wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:07 PM BST

PDB ID	:	3ZQ0
EMDB ID:	:	EMD-2326
Title	:	Visualizing GroEL-ES in the Act of Encapsulating a Non-Native Substrate Protein
Authors	:	Chen, D.-H.; Madan, D.; Weaver, J.; Lin, Z.; Schroder, G.F.; Chiu, W.; Rye, H.S.
Deposited on	:	2013-03-04
Resolution	:	9.20 Å(reported)
Based on PDB ID	:	1AON

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
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

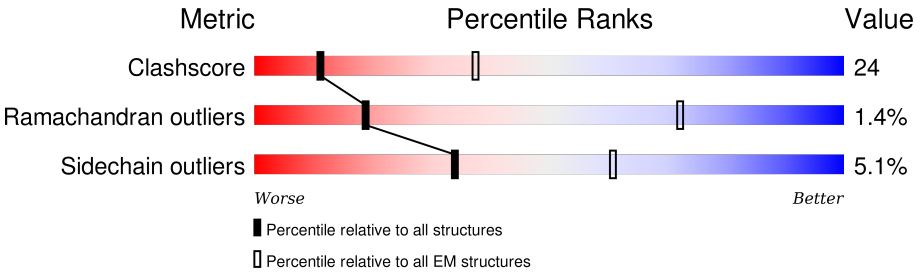
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.20 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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	524	58% 39% .
1	B	524	55% 41% .
1	C	524	56% 40% .
1	D	524	60% 37% .
1	E	524	55% 40% 5%
1	F	524	57% 40% .
1	G	524	55% 42% . .
1	H	524	62% 36% .
1	I	524	62% 36% .

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Mol	Chain	Length	Quality of chain
1	J	524	63% 34%
1	K	524	58% 40%
1	L	524	60% 38%
1	M	524	57% 41%
1	N	524	61% 37%
2	O	97	51% 39% 9%
2	P	97	47% 43% 9%
2	Q	97	63% 30% 6%
2	R	97	56% 37% 7%
2	S	97	39% 52% 9%
2	T	97	52% 37% 11%
2	U	97	53% 40% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 59276 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 60 KDA CHAPERONIN.

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

- Molecule 2 is a protein called 10 KDA CHAPERONIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	97	Total	C	N	O	S	0	0
			728	454	127	145	2		

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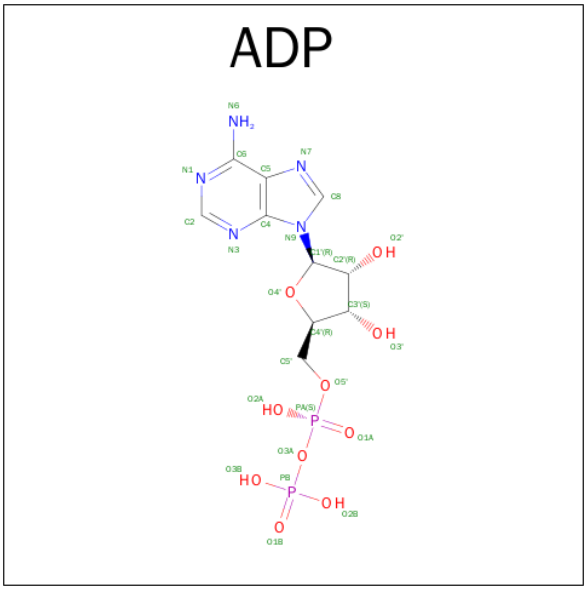
Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	Q	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	R	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	S	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	T	97	Total	C	N	O	S	0	0
			728	454	127	145	2		
2	U	97	Total	C	N	O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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

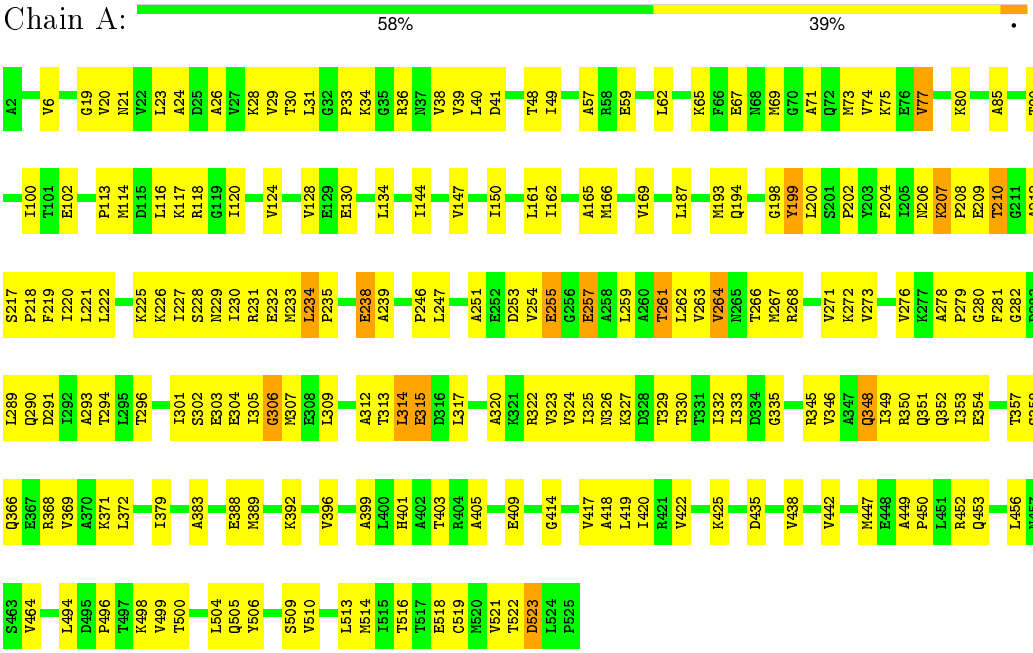
Mol	Chain	Residues	Atoms		AltConf
4	G	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	A	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

3 Residue-property plots (i)

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.

