



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:35 PM GMT

PDB ID : 1PCQ
Title : Crystal structure of groEL-groES
Authors : Chaudhry, C.; Farr, G.W.; Todd, M.J.; Rye, H.S.; Brunger, A.T.; Adams, P.D.; Horwich, A.L.; Sigler, P.B.
Deposited on : 2003-05-16
Resolution : 2.81 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

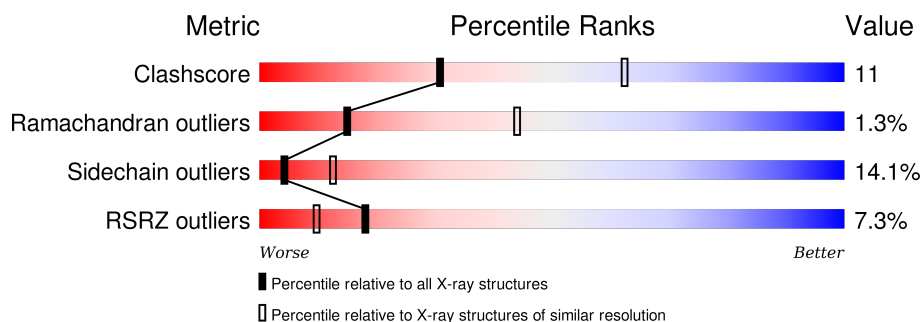
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	524	<div> <div>8%</div> <div>71% 23% 5%</div> </div>
1	B	524	<div> <div>10%</div> <div>73% 22% .</div> </div>
1	C	524	<div> <div>7%</div> <div>71% 23% 5%</div> </div>
1	D	524	<div> <div>9%</div> <div>70% 25% 5%</div> </div>
1	E	524	<div> <div>11%</div> <div>73% 23% .</div> </div>
1	F	524	<div> <div>14%</div> <div>74% 21% 5%</div> </div>
1	G	524	<div> <div>10%</div> <div>72% 23% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	524	<div><div></div><div>2%</div><div>67%</div><div>28%</div><div>5%</div></div>
1	I	524	<div><div></div><div>%</div><div>65%</div><div>30%</div><div>5%</div></div>
1	J	524	<div><div></div><div>2%</div><div>66%</div><div>28%</div><div>5%</div></div>
1	K	524	<div><div></div><div>%</div><div>67%</div><div>27%</div><div>5%</div></div>
1	L	524	<div><div></div><div>4%</div><div>67%</div><div>28%</div><div>.</div></div>
1	M	524	<div><div></div><div>3%</div><div>63%</div><div>30%</div><div>6%</div></div>
1	N	524	<div><div></div><div>2%</div><div>67%</div><div>27%</div><div>5%</div></div>
2	O	97	<div><div></div><div>22%</div><div>70%</div><div>24%</div><div>6%</div></div>
2	P	97	<div><div></div><div>12%</div><div>65%</div><div>28%</div><div>7%</div></div>
2	Q	97	<div><div></div><div>19%</div><div>67%</div><div>28%</div><div>.</div></div>
2	R	97	<div><div></div><div>31%</div><div>70%</div><div>24%</div><div>5%</div></div>
2	S	97	<div><div></div><div>21%</div><div>70%</div><div>25%</div><div>5%</div></div>
2	T	97	<div><div></div><div>24%</div><div>69%</div><div>26%</div><div>.</div></div>
2	U	97	<div><div></div><div>24%</div><div>68%</div><div>26%</div><div>6%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 59304 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	B	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	C	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	D	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	E	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	F	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	G	524	Total	C	N	O	S	0	0	0
			3855	2397	665	773	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

- Molecule 2 is a protein called groES protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	U	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

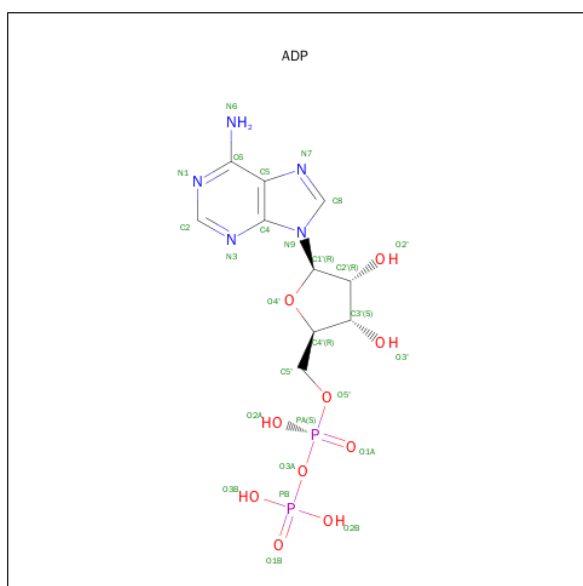
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	K	0	0
			1	1		
4	D	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		

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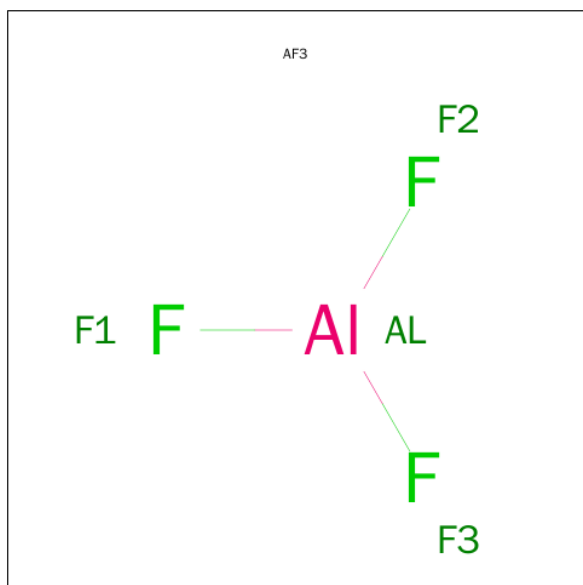
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	K	0	0
			1	1		
4	A	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).

