



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 18, 2023 – 09:19 PM EDT

PDB ID : 5DA8
Title : Crystal structure of chaperonin GroEL from
Authors : Chang, C.; Marshall, N.; Feldmann, B.; Joachimiak, A.; Midwest Center for
Structural Genomics (MCSG)
Deposited on : 2015-08-19
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

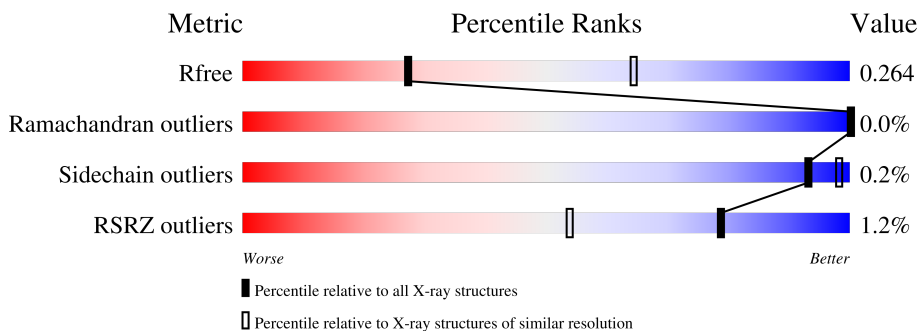
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



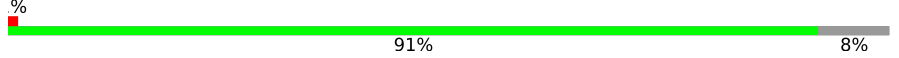
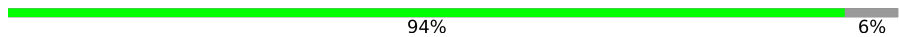
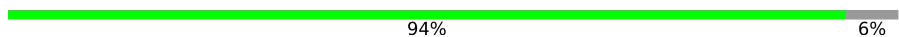
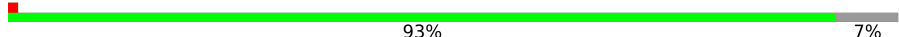






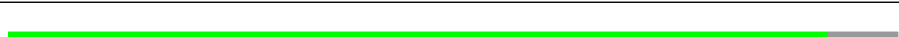


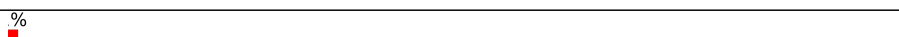
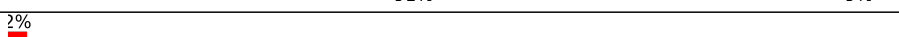
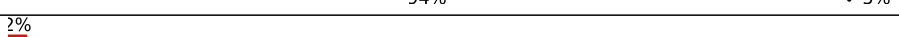
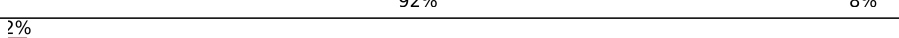
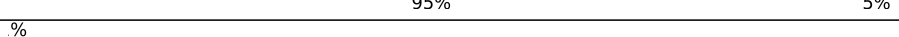
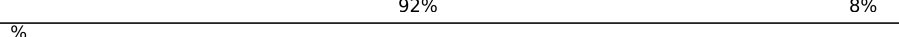
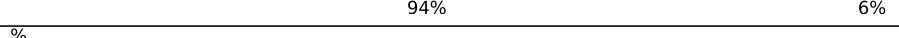
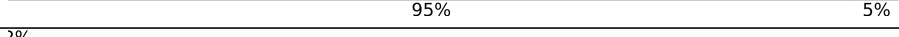
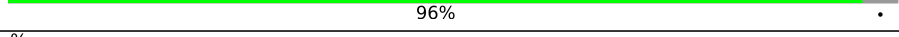
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	545	91% (green), 8% (grey)
1	B	545	95% (green), 5% (grey)
1	C	545	88% (green), 12% (grey), 1% (red)
1	D	545	95% (green), 5% (grey), 1% (red)
1	E	545	93% (green), 7% (grey), 1% (red)
1	F	545	91% (green), 9% (grey)

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Mol	Chain	Length	Quality of chain
1	G	545	 91% 8%
1	H	545	 94% 6%
1	I	545	 94% 6%
1	J	545	 93% 7%
1	K	545	 79% 21%
1	L	545	 89% 11%
1	M	545	 85% 15%
1	N	545	 94% 6%
1	O	545	 90% 10%
1	P	545	 96%
1	Q	545	 92% 8%
1	R	545	 92% 8%
1	S	545	 93% 6%
1	T	545	 91% 9%
1	U	545	 94% 5%
1	V	545	 92% 8%
1	W	545	 95% 5%
1	X	545	 92% 8%
1	Y	545	 94% 6%
1	Z	545	 95% 5%
1	a	545	 96%
1	b	545	 77% 22%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	K	601	-	-	-	X
4	MG	Q	601	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 99552 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 60 kDa chaperonin.

