



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:31 PM BST

PDB ID : 4V4O
Title : Crystal Structure of the Chaperonin Complex Cpn60/Cpn10/(ADP)7 from
Thermus Thermophilus
Authors : Shimamura, T.; Koike-Takeshita, A.; Yokoyama, K.; Masui, R.; Murai, N.;
Yoshida, M.; Taguchi, H.; Iwata, S.
Deposited on : 2004-05-23
Resolution : 2.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

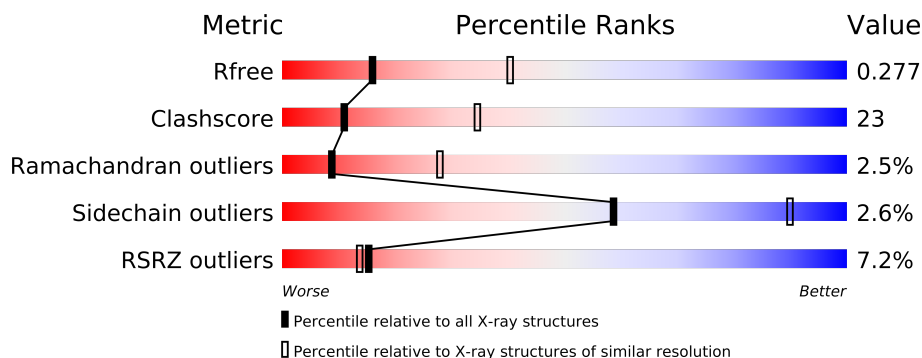
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	543	
1	B	543	
1	C	543	
1	D	543	
1	E	543	
1	F	543	
1	G	543	
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	

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Mol	Chain	Length	Quality of chain
1	a	543	
1	b	543	
1	c	543	
1	d	543	
1	e	543	
1	f	543	
1	g	543	
1	h	543	
1	i	543	
1	j	543	
1	k	543	
1	l	543	
1	m	543	
1	n	543	
2	O	100	
2	P	100	
2	Q	100	
2	R	100	
2	S	100	
2	T	100	
2	U	100	
2	o	100	
2	p	100	
2	q	100	
2	r	100	
2	s	100	
2	t	100	
2	u	100	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	601	-	X
3	MG	B	601	-	X
3	MG	D	601	-	X
3	MG	F	601	-	X
3	MG	a	601	-	X
3	MG	b	601	-	X
3	MG	c	601	-	X
3	MG	d	601	-	X
3	MG	e	601	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	MG	f	601	-	X
3	MG	g	601	-	X
4	ADP	f	602	-	X
5	DMS	H	601	-	X
5	DMS	J	601	-	X
5	DMS	h	601	-	X
5	DMS	j	601	-	X
5	DMS	k	601	-	X
5	DMS	l	601	-	X
5	DMS	m	601	-	X
5	DMS	n	701	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121267 atoms, of which 0 are hydrogen and 0 are deuterium.

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 cpn60(GroEL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	B	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	C	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	D	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	E	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	F	529	Total	C	N	O	S	0	0	0
			3974	2495	689	785	5			
1	G	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	H	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	I	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	J	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	K	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	L	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	M	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	N	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	a	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	b	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	d	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	e	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	f	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	g	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	h	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	i	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	j	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	k	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	l	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	m	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	n	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			

- Molecule 2 is a protein called cpn10(GroES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	P	94	Total	C	N	O		0	0	0
			723	460	123	140				
2	Q	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	R	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	S	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	T	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	U	96	Total	C	N	O		0	0	0
			739	470	126	143				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	o	96	Total 739	C 470	N 126	O 143	0	0	0
2	p	96	Total 739	C 470	N 126	O 143	0	0	0
2	q	96	Total 739	C 470	N 126	O 143	0	0	0
2	r	96	Total 739	C 470	N 126	O 143	0	0	0
2	s	96	Total 739	C 470	N 126	O 143	0	0	0
2	t	96	Total 739	C 470	N 126	O 143	0	0	0
2	u	96	Total 739	C 470	N 126	O 143	0	0	0

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

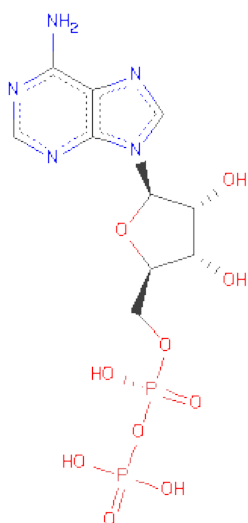
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0
3	g	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	e	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	a	1	Total 1	Mg 1	0	0
3	c	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0
3	f	1	Total 1	Mg 1	0	0
3	d	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	b	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



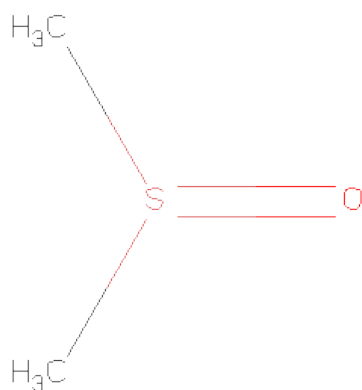
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		
5	L	1	Total	C	O	S	0	0
			4	2	1	1		
5	M	1	Total	C	O	S	0	0
			4	2	1	1		

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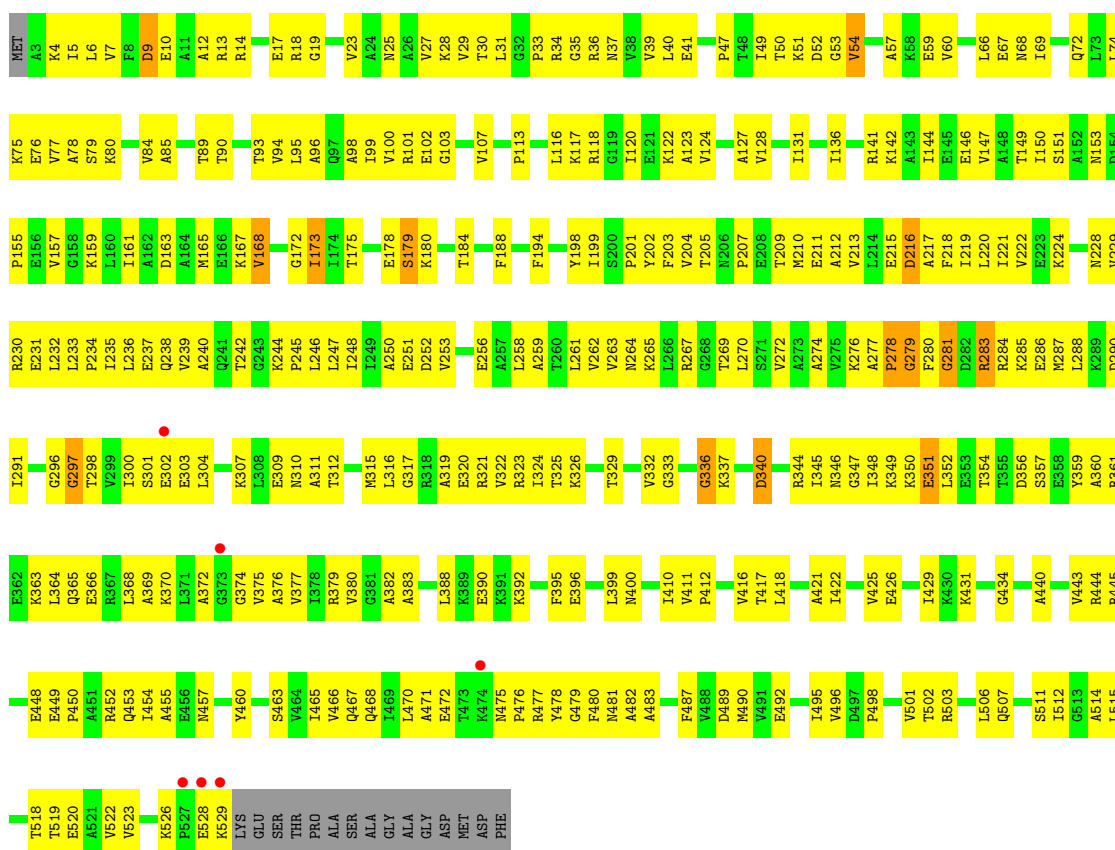
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total 4	C 2	O 1	S 1	0	0
5	h	1	Total 4	C 2	O 1	S 1	0	0
5	i	1	Total 4	C 2	O 1	S 1	0	0
5	j	1	Total 4	C 2	O 1	S 1	0	0
5	k	1	Total 4	C 2	O 1	S 1	0	0
5	l	1	Total 4	C 2	O 1	S 1	0	0
5	m	1	Total 4	C 2	O 1	S 1	0	0
5	n	1	Total 4	C 2	O 1	S 1	0	0

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.

