



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:46 PM BST

PDB ID : 1GRU  
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.; Hor-  
wich, A.L.; Saibil, H.R.  
Deposited on : 2001-12-16  
Resolution : 12.50 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could  
stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

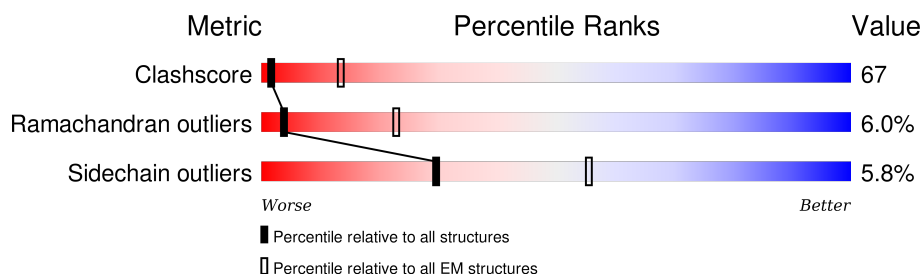


# 1 Overall quality at a glance

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)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

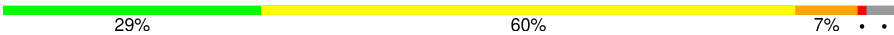
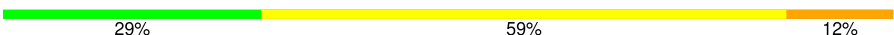
The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	547	
1	B	547	
1	C	547	
1	D	547	
1	E	547	
1	F	547	
1	G	547	
1	H	547	
1	I	547	

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Mol	Chain	Length	Quality of chain
1	J	547	 30% 59% 7% .
1	K	547	 29% 60% 6% . .
1	L	547	 28% 61% 7% . .
1	M	547	 29% 60% 7% . .
1	N	547	 29% 60% 7% . .
2	O	97	 33% 58% 9%
2	P	97	 34% 57% 9%
2	Q	97	 30% 59% 11%
2	R	97	 27% 61% 12%
2	S	97	 32% 60% 8%
2	T	97	 31% 56% 13%
2	U	97	 29% 59% 12%



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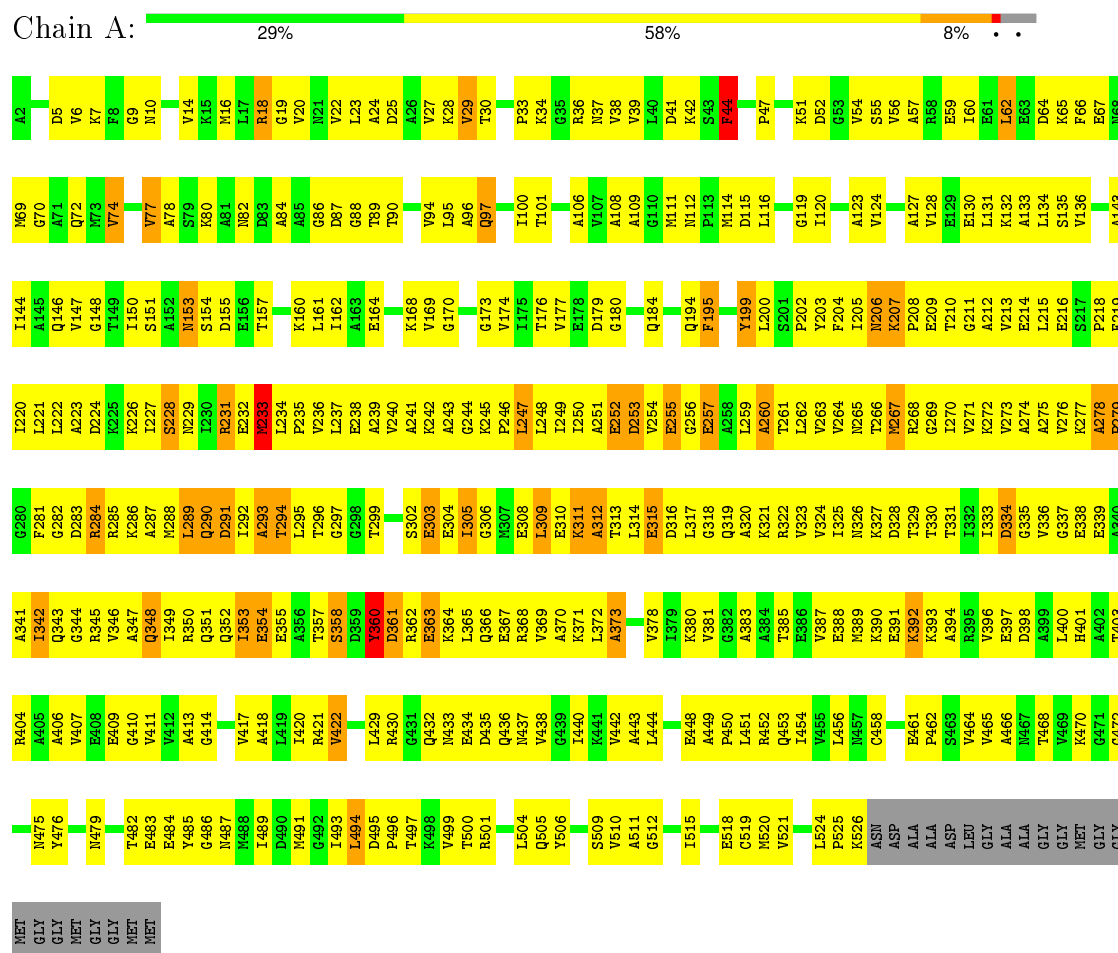
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	97	Total	C	N	O	S	0	0
			725	452	127	145	1		
2	Q	97	Total	C	N	O	S	0	0
			725	452	127	145	1		
2	R	97	Total	C	N	O	S	0	0
			725	452	127	145	1		
2	S	97	Total	C	N	O	S	0	0
			725	452	127	145	1		
2	T	97	Total	C	N	O	S	0	0
			725	452	127	145	1		
2	U	97	Total	C	N	O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