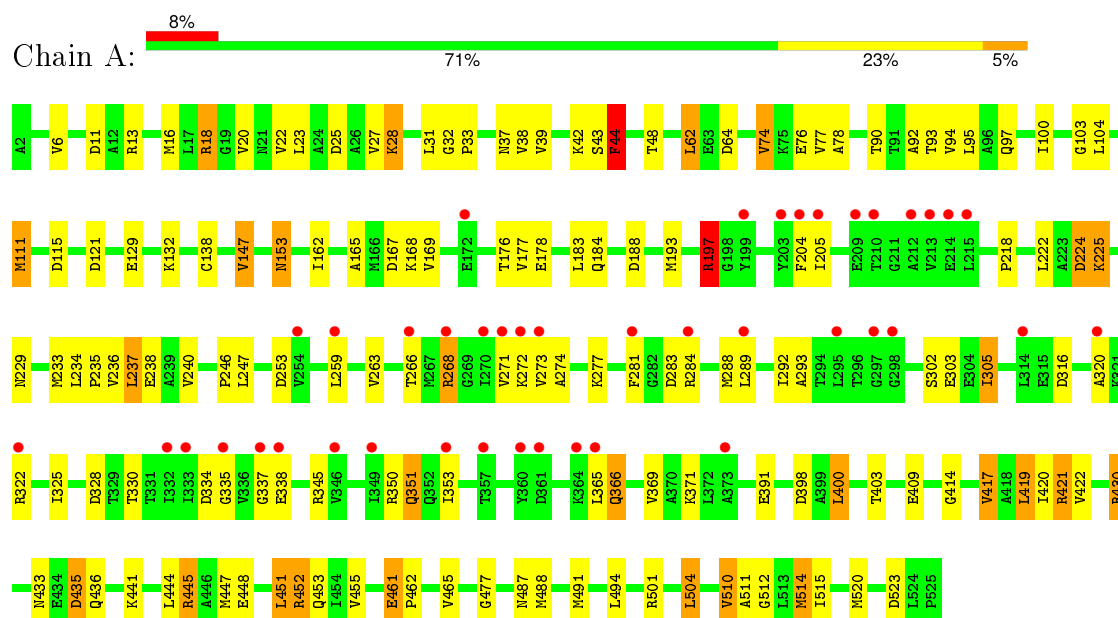


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F		
			4	1	3		
6	C	1	Total	Al	F		
			4	1	3		
6	D	1	Total	Al	F		
			4	1	3		
6	E	1	Total	Al	F	0	0
			4	1	3		
6	F	1	Total	Al	F		
			4	1	3		
6	G	1	Total	Al	F		
			4	1	3		

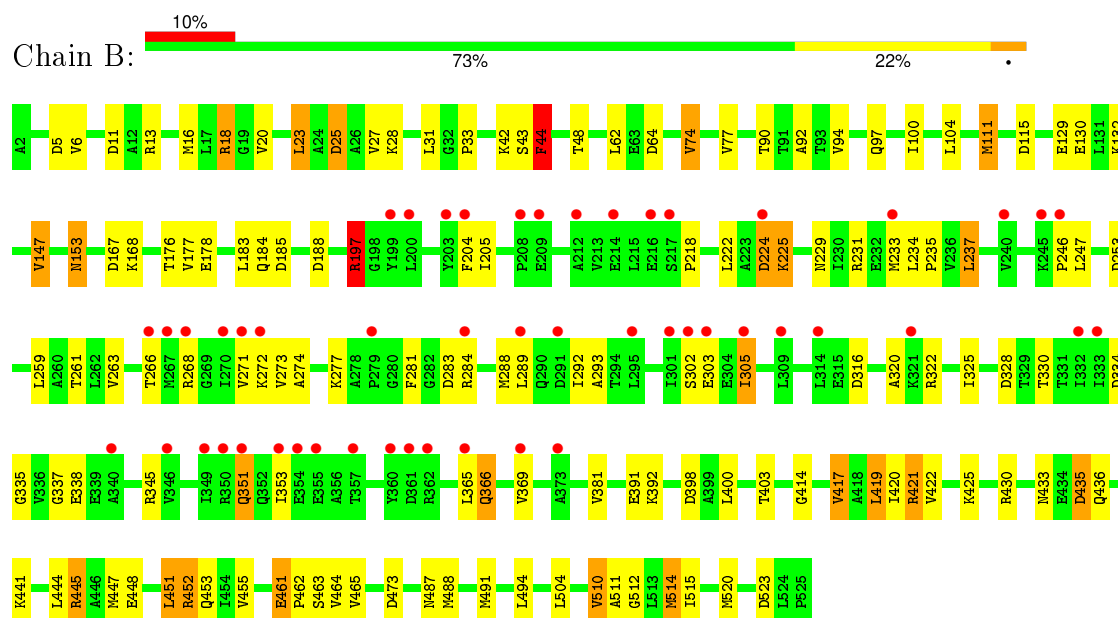
3 Residue-property plots

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 and electron 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 dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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 protein



• Molecule 1: groEL protein



Chain C: 71% 23% 5%

Item	Category
E434	Green
D435	Green
Q436	Green
K441	Green
L444	Green
R445	Green
A446	Green
M447	Green
E448	Green
L451	Green
R452	Green
Q453	Green
L454	Green
V455	Green
E461	Green
P462	Green
S463	Green
V464	Green
V465	Green
A466	Green
M467	Green
T468	Green
G477	Green
M487	Green
M488	Green
M491	Green
L494	Green
L504	Green
A508	Green
S509	Green
W510	Green
A511	Green
G512	Green
L513	Green
M514	Green
L515	Green
T516	Green
C519	Green
M520	Green
D523	Green
L524	Green
P525	Green
M233	Green
L234	Green
P235	Green
V236	Green
L237	Green
E238	Green
K242	Green
P246	Green
L247	Green
T250	Green
A251	Green
E252	Green
D253	Green
V254	Green
L259	Green
V263	Green
T266	Green
M267	Green
R268	Green
G269	Green
L270	Green
V271	Green
K272	Green
V273	Green
A274	Green
K277	Green
A278	Green
P279	Green
G280	Green
F281	Green
G282	Green
D283	Green
R284	Green
M288	Green
L289	Green
L292	Green
A293	Green
S302	Green
E303	Green
L305	Green
L309	Green
L314	Green
E315	Green
D316	Green
Q319	Green
A320	Green
R321	Green
K322	Green
L325	Green
T330	Green
D334	Green
G335	Green
V336	Green
G337	Green
E338	Green
R339	Green
A340	Green
L341	Green
V342	Green
E343	Green
L344	Green
V345	Green
T349	Green
R350	Green
Q351	Green
K352	Green
L353	Green
V354	Green
R355	Green
A356	Green
T357	Green
S358	Green
R359	Green
V360	Green
D361	Green
L365	Green
K366	Green
V369	Green
A370	Green
K371	Green
V381	Green
E391	Green
K392	Green
D398	Green
A399	Green
L400	Green
G414	Green
V417	Green
L418	Green
L419	Green
T420	Green
R421	Green
V422	Green
K425	Green
R430	Green
M432	Green
D115	Orange
V124	Orange
E129	Orange
E130	Orange
K132	Orange
C138	Orange
V147	Orange
N145	Orange
I162	Orange
K168	Orange
K171	Orange
E172	Orange

[illegible]

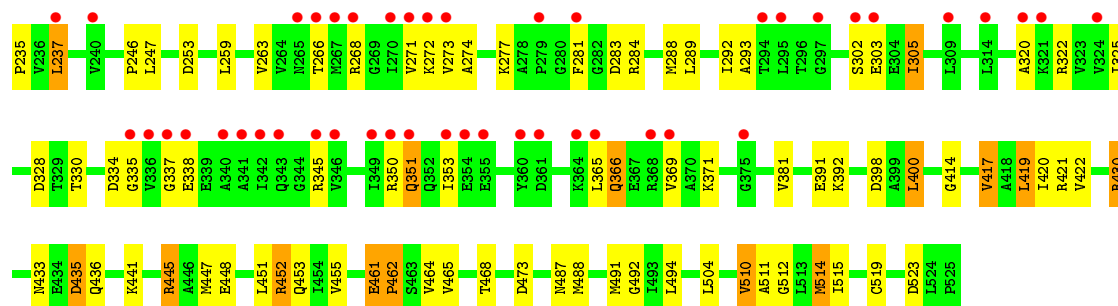
Chain E:

11% 73% 23%

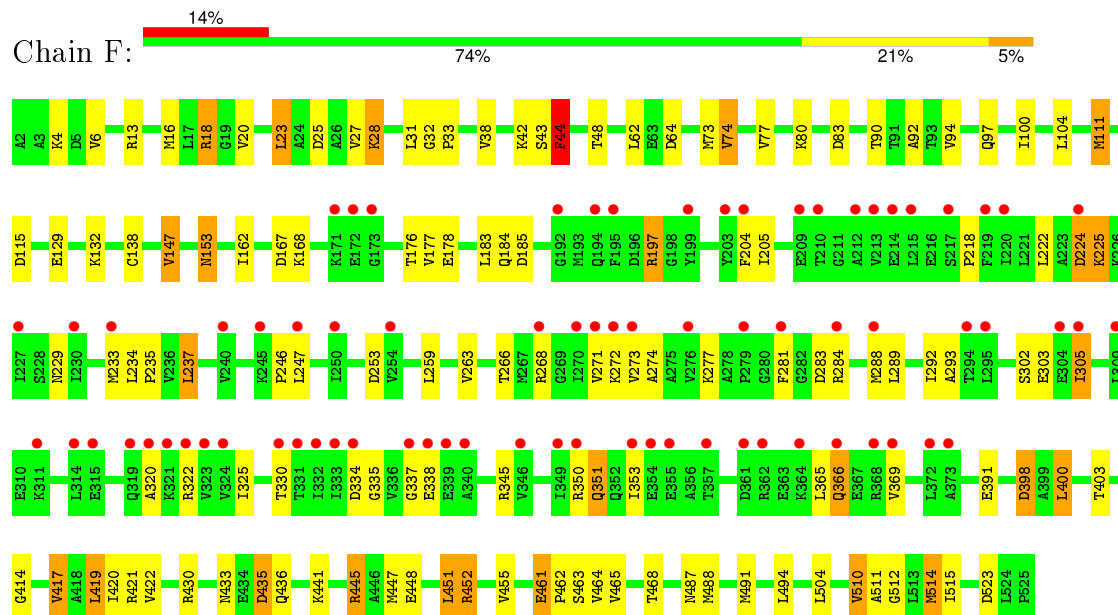
Legend: Green (11%), Yellow (73%), Orange (23%)

Nodes (top to bottom): A2, V6, D11, A12, R13, M16, L17, R18, G19, V20, L23, A24, D25, A26, V27, K28, L31, G32, P33, D41, K42, S43, F44, V54, R58, L62, B63, D64, V74, V77, R80, G88, T89, T90, T91, A92, T93, V94, Q97, I100, L104, M111

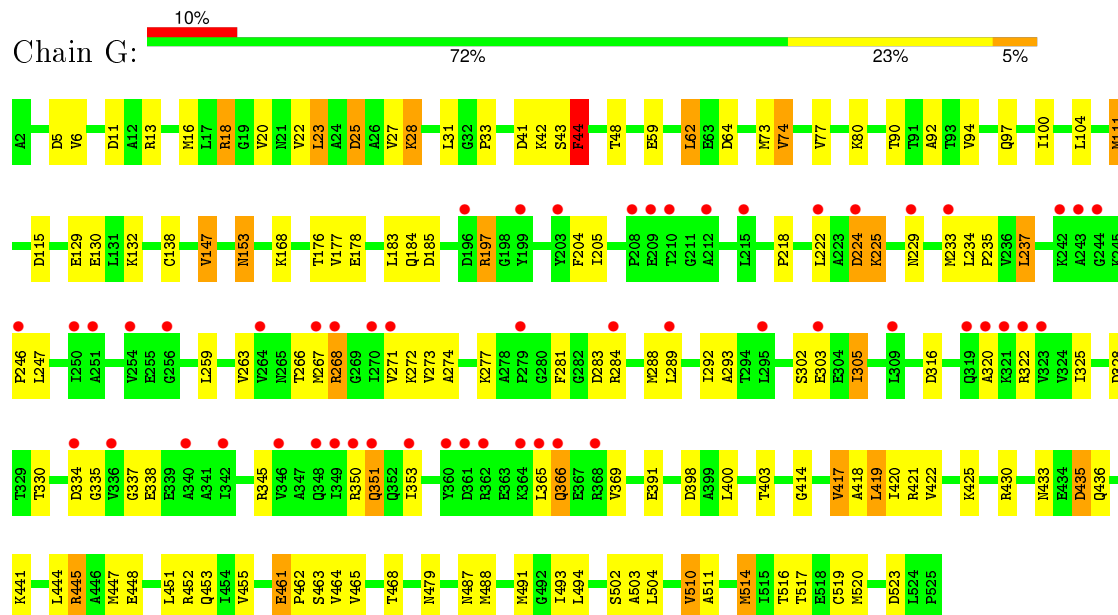
Nodes (bottom to top): D115, E129, E130, L131, K132, A133, C138, V147, I150, M153, I162, D167, K168, E172, T176, V177, E178, L183, Q184, D185, G192, M193, Q194, F195, D196, R197, G198, Y199, Y203, F204, I205, A212, L216, L215, E217, S217, P218, L222, A223, D224, K225, N229, M233, L234