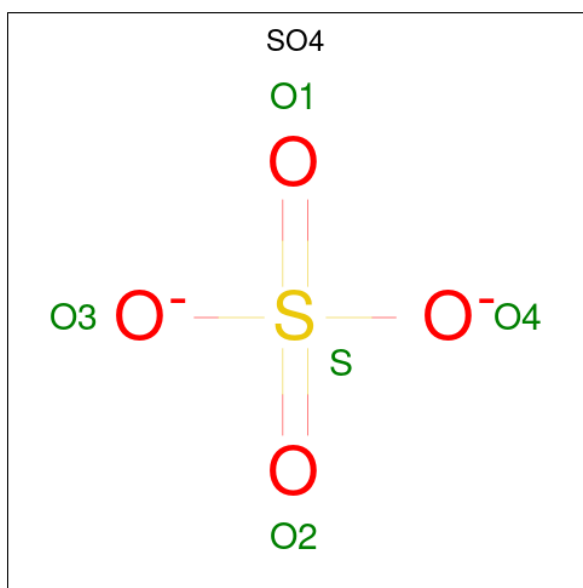
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			3601	2242	631	720	8			
1	B	519	Total	C	N	O	S	0	0	0
			3706	2296	655	745	10			
1	C	478	Total	C	N	O	S	0	0	0
			3335	2066	591	670	8			
1	D	517	Total	C	N	O	S	0	0	0
			3721	2316	654	743	8			
1	E	509	Total	C	N	O	S	0	0	0
			3631	2254	641	727	9			
1	F	497	Total	C	N	O	S	0	0	0
			3560	2201	630	720	9			
1	G	499	Total	C	N	O	S	0	0	0
			3500	2168	621	703	8			
1	H	515	Total	C	N	O	S	0	0	0
			3766	2342	659	757	8			
1	I	512	Total	C	N	O	S	0	0	0
			3697	2298	646	745	8			
1	J	507	Total	C	N	O	S	0	0	0
			3525	2175	624	719	7			
1	K	433	Total	C	N	O	S	0	0	0
			2968	1831	536	597	4			
1	L	484	Total	C	N	O	S	0	0	0
			3309	2033	591	679	6			
1	M	463	Total	C	N	O	S	0	0	0
			3247	2012	577	651	7			
1	N	511	Total	C	N	O	S	0	0	0
			3603	2232	638	725	8			
1	O	492	Total	C	N	O	S	0	0	0
			3451	2131	609	704	7			
1	P	522	Total	C	N	O	S	0	0	0
			3780	2350	661	760	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	502	Total	C	N	O	S	0	0	0
			3585	2229	633	715	8			
1	R	502	Total	C	N	O	S	0	0	0
			3576	2218	628	722	8			
1	S	512	Total	C	N	O	S	0	0	0
			3677	2286	646	737	8			
1	T	497	Total	C	N	O	S	0	0	0
			3494	2163	617	707	7			
1	U	518	Total	C	N	O	S	0	0	0
			3718	2315	648	746	9			
1	V	500	Total	C	N	O	S	0	0	0
			3575	2215	626	725	9			
1	W	517	Total	C	N	O	S	0	0	0
			3661	2269	647	737	8			
1	X	504	Total	C	N	O	S	0	0	0
			3581	2218	637	721	5			
1	Y	512	Total	C	N	O	S	0	0	0
			3695	2298	647	741	9			
1	Z	518	Total	C	N	O	S	0	0	0
			3703	2294	654	746	9			
1	a	522	Total	C	N	O	S	0	0	0
			3743	2324	658	752	9			
1	b	423	Total	C	N	O	S	0	0	0
			2961	1831	525	598	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		
2	U	1	Total	O	S	0	0
			5	4	1		
2	V	1	Total	O	S	0	0
			5	4	1		
2	Y	1	Total	O	S	0	0
			5	4	1		
2	Z	1	Total	O	S	0	0
			5	4	1		
2	a	1	Total	O	S	0	0
			5	4	1		
2	b	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	I	1	Total Ca 1 1	0	0
3	J	1	Total Ca 1 1	0	0
3	K	1	Total Ca 1 1	0	0
3	M	1	Total Ca 1 1	0	0
3	O	1	Total Ca 1 1	0	0
3	P	1	Total Ca 1 1	0	0
3	Q	1	Total Ca 1 1	0	0
3	R	1	Total Ca 1 1	0	0
3	T	1	Total Ca 1 1	0	0
3	U	1	Total Ca 1 1	0	0
3	V	1	Total Ca 1 1	0	0
3	Y	1	Total Ca 1 1	0	0
3	Z	1	Total Ca 1 1	0	0
3	a	1	Total Ca 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Mg 1 1	0	0
4	M	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total 1	Mg 1	0	0
4	R	1	Total 1	Mg 1	0	0
4	S	1	Total 1	Mg 1	0	0
4	T	1	Total 1	Mg 1	0	0
4	V	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	2	Total 2	O 2	0	0
5	C	1	Total 1	O 1	0	0
5	D	2	Total 2	O 2	0	0
5	E	2	Total 2	O 2	0	0
5	F	2	Total 2	O 2	0	0
5	H	1	Total 1	O 1	0	0
5	I	3	Total 3	O 3	0	0
5	J	3	Total 3	O 3	0	0
5	L	3	Total 3	O 3	0	0
5	N	2	Total 2	O 2	0	0
5	O	3	Total 3	O 3	0	0
5	P	2	Total 2	O 2	0	0
5	Q	3	Total 3	O 3	0	0

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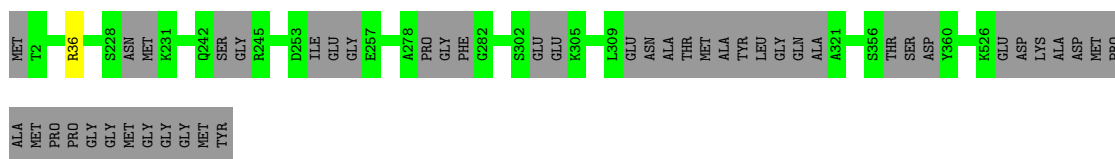
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	R	1	Total O 1 1	0	0
5	S	3	Total O 3 3	0	0
5	U	1	Total O 1 1	0	0
5	V	2	Total O 2 2	0	0
5	W	2	Total O 2 2	0	0
5	X	5	Total O 5 5	0	0
5	Y	3	Total O 3 3	0	0
5	Z	1	Total O 1 1	0	0
5	a	1	Total O 1 1	0	0
5	b	2	Total O 2 2	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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 ($RSRZ > 2$). 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: 60 kDa chaperonin

Chain A: 




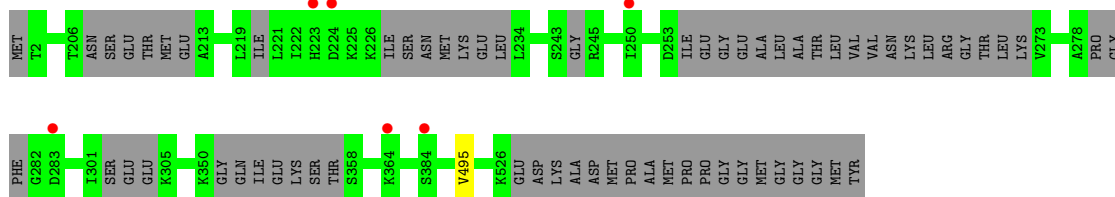
- Molecule 1: 60 kDa chaperonin

Chain B: 