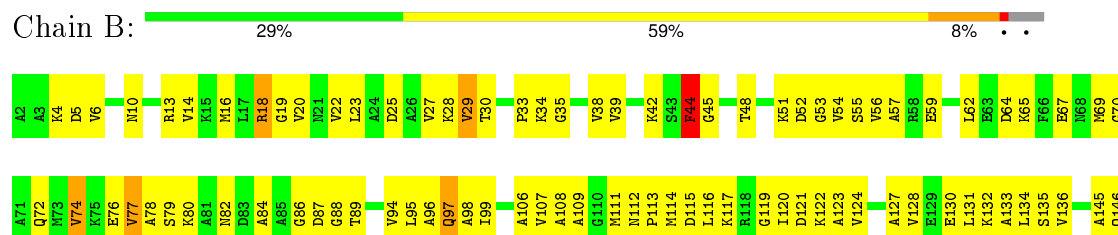
### 3 Residue-property plots

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



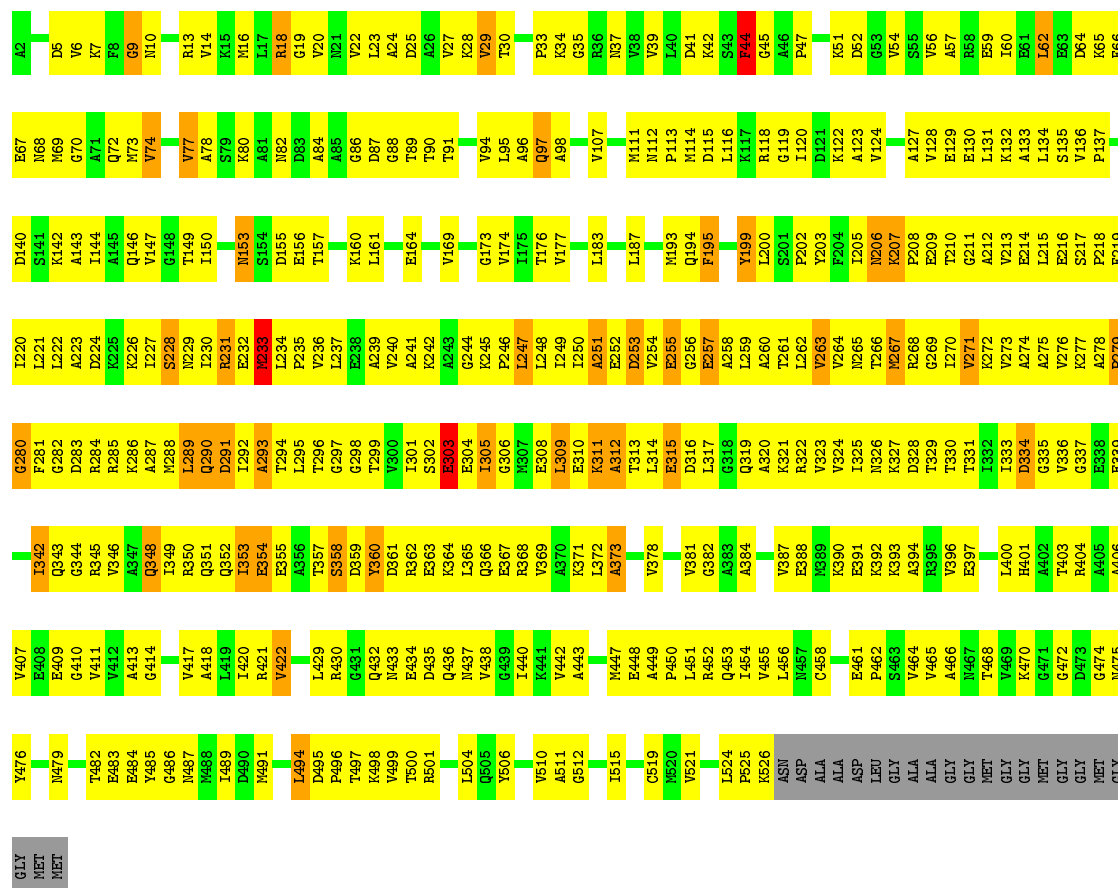


GLY	T468	H401	E338	A278	S217	A145	Q72	A2	MET	T492	G414	V346	K286	K225	V147
GLY	A402	A402	E339	P279	P218	Q146	M73	A3		E403	V417	A347	A287	K226	G146
MET	T403	T403	A340	G280	F219	V147	V74	K4		E404	V417	Q348	M288	I227	T149
GLY	R404	R404	A341	F281	F219	G148	K75	D5		Y485	A418	I349	L289	S228	I150
MET	G474	G474	I342	G283	L221	T149	E76	V6		G466	L419	Q350	Q290	N229	N153
GLY	N475	N475	Q343	D282	L222	I150	V77	K7		N467	L420	R351	D291	I230	N153
GLY	Y476	Y476	Q344	R284	A233	N153	A78	F8		M468	R421	Q352	L292	R231	E156
MET	E409	E409	R345	K285	D224	S154	N82	G9		I469	V422	I353	T294	E232	E156
GLY	G410	G410	V346	K286	K225	V158	D83	M10		M491	K425	E354	T294	K234	K160
GLY	V411	V411	A347	A287	K226	G159	A84	D11		G492	K425	E355	T296	P235	L161
MET	A480	A480	Q348	M288	I227	V158	G86	K15		I493	D428	A356	G297	V236	I162
MET	A481	A481	I349	L289	N229	G159	D87	M16		L494	L429	S357	G298	L237	A163
MET	A482	A482	Q351	Q290	I230	E164	G88	L17		D495	R430	D359	T299	E238	E164
MET	A483	A483	Q352	D231	R231	D167	T89	G19		P496	G432	Y360	V300	A239	A165
MET	A484	A484	I353	A293	E232	K168	T90	G19		K498	N433	R362	S302	K241	M166
MET	A485	A485	E354	T294	K234	V169	V94	V20		V499	E434	K363	S303	A241	D167
MET	A486	A486	E355	L295	L234	G169	L95	N21		T500	D435	K364	E304	K242	K168
MET	A487	A487	T357	T296	P235	G173	L96	V22		R501	Q436	L365	I305	K245	V169
MET	A488	A488	S358	G298	L237	V174	A96	K23		L504	M437	Q366	G306	P246	G173
MET	A489	A489	D359	T299	E238	I175	Q97	D25		G505	V438	R367	E307	L247	V174
MET	A490	A490	Y360	V300	A239	T176	G103	A26		Y506	T440	R368	E308	L248	G174
MET	A491	A491	D361	I301	V240	E178	V107	V27		S509	K441	A370	E310	I249	V177
MET	A492	A492	R362	S202	A241	E178	A108	K28		V510	V442	K371	E311	I250	E178
MET	A493	A493	E363	E303	K242	D179	V107	V29		G512	E448	A373	A312	E252	G180
MET	A494	A494	K364	E304	A283	G180	A108	K29		I515	A449	K380	A313	V254	L183
MET	A495	A495	L365	G306	G244	T181	M111	L31		C519	P450	V381	E315	E255	M193
MET	A496	A496	E367	G307	K245	G182	M112	G32		M520	R452	Q382	D316	E257	Q194
MET	A497	A497	R368	E308	L247	Q184	P113	P33		V521	Q453	A383	D319	A260	F195
MET	A498	A498	Y369	L309	L248	D185	M114	K34		L524	R452	E388	K321	T261	Y199
MET	A499	A499	A370	E310	I249	E186	D115	G35		P525	Q457	E388	R322	L262	L200
MET	A500	A500	K371	E311	I250	L187	L116	K42		K526	N457	E388	E322	T261	S201
MET	A501	A501	L372	A312	E252	V189	K117	R44		ASN	E461	E391	V323	V263	P202
MET	A502	A502	A373	L314	V254	V190	I120	T48		ASP	E461	E391	V324	V264	T203
MET	A503	A503	V376	E315	E255	M193	D121	K51		ALA	S463	K392	I325	V264	F204
MET	A504	A504	A377	D316	E255	Q194	K122	D52		ALA	P462	K393	I326	T266	T205
MET	A505	A505	V378	L317	G256	F195	A123	P51		ALA	S463	K393	I327	T266	T206
MET	A506	A506	I379	Q319	A258	E257	V124	D52		ALA	V464	K395	D328	R267	K207
MET	A507	A507	P450	Q319	A258	E257	V124	D52		ALA	V464	K395	D329	R268	K207
MET	A508	A508	L451	A320	L259	Y199	T125	G53		LEU	V465	V396	T329	G269	P208
MET	A509	A509	R452	K321	A260	S201	A127	V54		ALA	V466	E397	T330	I270	E209
MET	A510	A510	Q382	K322	K322	S201	E127	S55		ALA	V467	D398	T331	V271	T210
MET	A511	A511	A384	V323	L262	Y203	V128	A57		ALA	V468	A399	I332	K272	G211
MET	A512	A512	I325	V324	V263	Y203	E129	R58		GLY	V469	H401	D334	V273	A212
MET	A513	A513	L325	V324	V263	Y203	E130	R58		GLY	V470	H401	D334	V273	A212
MET	A514	A514	N265	L325	V264	I205	E130	R58		GLY	V470	H401	D334	V273	A212
MET	A515	A515	T266	K327	T266	N206	K132	E59		GLY	V471	A402	G335	A275	E214
MET	A516	A516	M267	K327	T266	N206	K132	E59		GLY	V472	A402	G335	A275	E214