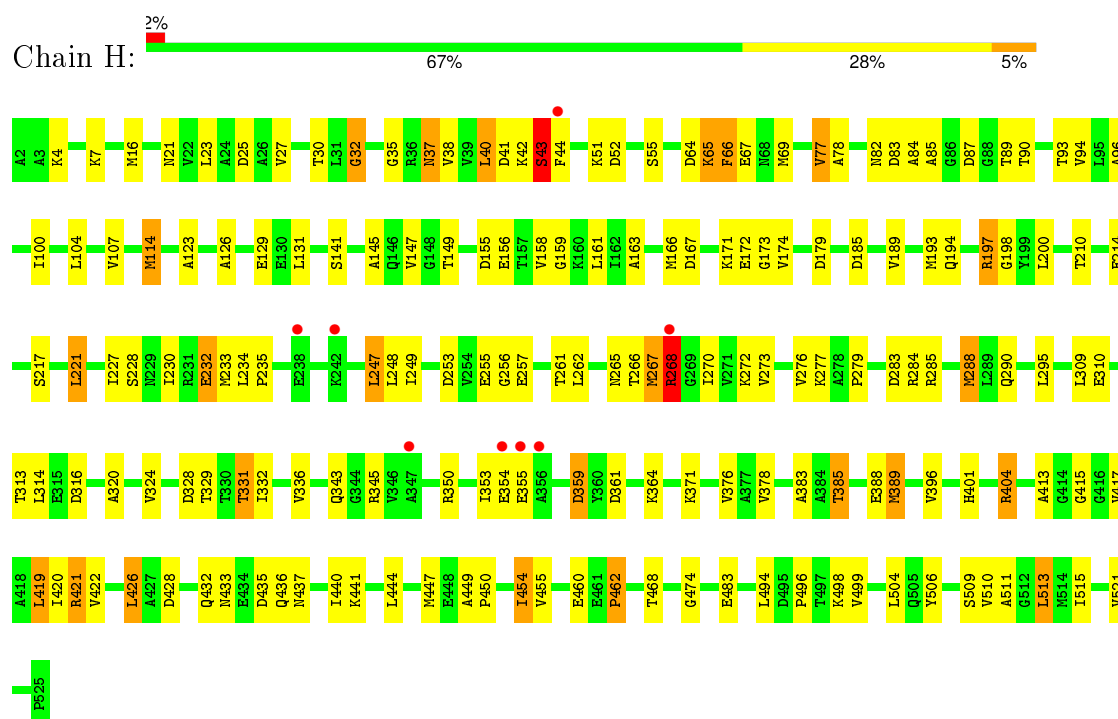
• Molecule 1: groEL protein



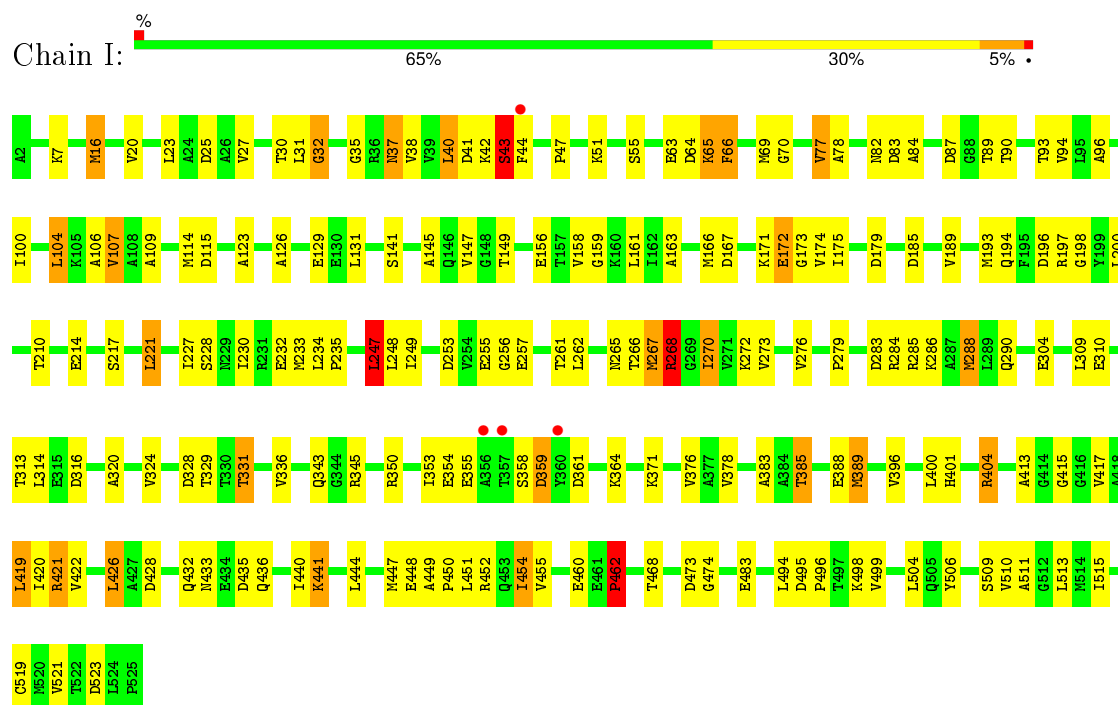
• Molecule 1: groEL protein



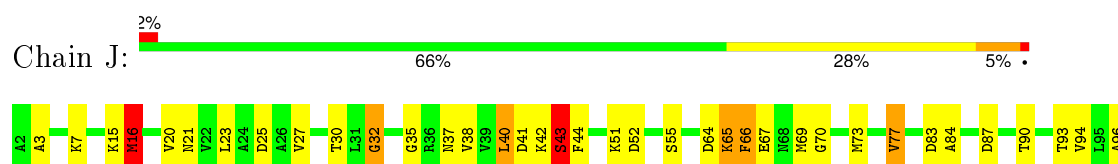
• Molecule 1: groEL protein

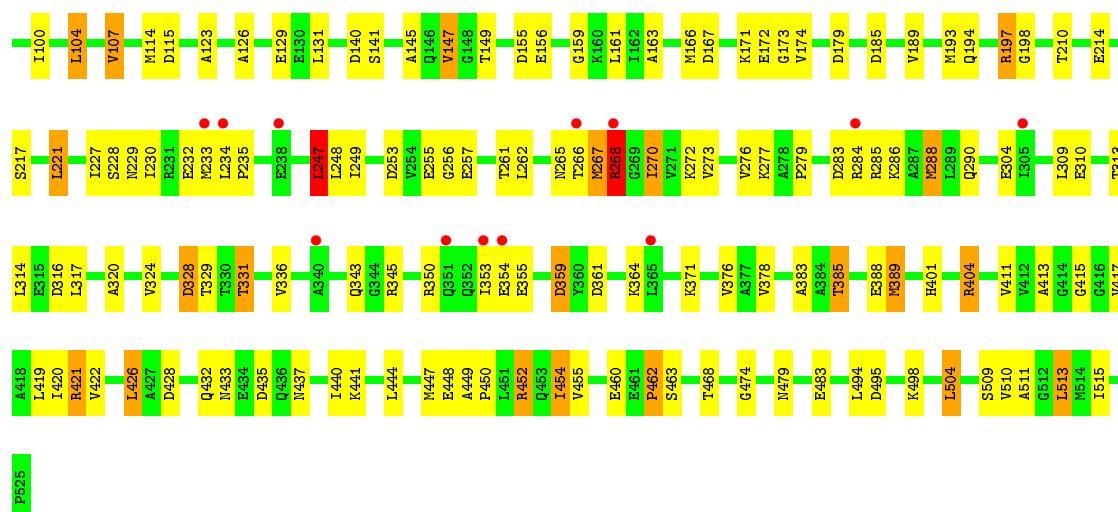


- Molecule 1: groEL protein

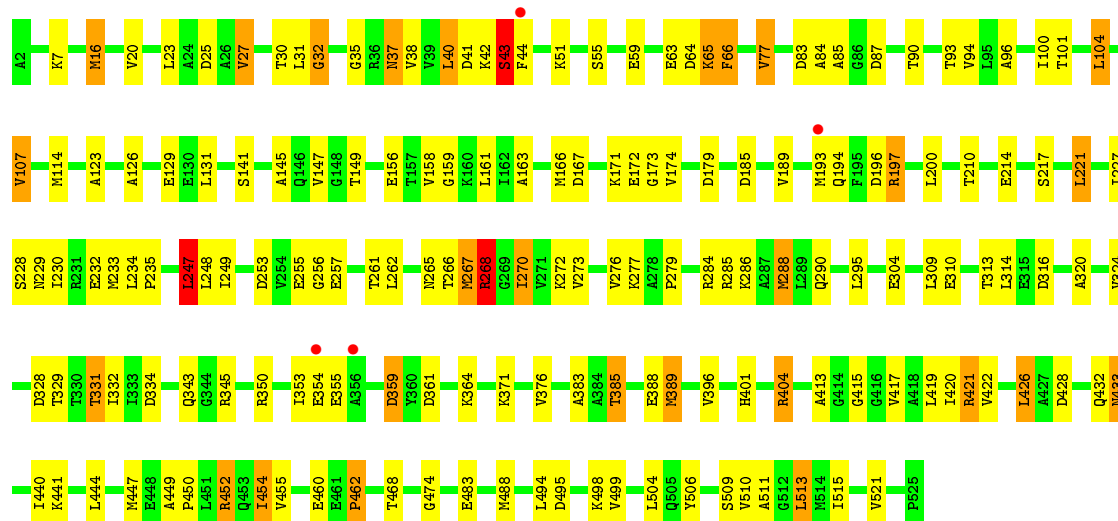


- Molecule 1: groEL protein

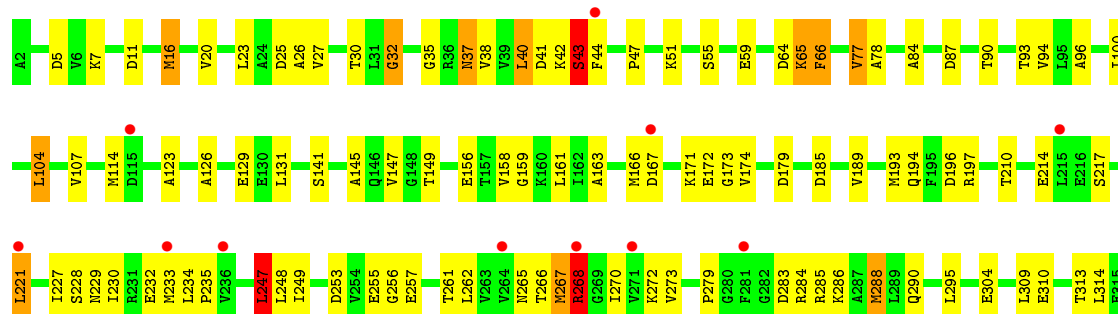


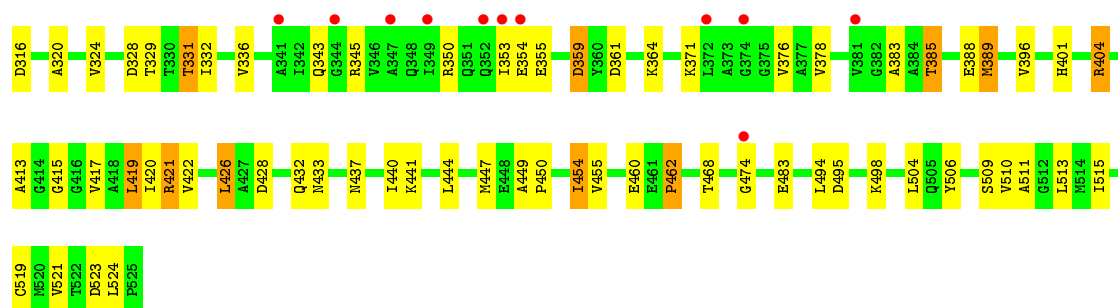


- Molecule 1: groEL protein

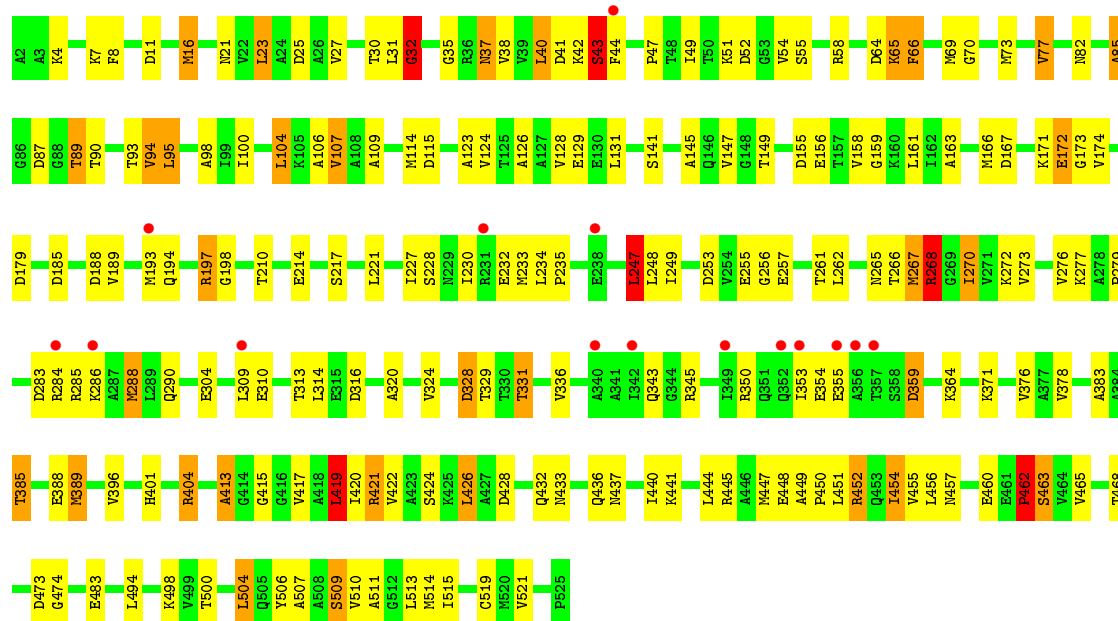


- Molecule 1: groEL protein

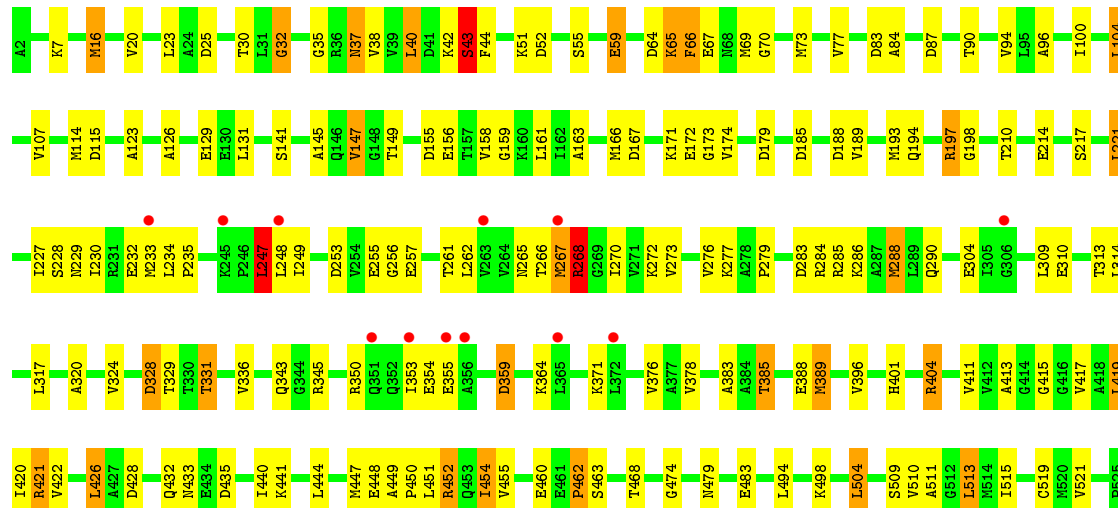