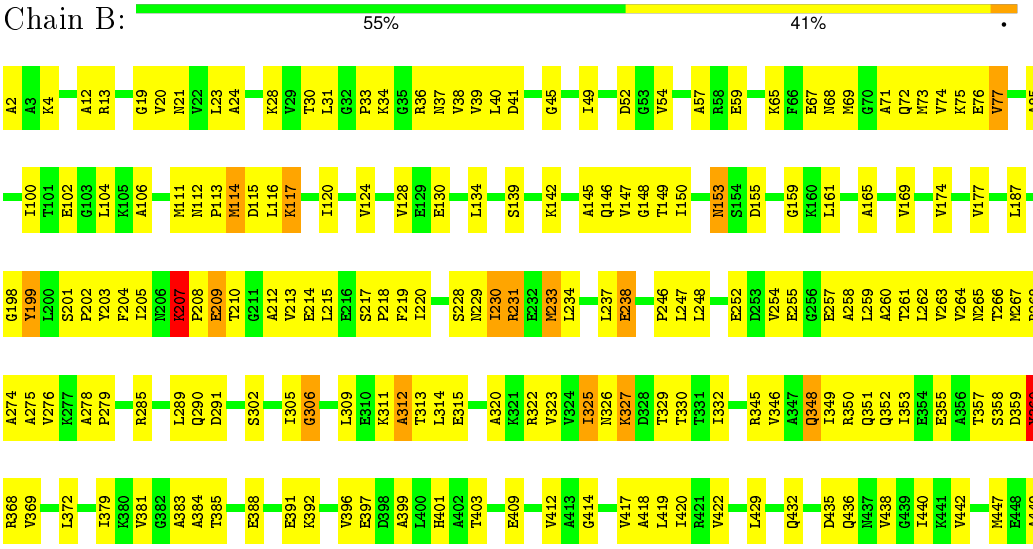
- Molecule 1: 60 KDA CHAPERONIN

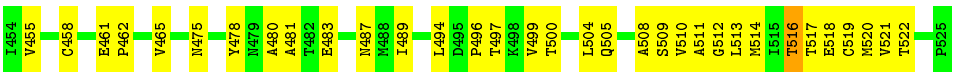
Chain A:



- Molecule 1: 60 KDA CHAPERONIN

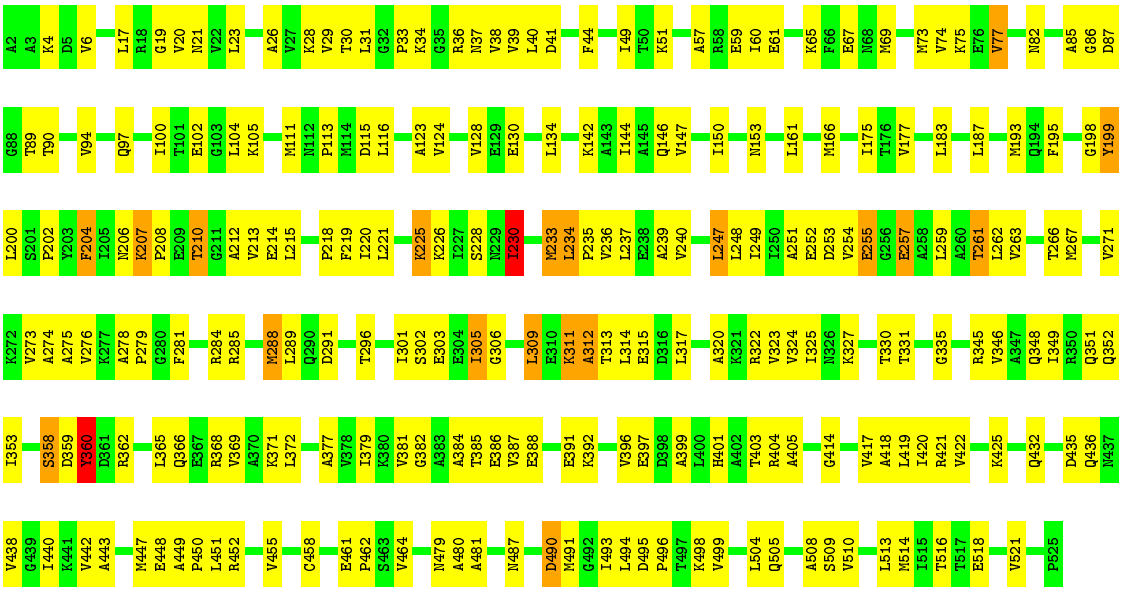
Chain B:





• Molecule 1: 60 KDA CHAPERONIN

Chain C:

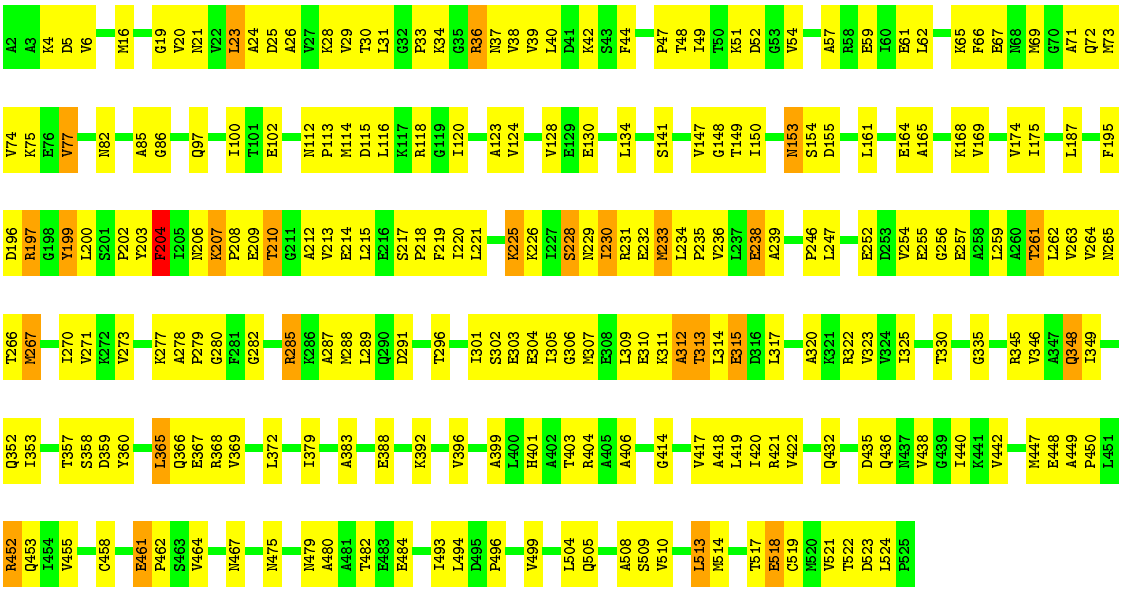


• Molecule 1: 60 KDA CHAPERONIN

Chain D:

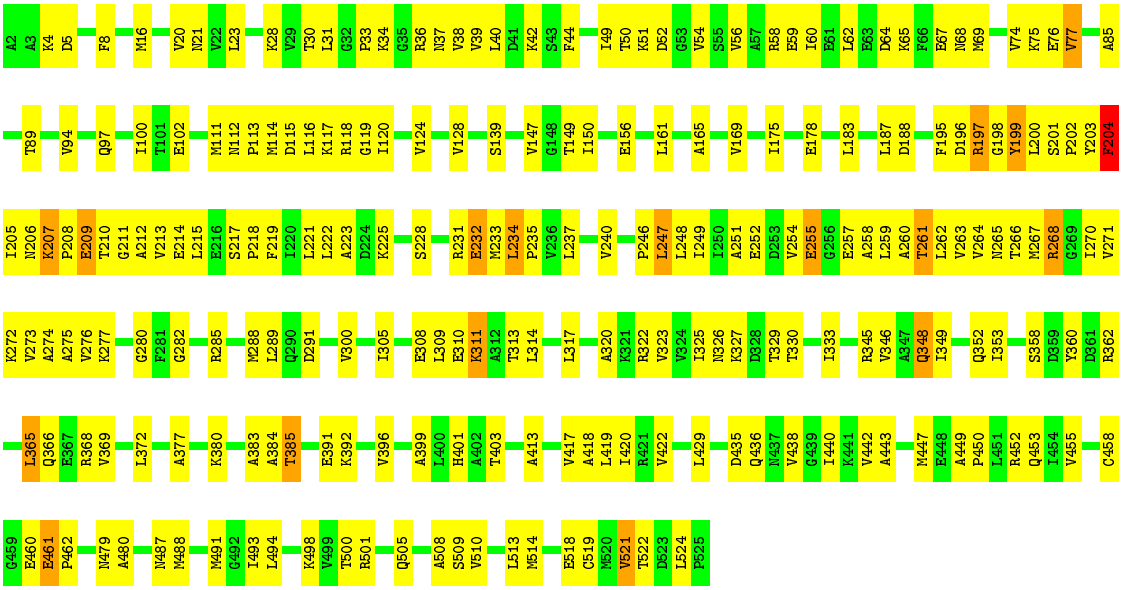
• Molecule 1: 60 KDA CHAPERONIN

Chain E:



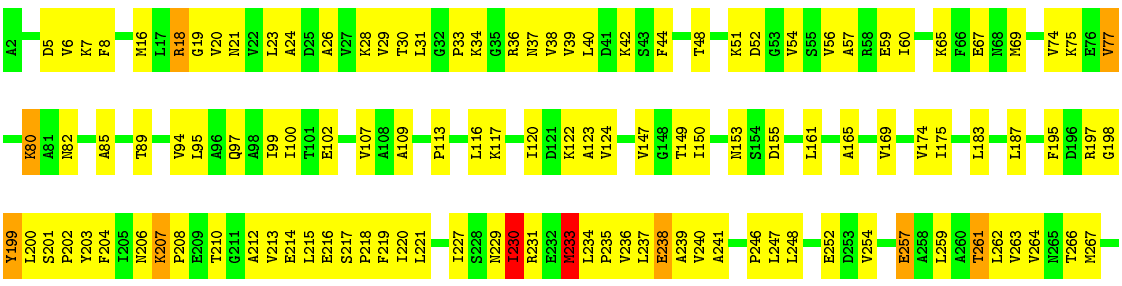
- Molecule 1: 60 KDA CHAPERONIN

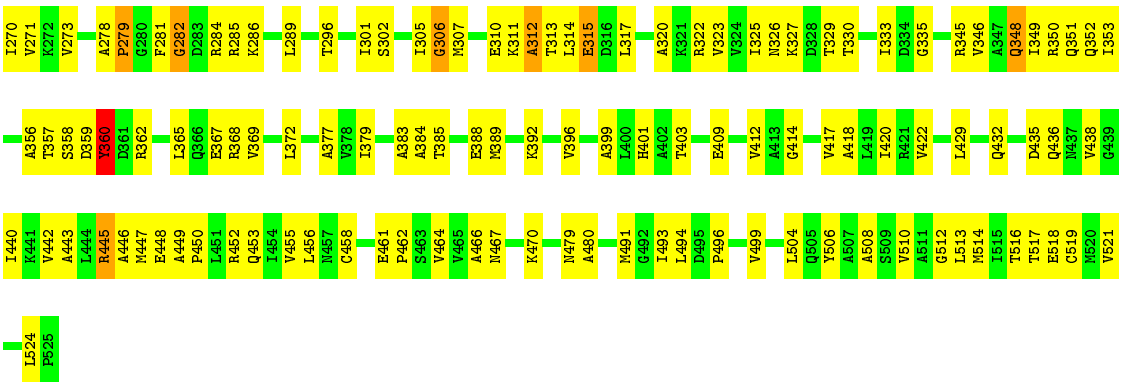
Chain F:



- Molecule 1: 60 KDA CHAPERONIN

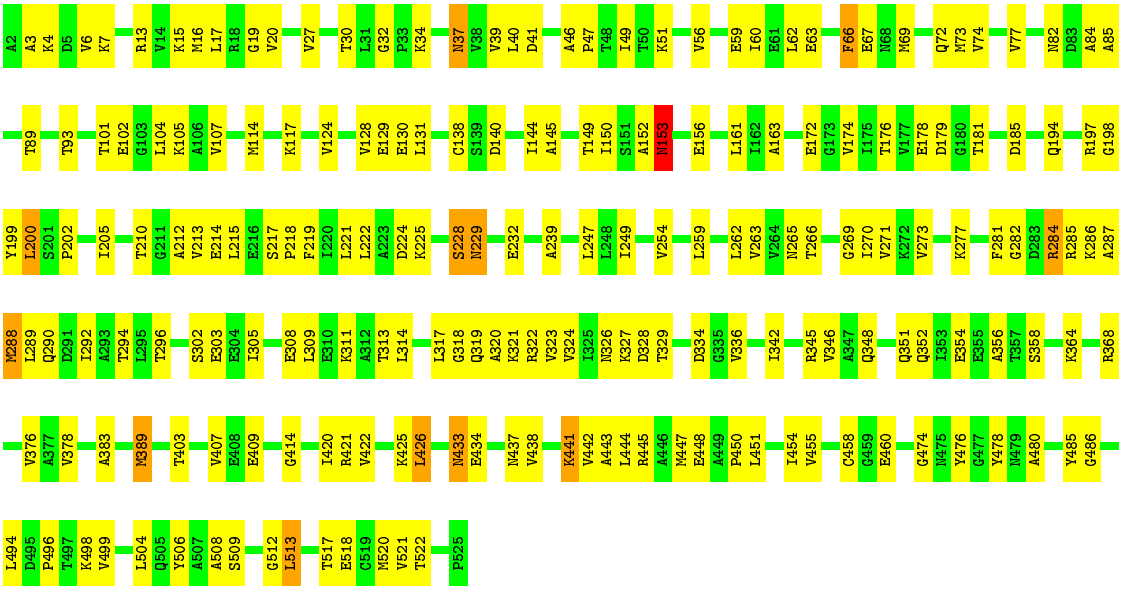
Chain G:





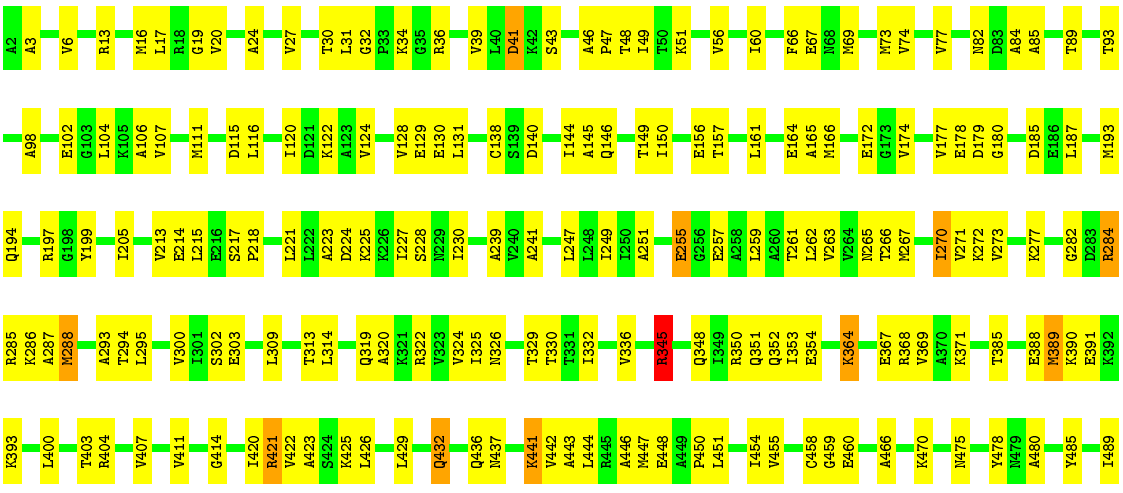
• Molecule 1: 60 KDA CHAPERONIN

Chain H:



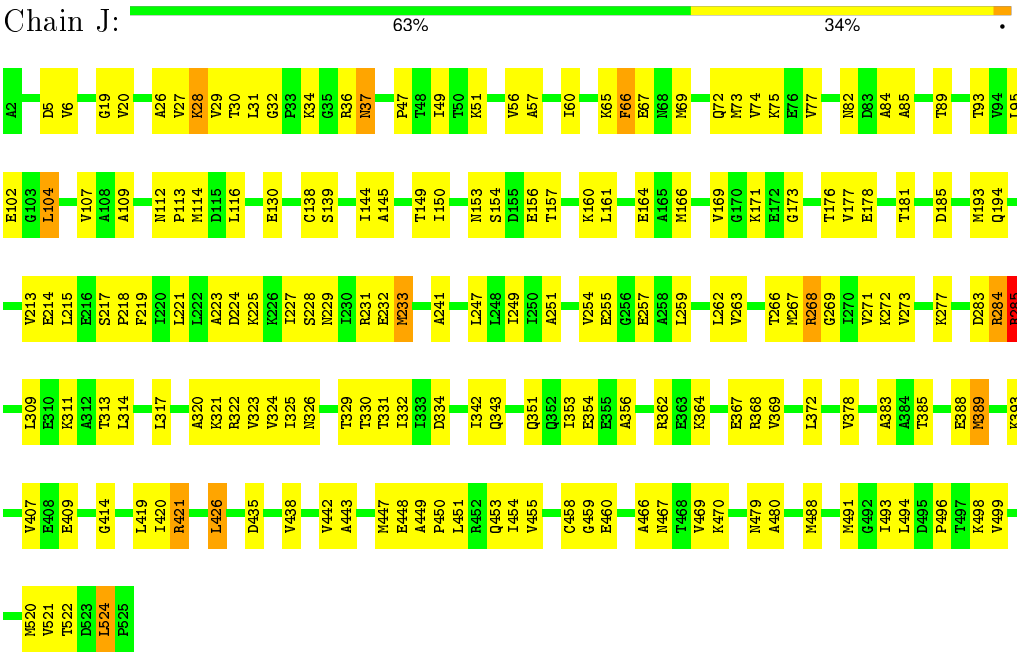
• Molecule 1: 60 KDA CHAPERONIN

Chain I:



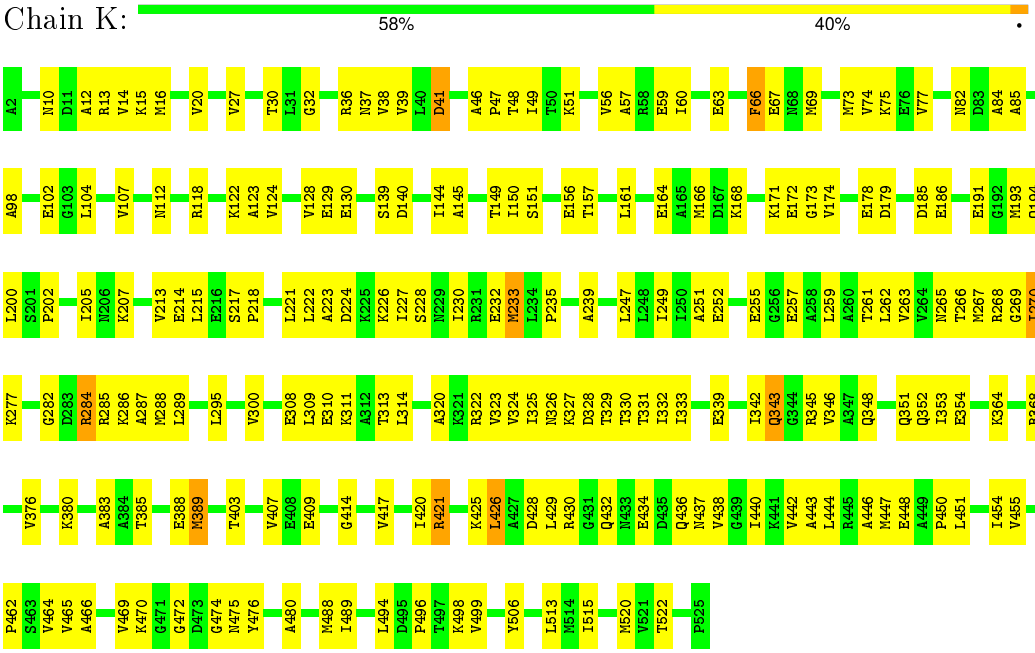
- Molecule 1: 60 KDA CHAPERONIN

Chain J:



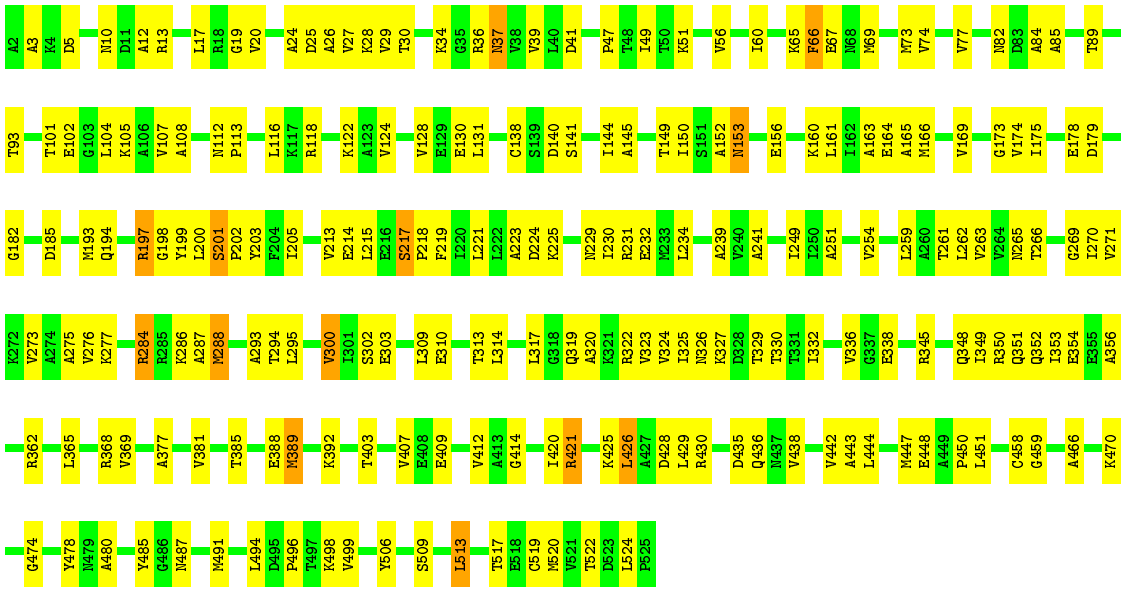
- Molecule 1: 60 KDA CHAPERONIN

Chain K:



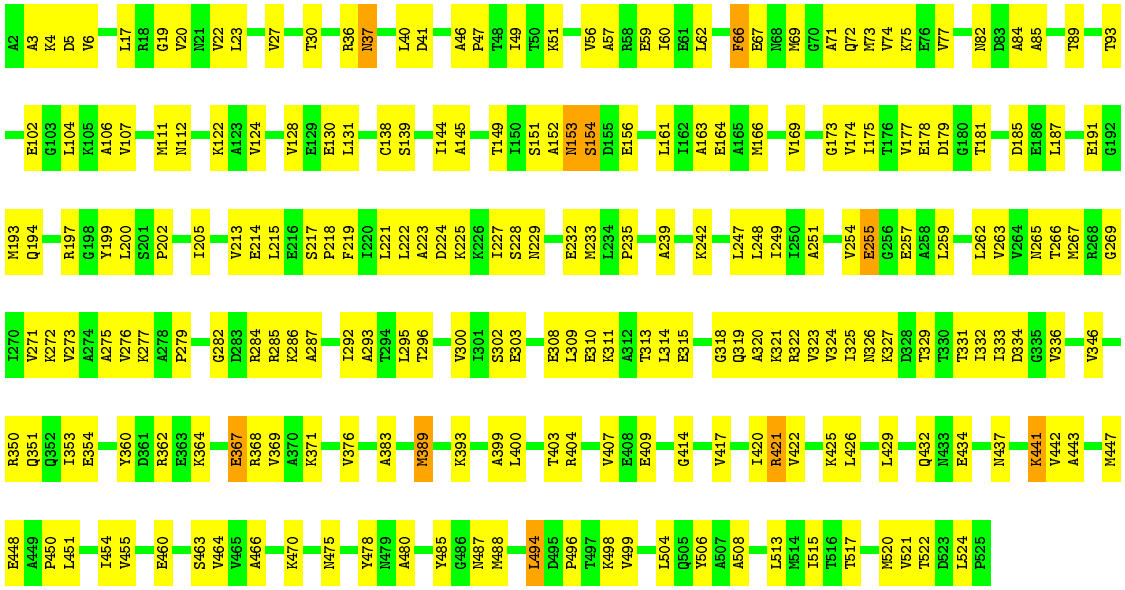
- Molecule 1: 60 KDA CHAPERONIN

Chain L:



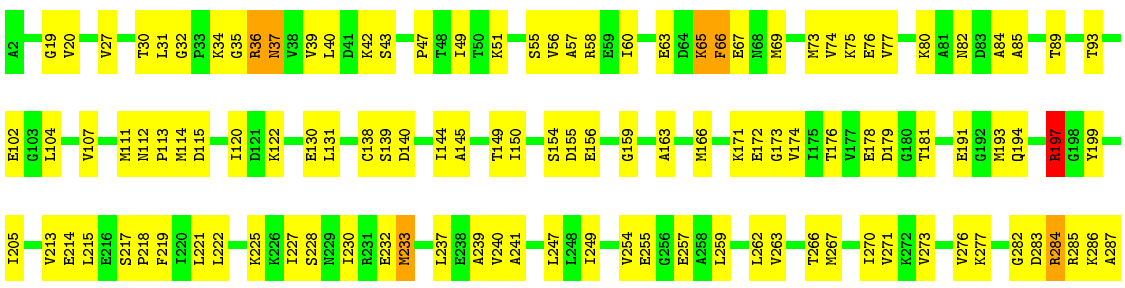
• Molecule 1: 60 KDA CHAPERONIN

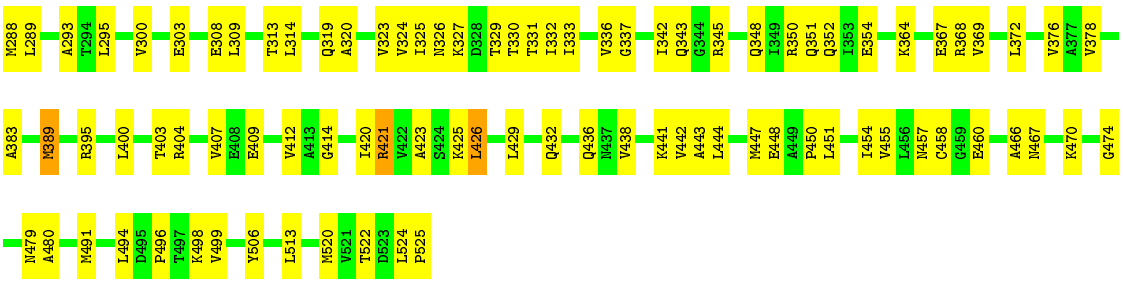
Chain M:



• Molecule 1: 60 KDA CHAPERONIN

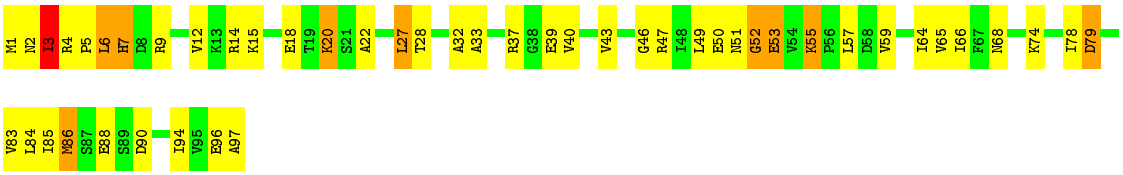
Chain N:





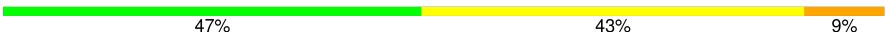
• Molecule 2: 10 KDA CHAPERONIN

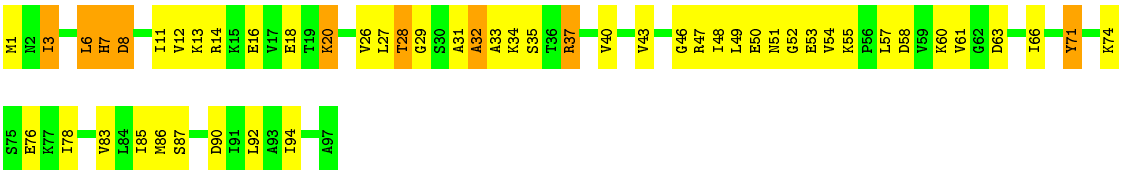
Chain O:



• Molecule 2: 10 KDA CHAPERONIN

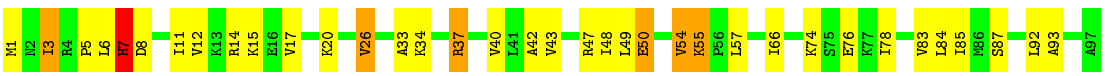
Chain P:





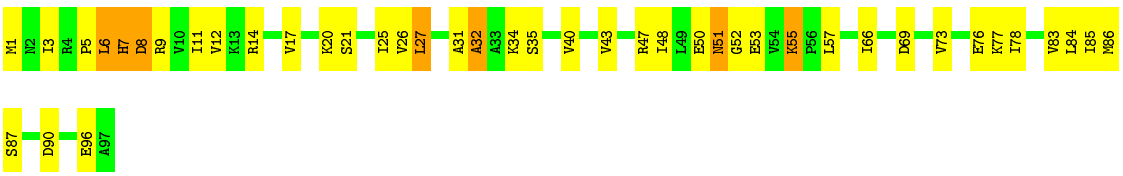
• Molecule 2: 10 KDA CHAPERONIN

Chain Q:



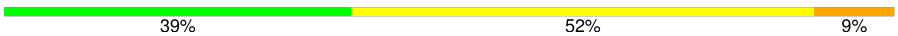
• Molecule 2: 10 KDA CHAPERONIN

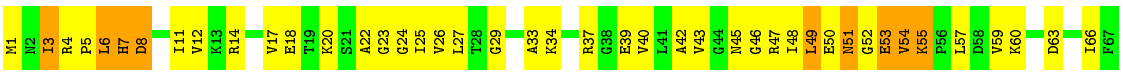
Chain R:

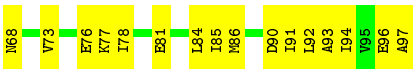


• Molecule 2: 10 KDA CHAPERONIN

Chain S:

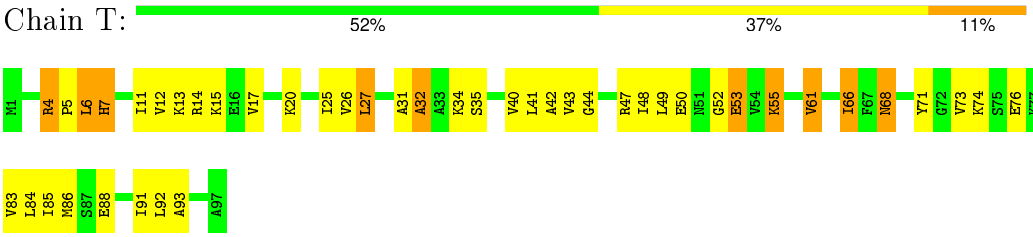






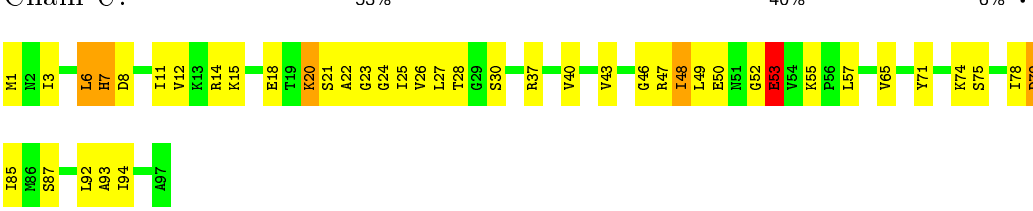
- Molecule 2: 10 KDA CHAPERONIN

Chain T:



- Molecule 2: 10 KDA CHAPERONIN

Chain U:



4 Experimental information (i)

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	EACH FRAME	Depositor
Microscope	JEOL KYOTO-3000SFF	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	4700	Depositor
Magnification	50000	Depositor
Image detector	GATAN CCD	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	#$\|Z\|$ >2	RMSZ	#$\|Z\|$ >2
1	A	0.37	0/3884	0.60	0/5243
1	B	0.37	0/3884	0.62	1/5243 (0.0%)
1	C	0.37	0/3884	0.62	0/5243
1	D	0.36	0/3884	0.61	0/5243
1	E	0.45	4/3884 (0.1%)	1.85	7/5243 (0.1%)
1	F	0.37	0/3884	0.61	0/5243
1	G	0.37	0/3884	0.63	0/5243
1	H	0.35	0/3884	0.60	0/5243
1	I	0.36	0/3884	0.62	1/5243 (0.0%)
1	J	0.36	0/3884	0.61	1/5243 (0.0%)
1	K	0.35	0/3884	0.60	0/5243
1	L	0.36	0/3884	0.60	0/5243
1	M	0.36	0/3884	0.61	0/5243
1	N	0.35	0/3884	0.60	0/5243
2	O	0.45	0/732	0.76	0/983
2	P	0.39	0/732	0.75	0/983
2	Q	0.40	0/732	0.69	0/983
2	R	0.45	0/732	0.74	0/983
2	S	0.43	0/732	0.73	0/983
2	T	0.42	0/732	0.75	2/983 (0.2%)
2	U	0.43	0/732	0.73	0/983
All	All	0.37	4/59500 (0.0%)	0.77	12/80283 (0.0%)

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	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	204	PHE	CB-CG	10.07	1.68	1.51
1	E	204	PHE	CG-CD1	7.69	1.50	1.38
1	E	204	PHE	CE1-CZ	5.70	1.48	1.37
1	E	204	PHE	CD1-CE1	-5.55	1.28	1.39

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	204	PHE	CD1-CE1-CZ	-75.38	29.65	120.10
1	E	204	PHE	CG-CD1-CE1	-61.55	53.10	120.80
1	E	204	PHE	CD1-CG-CD2	-40.88	65.15	118.30
1	E	204	PHE	CB-CG-CD1	38.19	147.53	120.80
1	E	204	PHE	CZ-CE2-CD2	-37.45	75.16	120.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	204	PHE	Sidechain

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	3856	0	3976	201	0
1	B	3856	0	3976	250	0
1	C	3856	0	3976	231	0
1	D	3856	0	3976	209	0
1	E	3856	0	3976	242	0
1	F	3856	0	3976	232	0
1	G	3856	0	3976	236	0
1	H	3856	0	3976	165	0
1	I	3856	0	3976	178	0
1	J	3856	0	3976	157	0
1	K	3856	0	3976	178	0
1	L	3856	0	3976	180	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	3856	0	3976	179	0
1	N	3856	0	3976	166	0
2	O	728	0	762	41	0
2	P	728	0	762	46	0
2	Q	728	0	762	39	0
2	R	728	0	762	40	0
2	S	728	0	762	61	0
2	T	728	0	762	52	0
2	U	728	0	762	59	0
3	A	27	0	12	4	0
3	B	27	0	12	5	0
3	C	27	0	12	7	0
3	D	27	0	12	3	0
3	E	27	0	12	7	0
3	F	27	0	12	4	0
3	G	27	0	12	3	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
All	All	59276	0	61082	2844	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 24.