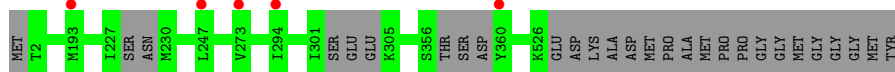
- Molecule 1: 60 kDa chaperonin

Chain C: 

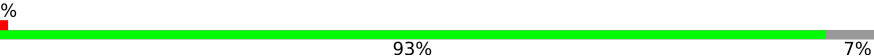


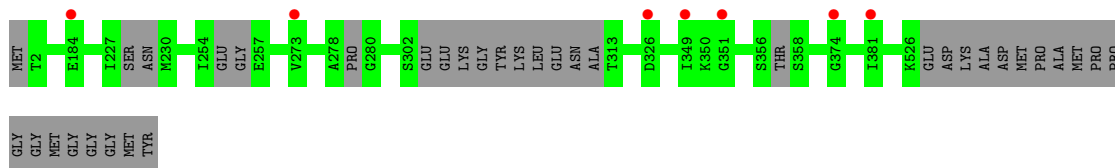
- Molecule 1: 60 kDa chaperonin

Chain D: 

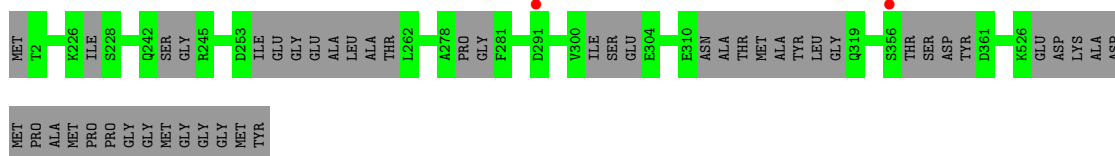


- Molecule 1: 60 kDa chaperonin

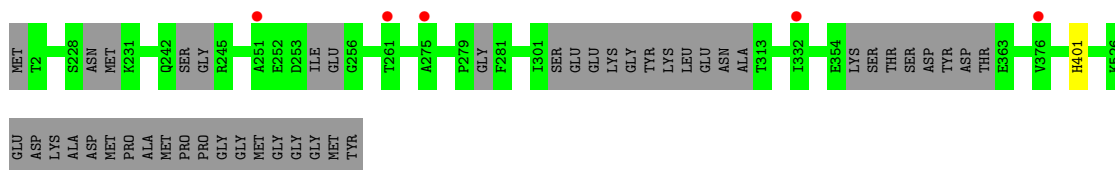
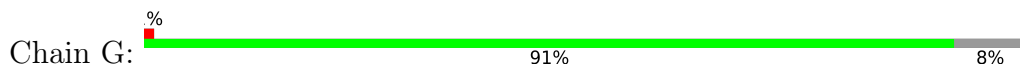
Chain E: 