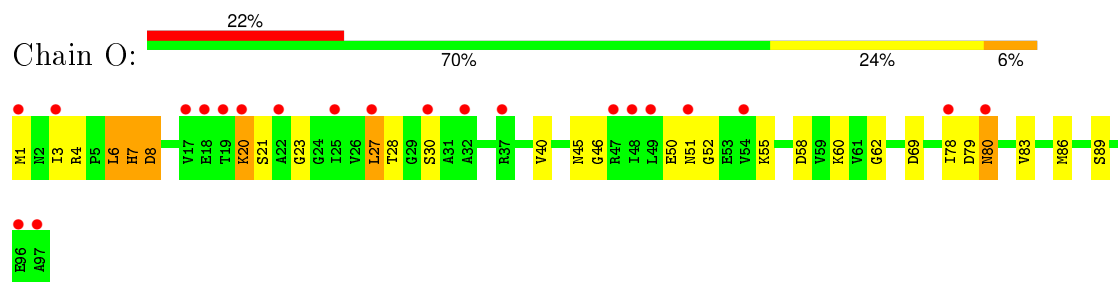
• Molecule 1: groEL protein



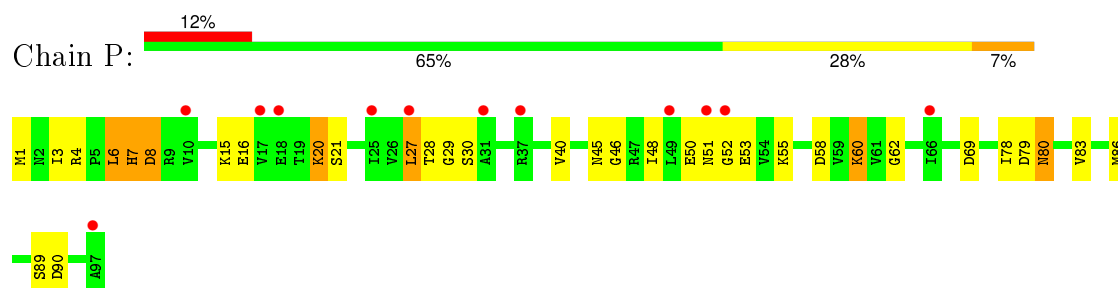
• Molecule 1: groEL protein



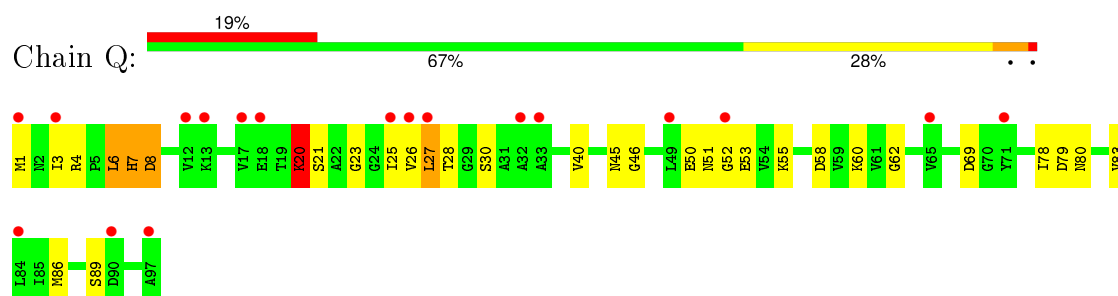
- Molecule 2: groES protein



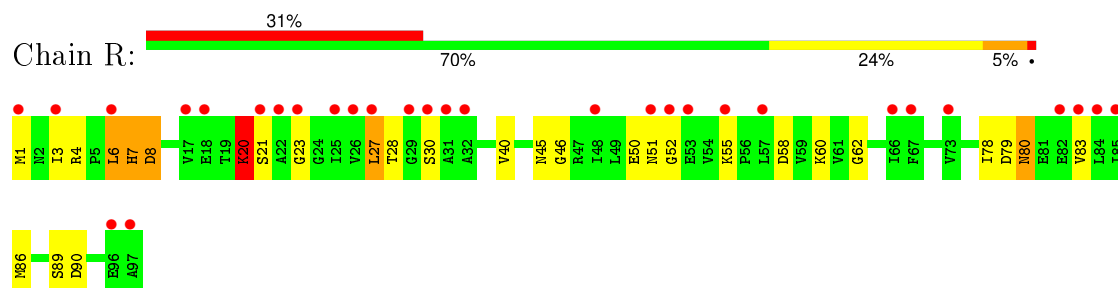
- Molecule 2: groES protein



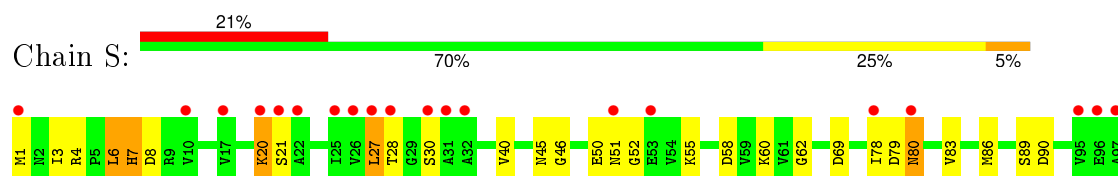
- Molecule 2: groES protein



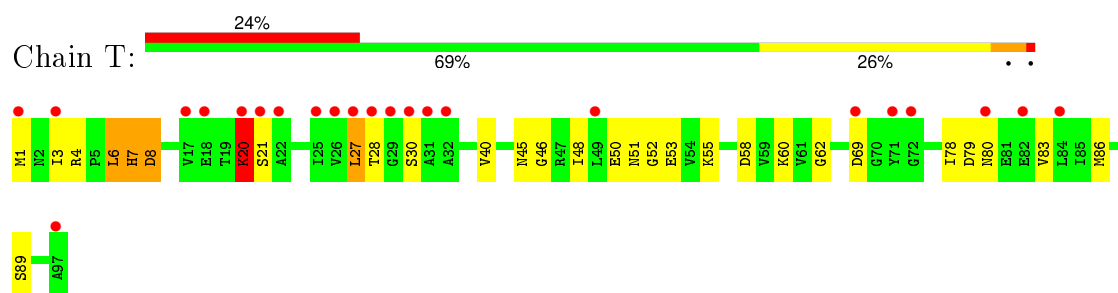
- Molecule 2: groES protein



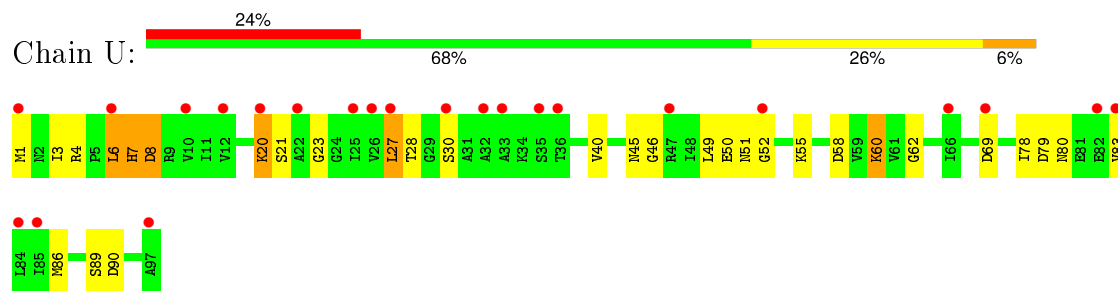
- Molecule 2: groES protein



- Molecule 2: groES protein



- Molecule 2: groES protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.55Å 266.86Å 187.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.81 49.44 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.39-2.81) 60.7 (49.44-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.262 , 0.278 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.958	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.2	EDS
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	6 of 345474 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	59304	wwPDB-VP
Average B, all atoms (Å ²)	2.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, MG, ADP, AF3

