 59% 11%



• Molecule 2: GROES

Chain U: 28% 61% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C7	Depositor
Number of particles used	1448	Depositor
Resolution determination method	Not provided	
CTF correction method	CLASS AVERAGES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.047	Depositor
Average map value	0.006	Depositor
Map value standard deviation	0.030	Depositor
Recommended contour level	0.029	Depositor
Map size ($\text{\AA}$)	358.4, 358.4, 358.4	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	2.8, 2.8, 2.8	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.69	2/3836 (0.1%)	1.11	20/5188 (0.4%)
1	B	0.66	0/3836	1.12	28/5188 (0.5%)
1	C	0.70	2/3836 (0.1%)	1.10	19/5188 (0.4%)
1	D	0.70	1/3836 (0.0%)	1.11	24/5188 (0.5%)
1	E	0.64	2/3836 (0.1%)	1.12	25/5188 (0.5%)
1	F	0.66	1/3836 (0.0%)	1.11	26/5188 (0.5%)
1	G	0.69	2/3836 (0.1%)	1.11	19/5188 (0.4%)
1	H	0.64	1/3876 (0.0%)	1.10	25/5232 (0.5%)
1	I	0.67	1/3876 (0.0%)	1.09	22/5232 (0.4%)
1	J	0.64	1/3876 (0.0%)	1.09	24/5232 (0.5%)
1	K	0.62	1/3876 (0.0%)	1.08	21/5232 (0.4%)
1	L	0.61	1/3876 (0.0%)	1.09	23/5232 (0.4%)
1	M	0.64	1/3876 (0.0%)	1.10	23/5232 (0.4%)
1	N	0.63	1/3876 (0.0%)	1.09	23/5232 (0.4%)
2	O	0.47	0/729	1.03	2/980 (0.2%)
2	P	0.45	0/729	1.04	5/980 (0.5%)
2	Q	0.46	0/729	1.08	4/980 (0.4%)
2	R	0.48	0/729	1.05	3/980 (0.3%)
2	S	0.48	0/729	1.07	3/980 (0.3%)
2	T	0.45	0/729	1.02	3/980 (0.3%)
2	U	0.46	0/729	1.02	4/980 (0.4%)
All	All	0.64	17/59087 (0.0%)	1.10	346/79800 (0.4%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	73	MET	SD-CE	7.88	1.99	1.79
1	C	73	MET	SD-CE	7.30	1.97	1.79
1	J	525	PRO	C-N	-5.81	1.25	1.33
1	I	525	PRO	C-N	-5.79	1.25	1.33
1	M	525	PRO	C-N	-5.74	1.25	1.33

The worst 5 of 346 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	416	GLY	N-CA-C	-9.66	101.65	115.27
1	N	416	GLY	N-CA-C	-9.60	102.07	115.32
1	J	416	GLY	N-CA-C	-9.42	102.32	115.32
1	K	33	PRO	N-CA-C	-9.42	102.09	113.86
1	K	65	LYS	N-CA-C	-9.29	98.99	110.41

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	3809	0	3890	605	0
1	B	3809	0	3890	561	0
1	C	3809	0	3890	559	0
1	D	3809	0	3890	570	0
1	E	3809	0	3890	579	0
1	F	3809	0	3890	584	0
1	G	3809	0	3890	576	0
1	H	3850	0	3959	561	0
1	I	3850	0	3959	572	0
1	J	3850	0	3958	556	0
1	K	3850	0	3960	573	0
1	L	3850	0	3961	604	0
1	M	3850	0	3960	578	0
1	N	3850	0	3960	555	0
2	O	725	0	755	123	0
2	P	725	0	755	99	0
2	Q	725	0	755	109	0
2	R	725	0	755	106	0
2	S	725	0	755	105	0
2	T	725	0	755	112	0
2	U	725	0	755	105	0
All	All	58688	0	60232	8590	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 72.