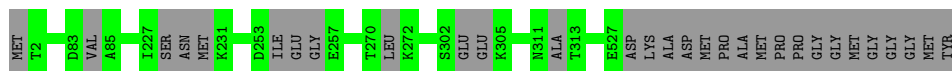
● Molecule 1: 60 kDa chaperonin



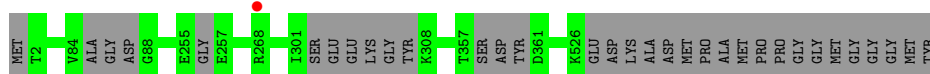
● Molecule 1: 60 kDa chaperonin



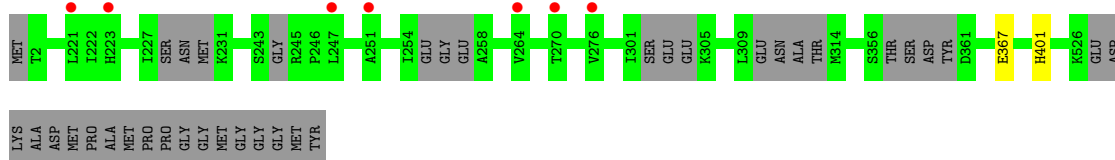
● Molecule 1: 60 kDa chaperonin



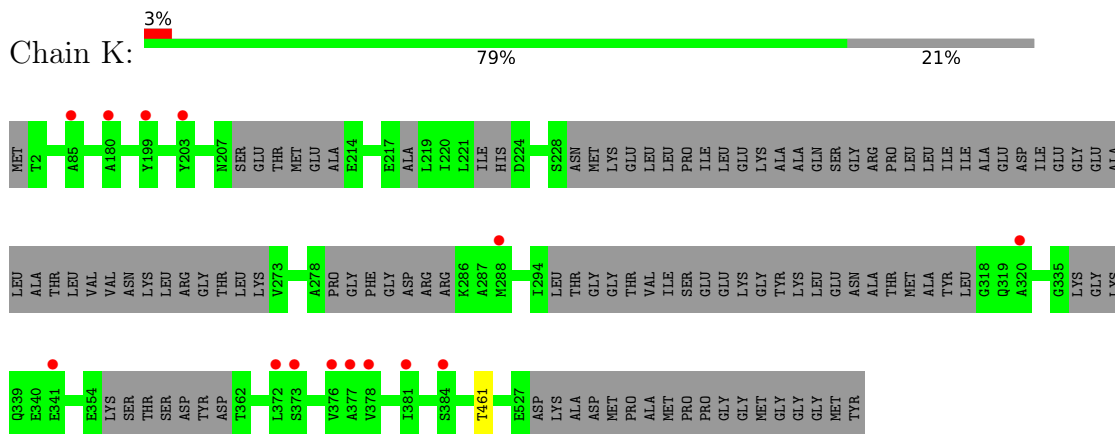
● Molecule 1: 60 kDa chaperonin



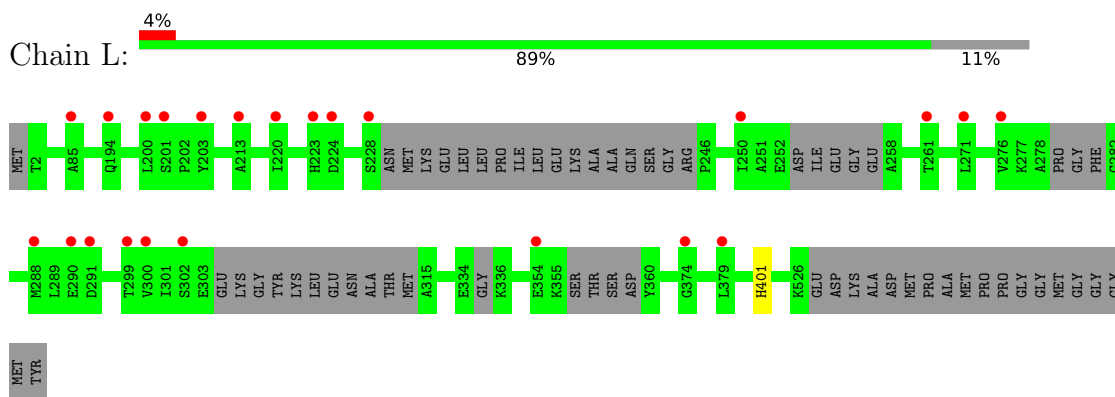
● Molecule 1: 60 kDa chaperonin



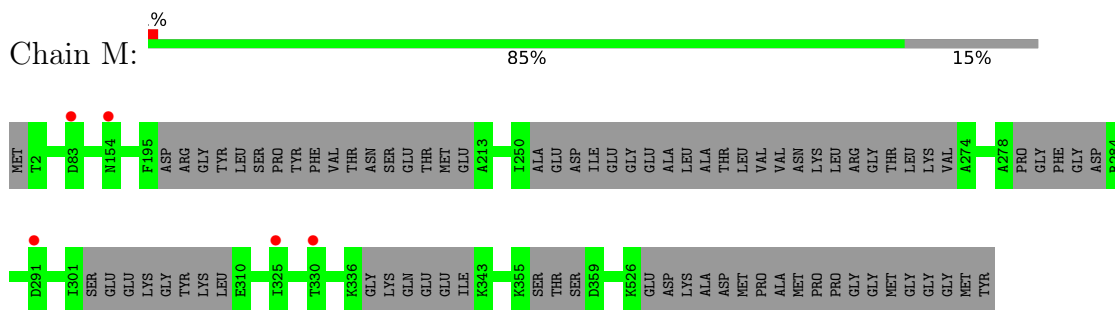
- Molecule 1: 60 kDa chaperonin



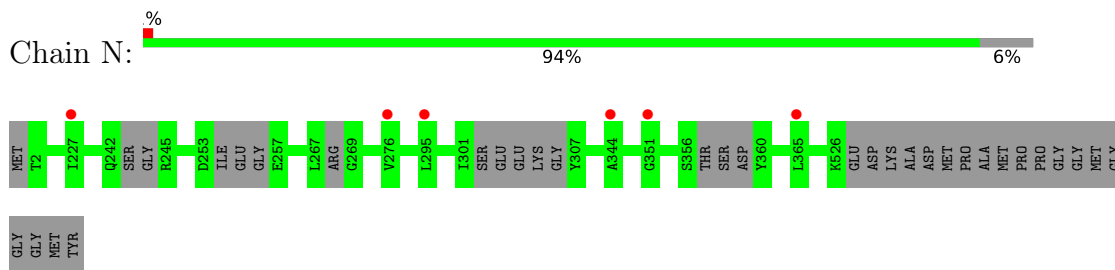
- Molecule 1: 60 kDa chaperonin



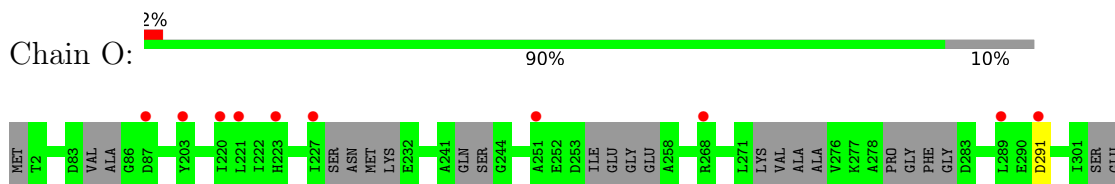
- Molecule 1: 60 kDa chaperonin



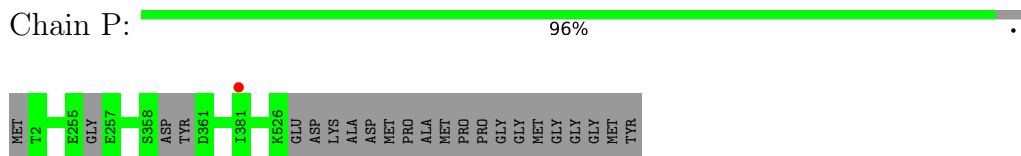
- Molecule 1: 60 kDa chaperonin