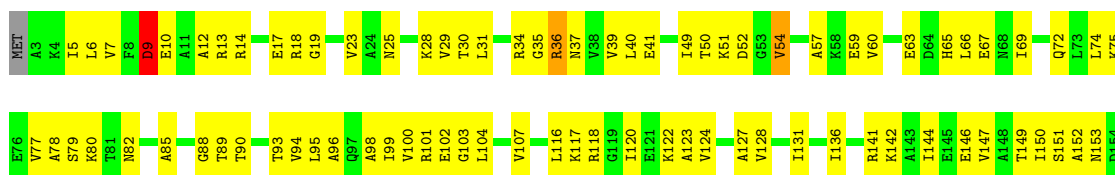
- Molecule 1: cpn60(GroEL)

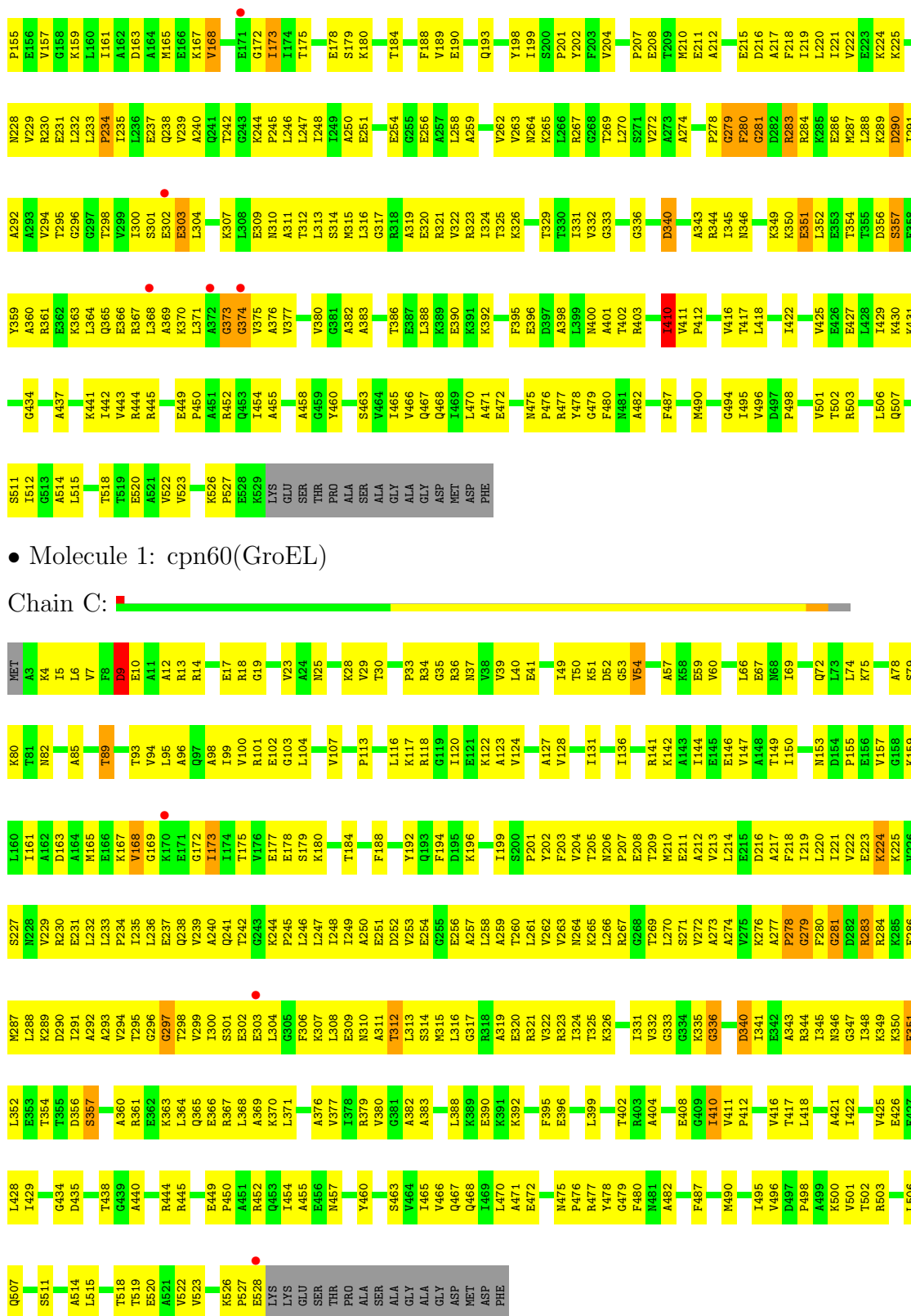
Chain A:

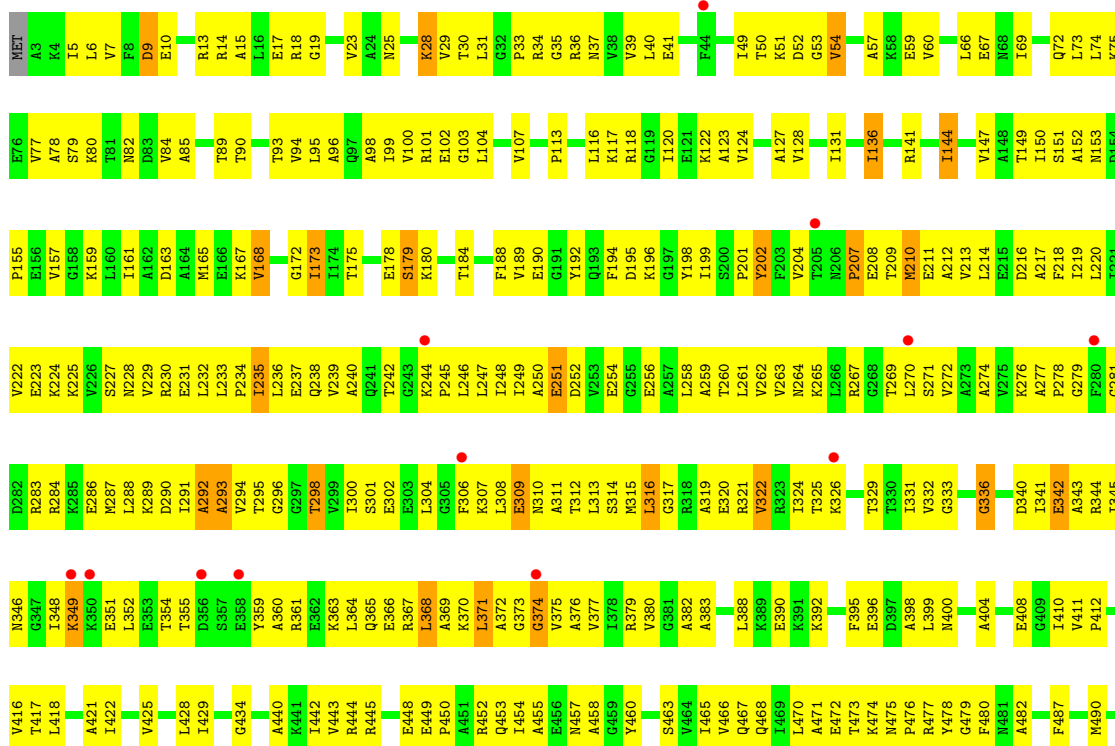


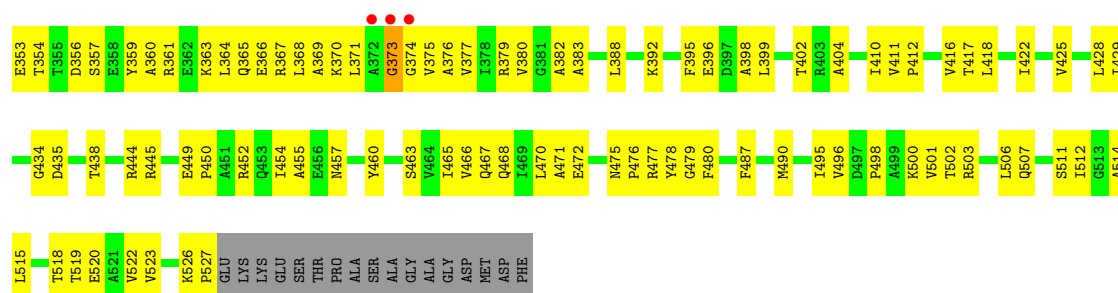
- Molecule 1: cpn60(GroEL)

Chain B:



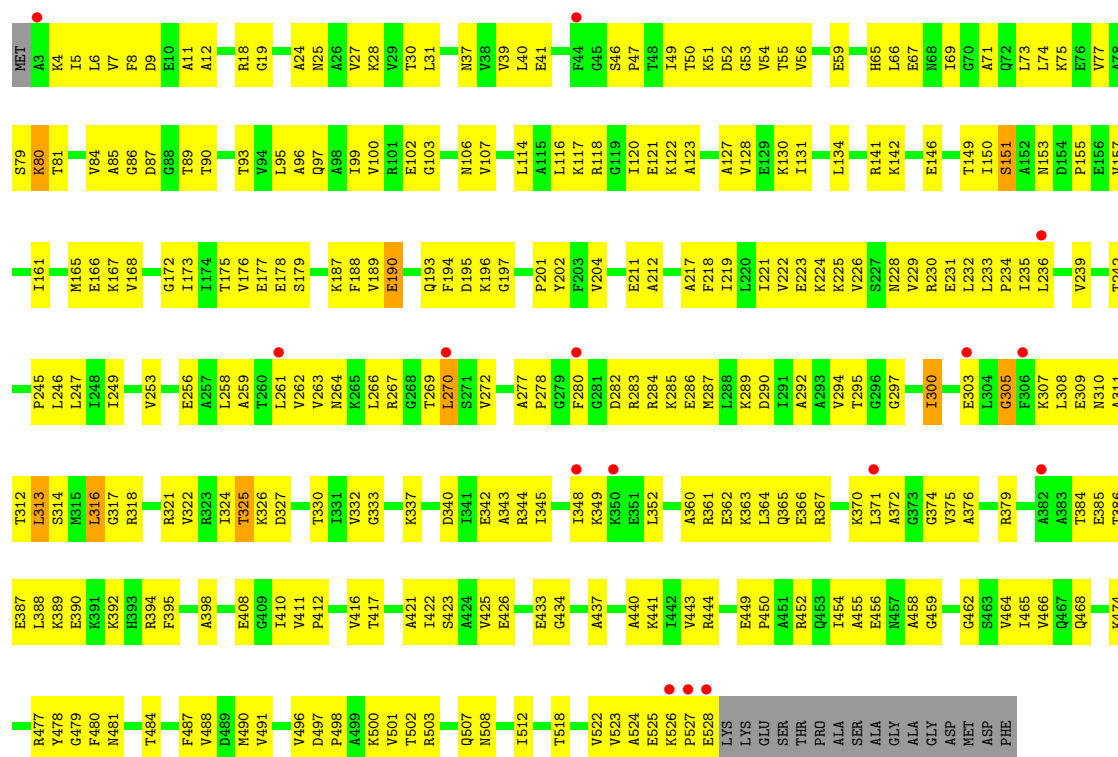






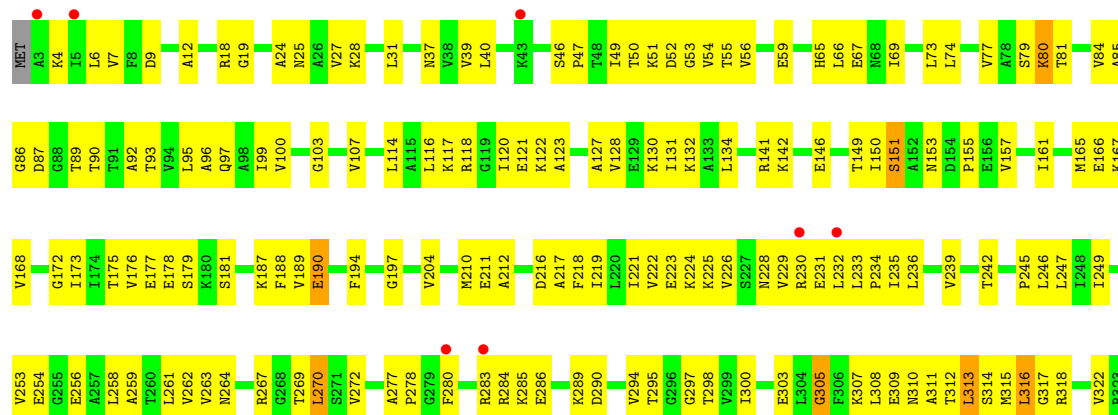
• Molecule 1: cpn60(GroEL)

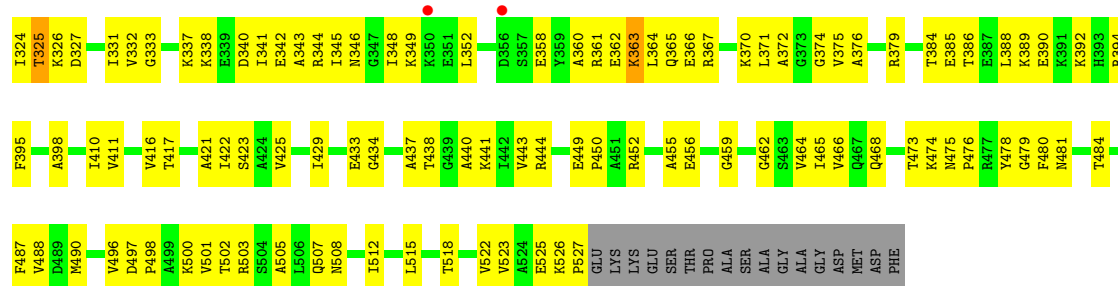
Chain H:



• Molecule 1: cpn60(GroEL)

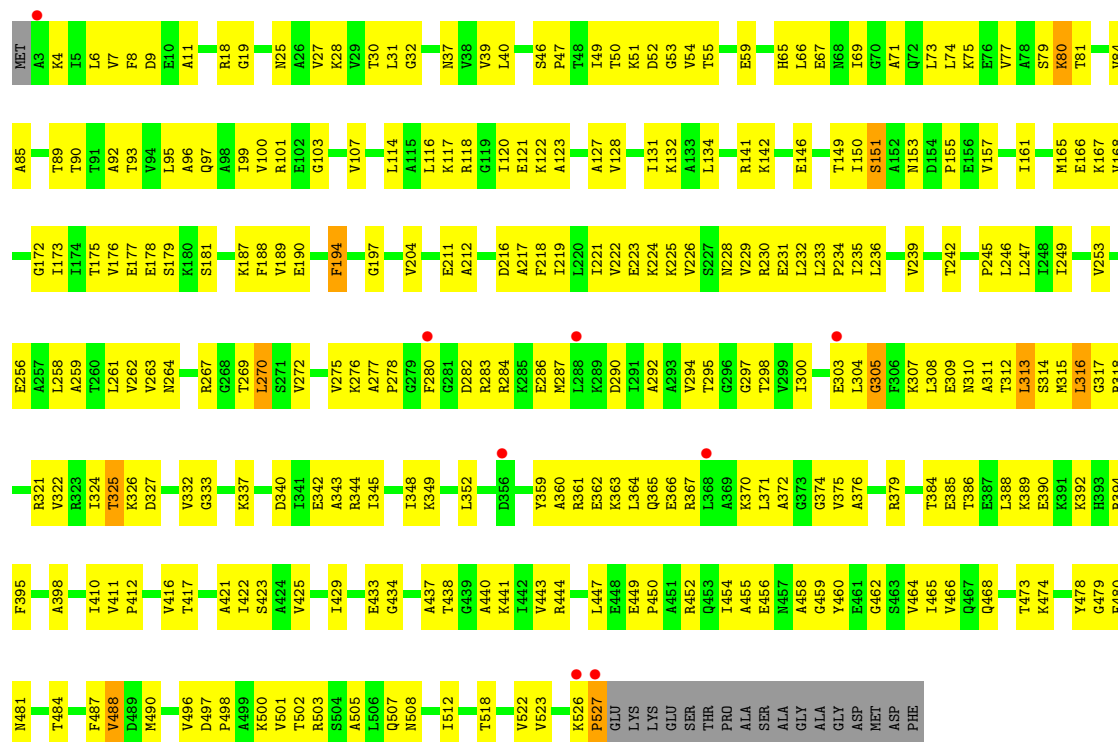
Chain I:





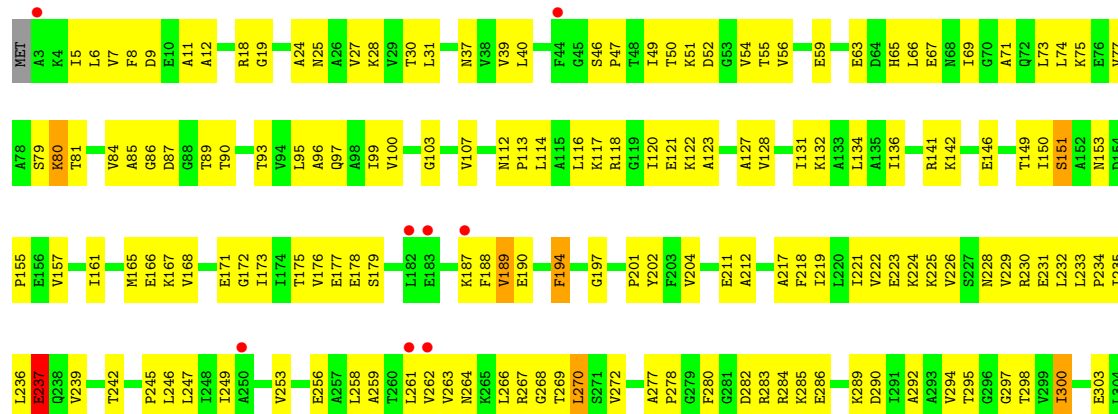
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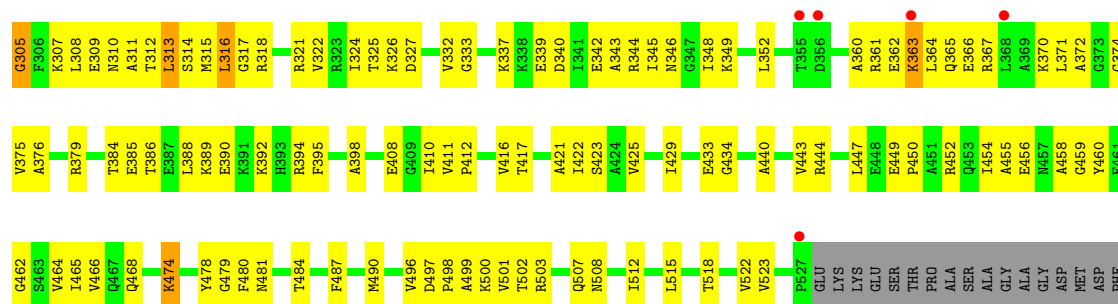
Chain J:



• Molecule 1: cpn60(GroEL)

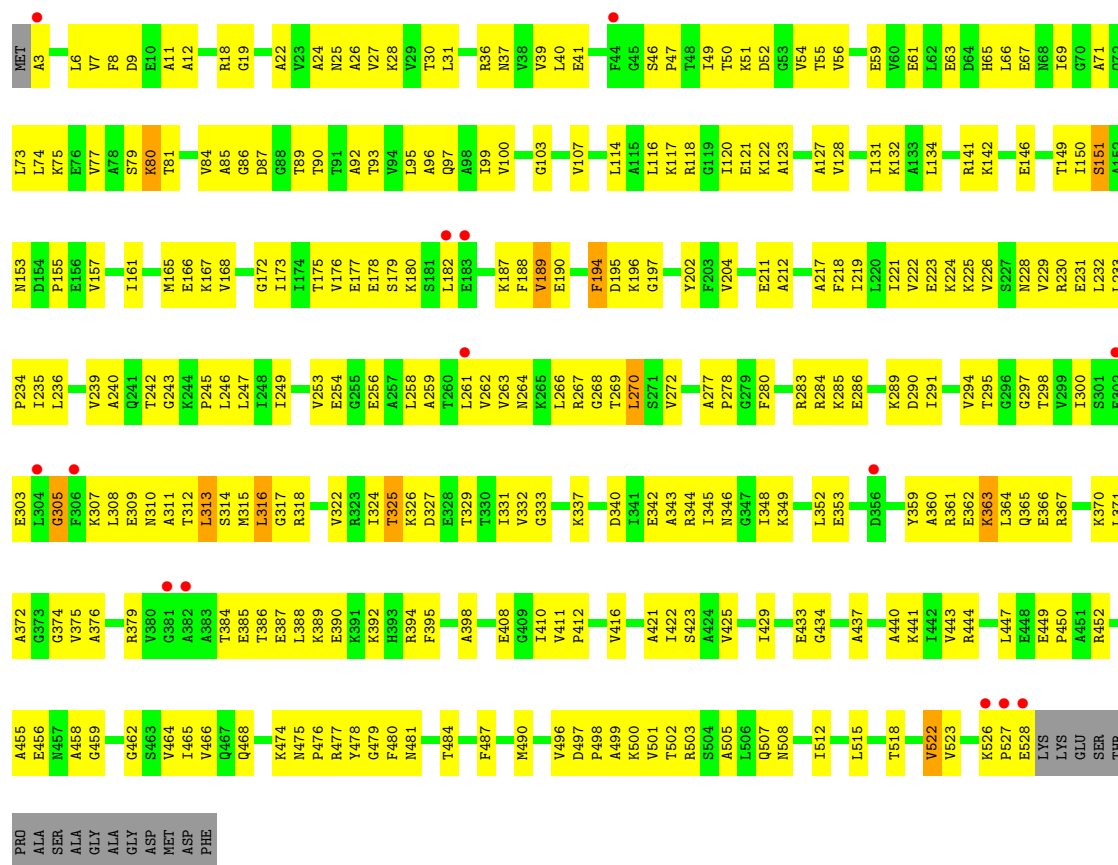
Chain K:





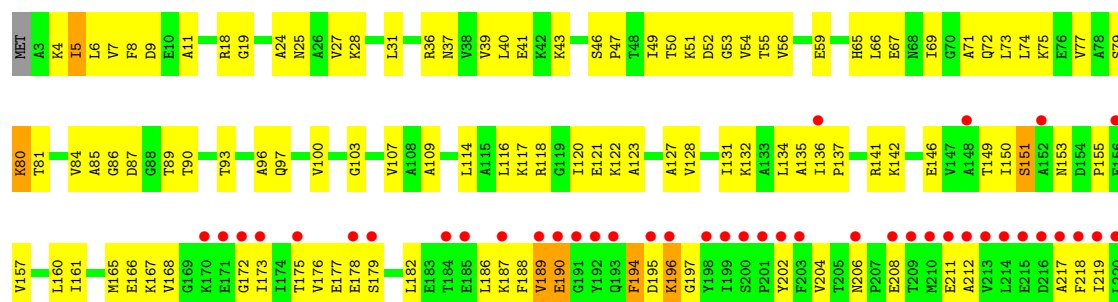
• Molecule 1: cpn60(GroEL)

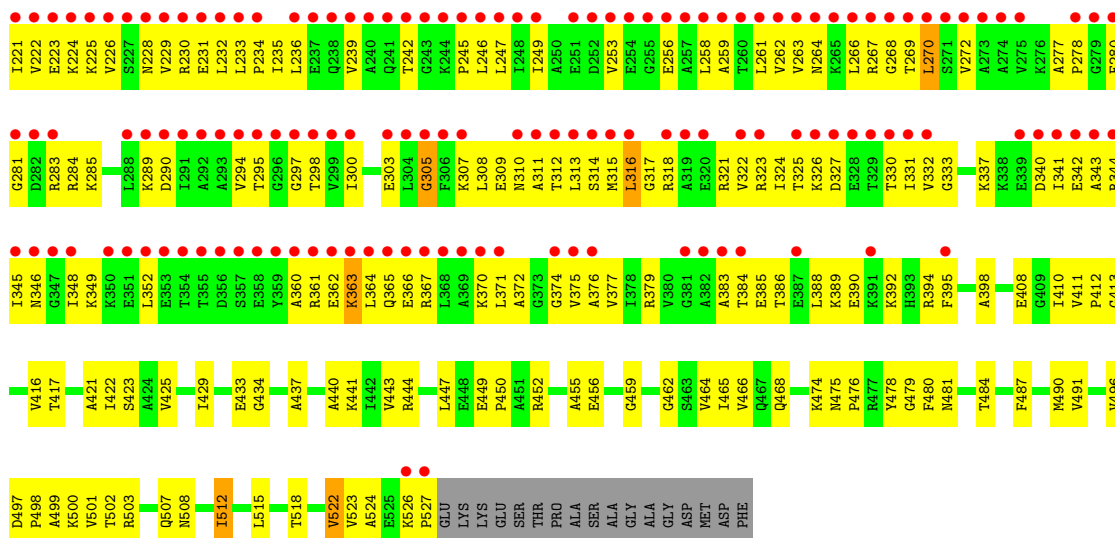
Chain L:



• Molecule 1: cpn60(GroEL)

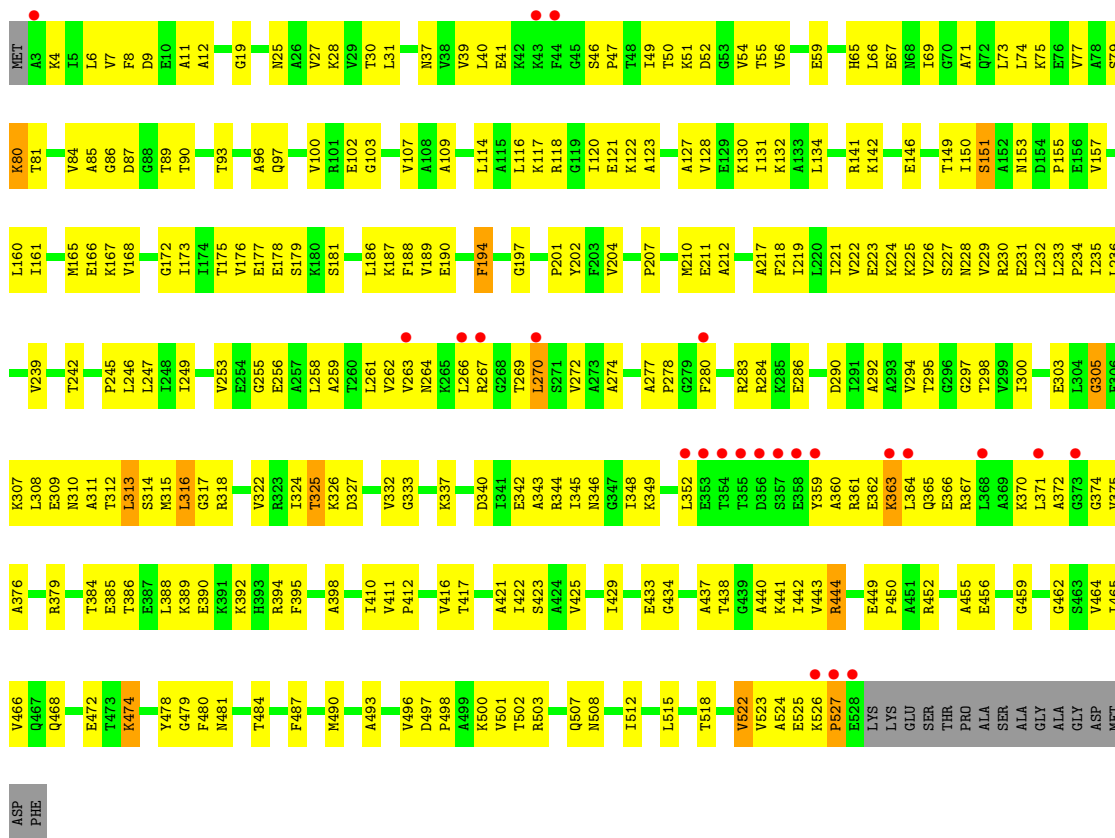
Chain M:





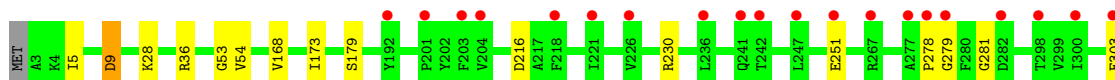
• Molecule 1: cpn60(GroEL)

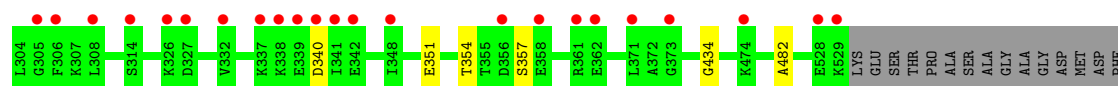
Chain N:



• Molecule 1: cpn60(GroEL)

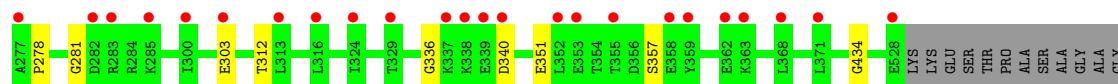
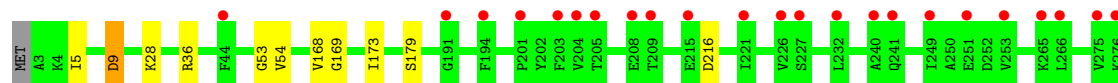
Chain a:





• Molecule 1: cpn60(GroEL)

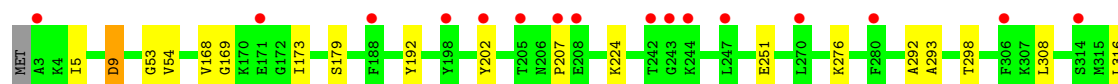
Chain b:



ASP
MET
ASP
PHE

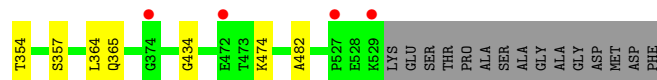
• Molecule 1: cpn60(GroEL)

Chain c:



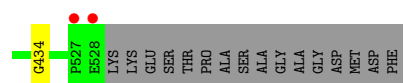
• Molecule 1: cpn60(GroEL)

Chain d:



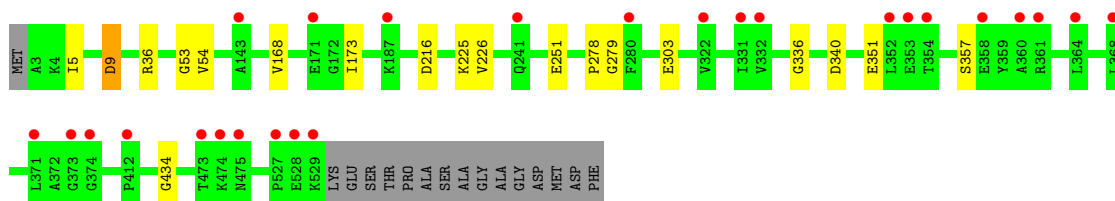
• Molecule 1: cpn60(GroEL)

Chain e:



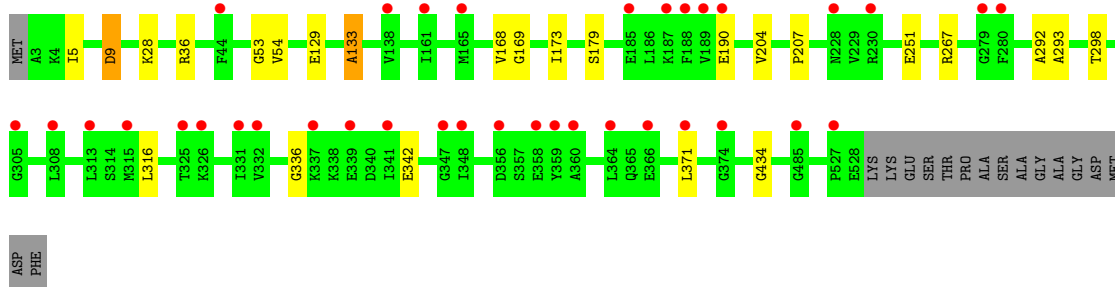
• Molecule 1: cpn60(GroEL)

Chain f:



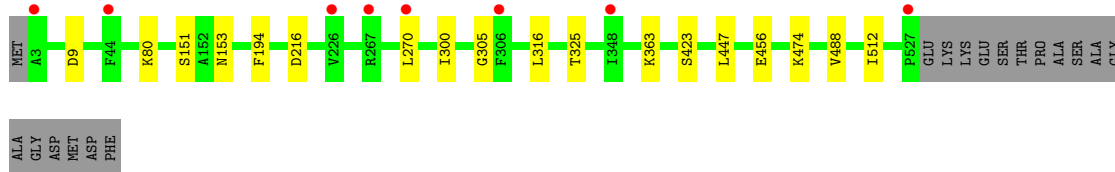
- Molecule 1: cpn60(GroEL)

Chain g:



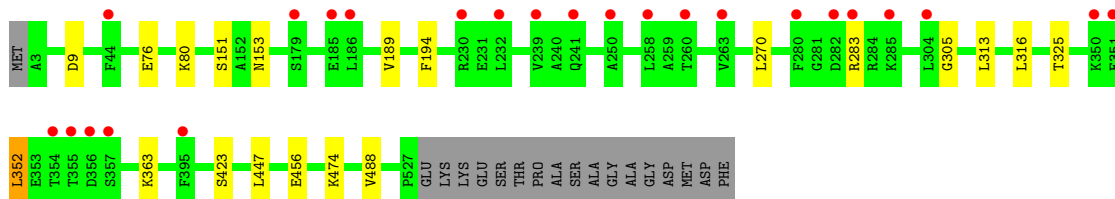
- Molecule 1: cpn60(GroEL)

Chain h:



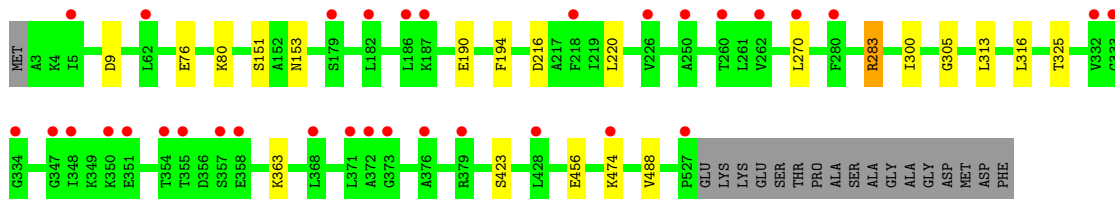
- Molecule 1: cpn60(GroEL)

Chain i:



- Molecule 1: cpn60(GroEL)

Chain j:



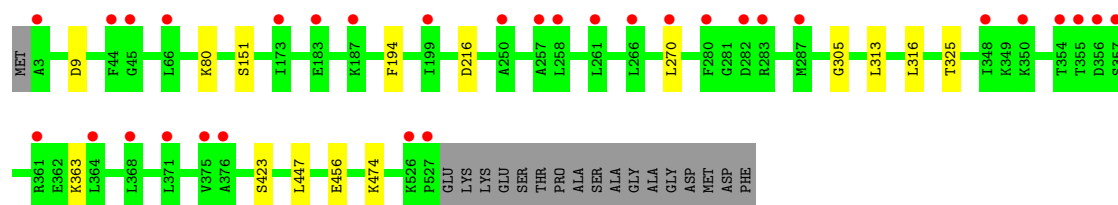
- Molecule 1: cpn60(GroEL)

[illegible]

- [illegible]

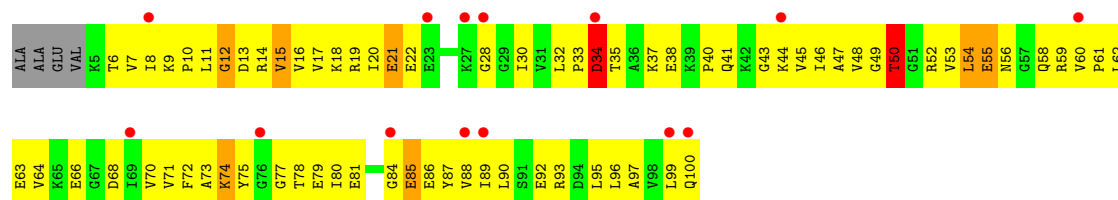
- | | | | | |
|--|------|------|------|-----|
| ALA
GLY
ASP
MET
ASP
PHE | T345 | S271 | E208 | MET |
| | N346 | A272 | T209 | A3 |
| | G347 | A273 | N210 | L6 |
| | I348 | A274 | E211 | V7 |
| | K349 | V275 | A212 | F8 |
| | K350 | K276 | V213 | D9 |
| | E351 | A277 | L214 | |
| | L352 | P278 | E215 | F44 |
| | E353 | G279 | D216 | L62 |
| | T354 | F280 | A217 | L66 |
| T355 | | F218 | | |
| D356 | R283 | L219 | L66 | |
| S357 | R284 | L220 | K80 | |
| E358 | | V222 | | |
| Y359 | M287 | E223 | I136 | |
| A360 | L288 | K224 | R141 | |
| R361 | K289 | E225 | K142 | |
| E362 | D290 | K226 | | |
| K363 | L291 | V226 | S151 | |
| L364 | A292 | S227 | A152 | |
| | A293 | | N153 | |
| L368 | V294 | L232 | | |
| L371 | T295 | L233 | K159 | |
| A372 | G296 | P234 | L160 | |
| G373 | G297 | L235 | | |
| G374 | T298 | L236 | E171 | |
| V375 | V299 | E237 | G172 | |
| | I300 | Q238 | I173 | |
| | S301 | Q239 | I174 | |
| V380 | E302 | A240 | T175 | |
| G381 | E303 | Q241 | E177 | |
| A382 | L304 | K242 | E178 | |
| A383 | G305 | G243 | L182 | |
| | F306 | K244 | T184 | |
| R394 | K307 | P245 | E185 | |
| F395 | L308 | L246 | L186 | |
| | | L247 | K187 | |
| T417 | A311 | L248 | F188 | |
| | T312 | L249 | V189 | |
| S423 | L313 | A250 | Y192 | |
| E456 | S314 | E251 | Q193 | |
| | M315 | D252 | F194 | |
| K474 | L316 | V253 | D195 | |
| | A319 | G255 | | |
| Y478 | E320 | E256 | Y198 | |
| K526 | R321 | A257 | I199 | |
| P527 | | L258 | S200 | |
| GLU | I324 | A259 | P201 | |
| LYS | T325 | T260 | Y202 | |
| LYS | K326 | L261 | F203 | |
| GLU | G334 | V262 | V204 | |
| SER | | V263 | | |
| THR | E339 | N264 | | |
| PRO | D340 | K265 | | |
| ALA | I341 | L266 | | |
| SER | E342 | R267 | | |
| ALA | A343 | Q268 | | |
| GLY | R344 | T269 | | |
| | | L270 | | |

- WORLDWIDE
 **PDB**
PROTEIN DATA BANK



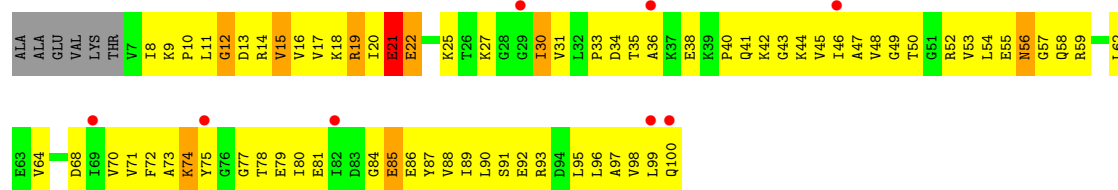
• Molecule 2: cpn10(GroES)

Chain O:



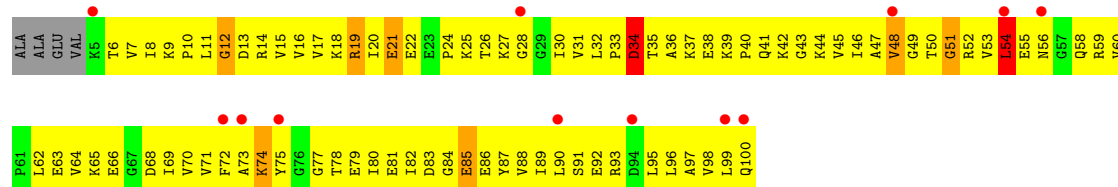
• Molecule 2: cpn10(GroES)