MET	A517	A517	I270	K327	T266	N206	K132	E59		GLY	V473	A402	G335	A275	E214
MET	A518	A518	E209	K327	T266	N206	K132	E59		GLY	V474	A402	G335	A275	E214
MET	A519	A519	T271	K327	T266	N206	K132	E59		GLY	V475	A402	G335	A275	E214
MET	A520	A520	K272	K327	T266	N206	K132	E59		GLY	V476	A402	G335	A275	E214
MET	A521	A521	G211	K327	T266	N206	K132	E59		GLY	V477	A402	G335	A275	E214
MET	A522	A522	V213	K327	T266	N206	K132	E59		GLY	V478	A402	G335	A275	E214
MET	A523	A523	E214	K327	T266	N206	K132	E59		GLY	V479	A402	G335	A275	E214
MET	A524	A524	A275	K327	T266	N206	K132	E59		GLY	V480	A402	G335	A275	E214
MET	A525	A525	V276	K327	T266	N206	K132	E59		GLY	V481	A402	G335	A275	E214
MET	A526	A526	K277	K327	T266	N206	K132	E59		GLY	V482	A402	G335	A275	E214
MET	A527	A527	E216	K327	T266	N206	K132	E59		GLY	V483	A402	G335	A275	E214
MET	A528	A528	E217	K327	T266	N206	K132	E59		GLY	V484	A402	G335	A275	E214
MET	A529	A529	E218	K327	T266	N206	K132	E59		GLY	V485	A402	G335	A275	E214
MET	A530	A530	E219	K327	T266	N206	K132	E59		GLY	V486	A402	G335	A275	E214
MET	A531	A531	E220	K327	T266	N206	K132	E59		GLY	V487	A402	G335	A275	E214
MET	A532	A532	E221	K327	T266	N206	K132	E59		GLY	V488	A402	G335	A275	E214
MET	A533	A533	E222	K327	T266	N206	K132	E59		GLY	V489	A402	G335	A275	E214
MET	A534	A534	E223	K327	T266	N206	K132	E59		GLY	V490	A402	G335	A275	E214
MET	A535	A535	E224	K327	T266	N206	K132	E59		GLY	V491	A402	G335	A275	E214
MET	A536	A536	E225	K327	T266	N206	K132	E59		GLY	V492	A402	G335	A275	E214
MET	A537	A537	E226	K327	T266	N206	K132	E59		GLY	V493	A402	G335	A275	E214
MET	A538	A538	E227	K327	T266	N206	K132	E59		GLY	V494	A402	G335	A275	E214
MET	A539	A539	E228	K327	T266	N206	K132	E59		GLY	V495	A402	G335	A275	E214
MET	A540	A540	E229	K327	T266	N206	K132	E59		GLY	V496	A402	G335	A275	E214
MET	A541	A541	E230	K327	T266	N206	K132	E59		GLY	V497	A402	G335	A275	E214
MET	A542	A542	E231	K327	T266	N206	K132	E59		GLY	V498	A402	G335	A275	E214
MET	A543	A543	E232	K327	T266	N206	K132	E59		GLY	V499	A402	G335	A275	E214
MET	A544	A544	E233	K327	T266	N206	K132	E59		GLY	V500	A402	G335	A275	E214
MET	A545	A545	E234	K327	T266	N206	K132	E59		GLY	V501	A402	G335	A275	E214
MET	A546	A546	E235	K327	T266	N206	K132	E59		GLY	V502	A402	G335	A275	E214
MET	A547	A547	E236	K327	T266	N206	K132	E59		GLY	V503	A402	G335	A275	E214
MET	A548	A548	E237	K327	T266	N206	K132	E59		GLY	V504	A402	G335	A275	E214
MET	A549	A549	E238	K327	T266	N206	K132	E59		GLY	V505	A402	G335	A275	E214
MET	A550	A550	E239	K327	T266	N206	K132	E59		GLY	V506	A402	G335	A275	E214
MET	A551	A551	E240	K327	T266	N206	K132	E59		GLY	V507	A402	G335	A275	E214
MET	A552	A552	E241	K327	T266	N206	K132	E59		GLY	V508	A402	G335	A275	E214
MET	A553	A553	E242	K327	T266	N206	K132	E59		GLY	V509	A402	G335	A275	E214
MET	A554	A554	E243	K327	T266	N206	K132	E59		GLY	V510	A402	G335	A275	E214
MET	A555	A555	E244	K327	T266	N206	K132	E59		GLY	V511	A402	G335	A275	E214
MET	A556	A556	E245	K327	T266	N206	K132	E59		GLY	V512	A402	G335	A275	E214
MET	A557	A557	E246	K327	T266	N206	K132	E59		GLY	V513	A402	G335	A275	E214
MET	A558	A558	E247	K327	T266	N206	K132	E59		GLY	V514	A402	G335	A275	E214
MET	A559	A559	E248	K327	T266	N206	K132	E59		GLY	V515	A402	G335	A275	E214
MET	A560	A560	E249	K327	T266	N206	K132	E59		GLY	V516	A402	G335	A275	E214
MET	A561	A561	E250	K327	T266	N206	K132	E59		GLY	V517	A402	G335	A275	E214
MET	A562	A562	E251	K327	T266	N206	K132	E59		GLY	V518	A402	G335	A275	E214
MET	A563	A563	E252	K327	T266	N206	K132	E59		GLY	V519	A402	G335	A275	E214
MET	A564	A564	E253	K327	T266	N206	K132	E59		GLY	V520	A402	G335	A275	E214
MET	A565	A565	E254	K327	T266	N206	K132	E59		GLY	V521	A402	G335	A275	E214
MET	A566	A566	E255	K327	T266	N206	K132	E59		GLY	V522	A402	G335	A275	E2