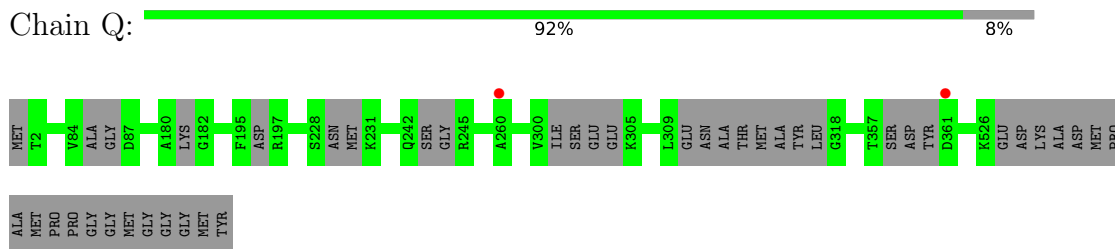
- Molecule 1: 60 kDa chaperonin



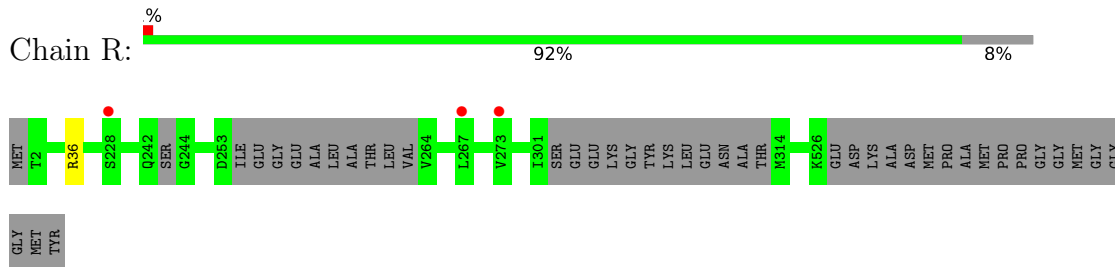
• Molecule 1: 60 kDa chaperonin



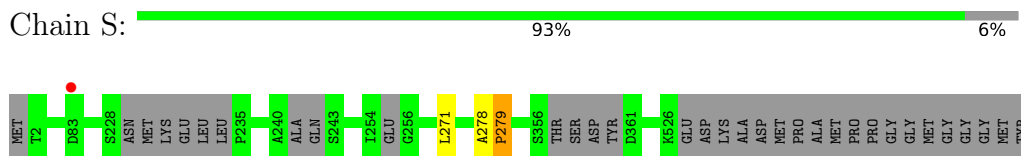
• Molecule 1: 60 kDa chaperonin



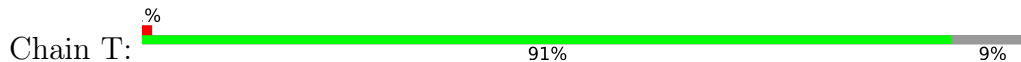
• Molecule 1: 60 kDa chaperonin

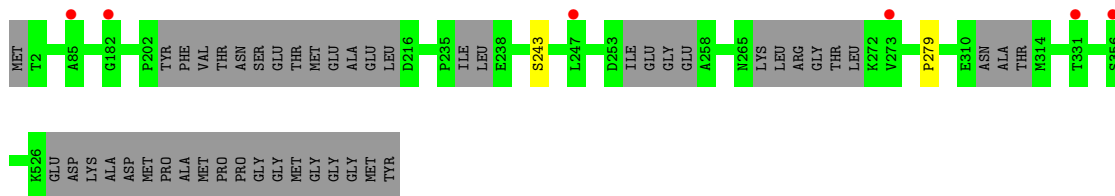


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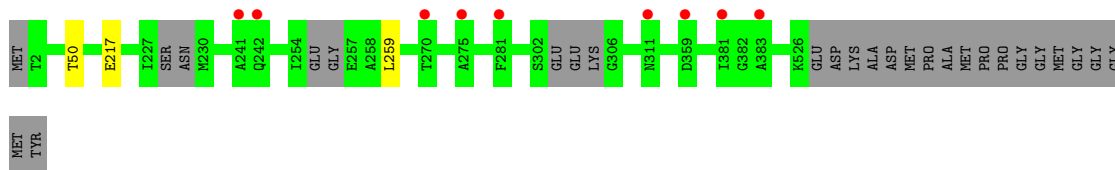


• Molecule 1: 60 kDa chaperonin

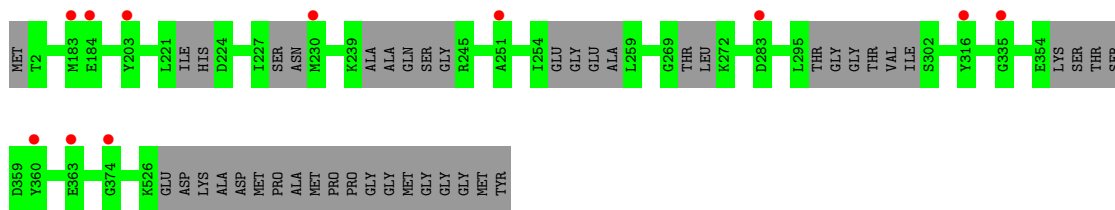




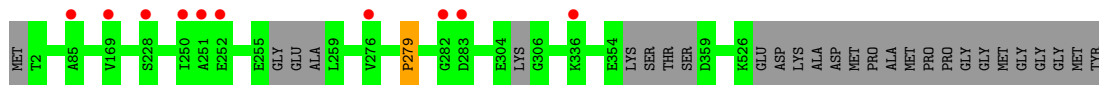
• Molecule 1: 60 kDa chaperonin



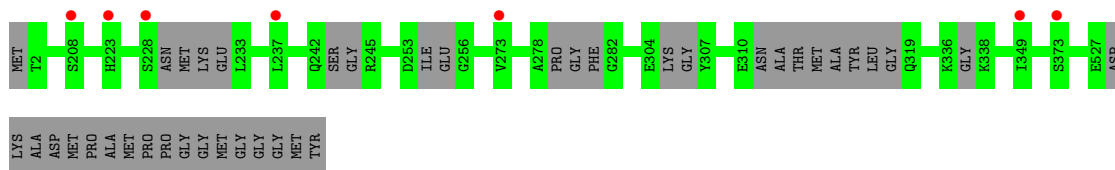
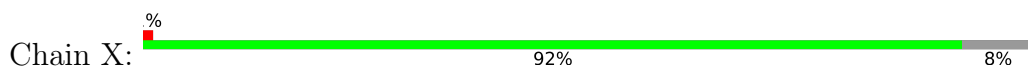
• Molecule 1: 60 kDa chaperonin