The worst 5 of 8590 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:L:191:GLU:CB	1:L:342:ILE:HG21	1.14	1.61
1:I:191:GLU:CG	1:I:342:ILE:HG22	1.26	1.59
1:I:191:GLU:CB	1:I:342:ILE:CG2	1.77	1.58
1:L:373:ALA:C	1:L:375:GLY:HA3	1.20	1.54
1:J:174:VAL:HG21	1:J:371:LYS:CD	1.38	1.53

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	523/547 (96%)	396 (76%)	92 (18%)	35 (7%)	1	12
1	B	523/547 (96%)	398 (76%)	95 (18%)	30 (6%)	1	14
1	C	523/547 (96%)	397 (76%)	88 (17%)	38 (7%)	1	10
1	D	523/547 (96%)	397 (76%)	93 (18%)	33 (6%)	1	13
1	E	523/547 (96%)	390 (75%)	98 (19%)	35 (7%)	1	12
1	F	523/547 (96%)	399 (76%)	93 (18%)	31 (6%)	1	13
1	G	523/547 (96%)	390 (75%)	99 (19%)	34 (6%)	1	12
1	H	519/547 (95%)	374 (72%)	116 (22%)	29 (6%)	1	14
1	I	519/547 (95%)	377 (73%)	115 (22%)	27 (5%)	1	15
1	J	519/547 (95%)	376 (72%)	117 (22%)	26 (5%)	1	16
1	K	519/547 (95%)	372 (72%)	120 (23%)	27 (5%)	1	15
1	L	519/547 (95%)	372 (72%)	116 (22%)	31 (6%)	1	13
1	M	519/547 (95%)	375 (72%)	117 (22%)	27 (5%)	1	15
1	N	519/547 (95%)	377 (73%)	114 (22%)	28 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	95/97 (98%)	69 (73%)	20 (21%)	6 (6%)	1	13
2	P	95/97 (98%)	65 (68%)	24 (25%)	6 (6%)	1	13
2	Q	95/97 (98%)	67 (70%)	21 (22%)	7 (7%)	1	10
2	R	95/97 (98%)	68 (72%)	18 (19%)	9 (10%)	0	8
2	S	95/97 (98%)	73 (77%)	16 (17%)	6 (6%)	1	13
2	T	95/97 (98%)	67 (70%)	20 (21%)	8 (8%)	0	9
2	U	95/97 (98%)	64 (67%)	24 (25%)	7 (7%)	1	10
All	All	7959/8337 (96%)	5863 (74%)	1616 (20%)	480 (6%)	2	13

5 of 480 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	44	PHE
1	A	233	MET
1	A	279	PRO
1	A	309	LEU

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	393/414 (95%)	362 (92%)	31 (8%)	11	32
1	B	393/414 (95%)	358 (91%)	35 (9%)	9	28
1	C	393/414 (95%)	364 (93%)	29 (7%)	13	33
1	D	393/414 (95%)	364 (93%)	29 (7%)	13	33
1	E	393/414 (95%)	365 (93%)	28 (7%)	13	35
1	F	393/414 (95%)	360 (92%)	33 (8%)	10	30
1	G	393/414 (95%)	359 (91%)	34 (9%)	9	29
1	H	403/414 (97%)	381 (94%)	22 (6%)	19	41
1	I	403/414 (97%)	378 (94%)	25 (6%)	16	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	403/414 (97%)	379 (94%)	24 (6%)	17	39
1	K	403/414 (97%)	380 (94%)	23 (6%)	18	40
1	L	403/414 (97%)	379 (94%)	24 (6%)	17	39
1	M	403/414 (97%)	380 (94%)	23 (6%)	18	40
1	N	403/414 (97%)	380 (94%)	23 (6%)	18	40
2	O	79/80 (99%)	76 (96%)	3 (4%)	29	50
2	P	79/80 (99%)	75 (95%)	4 (5%)	21	42
2	Q	79/80 (99%)	73 (92%)	6 (8%)	12	33
2	R	79/80 (99%)	74 (94%)	5 (6%)	16	37
2	S	79/80 (99%)	74 (94%)	5 (6%)	16	37
2	T	79/80 (99%)	72 (91%)	7 (9%)	9	28
2	U	79/80 (99%)	75 (95%)	4 (5%)	21	42
All	All	6125/6356 (96%)	5708 (93%)	417 (7%)	16	36

5 of 417 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	284	ARG
1	J	426	LEU
2	R	55	LYS
1	H	426	LEU
1	I	364	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	21	ASN
1	K	37	ASN
2	R	45	ASN
1	I	146	GLN
1	J	37	ASN

5.3.3 RNA ⓘ

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](#)

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	2
1	J	2
1	N	2
1	H	2
1	K	2
1	M	2
1	L	2