Chain P:



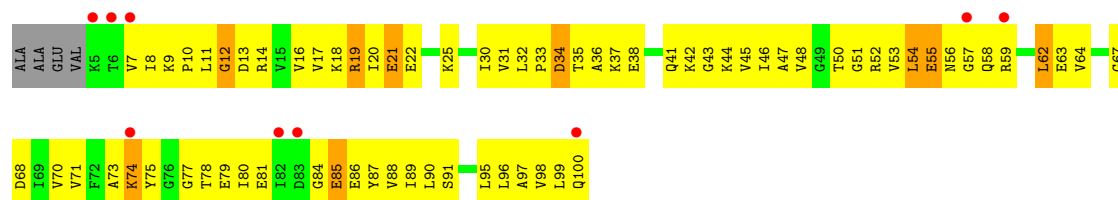
• Molecule 2: cpn10(GroES)

Chain Q:



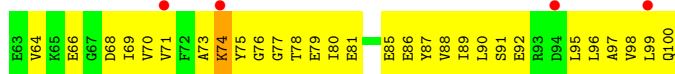
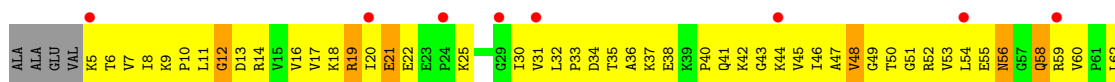
• Molecule 2: cpn10(GroES)

Chain R:



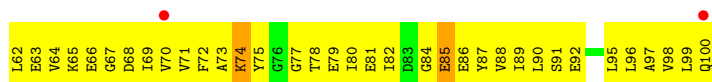
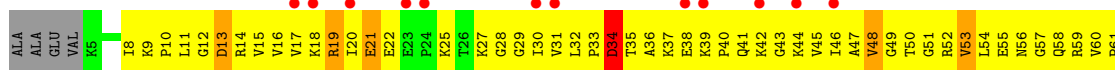
• Molecule 2: cpn10(GroES)

Chain S:



• Molecule 2: cpn10(GroES)

Chain T:



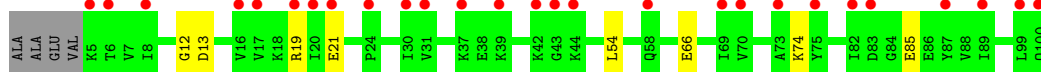
• Molecule 2: cpn10(GroES)

Chain U:



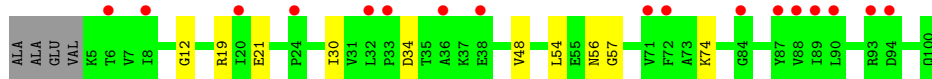
• Molecule 2: cpn10(GroES)

Chain o:



• Molecule 2: cpn10(GroES)

Chain p:



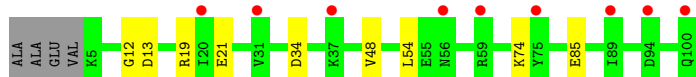
• Molecule 2: cpn10(GroES)

Chain q:



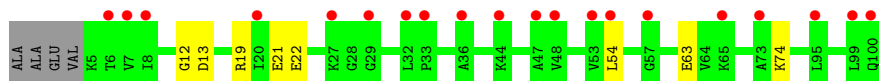
• Molecule 2: cpn10(GroES)

Chain r:



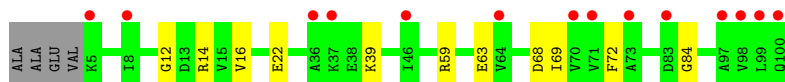
- Molecule 2: cpn10(GroES)

Chain s:



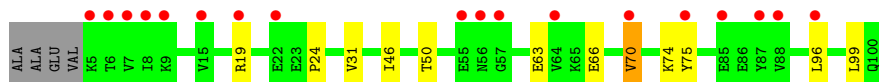
- Molecule 2: cpn10(GroES)

Chain t:



- Molecule 2: cpn10(GroES)

Chain u:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 156.42Å 273.15Å 82.88° 85.35° 68.52°	Depositor
Resolution (Å)	39.98 – 2.80 39.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.3 (39.98-2.80) 81.4 (39.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279 0.238 , 0.277	Depositor DCC
R_{free} test set	12690 reflections (3.04%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 429625 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	121267	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.44	0/3989	0.65	0/5383
1	B	0.43	1/3989 (0.0%)	0.65	1/5383 (0.0%)
1	C	0.45	0/3980	0.67	0/5372
1	D	0.42	0/3980	0.65	1/5372 (0.0%)
1	E	0.43	0/3980	0.64	0/5372
1	F	0.39	0/4007	0.63	0/5406
1	G	0.41	0/3971	0.64	0/5360
1	H	0.36	0/3980	0.60	0/5372
1	I	0.37	0/3971	0.60	0/5360
1	J	0.40	0/3971	0.62	0/5360
1	K	0.39	1/3971 (0.0%)	0.62	0/5360
1	L	0.38	0/3980	0.60	0/5372
1	M	0.39	1/3971 (0.0%)	0.62	1/5360 (0.0%)
1	N	0.38	0/3980	0.63	1/5372 (0.0%)
1	a	0.41	0/3989	0.64	0/5383
1	b	0.40	0/3980	0.63	0/5372
1	c	0.39	0/3989	0.64	0/5383
1	d	0.39	0/3989	0.62	0/5383
1	e	0.37	0/3980	0.62	0/5372
1	f	0.34	0/3989	0.59	0/5383
1	g	0.41	1/3980 (0.0%)	0.62	1/5372 (0.0%)
1	h	0.40	0/3971	0.62	1/5360 (0.0%)
1	i	0.36	1/3971 (0.0%)	0.60	0/5360
1	j	0.35	0/3971	0.61	1/5360 (0.0%)
1	k	0.34	0/3971	0.59	0/5360
1	l	0.33	0/3971	0.59	0/5360
1	m	0.36	1/3971 (0.0%)	0.59	0/5360
1	n	0.34	0/3971	0.58	0/5360
2	O	0.40	0/746	0.68	0/1003
2	P	0.54	0/730	0.77	0/982
2	Q	0.39	0/746	0.70	2/1003 (0.2%)
2	R	0.42	0/746	0.69	0/1003

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	S	0.42	0/746	0.72	1/1003 (0.1%)
2	T	0.39	0/746	0.67	0/1003
2	U	0.46	0/746	0.72	0/1003
2	o	0.52	0/746	0.71	0/1003
2	p	0.40	0/746	0.68	0/1003
2	q	0.38	0/746	0.72	0/1003
2	r	0.41	0/746	0.67	0/1003
2	s	0.53	0/746	0.76	0/1003
2	t	0.31	0/746	0.64	0/1003
2	u	0.30	0/746	0.62	0/1003
All	All	0.39	6/121841 (0.0%)	0.63	10/164393 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	133	ALA	CA-CB	-13.30	1.24	1.52
1	m	394	ARG	CZ-NH2	-8.93	1.21	1.33
1	K	237	GLU	CD-OE1	-5.26	1.19	1.25
1	M	512	ILE	CB-CG2	5.16	1.68	1.52
1	B	410	ILE	CB-CG2	5.08	1.68	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	444	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	g	133	ALA	CB-CA-C	-7.31	99.13	110.10
1	j	283	ARG	CG-CD-NE	5.69	123.75	111.80
2	Q	51	GLY	N-CA-C	-5.32	99.81	113.10
1	M	512	ILE	CG1-CB-CG2	5.29	123.03	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3956	0	4129	361	0
1	B	3956	0	4129	347	0
1	C	3947	0	4116	427	1
1	D	3947	0	4116	335	0
1	E	3947	0	4116	419	3
1	F	3974	0	4148	316	0
1	G	3938	0	4110	376	0
1	H	3947	0	4116	322	0
1	I	3938	0	4110	306	0
1	J	3938	0	4110	317	0
1	K	3938	0	4110	314	1
1	L	3947	0	4116	367	1
1	M	3938	0	4110	426	0
1	N	3947	0	4116	335	4
1	a	3956	0	4129	0	0
1	b	3947	0	4116	0	0
1	c	3956	0	4129	0	0
1	d	3956	0	4129	0	4
1	e	3947	0	4116	0	0
1	f	3956	0	4129	0	0
1	g	3947	0	4116	0	4
1	h	3938	0	4110	0	0
1	i	3938	0	4110	0	0
1	j	3938	0	4110	0	0
1	k	3938	0	4110	0	0
1	l	3938	0	4110	0	0
1	m	3938	0	4110	0	0
1	n	3938	0	4110	0	0
2	O	739	0	786	153	0
2	P	723	0	766	154	0
2	Q	739	0	786	217	0
2	R	739	0	786	137	0
2	S	739	0	786	158	0
2	T	739	0	786	196	0
2	U	739	0	786	171	0
2	o	739	0	786	0	0
2	p	739	0	786	0	0
2	q	739	0	786	0	0
2	r	739	0	786	0	0
2	s	739	0	786	0	0
2	t	739	0	786	0	0
2	u	739	0	786	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	27	0	12	1	0
4	B	27	0	12	1	0
4	C	27	0	12	1	0
4	D	27	0	12	1	0
4	E	27	0	12	5	0
4	F	27	0	12	2	0
4	G	27	0	12	1	0
4	a	27	0	12	0	0
4	b	27	0	12	0	0
4	c	27	0	12	0	0
4	d	27	0	12	0	0
4	e	27	0	12	0	0
4	f	27	0	12	0	0
4	g	27	0	12	0	0
5	H	4	0	6	3	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	4	0	6	0	0
5	L	4	0	6	0	0
5	M	4	0	6	0	0
5	N	4	0	6	0	0
5	h	4	0	6	0	0
5	i	4	0	6	0	0
5	j	4	0	6	0	0
5	k	4	0	6	0	0
5	l	4	0	6	0	0
5	m	4	0	6	0	0
5	n	4	0	6	0	0
All	All	121267	0	126522	5603	9