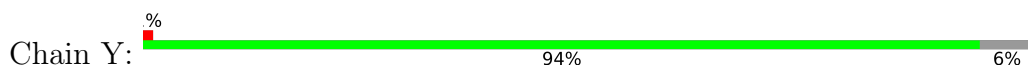
• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	139.00Å 159.78Å 228.82Å 75.46° 90.51° 91.22°	Depositor
Resolution (Å)	48.60 – 3.00 49.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (48.60-3.00) 95.9 (49.65-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 3.01Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.230 , 0.263 0.231 , 0.264	Depositor DCC
R_{free} test set	18192 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.7	Xtrriage
Anisotropy	0.082	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	99552	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, SO4, MG

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	0.23	0/3615	0.40	0/4880
1	B	0.23	0/3727	0.41	0/5041
1	C	0.23	0/3344	0.40	0/4527
1	D	0.23	0/3742	0.41	0/5062
1	E	0.23	0/3647	0.41	0/4933
1	F	0.23	0/3574	0.41	0/4827
1	G	0.23	0/3514	0.42	0/4756
1	H	0.23	0/3785	0.40	0/5106
1	I	0.23	0/3715	0.41	0/5024
1	J	0.23	0/3541	0.41	0/4799
1	K	0.23	0/2974	0.41	0/4025
1	L	0.23	0/3319	0.40	0/4501
1	M	0.23	0/3257	0.40	0/4407
1	N	0.23	0/3620	0.41	0/4902
1	O	0.23	0/3462	0.41	0/4684
1	P	0.23	0/3803	0.41	0/5142
1	Q	0.23	0/3600	0.41	0/4862
1	R	0.23	0/3595	0.41	0/4867
1	S	0.23	0/3697	0.42	1/5001 (0.0%)
1	T	0.23	0/3508	0.43	1/4751 (0.0%)
1	U	0.23	0/3739	0.42	0/5062
1	V	0.23	0/3591	0.42	0/4854
1	W	0.23	0/3679	0.42	1/4981 (0.0%)
1	X	0.23	0/3597	0.40	0/4865
1	Y	0.23	0/3715	0.41	0/5017
1	Z	0.23	0/3723	0.42	0/5039
1	a	0.23	0/3766	0.42	0/5099
1	b	0.22	0/2965	0.40	0/4007
All	All	0.23	0/99814	0.41	3/135021 (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	J	0	1
1	T	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	279	PRO	N-CA-CB	6.36	110.93	103.30
1	W	279	PRO	N-CA-CB	6.24	110.78	103.30
1	T	279	PRO	N-CA-CB	6.05	110.56	103.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	J	367	GLU	Peptide
1	T	243	SER	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	483/545 (89%)	472 (98%)	11 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	511/545 (94%)	496 (97%)	15 (3%)	0	100	100
1	C	460/545 (84%)	448 (97%)	12 (3%)	0	100	100
1	D	509/545 (93%)	497 (98%)	12 (2%)	0	100	100
1	E	497/545 (91%)	479 (96%)	18 (4%)	0	100	100
1	F	481/545 (88%)	468 (97%)	13 (3%)	0	100	100
1	G	485/545 (89%)	467 (96%)	18 (4%)	0	100	100
1	H	501/545 (92%)	489 (98%)	12 (2%)	0	100	100
1	I	502/545 (92%)	490 (98%)	12 (2%)	0	100	100
1	J	493/545 (90%)	477 (97%)	16 (3%)	0	100	100
1	K	415/545 (76%)	399 (96%)	16 (4%)	0	100	100
1	L	470/545 (86%)	456 (97%)	14 (3%)	0	100	100
1	M	449/545 (82%)	434 (97%)	15 (3%)	0	100	100
1	N	499/545 (92%)	480 (96%)	19 (4%)	0	100	100
1	O	472/545 (87%)	449 (95%)	23 (5%)	0	100	100
1	P	516/545 (95%)	497 (96%)	19 (4%)	0	100	100
1	Q	484/545 (89%)	469 (97%)	15 (3%)	0	100	100
1	R	494/545 (91%)	475 (96%)	19 (4%)	0	100	100
1	S	502/545 (92%)	485 (97%)	15 (3%)	2 (0%)	34	72
1	T	485/545 (89%)	466 (96%)	19 (4%)	0	100	100
1	U	510/545 (94%)	498 (98%)	12 (2%)	0	100	100
1	V	484/545 (89%)	465 (96%)	19 (4%)	0	100	100
1	W	509/545 (93%)	476 (94%)	32 (6%)	1 (0%)	47	82
1	X	488/545 (90%)	469 (96%)	19 (4%)	0	100	100
1	Y	500/545 (92%)	486 (97%)	14 (3%)	0	100	100
1	Z	510/545 (94%)	487 (96%)	23 (4%)	0	100	100
1	a	518/545 (95%)	497 (96%)	21 (4%)	0	100	100
1	b	401/545 (74%)	386 (96%)	15 (4%)	0	100	100
All	All	13628/15260 (89%)	13157 (96%)	468 (3%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	S	279	PRO

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Mol	Chain	Res	Type
1	W	279	PRO
1	S	278	ALA

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 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	360/427 (84%)	359 (100%)	1 (0%)	92	97
1	B	358/427 (84%)	357 (100%)	1 (0%)	92	97
1	C	310/427 (73%)	309 (100%)	1 (0%)	92	97
1	D	367/427 (86%)	367 (100%)	0	100	100
1	E	353/427 (83%)	353 (100%)	0	100	100
1	F	347/427 (81%)	347 (100%)	0	100	100
1	G	331/427 (78%)	330 (100%)	1 (0%)	92	97
1	H	381/427 (89%)	381 (100%)	0	100	100
1	I	369/427 (86%)	369 (100%)	0	100	100
1	J	328/427 (77%)	327 (100%)	1 (0%)	92	97
1	K	266/427 (62%)	265 (100%)	1 (0%)	91	97
1	L	299/427 (70%)	298 (100%)	1 (0%)	92	97
1	M	307/427 (72%)	307 (100%)	0	100	100
1	N	343/427 (80%)	343 (100%)	0	100	100
1	O	324/427 (76%)	323 (100%)	1 (0%)	92	97
1	P	378/427 (88%)	378 (100%)	0	100	100
1	Q	349/427 (82%)	349 (100%)	0	100	100
1	R	347/427 (81%)	346 (100%)	1 (0%)	92	97
1	S	362/427 (85%)	361 (100%)	1 (0%)	92	97
1	T	332/427 (78%)	332 (100%)	0	100	100
1	U	366/427 (86%)	363 (99%)	3 (1%)	81	93
1	V	345/427 (81%)	345 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	W	348/427 (82%)	348 (100%)	0	100	100
1	X	340/427 (80%)	340 (100%)	0	100	100
1	Y	362/427 (85%)	362 (100%)	0	100	100
1	Z	359/427 (84%)	358 (100%)	1 (0%)	92	97
1	a	368/427 (86%)	367 (100%)	1 (0%)	92	97
1	b	279/427 (65%)	278 (100%)	1 (0%)	91	97
All	All	9578/11956 (80%)	9562 (100%)	16 (0%)	93	98