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	373:ALA	C	374:GLY	N	6.88
1	J	373:ALA	C	374:GLY	N	6.54
1	N	373:ALA	C	374:GLY	N	6.51
1	H	373:ALA	C	374:GLY	N	6.50
1	K	373:ALA	C	374:GLY	N	6.07

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1046. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

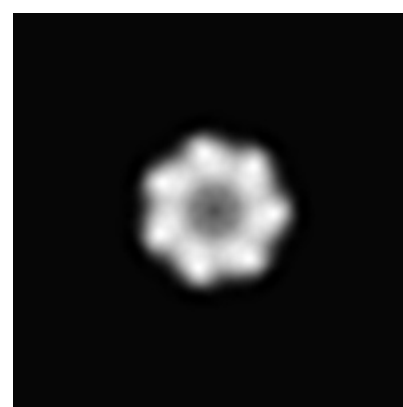
6.1.1 Primary map



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: 64



Y Index: 64



Z Index: 64

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

6.3 Largest variance slices [i](#)

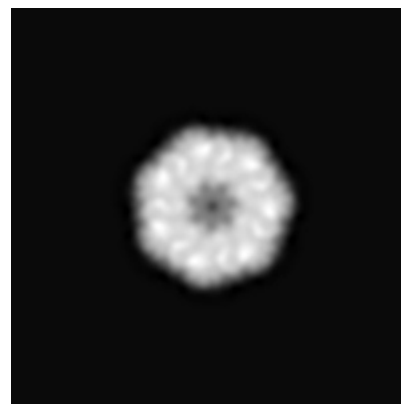
6.3.1 Primary map



X Index: 76



Y Index: 74



Z Index: 61

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

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

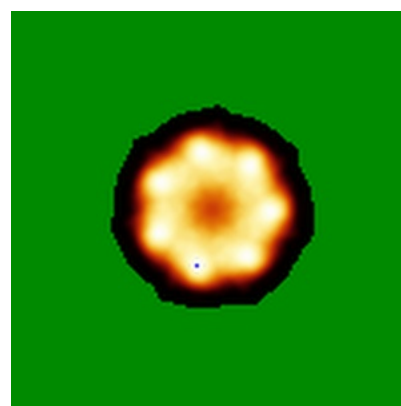
6.4.1 Primary map



X



Y

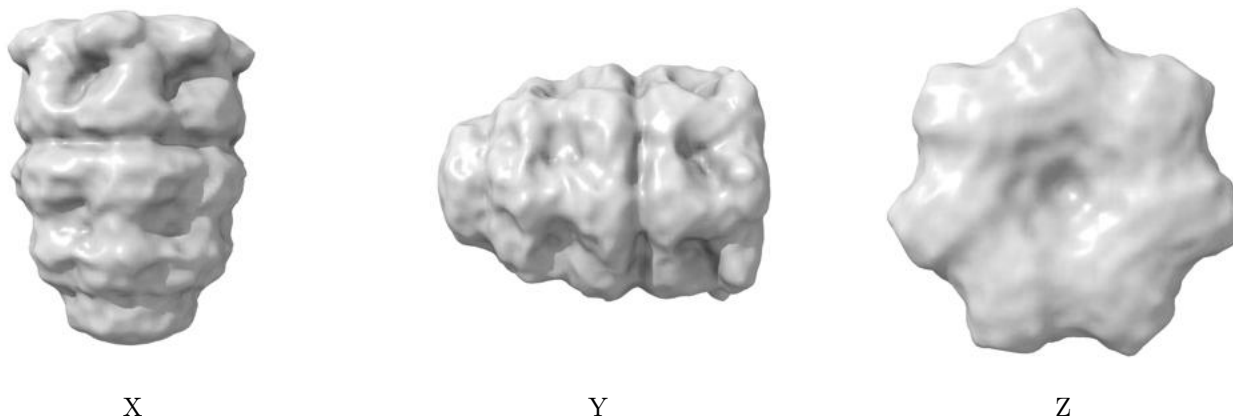


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

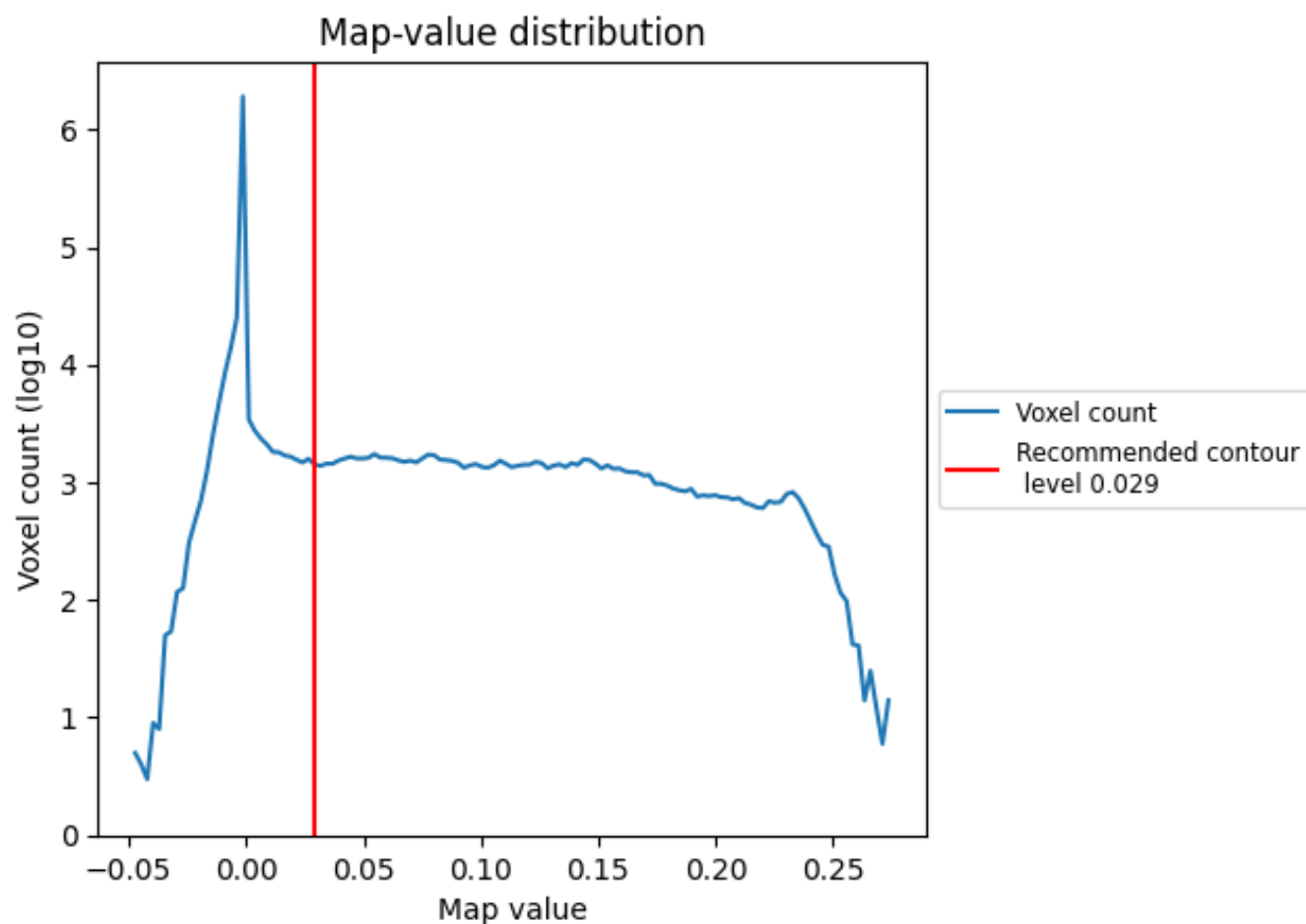
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