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

The worst 5 of 5603 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:150:ILE:HD11	1:D:495:ILE:HA	1.22	1.21
1:K:283:ARG:NH2	1:K:367:ARG:HD3	2.09	1.20
1:K:283:ARG:HH21	1:K:367:ARG:CD	2.35	1.19
1:I:283:ARG:NH2	1:I:367:ARG:HD3	2.14	1.18
1:E:229:VAL:HG21	2:S:36:ALA:HB2	2.51	1.15

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:474:LYS:CE	1:N:472:GLU:OE1[1_455]	1.85	0.35
1:K:474:LYS:NZ	1:N:493:ALA:O[1_455]	1.93	0.27
1:d:474:LYS:CE	1:g:133:ALA:CB[1_455]	1.93	0.27
1:d:474:LYS:NZ	1:g:133:ALA:CB[1_455]	1.95	0.25
1:C:141:ARG:NH2	1:L:353:GLU:OE1[1_565]	2.11	0.09

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 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	525/543 (97%)	456 (87%)	56 (11%)	13 (2%)	9	28
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	10	31
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	7	23
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	7	21
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	5	17
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	8	25
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	11	33
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	22	60
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	14	42
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	15	46
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	18	51
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	18	51
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	21	57
1	a	525/543 (97%)	453 (86%)	57 (11%)	15 (3%)	7	23
1	b	524/543 (96%)	452 (86%)	61 (12%)	11 (2%)	11	33
1	c	525/543 (97%)	446 (85%)	61 (12%)	18 (3%)	6	19
1	d	525/543 (97%)	451 (86%)	56 (11%)	18 (3%)	6	19
1	e	524/543 (96%)	455 (87%)	57 (11%)	12 (2%)	10	31
1	f	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	10	31
1	g	524/543 (96%)	450 (86%)	60 (12%)	14 (3%)	8	25
1	h	523/543 (96%)	459 (88%)	57 (11%)	7 (1%)	18	51
1	i	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	14	42
1	j	523/543 (96%)	454 (87%)	60 (12%)	9 (2%)	14	42
1	k	523/543 (96%)	456 (87%)	61 (12%)	6 (1%)	21	57
1	l	523/543 (96%)	457 (87%)	59 (11%)	7 (1%)	18	51
1	m	523/543 (96%)	465 (89%)	51 (10%)	7 (1%)	18	51
1	n	523/543 (96%)	459 (88%)	58 (11%)	6 (1%)	21	57
2	O	94/100 (94%)	74 (79%)	13 (14%)	7 (7%)	2	3
2	P	92/100 (92%)	72 (78%)	13 (14%)	7 (8%)	2	3
2	Q	94/100 (94%)	75 (80%)	12 (13%)	7 (7%)	2	3
2	R	94/100 (94%)	75 (80%)	11 (12%)	8 (8%)	1	2
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	3	9
2	T	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	2	3
2	U	94/100 (94%)	77 (82%)	10 (11%)	7 (7%)	2	3
2	o	94/100 (94%)	75 (80%)	13 (14%)	6 (6%)	2	5
2	p	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	2	3
2	q	94/100 (94%)	58 (62%)	21 (22%)	15 (16%)	0	1
2	r	94/100 (94%)	71 (76%)	17 (18%)	6 (6%)	2	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	s	94/100 (94%)	76 (81%)	13 (14%)	5 (5%)	3	9
2	t	94/100 (94%)	69 (73%)	17 (18%)	8 (8%)	1	2
2	u	94/100 (94%)	66 (70%)	18 (19%)	10 (11%)	1	1
All	All	15983/16604 (96%)	13715 (86%)	1863 (12%)	405 (2%)	9	28

5 of 405 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	278	PRO
1	B	9	ASP
1	B	278	PRO
1	C	9	ASP

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	412/423 (97%)	402 (98%)	10 (2%)	61	91
1	B	412/423 (97%)	399 (97%)	13 (3%)	51	85
1	C	411/423 (97%)	399 (97%)	12 (3%)	55	88
1	D	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	E	411/423 (97%)	395 (96%)	16 (4%)	43	80
1	F	414/423 (98%)	405 (98%)	9 (2%)	64	92
1	G	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	H	411/423 (97%)	403 (98%)	8 (2%)	69	94
1	I	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	J	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	K	410/423 (97%)	401 (98%)	9 (2%)	64	92
1	L	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	M	410/423 (97%)	399 (97%)	11 (3%)	57	89
1	N	411/423 (97%)	401 (98%)	10 (2%)	61	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	412/423 (97%)	404 (98%)	8 (2%)	69	94
1	b	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	c	412/423 (97%)	400 (97%)	12 (3%)	55	88
1	d	412/423 (97%)	401 (97%)	11 (3%)	57	89
1	e	411/423 (97%)	403 (98%)	8 (2%)	69	94
1	f	412/423 (97%)	404 (98%)	8 (2%)	69	94
1	g	411/423 (97%)	401 (98%)	10 (2%)	61	91
1	h	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	i	410/423 (97%)	399 (97%)	11 (3%)	57	89
1	j	410/423 (97%)	398 (97%)	12 (3%)	55	88
1	k	410/423 (97%)	399 (97%)	11 (3%)	57	89
1	l	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	m	410/423 (97%)	400 (98%)	10 (2%)	61	91
1	n	410/423 (97%)	401 (98%)	9 (2%)	64	92
2	O	81/83 (98%)	76 (94%)	5 (6%)	26	60
2	P	79/83 (95%)	76 (96%)	3 (4%)	44	80
2	Q	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	R	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	S	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	T	81/83 (98%)	77 (95%)	4 (5%)	35	71
2	U	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	o	81/83 (98%)	79 (98%)	2 (2%)	60	90
2	p	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	q	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	r	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	s	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	t	81/83 (98%)	78 (96%)	3 (4%)	45	81
2	u	81/83 (98%)	78 (96%)	3 (4%)	45	81
All	All	12637/13006 (97%)	12305 (97%)	332 (3%)	59	90

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	O	34	ASP
1	b	216	ASP
1	n	270	LEU
2	P	21	GLU
2	T	48	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 271 such sidechains are listed below:

Mol	Chain	Res	Type
1	N	310	ASN
1	d	310	ASN
1	m	507	GLN
1	N	468	GLN
1	a	457	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 42 ligands modelled in this entry, 14 are monoatomic - leaving 28 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
4	ADP	A	602	3	29,29,29	1.40	4 (13%)	45,45,45	2.35	7 (15%)
4	ADP	B	602	3	29,29,29	1.49	6 (20%)	45,45,45	2.48	9 (20%)
4	ADP	C	602	3	29,29,29	1.60	6 (20%)	45,45,45	2.45	6 (13%)
4	ADP	D	602	3	29,29,29	1.63	7 (24%)	45,45,45	2.37	7 (15%)
4	ADP	E	602	3	29,29,29	1.45	5 (17%)	45,45,45	2.55	9 (20%)
4	ADP	F	602	3	29,29,29	1.66	5 (17%)	45,45,45	2.47	9 (20%)
4	ADP	G	602	3	29,29,29	1.55	7 (24%)	45,45,45	2.49	7 (15%)
5	DMS	H	601	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	I	601	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	J	601	-	3,3,3	0.36	0	3,3,3	0.70	0
5	DMS	K	601	-	3,3,3	0.28	0	3,3,3	0.64	0
5	DMS	L	601	-	3,3,3	0.30	0	3,3,3	0.64	0
5	DMS	M	601	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.61	0
4	ADP	a	602	3	29,29,29	1.60	5 (17%)	45,45,45	2.42	7 (15%)
4	ADP	b	602	3	29,29,29	1.68	6 (20%)	45,45,45	2.47	6 (13%)
4	ADP	c	602	3	29,29,29	1.91	7 (24%)	45,45,45	2.69	8 (17%)
4	ADP	d	602	3	29,29,29	1.69	6 (20%)	45,45,45	2.49	9 (20%)
4	ADP	e	602	3	29,29,29	1.70	8 (27%)	45,45,45	2.48	7 (15%)
4	ADP	f	602	3	29,29,29	1.57	6 (20%)	45,45,45	2.50	7 (15%)
4	ADP	g	602	3	29,29,29	1.59	7 (24%)	45,45,45	2.46	8 (17%)
5	DMS	h	601	-	3,3,3	0.34	0	3,3,3	0.66	0
5	DMS	i	601	-	3,3,3	0.33	0	3,3,3	0.65	0
5	DMS	j	601	-	3,3,3	0.29	0	3,3,3	0.61	0
5	DMS	k	601	-	3,3,3	0.30	0	3,3,3	0.63	0
5	DMS	l	601	-	3,3,3	0.32	0	3,3,3	0.63	0
5	DMS	m	601	-	3,3,3	0.25	0	3,3,3	0.57	0
5	DMS	n	701	-	3,3,3	0.25	0	3,3,3	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	602	3	-	0/16/32/32	0/3/3/3
4	ADP	B	602	3	-	0/16/32/32	0/3/3/3
4	ADP	C	602	3	-	0/16/32/32	0/3/3/3
4	ADP	D	602	3	-	0/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	E	602	3	-	0/16/32/32	0/3/3/3
4	ADP	F	602	3	-	0/16/32/32	0/3/3/3
4	ADP	G	602	3	-	0/16/32/32	0/3/3/3
5	DMS	H	601	-	-	0/0/0/0	0/0/0/0
5	DMS	I	601	-	-	0/0/0/0	0/0/0/0
5	DMS	J	601	-	-	0/0/0/0	0/0/0/0
5	DMS	K	601	-	-	0/0/0/0	0/0/0/0
5	DMS	L	601	-	-	0/0/0/0	0/0/0/0
5	DMS	M	601	-	-	0/0/0/0	0/0/0/0
5	DMS	N	701	-	-	0/0/0/0	0/0/0/0
4	ADP	a	602	3	-	0/16/32/32	0/3/3/3
4	ADP	b	602	3	-	0/16/32/32	0/3/3/3
4	ADP	c	602	3	-	0/16/32/32	0/3/3/3
4	ADP	d	602	3	-	0/16/32/32	0/3/3/3
4	ADP	e	602	3	-	0/16/32/32	0/3/3/3
4	ADP	f	602	3	-	0/16/32/32	0/3/3/3
4	ADP	g	602	3	-	0/16/32/32	0/3/3/3
5	DMS	h	601	-	-	0/0/0/0	0/0/0/0
5	DMS	i	601	-	-	0/0/0/0	0/0/0/0
5	DMS	j	601	-	-	0/0/0/0	0/0/0/0
5	DMS	k	601	-	-	0/0/0/0	0/0/0/0
5	DMS	l	601	-	-	0/0/0/0	0/0/0/0
5	DMS	m	601	-	-	0/0/0/0	0/0/0/0
5	DMS	n	701	-	-	0/0/0/0	0/0/0/0