• Molecule 1: GROEL

Chain D:  30% 58% 8%





GLY	Y476	G410
GLY	G477	V411
MET	Y478	V412
GLY	N479	A413
GLY	A480	G414
MET	A481	
GLY	T482	V417
GLY	E483	A418
MET	E484	L419
MET	Y485	I420
	G486	R421
	N487	V422
	Y488	
	T489	K425
	D490	
	N491	D428
	G492	L429
	L493	R430
	L494	G431
	D495	Q432
	P496	N433
	T497	E434
	K498	D435
	Y499	Q436
	T500	N437
	R501	V438
		G439
	L504	T440
	Q505	K441
	Y506	V442
		A443
	S509	
	V510	N447
	A511	E448
	G512	A449
		P450
	T515	L451
	T516	R452
	T517	Q453
	E518	T454
	C519	V455
	M520	L456
	T521	N457
	T522	C458
	D523	G459
	L524	E460
	P525	E461
	K526	P462
	ASN	S463
	ASP	V464
	ALA	V465
	ALA	A466
	ASP	N467
	LEU	T468
	GLY	V469
	ALA	K470
	ALA	G471
	GLY	G472
	GLY	
	MET	N475

• Molecule 1: GROEL

Chain F: 28% 59% 8% . .

GLY	E409	A341	P279	P218	Q146	G70	A2
GLY	G410	I342	G280	F219	V147	A71	A3
MET	Y476	Q343	G281	T220	G148	Q72	K4
GLY	Y478	G344	G282	L221	T149	M73	D5
GLY	A412	R345	D283	L222	I150	V74	V6
MET	G414	V346	R284	A223	S151	K75	K7
MET	A481	A347	R285	D224	A152	E76	F8
	Y417	Q348	K286	K225	N153	V77	G9
E483	A418	L349	A287	K226	S154	A78	N10
E484	L419	R350	N288	I227	D155	S79	Y14
Y485	T420	Q351	L289	S228	K80		
G486	R421	Q352	Q290	N229	V158	A81	K15
N487	V422	L353	D291	I230	G159	N82	M16
M488		E354	L292	R231	L160	D83	L17
Y491	D428	E355	A293	E232	L161	A84	R18
	L429	A356	T294	R233	I162	A85	G19
R430	R430	T357	L295	L234	A163	G86	V20
G431	G431	S358	T296	P235	E164	D87	N21
D495	Q432	V359		V236	A165	G88	V22
P496	N433	D360		L237	M166	T89	L23
T497	A434	R361	I301	E238	D167		A24
K498	D435	R362	S302	A239	K168	V94	D25
Y499	Q436	E363	E303	V240	G169	L95	A26
T500	N437	K364	E304	A241	V169	A96	V27
R501	V438	L365	L305	K242		Q97	K28
L504	G439	Q366	G306	G243	G173		V29
	T440	E367	P307	G244	I175	I100	T30
Q505	K441	R368	K308	K245	T176	T101	P33
Y506	V442	V369	L309	P246	E177	V107	K34
V510	A443		E310	L247	E178	A108	G35
A511	L444	L372	K311	L248	D179	A109	Y39
G512		A373	A312	T249	G180		
I515	N447		T313	T250		G110	L40
	E448	K360	L314	A251	L183	M11	L40
E518	A449	V361	E315	E252	Q184	N112	M11
	P450	G382	D316	D253	D185	P113	K42
	L451	A383	L317	V254		M114	S43
	C519	A384	G318	E255	M193	D115	F44
M520	Q453	T385	Q319	G256	Q194	L116	Y48
V521	T454		A320	E257	F195		
T522	V455	E388	K321	A258		I120	
E523	L456	K389	R322	L259	Y199	D121	K51
L524	P457	A390	V323	A260	L200	K122	D52
P525	C458	E391	V324	T261	S201	G53	G32
K526	G459	K392	L325	L262	P202	V124	V54
ASN	E460	K393	N326	V263	Y203	S55	S55
ASP	P461	A394	K327	V264	F204	A127	V56
ALA	P462	K395	D328	N265	T205	V128	A57
ALA	S463	V396	T329	T266	N206	E129	R58
ALA	V464	E397	T330	M267	K207	E130	E59
LEU	V465		T331		P208	L131	I60
GLY	A466	L400	L332	I270	E209	K132	E61
ALA	Y467	H401	T333	V271	A209	A133	L62
ALA	T468	A402	D334	K272	T210	L134	E63
GLY	Y469	T403	G335	V273	G211	S135	D64
GLY	K470	R404	V336	A274	V213	V136	K65
MET	G471	A405	G337	A275	E214		F66
GLY	G472	A406	E338	V276	L215	A143	E67
GLY	D473	V407	E339	K277	E216	T144	N68
MET	C474	E408	L439	A278	S217	A146	M69