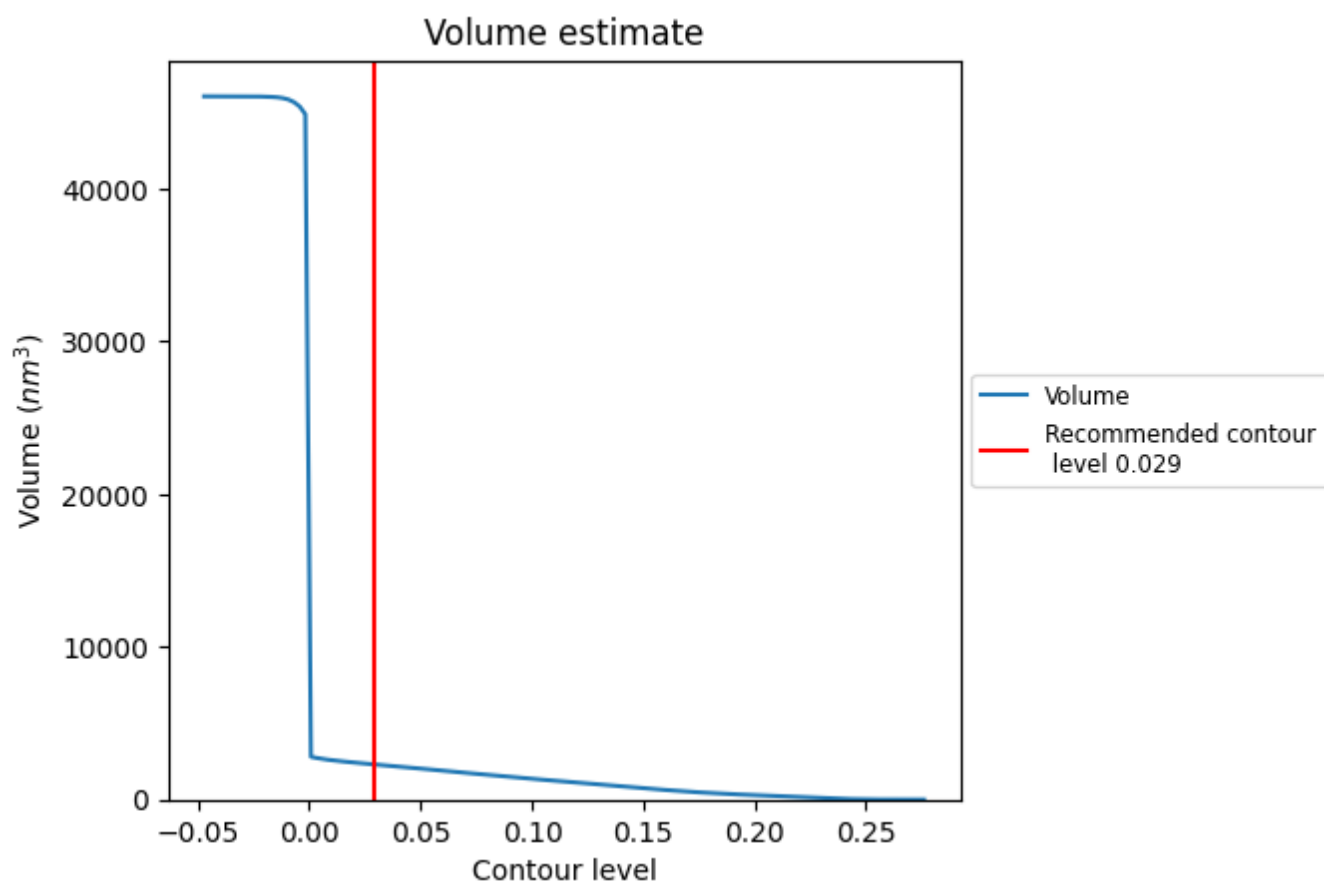
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