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	B	401	HIS
1	C	495	VAL
1	G	401	HIS
1	J	401	HIS
1	K	461	THR
1	L	401	HIS
1	O	291	ASP
1	R	36	ARG
1	S	271	LEU
1	U	50	THR
1	U	217	GLU
1	U	259	LEU
1	Z	401	HIS
1	a	401	HIS
1	b	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	507	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 25 are monoatomic - leaving 21 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	$\# Z > 2$
2	SO4	F	601	-	4,4,4	0.15	0	6,6,6	0.04	0
2	SO4	Y	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	D	601	-	4,4,4	0.15	0	6,6,6	0.07	0
2	SO4	C	601	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	K	601	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	P	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	L	601	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	N	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	U	601	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	B	601	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	M	602	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	b	601	-	4,4,4	0.14	0	6,6,6	0.07	0
2	SO4	T	602	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	G	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	a	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	E	601	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	J	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	Z	601	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	A	601	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	V	602	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	R	602	-	4,4,4	0.15	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 i

6.1 Protein, DNA and RNA chains i

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	499/545 (91%)	-0.21	0 100 100	18, 51, 104, 115	0
1	B	519/545 (95%)	-0.25	1 (0%) 95 87	14, 44, 104, 121	0
1	C	478/545 (87%)	-0.13	6 (1%) 77 51	18, 52, 103, 127	0
1	D	517/545 (94%)	-0.11	5 (0%) 82 59	18, 58, 110, 129	0
1	E	509/545 (93%)	-0.12	7 (1%) 75 49	20, 66, 110, 123	0
1	F	497/545 (91%)	-0.21	2 (0%) 92 79	16, 46, 102, 122	0
1	G	499/545 (91%)	-0.16	5 (1%) 82 59	19, 59, 113, 125	0
1	H	515/545 (94%)	-0.20	0 100 100	18, 60, 102, 111	0
1	I	512/545 (93%)	-0.28	1 (0%) 95 87	17, 52, 97, 116	0
1	J	507/545 (93%)	-0.11	7 (1%) 75 49	18, 63, 116, 133	0
1	K	433/545 (79%)	-0.04	14 (3%) 47 20	20, 54, 121, 138	0
1	L	484/545 (88%)	-0.03	23 (4%) 30 11	21, 53, 125, 136	0
1	M	463/545 (84%)	-0.14	5 (1%) 80 56	24, 55, 108, 129	0
1	N	511/545 (93%)	-0.08	6 (1%) 79 54	21, 65, 112, 128	0
1	O	492/545 (90%)	-0.08	12 (2%) 59 30	20, 50, 122, 132	0
1	P	522/545 (95%)	-0.29	1 (0%) 95 87	15, 49, 92, 116	0
1	Q	502/545 (92%)	-0.24	2 (0%) 92 79	11, 44, 110, 134	0
1	R	502/545 (92%)	-0.25	3 (0%) 89 72	11, 37, 106, 125	0
1	S	512/545 (93%)	-0.22	1 (0%) 95 87	15, 61, 100, 118	0
1	T	497/545 (91%)	-0.15	6 (1%) 79 54	23, 62, 98, 111	0
1	U	518/545 (95%)	-0.12	9 (1%) 70 41	24, 74, 106, 124	0
1	V	500/545 (91%)	-0.07	11 (2%) 62 33	15, 49, 119, 139	0
1	W	517/545 (94%)	-0.08	10 (1%) 66 37	14, 55, 119, 127	0
1	X	504/545 (92%)	-0.09	7 (1%) 75 49	15, 61, 124, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	512/545 (93%)	-0.11	6 (1%) 79 54	21, 58, 110, 139	0
1	Z	518/545 (95%)	-0.05	6 (1%) 79 54	25, 75, 113, 124	0
1	a	522/545 (95%)	-0.01	9 (1%) 70 41	27, 74, 111, 126	0
1	b	423/545 (77%)	-0.09	5 (1%) 79 54	19, 49, 119, 136	0
All	All	13984/15260 (91%)	-0.14	170 (1%) 79 54	11, 56, 113, 144	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	W	282	GLY	4.6
1	S	83	ASP	4.4
1	V	335	GLY	4.2
1	a	384	SER	4.0
1	X	373	SER	3.9
1	E	374	GLY	3.9
1	X	208	SER	3.8