• Molecule 1: GROEL

Chain G: 28% 59% 9% . .

L134	F66	A2
S135	E67	A3
V136	M68	K4
	M69	D5
D140	G70	V6
S141	A71	K7
K142	Q72	F8
	V73	G9
A145	V74	M10
Q146	E76	
V147	V77	R13
	A78	V14
I150	S79	K15
S151	K80	M16
A152	N81	L17
M153	N82	R18
	D83	G19
V158	A84	V20
G159	A85	M21
K160	G86	V22
L161	D87	L23
L162	G88	A24
A163	T89	D25
E164	T90	A26
		V27
D167	V94	K28
K168	L95	V29
V169	A96	T30
G170	Q97	L31
	A98	G32
G173	I99	P33
V174	I98	K34
I175	I100	G35
T176	T101	R36
V177		N37
E178	A108	V38
D179		V39
G180	M111	L40
L183	N112	D41
Q184	P113	K42
D185	M114	S43
	D115	P44
	L116	G45
M193	K117	
Q194	R118	T48
F195	G119	
	I120	K51
Y199	D121	D52
L200	K122	G53
S201	A123	V54
P202	V124	S55
Y203	T125	V56
F204	A126	A57
L205	A127	R58
N206	L128	E59
K207	E129	
	E130	L62
E208	L131	D63
P209	K132	D64
T210	A133	V65
T211		



LEU	D398	A466	V273	A212
GLY	A399	P467	A274	V213
ALA	L400	T468	A275	E214
ALA	L401	V469	V276	L215
GLY	A402	G470	K277	E216
GLY	T403	G471	A278	S217
MET	R404	G472	P279	P218
GLY	A405	D473	G280	F219
GLY	A406	G474	F281	L220
MET	E409	M475	G282	L221
GLY	G410	G477	D283	L222
MET	V411	G478	R284	A223
GLY	V412	M479	R285	D224
GLY	A413	A480	K286	K225
MET	G414	A481	A287	K226
		L482	M288	L227
		V483	L289	
		G484	Q290	
		E485	D291	
		G486	L292	
		M487	A293	
		L488	T294	
		K489	L295	
		D490	L296	
		M491	T297	
		L494	G298	
		D495	V299	
		P496	V300	
		G497	I301	
		M498	S302	
		L499	K303	
		G500	E304	
		M501	I305	
		L504	G306	
		Q505	E307	
		V506	M307	
		S509	E308	
		A511	I309	
		G512	E310	
		T515	K311	
		T516	A312	
		T517	T313	
		K518	L314	
		C519	E315	
		M520	D316	
		K142	L317	
		A143	G318	
		I144	Q319	
		T210	A320	
		G211	K321	
		A212	R322	
		V213	V323	
		E214	V324	
		L215	I325	
		L150	N326	
		S151	K327	
			D328	
			T329	
			T330	
			T331	
			V332	
			K333	
			E334	
			L335	
			T336	
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			V339	
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			V579	
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			E581	
			V582	
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			V585	
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			L619	
			E620	
			V621	
			L622	
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			V624	
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			V627	
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			E629	
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			L655	
			E656	
			V657	
			L658	
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			V660	
			L661	
			E662	
			V663	
			L664	
			E665	
			V666	