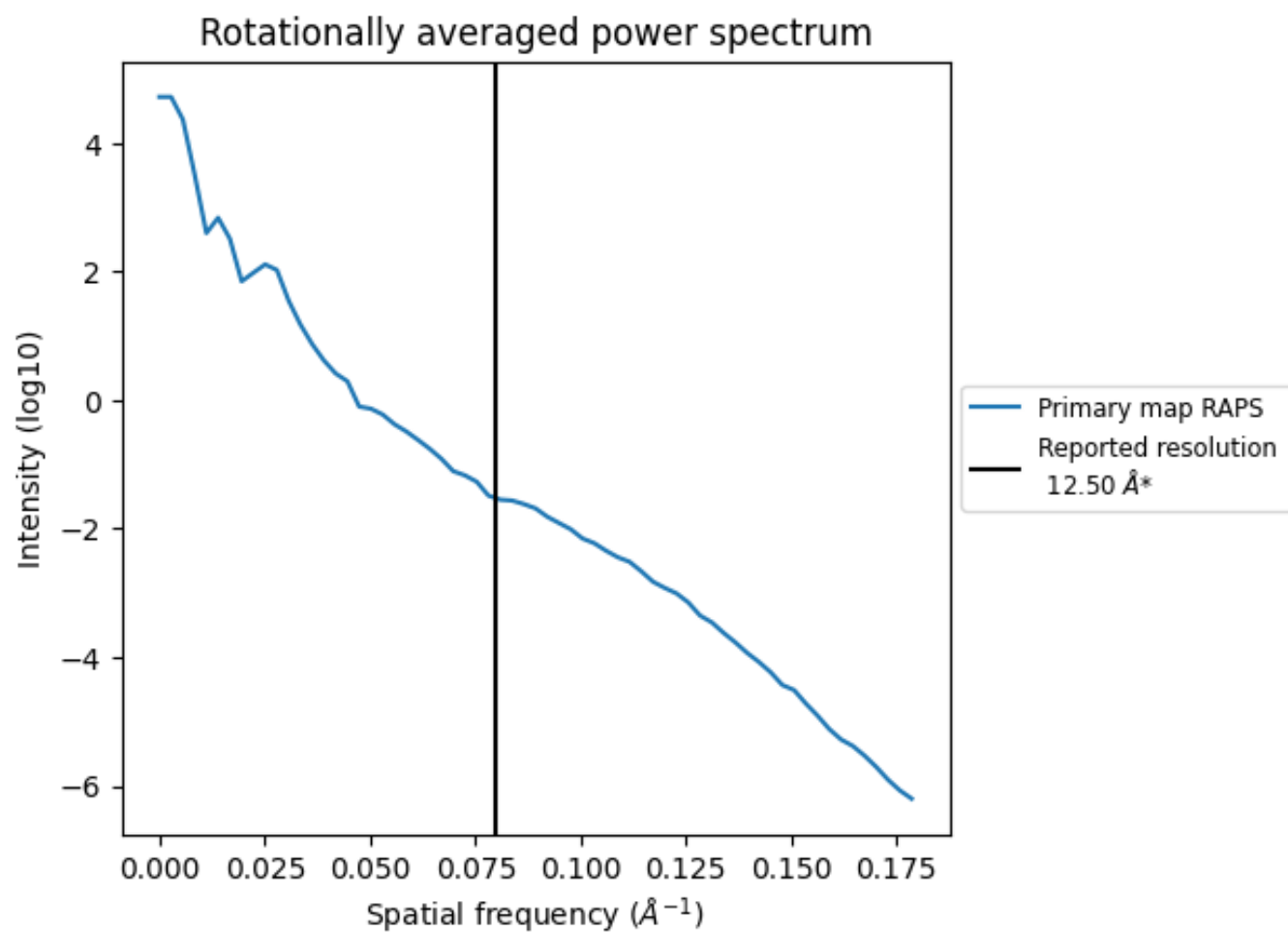
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2303 nm³; this corresponds to an approximate mass of 2080 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.080 Å⁻¹

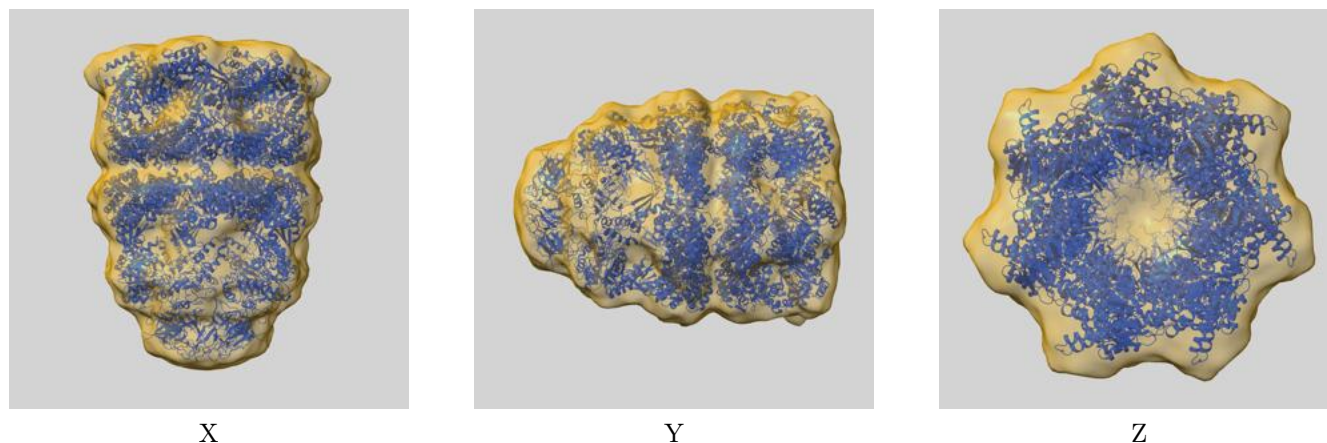
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