The worst 5 of 2844 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:G:237:LEU:HD22	2:U:26:VAL:HG22	1.23	1.14
1:A:352:GLN:HB3	1:A:365:LEU:HD11	1.33	1.08
1:D:322:ARG:HB3	1:D:333:ILE:HD12	1.37	1.00
1:C:306:GLY:HA3	1:D:264:VAL:HG21	1.45	0.98
1:C:352:GLN:HB3	1:C:365:LEU:HD11	1.45	0.98

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/524 (100%)	502 (96%)	12 (2%)	8 (2%)	13	57
1	B	522/524 (100%)	503 (96%)	9 (2%)	10 (2%)	10	52
1	C	522/524 (100%)	505 (97%)	7 (1%)	10 (2%)	10	52
1	D	522/524 (100%)	499 (96%)	17 (3%)	6 (1%)	17	63
1	E	522/524 (100%)	501 (96%)	13 (2%)	8 (2%)	13	57
1	F	522/524 (100%)	500 (96%)	13 (2%)	9 (2%)	11	55
1	G	522/524 (100%)	503 (96%)	9 (2%)	10 (2%)	10	52
1	H	522/524 (100%)	507 (97%)	11 (2%)	4 (1%)	24	69
1	I	522/524 (100%)	513 (98%)	7 (1%)	2 (0%)	39	80
1	J	522/524 (100%)	515 (99%)	5 (1%)	2 (0%)	39	80
1	K	522/524 (100%)	511 (98%)	8 (2%)	3 (1%)	30	74
1	L	522/524 (100%)	513 (98%)	6 (1%)	3 (1%)	30	74
1	M	522/524 (100%)	511 (98%)	8 (2%)	3 (1%)	30	74
1	N	522/524 (100%)	508 (97%)	10 (2%)	4 (1%)	24	69
2	O	95/97 (98%)	85 (90%)	3 (3%)	7 (7%)	1	21
2	P	95/97 (98%)	85 (90%)	4 (4%)	6 (6%)	2	25
2	Q	95/97 (98%)	89 (94%)	3 (3%)	3 (3%)	5	41
2	R	95/97 (98%)	89 (94%)	2 (2%)	4 (4%)	3	34
2	S	95/97 (98%)	84 (88%)	7 (7%)	4 (4%)	3	34
2	T	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	9	50
2	U	95/97 (98%)	86 (90%)	3 (3%)	6 (6%)	2	25
All	All	7973/8015 (100%)	7694 (96%)	165 (2%)	114 (1%)	19	58

5 of 114 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	GLY
1	A	358	SER
1	B	312	ALA
1	B	360	TYR
1	C	233	MET

5.3.2 Protein sidechains (i)

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	404/404 (100%)	386 (96%)	18 (4%)	34 69
1	B	404/404 (100%)	387 (96%)	17 (4%)	36 70
1	C	404/404 (100%)	388 (96%)	16 (4%)	38 71
1	D	404/404 (100%)	384 (95%)	20 (5%)	30 66
1	E	404/404 (100%)	372 (92%)	32 (8%)	15 51
1	F	404/404 (100%)	386 (96%)	18 (4%)	34 69
1	G	404/404 (100%)	382 (95%)	22 (5%)	27 64
1	H	404/404 (100%)	384 (95%)	20 (5%)	30 66
1	I	404/404 (100%)	389 (96%)	15 (4%)	41 73
1	J	404/404 (100%)	385 (95%)	19 (5%)	32 68
1	K	404/404 (100%)	387 (96%)	17 (4%)	36 70
1	L	404/404 (100%)	392 (97%)	12 (3%)	48 77
1	M	404/404 (100%)	388 (96%)	16 (4%)	38 71
1	N	404/404 (100%)	385 (95%)	19 (5%)	32 68
2	O	80/80 (100%)	71 (89%)	9 (11%)	7 33
2	P	80/80 (100%)	69 (86%)	11 (14%)	4 27
2	Q	80/80 (100%)	72 (90%)	8 (10%)	9 38
2	R	80/80 (100%)	74 (92%)	6 (8%)	17 53
2	S	80/80 (100%)	73 (91%)	7 (9%)	12 45
2	T	80/80 (100%)	70 (88%)	10 (12%)	6 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	U	80/80 (100%)	72 (90%)	8 (10%)	9 38
All	All	6216/6216 (100%)	5896 (95%)	320 (5%)	34 66

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	7	LYS
1	J	37	ASN
2	S	1	MET
1	H	172	GLU
1	H	513	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	352	GLN
1	H	21	ASN
1	N	343	GLN
1	F	457	ASN
1	G	366	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)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	ADP	A	1	4	24,29,29	1.27	3 (12%)	23,45,45	3.27	6 (26%)
3	ADP	B	1	4	24,29,29	1.26	3 (12%)	23,45,45	3.26	6 (26%)
3	ADP	C	1	4	24,29,29	1.25	3 (12%)	23,45,45	3.19	5 (21%)
3	ADP	D	1	4	24,29,29	1.27	3 (12%)	23,45,45	3.18	5 (21%)
3	ADP	E	1	4	24,29,29	1.26	3 (12%)	23,45,45	3.27	5 (21%)
3	ADP	F	1	4	24,29,29	1.27	3 (12%)	23,45,45	3.21	5 (21%)
3	ADP	G	1	4	24,29,29	1.28	3 (12%)	23,45,45	3.30	6 (26%)

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
3	ADP	A	1	4	-	0/12/32/32	0/3/3/3
3	ADP	B	1	4	-	0/12/32/32	0/3/3/3
3	ADP	C	1	4	-	0/12/32/32	0/3/3/3
3	ADP	D	1	4	-	0/12/32/32	0/3/3/3
3	ADP	E	1	4	-	0/12/32/32	0/3/3/3
3	ADP	F	1	4	-	0/12/32/32	0/3/3/3
3	ADP	G	1	4	-	0/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	ADP	C5-N7	-2.19	1.31	1.39
3	E	1	ADP	C5-N7	-2.17	1.31	1.39
3	G	1	ADP	C5-N7	-2.16	1.31	1.39
3	A	1	ADP	C5-N7	-2.15	1.31	1.39
3	C	1	ADP	C5-N7	-2.15	1.31	1.39

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	ADP	N3-C2-N1	-13.20	118.50	128.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1	ADP	N3-C2-N1	-13.12	118.57	128.87
3	F	1	ADP	N3-C2-N1	-13.09	118.59	128.87
3	B	1	ADP	N3-C2-N1	-13.08	118.60	128.87
3	A	1	ADP	N3-C2-N1	-13.07	118.60	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	ADP	4	0
3	B	1	ADP	5	0
3	C	1	ADP	7	0
3	D	1	ADP	3	0
3	E	1	ADP	7	0
3	F	1	ADP	4	0
3	G	1	ADP	3	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.