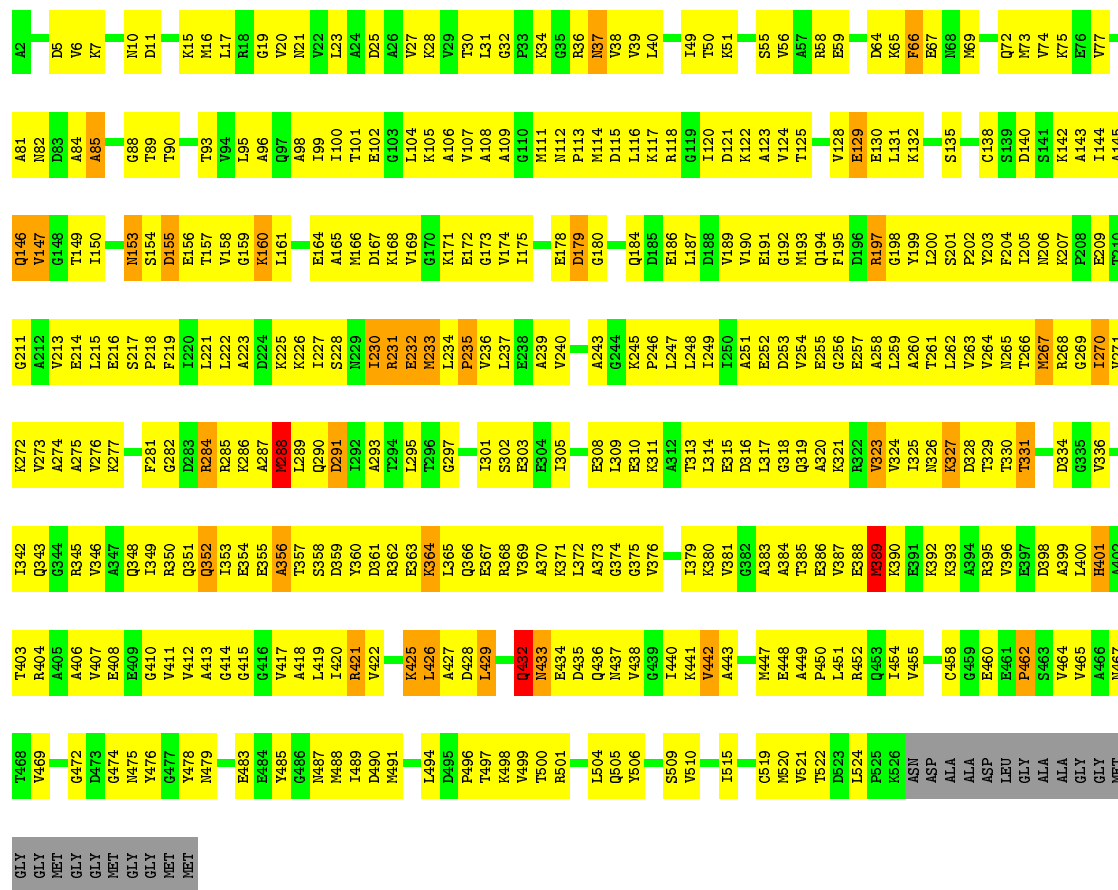






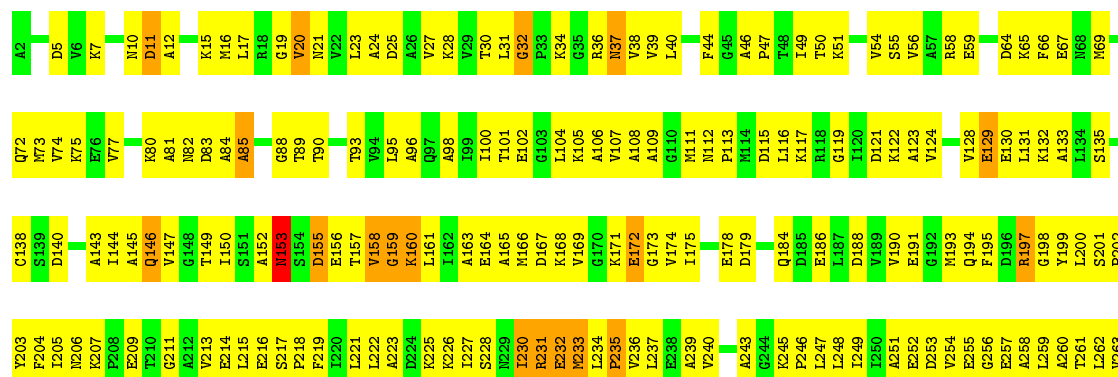
- Molecule 1: GROEL

Chain K:  29% 60% 6% . .

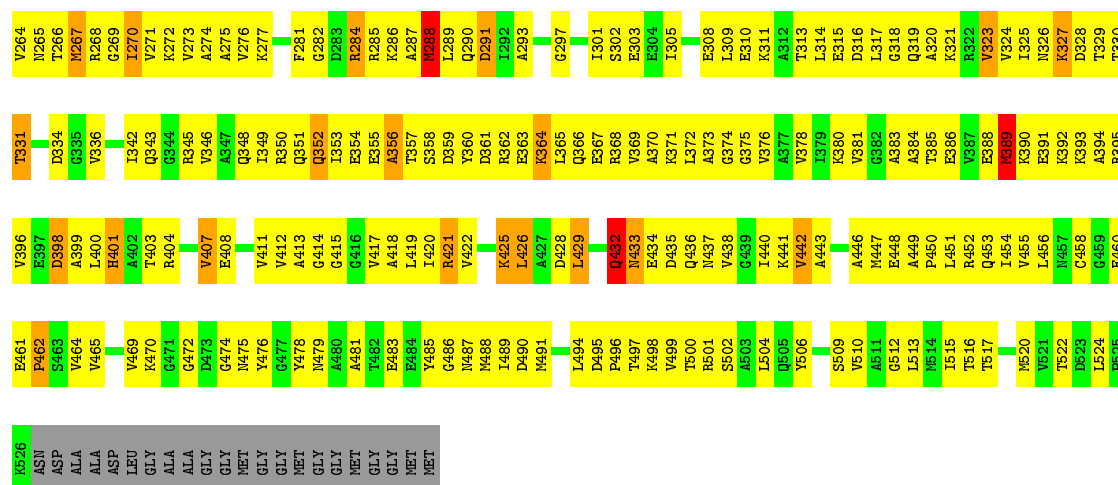


- Molecule 1: GROEL

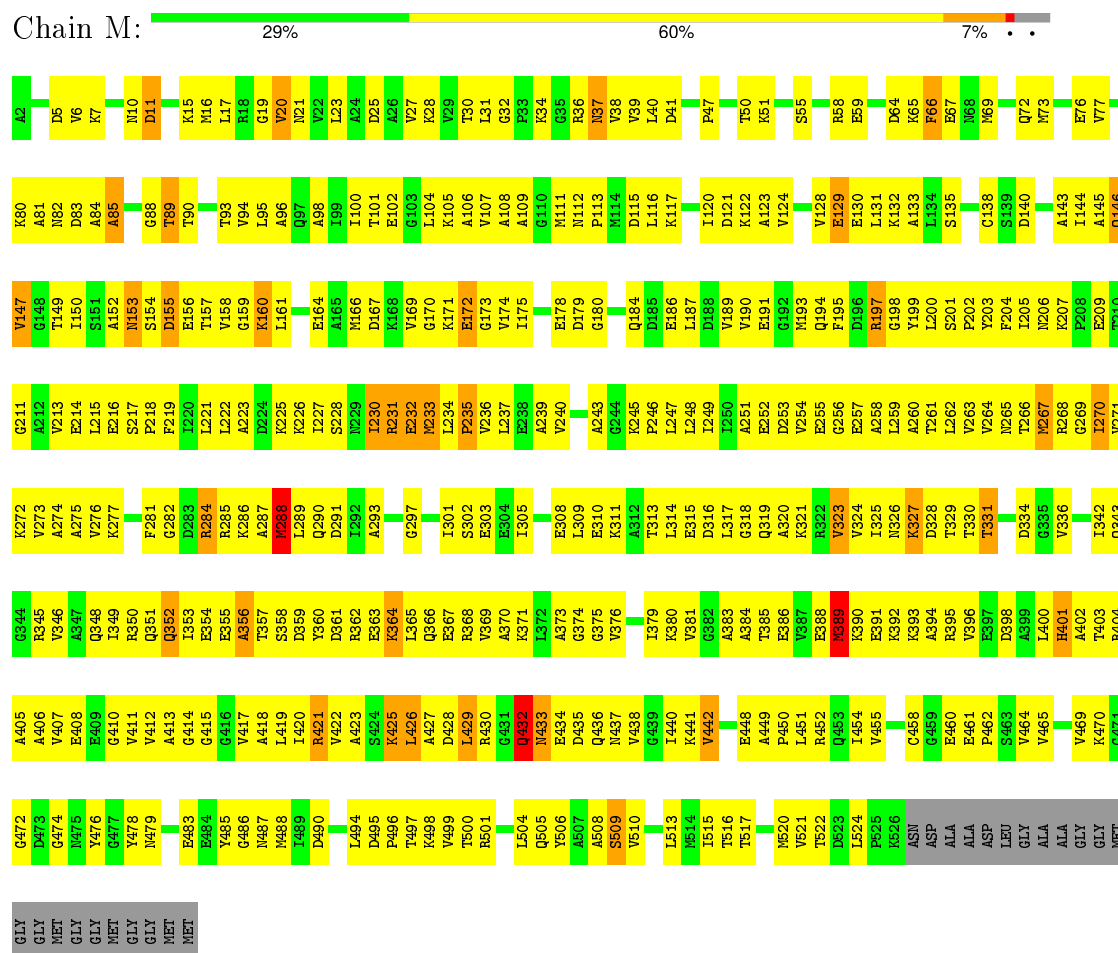
Chain L:  28% 61% 7% . .