The worst 5 of 85 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c	602	ADP	C4-N9	-6.02	1.29	1.37
4	b	602	ADP	C2'-C1'	-4.61	1.46	1.53
4	F	602	ADP	C4-N9	-4.40	1.31	1.37
4	g	602	ADP	C4-N9	-4.34	1.31	1.37
4	C	602	ADP	C2'-C1'	-4.33	1.47	1.53

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	602	ADP	N3-C2-N1	-12.95	117.50	128.89
4	f	602	ADP	N3-C2-N1	-12.69	117.72	128.89
4	b	602	ADP	N3-C2-N1	-12.64	117.77	128.89
4	d	602	ADP	N3-C2-N1	-12.63	117.78	128.89
4	C	602	ADP	N3-C2-N1	-12.53	117.86	128.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	527/543 (97%)	-0.21	6 (1%) 77 78	16, 51, 95, 147	0
1	B	527/543 (97%)	-0.16	5 (0%) 81 81	15, 52, 101, 146	0
1	C	526/543 (96%)	-0.23	3 (0%) 86 88	14, 50, 101, 140	0
1	D	526/543 (96%)	-0.07	12 (2%) 57 58	14, 55, 120, 154	0
1	E	526/543 (96%)	-0.01	13 (2%) 54 55	9, 51, 127, 164	0
1	F	529/543 (97%)	-0.07	9 (1%) 67 68	17, 58, 108, 159	0
1	G	525/543 (96%)	-0.12	4 (0%) 83 83	19, 57, 106, 140	0
1	H	526/543 (96%)	-0.01	15 (2%) 49 50	26, 70, 120, 163	0
1	I	525/543 (96%)	-0.08	9 (1%) 67 68	24, 67, 121, 151	0
1	J	525/543 (96%)	-0.11	8 (1%) 70 71	14, 55, 110, 163	0
1	K	525/543 (96%)	-0.05	13 (2%) 54 55	16, 63, 120, 157	0
1	L	526/543 (96%)	-0.05	14 (2%) 52 52	23, 62, 115, 154	0
1	M	525/543 (96%)	2.03	182 (34%) 1 1	25, 95, 150, 167	0
1	N	526/543 (96%)	0.11	24 (4%) 31 31	25, 70, 124, 167	0
1	a	527/543 (97%)	0.31	43 (8%) 12 10	18, 71, 128, 157	0
1	b	526/543 (96%)	0.24	47 (8%) 10 8	18, 66, 121, 163	0
1	c	527/543 (97%)	0.18	28 (5%) 25 26	23, 72, 134, 166	0
1	d	527/543 (97%)	0.08	14 (2%) 52 52	29, 77, 118, 146	0
1	e	526/543 (96%)	0.20	19 (3%) 41 41	42, 81, 116, 155	0
1	f	527/543 (97%)	0.32	26 (4%) 28 29	45, 88, 123, 149	0
1	g	526/543 (96%)	0.25	36 (6%) 17 15	27, 88, 136, 163	0
1	h	525/543 (96%)	-0.06	8 (1%) 70 71	24, 61, 112, 150	0
1	i	525/543 (96%)	0.10	24 (4%) 31 31	28, 76, 125, 160	0
1	j	525/543 (96%)	0.27	33 (6%) 19 18	32, 79, 125, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	k	525/543 (96%)	0.54	59 (11%) 6 5	37, 94, 135, 158	0
1	l	525/543 (96%)	1.05	118 (22%) 1 1	48, 106, 143, 162	0
1	m	525/543 (96%)	1.57	167 (31%) 1 1	56, 104, 146, 174	0
1	n	525/543 (96%)	0.15	32 (6%) 21 20	37, 79, 130, 158	0
2	O	96/100 (96%)	0.63	14 (14%) 3 3	59, 109, 142, 146	0
2	P	94/100 (94%)	0.59	8 (8%) 11 9	69, 108, 142, 146	0
2	Q	96/100 (96%)	0.69	12 (12%) 5 4	60, 108, 142, 149	0
2	R	96/100 (96%)	0.48	9 (9%) 9 7	60, 99, 134, 151	0
2	S	96/100 (96%)	0.73	12 (12%) 5 4	61, 107, 140, 150	0
2	T	96/100 (96%)	0.82	14 (14%) 3 3	65, 106, 141, 154	0
2	U	96/100 (96%)	0.70	7 (7%) 15 13	55, 107, 142, 148	0
2	o	96/100 (96%)	1.35	27 (28%) 1 1	86, 116, 152, 164	0
2	p	96/100 (96%)	0.98	17 (17%) 2 2	80, 112, 146, 150	0
2	q	96/100 (96%)	0.51	6 (6%) 19 18	45, 101, 141, 157	0
2	r	96/100 (96%)	0.71	9 (9%) 9 7	60, 109, 141, 150	0
2	s	96/100 (96%)	0.97	20 (20%) 1 1	73, 114, 143, 150	0
2	t	96/100 (96%)	0.69	14 (14%) 3 3	82, 118, 147, 159	0
2	u	96/100 (96%)	0.92	18 (18%) 2 2	83, 122, 153, 167	0
All	All	16067/16604 (96%)	0.27	1158 (7%) 15 14	9, 76, 133, 174	0

The worst 5 of 1158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	273	ALA	20.1
1	M	294	VAL	19.6
1	M	291	ILE	17.8
1	M	247	LEU	17.3
1	M	246	LEU	14.8

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	g	601	1/1	0.54	14.41	66,66,66,66	0
3	MG	F	601	1/1	0.27	10.85	25,25,25,25	0
3	MG	d	601	1/1	0.38	10.22	68,68,68,68	0
3	MG	D	601	1/1	0.22	8.61	29,29,29,29	0
3	MG	f	601	1/1	0.46	7.13	70,70,70,70	0
3	MG	c	601	1/1	0.31	5.95	51,51,51,51	0
3	MG	A	601	1/1	0.23	5.36	27,27,27,27	0
5	DMS	k	601	4/4	0.28	4.50	89,96,103,115	0
5	DMS	n	701	4/4	0.27	4.45	69,85,87,99	0
3	MG	e	601	1/1	0.32	4.44	62,62,62,62	0
3	MG	B	601	1/1	0.29	3.49	44,44,44,44	0
3	MG	a	601	1/1	0.32	3.44	54,54,54,54	0
5	DMS	j	601	4/4	0.27	3.07	82,83,101,117	0
5	DMS	h	601	4/4	0.22	3.01	52,58,85,96	0
5	DMS	H	601	4/4	0.26	2.78	24,28,74,96	0
5	DMS	m	601	4/4	0.23	2.67	82,92,95,105	0
5	DMS	l	601	4/4	0.27	2.66	63,95,106,125	0
5	DMS	J	601	4/4	0.23	2.63	39,53,65,90	0
3	MG	b	601	1/1	0.25	2.16	53,53,53,53	0
4	ADP	f	602	27/27	0.28	2.01	47,93,109,116	0
3	MG	E	601	1/1	0.22	1.84	20,20,20,20	0
5	DMS	I	601	4/4	0.19	1.67	37,58,66,93	0
5	DMS	L	601	4/4	0.22	1.53	39,58,61,94	0
4	ADP	B	602	27/27	0.22	1.53	18,54,75,80	0
4	ADP	d	602	27/27	0.23	1.52	45,72,87,93	0
4	ADP	g	602	27/27	0.25	1.46	56,84,98,103	0
4	ADP	a	602	27/27	0.24	1.36	21,70,81,90	0
3	MG	G	601	1/1	0.20	1.25	29,29,29,29	0
4	ADP	D	602	27/27	0.20	1.21	1,38,64,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ADP	G	602	27/27	0.21	1.19	1,61,76,85	0
4	ADP	e	602	27/27	0.24	1.16	48,78,103,108	0
4	ADP	c	602	27/27	0.22	1.10	24,67,80,102	0
5	DMS	M	601	4/4	0.18	1.05	26,29,60,79	0
3	MG	C	601	1/1	0.20	0.97	28,28,28,28	0
4	ADP	F	602	27/27	0.21	0.91	23,51,75,88	0
5	DMS	i	601	4/4	0.19	0.80	27,32,40,87	0
4	ADP	E	602	27/27	0.20	0.71	12,44,74,80	0
4	ADP	b	602	27/27	0.19	0.61	13,58,79,85	0
4	ADP	A	602	27/27	0.20	0.49	1,47,68,77	0
5	DMS	K	601	4/4	0.17	0.47	43,44,76,91	0
4	ADP	C	602	27/27	0.19	0.40	1,34,70,78	0
5	DMS	N	701	4/4	0.15	-0.45	53,57,64,90	0

6.5 Other polymers ⓘ

There are no such residues in this entry.