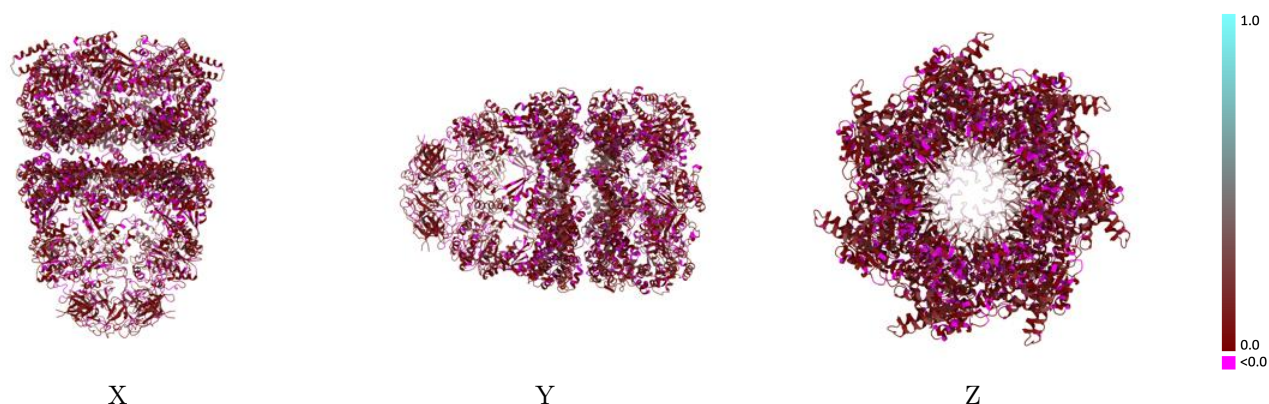
This section contains information regarding the fit between EMDB map EMD-1046 and PDB model 1GRU. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



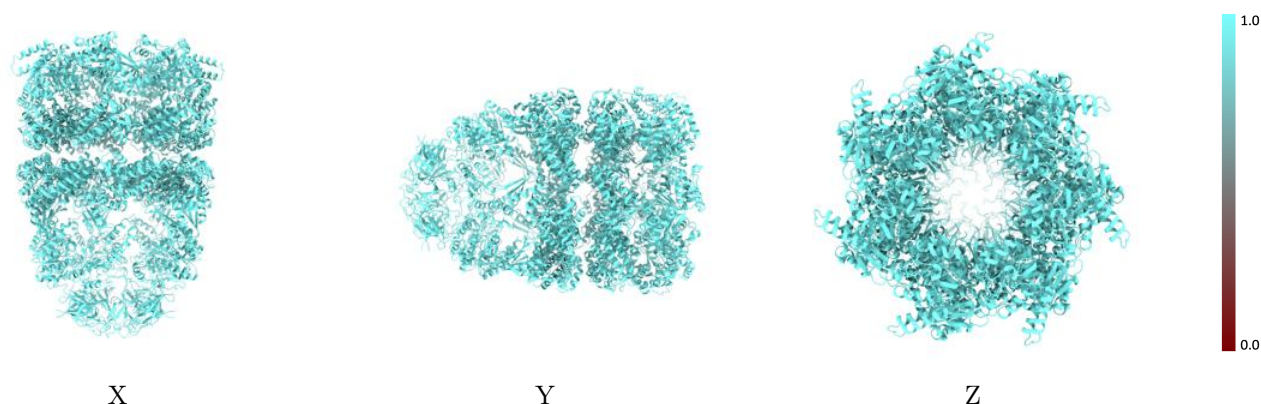
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