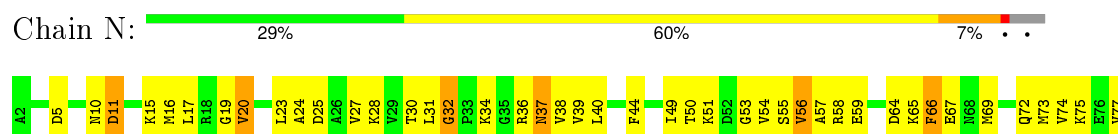




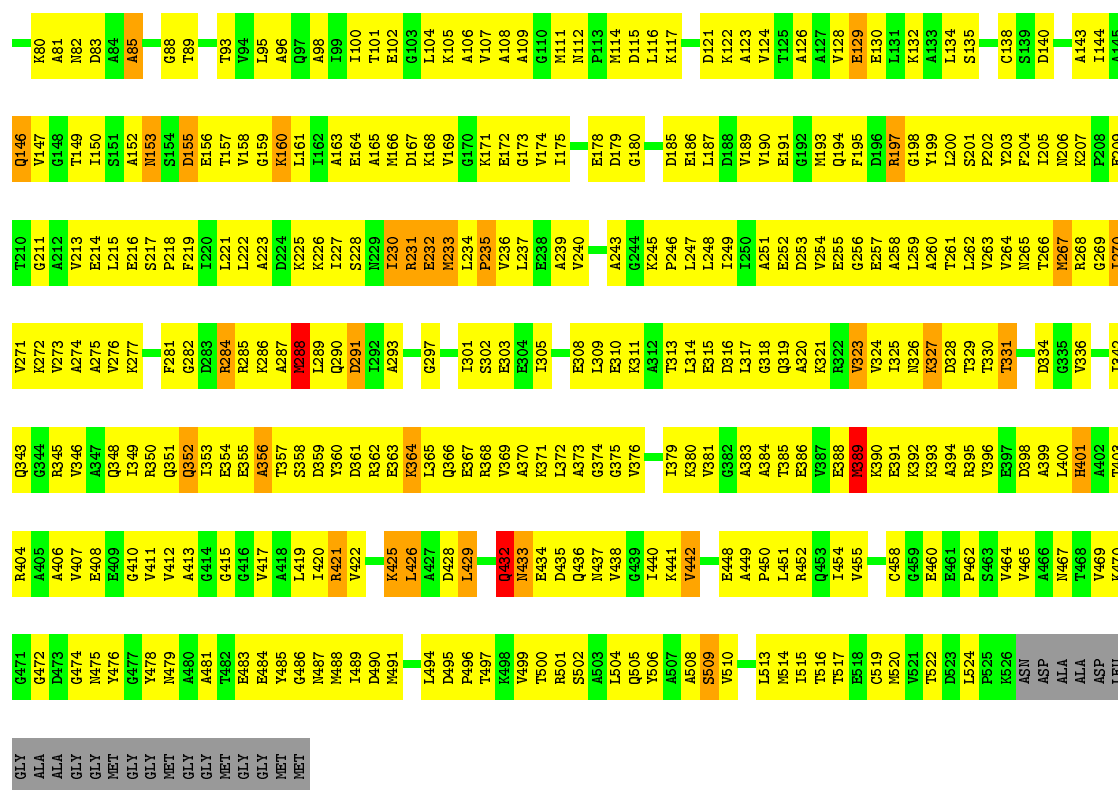
### • Molecule 1: GROEL



### • Molecule 1: GROEL











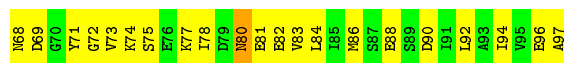
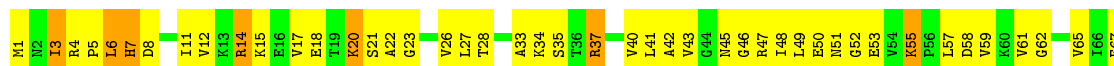
- Molecule 2: GROES

Chain R: 27% 61% 12%



- Molecule 2: GROES

Chain S: 32% 60% 8%



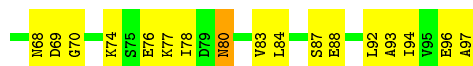
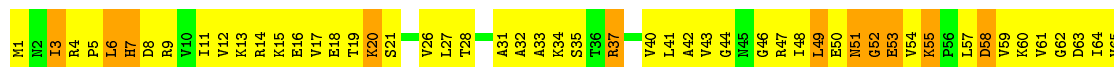
- Molecule 2: GROES