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	0.70	1/3883 (0.0%)	0.93	19/5243 (0.4%)
1	B	0.61	0/3883	0.96	23/5243 (0.4%)
1	C	0.66	0/3883	0.91	19/5243 (0.4%)
1	D	0.68	1/3883 (0.0%)	0.92	19/5243 (0.4%)
1	E	0.54	0/3883	0.86	17/5243 (0.3%)
1	F	0.54	0/3883	0.87	17/5243 (0.3%)
1	G	0.62	0/3883	0.92	20/5243 (0.4%)
1	H	0.60	0/3884	0.83	15/5243 (0.3%)
1	I	0.64	0/3884	0.87	19/5243 (0.4%)
1	J	0.60	1/3884 (0.0%)	0.85	20/5243 (0.4%)
1	K	0.52	0/3884	0.86	16/5243 (0.3%)
1	L	0.49	0/3884	0.81	17/5243 (0.3%)
1	M	0.83	4/3884 (0.1%)	0.99	24/5243 (0.5%)
1	N	0.60	0/3884	0.85	16/5243 (0.3%)
2	O	0.35	0/732	0.69	4/983 (0.4%)
2	P	0.35	0/732	0.69	5/983 (0.5%)
2	Q	0.34	0/732	0.69	4/983 (0.4%)
2	R	0.34	0/732	0.69	4/983 (0.4%)
2	S	0.35	0/732	0.69	4/983 (0.4%)
2	T	0.35	0/732	0.69	4/983 (0.4%)
2	U	0.35	0/732	0.69	5/983 (0.5%)
All	All	0.60	7/59493 (0.0%)	0.87	291/80283 (0.4%)

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	M	0	1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	95	LEU	CG-CD1	7.61	1.80	1.51
1	D	130	GLU	CD-OE1	5.75	1.31	1.25
1	M	94	VAL	C-O	5.54	1.33	1.23
1	M	85	ALA	CA-CB	5.50	1.64	1.52
1	A	76	GLU	CD-OE1	5.26	1.31	1.25

The worst 5 of 291 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-19.61	110.50	120.30
1	B	231	ARG	NE-CZ-NH2	18.76	129.68	120.30
1	K	268	ARG	NE-CZ-NH2	-14.05	113.28	120.30
1	M	268	ARG	NE-CZ-NH2	-13.54	113.53	120.30
1	K	268	ARG	NE-CZ-NH1	13.45	127.03	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	32	GLY	Peptide

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	3855	0	3976	91	0
1	B	3855	0	3976	75	0
1	C	3855	0	3976	95	0
1	D	3855	0	3976	90	0
1	E	3855	0	3976	75	0
1	F	3855	0	3976	72	0
1	G	3855	0	3976	83	0
1	H	3856	0	3976	92	0
1	I	3856	0	3976	97	0
1	J	3856	0	3976	98	0
1	K	3856	0	3976	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	3856	0	3976	81	0
1	M	3856	0	3976	129	0
1	N	3856	0	3976	102	0
2	O	728	0	762	13	0
2	P	728	0	762	19	0
2	Q	728	0	762	16	0
2	R	728	0	762	12	0
2	S	728	0	762	11	0
2	T	728	0	762	13	0
2	U	728	0	762	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	27	0	12	4	0
5	B	27	0	12	1	0
5	C	27	0	12	5	0
5	D	27	0	12	2	0
5	E	27	0	12	1	0
5	F	27	0	12	3	0
5	G	27	0	12	1	0
6	A	4	0	0	1	0
6	B	4	0	0	0	0
6	C	4	0	0	1	0
6	D	4	0	0	0	0
6	E	4	0	0	0	0
6	F	4	0	0	0	0
6	G	4	0	0	1	0
All	All	59304	0	61082	1315	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 11.

The worst 5 of 1315 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:M:95:LEU:CG	1:M:95:LEU:CD1	1.80	1.60
1:F:73:MET:CE	1:F:73:MET:SD	2.01	1.48
1:H:114:MET:CE	1:H:114:MET:SD	2.02	1.48
1:G:73:MET:SD	1:G:73:MET:CE	2.01	1.48
1:N:16:MET:SD	1:N:16:MET:CE	2.01	1.47

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 X-ray entries followed by that with respect to entries of similar resolution.

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	522/524 (100%)	486 (93%)	32 (6%)	4 (1%)	24	58
1	B	522/524 (100%)	486 (93%)	32 (6%)	4 (1%)	24	58
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	24	58
1	D	522/524 (100%)	486 (93%)	31 (6%)	5 (1%)	19	52
1	E	522/524 (100%)	488 (94%)	30 (6%)	4 (1%)	24	58
1	F	522/524 (100%)	487 (93%)	31 (6%)	4 (1%)	24	58
1	G	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	24	58
1	H	522/524 (100%)	483 (92%)	33 (6%)	6 (1%)	17	50
1	I	522/524 (100%)	480 (92%)	36 (7%)	6 (1%)	17	50
1	J	522/524 (100%)	477 (91%)	39 (8%)	6 (1%)	17	50
1	K	522/524 (100%)	483 (92%)	33 (6%)	6 (1%)	17	50
1	L	522/524 (100%)	485 (93%)	31 (6%)	6 (1%)	17	50
1	M	522/524 (100%)	468 (90%)	42 (8%)	12 (2%)	8	26
1	N	522/524 (100%)	479 (92%)	37 (7%)	6 (1%)	17	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	95/97 (98%)	74 (78%)	18 (19%)	3 (3%)	5	17
2	P	95/97 (98%)	74 (78%)	17 (18%)	4 (4%)	3	11
2	Q	95/97 (98%)	74 (78%)	16 (17%)	5 (5%)	2	7
2	R	95/97 (98%)	74 (78%)	17 (18%)	4 (4%)	3	11
2	S	95/97 (98%)	74 (78%)	18 (19%)	3 (3%)	5	17
2	T	95/97 (98%)	74 (78%)	16 (17%)	5 (5%)	2	7
2	U	95/97 (98%)	73 (77%)	18 (19%)	4 (4%)	3	11
All	All	7973/8015 (100%)	7278 (91%)	590 (7%)	105 (1%)	15	44

5 of 105 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	A	337	GLY
1	B	44	PHE
1	B	337	GLY
1	C	44	PHE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	B	404/404 (100%)	354 (88%)	50 (12%)	6	17
1	C	404/404 (100%)	353 (87%)	51 (13%)	5	17
1	D	404/404 (100%)	351 (87%)	53 (13%)	5	15
1	E	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	F	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	G	404/404 (100%)	352 (87%)	52 (13%)	5	16
1	H	404/404 (100%)	344 (85%)	60 (15%)	4	11
1	I	404/404 (100%)	343 (85%)	61 (15%)	3	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	J	404/404 (100%)	344 (85%)	60 (15%)	4	11
1	K	404/404 (100%)	342 (85%)	62 (15%)	3	10
1	L	404/404 (100%)	345 (85%)	59 (15%)	4	11
1	M	404/404 (100%)	342 (85%)	62 (15%)	3	10
1	N	404/404 (100%)	345 (85%)	59 (15%)	4	11
2	O	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	P	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	Q	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	R	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	S	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	T	80/80 (100%)	67 (84%)	13 (16%)	3	8
2	U	80/80 (100%)	67 (84%)	13 (16%)	3	8
All	All	6216/6216 (100%)	5340 (86%)	876 (14%)	4	12