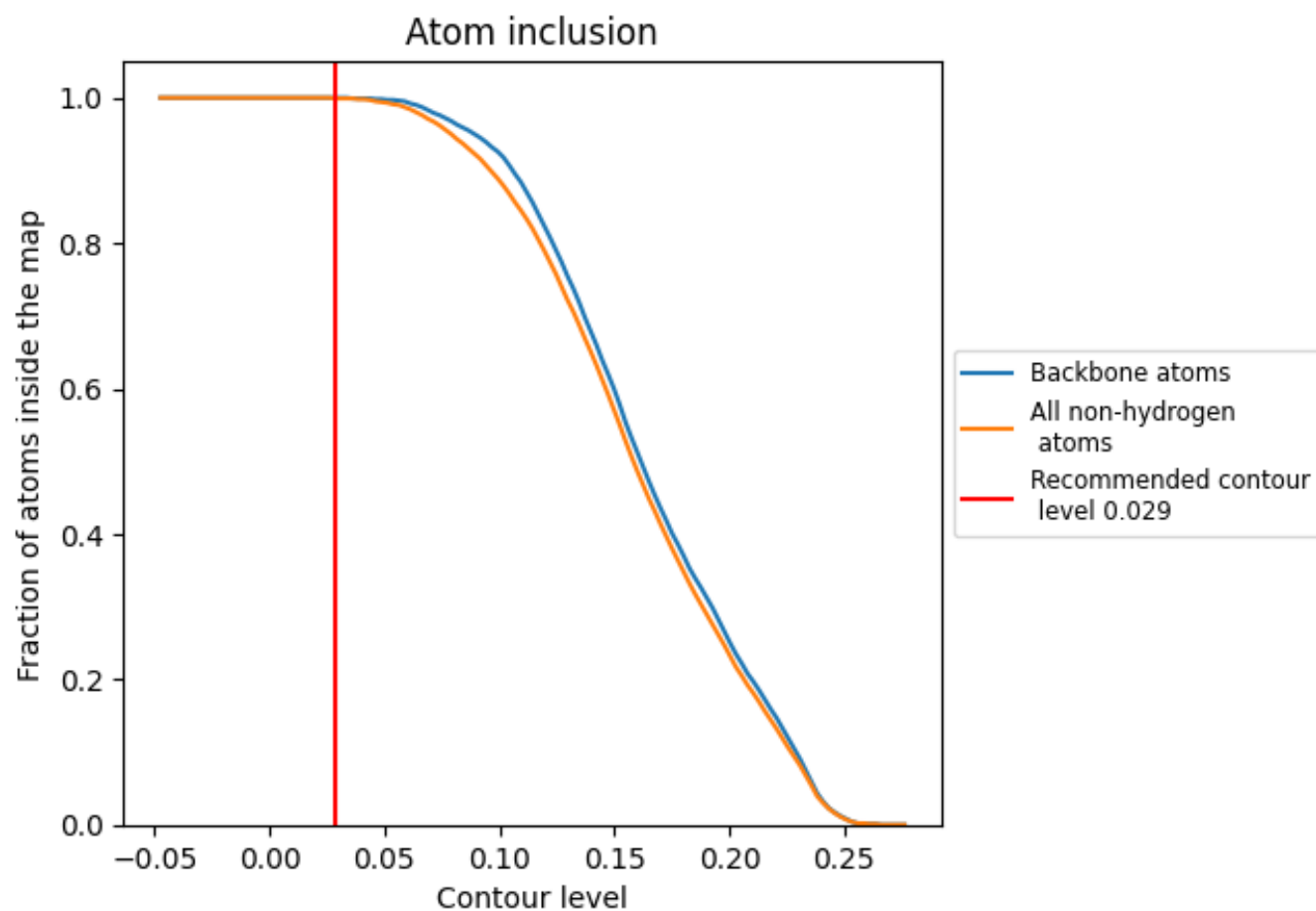
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9990	 0.0700
A	 1.0000	 0.0690
B	 1.0000	 0.0700
C	 1.0000	 0.0710
D	 1.0000	 0.0680
E	 1.0000	 0.0670
F	 1.0000	 0.0670
G	 1.0000	 0.0690
H	 1.0000	 0.0740
I	 1.0000	 0.0740
J	 1.0000	 0.0720
K	 1.0000	 0.0720
L	 0.9990	 0.0720
M	 1.0000	 0.0730
N	 1.0000	 0.0740
O	 0.9960	 0.0620
P	 0.9930	 0.0640
Q	 0.9940	 0.0690
R	 0.9960	 0.0630
S	 0.9940	 0.0580
T	 0.9970	 0.0570
U	 0.9960	 0.0600