Chain T: 31% 56% 13%



- Molecule 2: GROES

Chain U: 29% 59% 12%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CLASS AVERAGES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.52	0/3836	0.76	0/5188
1	B	0.52	0/3836	0.75	0/5188
1	C	0.52	0/3836	0.74	0/5188
1	D	0.53	0/3836	0.74	0/5188
1	E	0.52	0/3836	0.76	0/5188
1	F	0.53	0/3836	0.75	0/5188
1	G	0.53	0/3836	0.75	0/5188
1	H	0.48	0/3876	0.73	0/5232
1	I	0.49	0/3876	0.72	0/5232
1	J	0.48	0/3876	0.72	0/5232
1	K	0.48	0/3876	0.72	0/5232
1	L	0.47	0/3876	0.72	0/5232
1	M	0.48	0/3876	0.72	0/5232
1	N	0.48	0/3876	0.72	0/5232
2	O	0.39	0/729	0.68	0/980
2	P	0.36	0/729	0.68	0/980
2	Q	0.37	0/729	0.69	0/980
2	R	0.39	0/729	0.69	0/980
2	S	0.37	0/729	0.69	0/980
2	T	0.39	0/729	0.69	0/980
2	U	0.36	0/729	0.68	0/980
All	All	0.49	0/59087	0.73	0/79800

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [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	3809	0	3890	559	0
1	B	3809	0	3890	514	0
1	C	3809	0	3890	524	0
1	D	3809	0	3890	530	0
1	E	3809	0	3890	542	0
1	F	3809	0	3890	542	0
1	G	3809	0	3890	528	0
1	H	3850	0	3959	527	0
1	I	3850	0	3959	528	0
1	J	3850	0	3958	512	0
1	K	3850	0	3960	531	0
1	L	3850	0	3961	564	0
1	M	3850	0	3960	538	0
1	N	3850	0	3960	518	0
2	O	725	0	755	119	0
2	P	725	0	755	98	0
2	Q	725	0	755	103	0
2	R	725	0	755	107	0
2	S	725	0	755	100	0
2	T	725	0	755	109	0
2	U	725	0	755	102	0
All	All	58688	0	60232	7994	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 67.

The worst 5 of 7994 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:J:174:VAL:HG21	1:J:371:LYS:CD	1.38	1.53
1:H:373:ALA:N	1:H:375:GLY:HA2	1.25	1.50

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	24
1	B	523/547 (96%)	398 (76%)	95 (18%)	30 (6%)	2	28
1	C	523/547 (96%)	397 (76%)	88 (17%)	38 (7%)	1	21
1	D	523/547 (96%)	397 (76%)	93 (18%)	33 (6%)	2	25
1	E	523/547 (96%)	390 (75%)	98 (19%)	35 (7%)	1	24
1	F	523/547 (96%)	399 (76%)	93 (18%)	31 (6%)	2	27
1	G	523/547 (96%)	390 (75%)	99 (19%)	34 (6%)	1	25
1	H	519/547 (95%)	374 (72%)	116 (22%)	29 (6%)	2	28
1	I	519/547 (95%)	377 (73%)	115 (22%)	27 (5%)	2	30
1	J	519/547 (95%)	376 (72%)	117 (22%)	26 (5%)	3	31
1	K	519/547 (95%)	372 (72%)	120 (23%)	27 (5%)	2	30
1	L	519/547 (95%)	372 (72%)	116 (22%)	31 (6%)	2	26
1	M	519/547 (95%)	375 (72%)	117 (22%)	27 (5%)	2	30
1	N	519/547 (95%)	377 (73%)	114 (22%)	28 (5%)	2	29
2	O	95/97 (98%)	69 (73%)	20 (21%)	6 (6%)	2	25
2	P	95/97 (98%)	65 (68%)	24 (25%)	6 (6%)	2	25
2	Q	95/97 (98%)	67 (70%)	21 (22%)	7 (7%)	1	21
2	R	95/97 (98%)	68 (72%)	18 (19%)	9 (10%)	1	15
2	S	95/97 (98%)	73 (77%)	16 (17%)	6 (6%)	2	25
2	T	95/97 (98%)	67 (70%)	20 (21%)	8 (8%)	1	18
2	U	95/97 (98%)	64 (67%)	24 (25%)	7 (7%)	1	21
All	All	7959/8337 (96%)	5863 (74%)	1616 (20%)	480 (6%)	4	26

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%)	369 (94%)	24 (6%)	23	60
1	B	393/414 (95%)	368 (94%)	25 (6%)	22	58
1	C	393/414 (95%)	369 (94%)	24 (6%)	23	60
1	D	393/414 (95%)	369 (94%)	24 (6%)	23	60
1	E	393/414 (95%)	368 (94%)	25 (6%)	22	58
1	F	393/414 (95%)	368 (94%)	25 (6%)	22	58
1	G	393/414 (95%)	367 (93%)	26 (7%)	21	57
1	H	403/414 (97%)	385 (96%)	18 (4%)	34	69
1	I	403/414 (97%)	382 (95%)	21 (5%)	29	65
1	J	403/414 (97%)	383 (95%)	20 (5%)	30	66
1	K	403/414 (97%)	384 (95%)	19 (5%)	32	68
1	L	403/414 (97%)	384 (95%)	19 (5%)	32	68
1	M	403/414 (97%)	383 (95%)	20 (5%)	30	66
1	N	403/414 (97%)	384 (95%)	19 (5%)	32	68
2	O	79/80 (99%)	73 (92%)	6 (8%)	16	53
2	P	79/80 (99%)	74 (94%)	5 (6%)	22	59
2	Q	79/80 (99%)	72 (91%)	7 (9%)	12	44
2	R	79/80 (99%)	70 (89%)	9 (11%)	7	33
2	S	79/80 (99%)	73 (92%)	6 (8%)	16	53
2	T	79/80 (99%)	71 (90%)	8 (10%)	9	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	U	79/80 (99%)	72 (91%)	7 (9%)	12	44
All	All	6125/6356 (96%)	5768 (94%)	357 (6%)	29	61

5 of 357 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	257	GLU
1	I	197	ARG
2	R	20	LYS
1	G	315	GLU
1	H	233	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 195 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	348	GLN
1	I	146	GLN
2	Q	45	ASN
1	G	352	GLN
1	H	319	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

There are no chain breaks in this entry.