5 of 876 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	329	THR
1	J	55	SER
2	P	86	MET
1	H	404	ARG
1	I	230	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	153	ASN
1	I	37	ASN
2	R	45	ASN
1	G	348	GLN
1	H	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 14 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	ADP	A	600	3,4,6	22,29,29	1.11	2 (9%)	27,45,45	3.01	9 (33%)
6	AF3	A	602	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	B	700	3,4,6	22,29,29	1.02	2 (9%)	27,45,45	2.79	7 (25%)
6	AF3	B	702	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	C	800	3,4,6	22,29,29	1.05	2 (9%)	27,45,45	2.86	5 (18%)
6	AF3	C	802	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	D	900	3,4,6	22,29,29	1.10	3 (13%)	27,45,45	3.11	7 (25%)
6	AF3	D	902	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	E	1000	3,4,6	22,29,29	1.09	2 (9%)	27,45,45	3.10	8 (29%)
6	AF3	E	1002	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	F	1100	3,4,6	22,29,29	1.14	2 (9%)	27,45,45	2.83	5 (18%)
6	AF3	F	1102	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	G	1200	3,4,6	22,29,29	1.19	2 (9%)	27,45,45	2.99	8 (29%)
6	AF3	G	1202	1,3,5,4	0,3,3	0.00	-	0,3,3	0.00	-

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
5	ADP	A	600	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	A	602	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	B	700	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	B	702	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	C	800	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	C	802	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	D	900	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	D	902	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	E	1000	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	E	1002	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	F	1100	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	F	1102	1,3,5,4	-	0/0/0/0	0/0/0/0
5	ADP	G	1200	3,4,6	-	0/12/32/32	0/3/3/3
6	AF3	G	1202	1,3,5,4	-	0/0/0/0	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	900	ADP	O4'-C4'	-2.03	1.40	1.45
5	E	1000	ADP	C2-N1	2.15	1.38	1.33
5	D	900	ADP	C2-N1	2.33	1.38	1.33
5	A	600	ADP	C2-N1	2.40	1.38	1.33
5	F	1100	ADP	C2-N1	2.58	1.38	1.33

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1000	ADP	N3-C2-N1	-12.68	119.18	128.89
5	D	900	ADP	N3-C2-N1	-12.37	119.42	128.89
5	F	1100	ADP	N3-C2-N1	-11.63	119.99	128.89
5	B	700	ADP	N3-C2-N1	-11.55	120.05	128.89
5	A	600	ADP	N3-C2-N1	-11.45	120.13	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	4	0
6	A	602	AF3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	700	ADP	1	0
5	C	800	ADP	5	0
6	C	802	AF3	1	0
5	D	900	ADP	2	0
5	E	1000	ADP	1	0
5	F	1100	ADP	3	0
5	G	1200	ADP	1	0
6	G	1202	AF3	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	524/524 (100%)	0.32	42 (8%) 15 7	2, 2, 4, 6	0
1	B	524/524 (100%)	0.37	50 (9%) 10 5	2, 2, 4, 6	0
1	C	524/524 (100%)	0.37	39 (7%) 17 9	2, 2, 4, 6	0
1	D	524/524 (100%)	0.34	47 (8%) 12 6	2, 2, 4, 6	0
1	E	524/524 (100%)	0.40	58 (11%) 7 3	2, 2, 4, 6	0
1	F	524/524 (100%)	0.66	75 (14%) 4 2	2, 2, 4, 6	0
1	G	524/524 (100%)	0.44	53 (10%) 9 4	2, 2, 4, 6	0
1	H	524/524 (100%)	-0.05	8 (1%) 76 68	2, 2, 4, 6	0
1	I	524/524 (100%)	-0.07	4 (0%) 87 81	2, 2, 4, 6	0
1	J	524/524 (100%)	-0.02	12 (2%) 64 52	2, 2, 4, 6	0
1	K	524/524 (100%)	0.02	4 (0%) 87 81	2, 2, 4, 6	0
1	L	524/524 (100%)	0.21	22 (4%) 40 28	2, 2, 4, 6	0
1	M	524/524 (100%)	0.03	15 (2%) 55 43	2, 2, 4, 6	0
1	N	524/524 (100%)	0.00	12 (2%) 64 52	2, 2, 4, 6	0
2	O	97/97 (100%)	1.27	21 (21%) 1 1	2, 2, 2, 3	0
2	P	97/97 (100%)	0.77	12 (12%) 5 2	2, 2, 2, 3	0
2	Q	97/97 (100%)	0.89	18 (18%) 2 1	2, 2, 2, 2	0
2	R	97/97 (100%)	1.34	30 (30%) 1 0	2, 2, 2, 3	0
2	S	97/97 (100%)	1.08	20 (20%) 1 1	2, 2, 2, 3	0
2	T	97/97 (100%)	1.11	23 (23%) 1 1	2, 2, 2, 3	0
2	U	97/97 (100%)	1.02	23 (23%) 1 1	2, 2, 2, 2	0
All	All	8015/8015 (100%)	0.29	588 (7%) 18 10	2, 2, 4, 6	0

The worst 5 of 588 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	ALA	12.1
2	S	1	MET	10.3
1	F	212	ALA	9.8
2	O	1	MET	9.7
2	O	17	VAL	9.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	K	E	1003	1/1	0.98	0.27	1.38	24,24,24,24	0
4	K	D	903	1/1	0.98	0.22	0.02	24,24,24,24	0
5	ADP	E	1000	27/27	0.95	0.18	-0.33	2,2,5,8	0
5	ADP	F	1100	27/27	0.95	0.18	-0.62	2,2,5,8	0
4	K	G	1203	1/1	0.97	0.17	-0.84	24,24,24,24	0
5	ADP	B	700	27/27	0.95	0.15	-0.98	2,2,5,8	0
4	K	B	703	1/1	0.98	0.16	-1.03	24,24,24,24	0
5	ADP	A	600	27/27	0.96	0.12	-1.26	2,2,6,8	0
5	ADP	G	1200	27/27	0.96	0.16	-1.41	2,2,6,8	0
5	ADP	C	800	27/27	0.95	0.15	-1.45	2,2,5,8	0
4	K	A	603	1/1	0.98	0.16	-1.49	24,24,24,24	0
6	AF3	F	1102	4/4	0.86	0.18	-1.59	5,7,8,12	0
4	K	F	1103	1/1	0.98	0.15	-1.60	24,24,24,24	0
6	AF3	D	902	4/4	0.94	0.15	-1.70	5,7,8,12	0
6	AF3	A	602	4/4	0.91	0.14	-1.71	5,7,8,12	0
5	ADP	D	900	27/27	0.97	0.13	-2.02	2,2,5,8	0
6	AF3	C	802	4/4	0.89	0.13	-2.29	5,7,8,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	K	C	803	1/1	0.98	0.12	-2.32	24,24,24,24	0
6	AF3	G	1202	4/4	0.94	0.10	-2.74	5,7,8,12	0
6	AF3	B	702	4/4	0.90	0.11	-2.90	5,7,8,12	0
6	AF3	E	1002	4/4	0.89	0.12	-3.21	5,7,8,12	0
3	MG	B	701	1/1	0.97	0.06	-	2,2,2,2	0
3	MG	F	1101	1/1	0.97	0.08	-	2,2,2,2	0
3	MG	A	601	1/1	0.98	0.06	-	2,2,2,2	0
3	MG	C	801	1/1	0.97	0.06	-	2,2,2,2	0
3	MG	E	1001	1/1	0.98	0.05	-	2,2,2,2	0
3	MG	D	901	1/1	0.98	0.05	-	2,2,2,2	0
3	MG	G	1201	1/1	0.96	0.06	-	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.