1	L	201	SER	3.8
1	K	180	ALA	3.7
1	T	85	ALA	3.7
1	K	320	ALA	3.6
1	K	199	TYR	3.4
1	U	359	ASP	3.4
1	X	237	LEU	3.4
1	L	220	ILE	3.4
1	L	250	ILE	3.3
1	W	283	ASP	3.3
1	G	376	VAL	3.3
1	C	223	HIS	3.3
1	Q	260	ALA	3.2
1	a	183	MET	3.2
1	U	281	PHE	3.2
1	L	290	GLU	3.1
1	L	194	GLN	3.1
1	E	381	ILE	3.1
1	L	213	ALA	3.0
1	V	251	ALA	3.0
1	N	365	LEU	3.0
1	J	264	VAL	3.0
1	a	361	ASP	2.9
1	T	247	LEU	2.9
1	W	252	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	85	ALA	2.8
1	C	283	ASP	2.8
1	X	273	VAL	2.8
1	U	383	ALA	2.8
1	b	218	ALA	2.7
1	J	221	LEU	2.7
1	U	275	ALA	2.7
1	Z	85	ALA	2.7
1	J	251	ALA	2.7
1	E	273	VAL	2.7
1	Y	295	LEU	2.7
1	W	251	ALA	2.7
1	N	351	GLY	2.7
1	O	203	TYR	2.7
1	V	363	GLU	2.6
1	Z	264	VAL	2.6
1	a	216	ASP	2.6
1	G	251	ALA	2.6
1	L	374	GLY	2.6
1	O	251	ALA	2.6
1	V	374	GLY	2.6
1	E	184	GLU	2.6
1	L	200	LEU	2.6
1	X	228	SER	2.6
1	W	336	LYS	2.6
1	L	223	HIS	2.6
1	V	184	GLU	2.6
1	V	203	TYR	2.5
1	O	289	LEU	2.5
1	U	270	THR	2.5
1	K	288	MET	2.5
1	K	381	ILE	2.5
1	L	261	THR	2.5
1	K	377	ALA	2.5
1	J	223	HIS	2.5
1	O	220	ILE	2.5
1	L	276	VAL	2.5
1	a	182	GLY	2.5
1	O	221	LEU	2.4
1	Y	141	LYS	2.4
1	O	227	ILE	2.4
1	O	291	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	349	ILE	2.4
1	L	354	GLU	2.4
1	T	356	SER	2.4
1	Z	381	ILE	2.4
1	a	295	LEU	2.4
1	D	294	ILE	2.4
1	O	223	HIS	2.4
1	I	268	ARG	2.4
1	V	360	TYR	2.4
1	K	372	LEU	2.4
1	C	364	LYS	2.4
1	N	227	ILE	2.4
1	L	271	LEU	2.3
1	M	325	ILE	2.3
1	L	224	ASP	2.3
1	K	373	SER	2.3
1	L	302	SER	2.3
1	P	381	ILE	2.3
1	a	360	TYR	2.3
1	K	384	SER	2.3
1	T	331	THR	2.3
1	W	169	VAL	2.3
1	L	300	VAL	2.3
1	L	288	MET	2.3
1	N	344	ALA	2.3
1	W	85	ALA	2.3
1	V	230	MET	2.3
1	R	267	LEU	2.3
1	D	360	TYR	2.3
1	M	330	THR	2.3
1	J	247	LEU	2.3
1	Z	203	TYR	2.3
1	b	290	GLU	2.3
1	D	247	LEU	2.3
1	M	83	ASP	2.2
1	M	291	ASP	2.2
1	a	264	VAL	2.2
1	L	299	THR	2.2
1	W	228	SER	2.2
1	T	273	VAL	2.2
1	V	316	TYR	2.2
1	R	228	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	250	ILE	2.2
1	K	376	VAL	2.2
1	U	381	ILE	2.2
1	O	362	THR	2.2
1	L	228	SER	2.2
1	K	341	GLU	2.2
1	O	268	ARG	2.2
1	X	223	HIS	2.2
1	D	273	VAL	2.2
1	W	250	ILE	2.2
1	F	291	ASP	2.2
1	K	378	VAL	2.2
1	L	291	ASP	2.2
1	V	183	MET	2.2
1	U	241	ALA	2.1
1	F	356	SER	2.1
1	L	203	TYR	2.1
1	Y	168	LYS	2.1
1	D	193	MET	2.1
1	N	295	LEU	2.1
1	N	276	VAL	2.1
1	Y	182	GLY	2.1
1	C	224	ASP	2.1
1	J	270	THR	2.1
1	Z	379	LEU	2.1
1	B	349	ILE	2.1
1	V	283	ASP	2.1
1	O	87	ASP	2.1
1	M	154	ASN	2.1
1	U	311	ASN	2.1
1	b	347	ASN	2.1
1	O	344	ALA	2.1
1	b	348	GLU	2.1
1	J	276	VAL	2.1
1	W	276	VAL	2.1
1	Y	273	VAL	2.1
1	b	293	ALA	2.1
1	E	326	ASP	2.1
1	Q	361	ASP	2.1
1	G	275	ALA	2.0
1	R	273	VAL	2.0
1	a	85	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	X	349	ILE	2.0
1	K	85	ALA	2.0
1	Z	295	LEU	2.0
1	K	203	TYR	2.0
1	L	379	LEU	2.0
1	E	351	GLY	2.0
1	G	332	ILE	2.0
1	T	182	GLY	2.0
1	G	261	THR	2.0
1	U	242	GLN	2.0
1	C	384	SER	2.0
1	Y	224	ASP	2.0

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 monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
4	MG	Q	601	1/1	0.31	0.53	67,67,67,67	0
4	MG	S	601	1/1	0.48	0.30	54,54,54,54	0
4	MG	M	601	1/1	0.59	0.26	53,53,53,53	0
2	SO4	K	601	5/5	0.61	0.45	42,55,61,61	5
2	SO4	A	601	5/5	0.70	0.36	37,61,63,70	5
3	CA	B	602	1/1	0.71	0.13	77,77,77,77	0
2	SO4	U	601	5/5	0.72	0.27	55,62,75,80	5
2	SO4	P	601	5/5	0.74	0.34	29,35,57,64	5
2	SO4	T	602	5/5	0.77	0.31	37,47,50,59	5
2	SO4	L	601	5/5	0.77	0.29	38,55,60,64	5
3	CA	P	602	1/1	0.78	0.14	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	Z	601	5/5	0.78	0.38	49,51,72,74	5
4	MG	R	601	1/1	0.79	0.23	34,34,34,34	0
2	SO4	V	602	5/5	0.79	0.34	34,35,45,48	5
3	CA	Q	602	1/1	0.80	0.08	78,78,78,78	0
3	CA	Y	602	1/1	0.80	0.09	72,72,72,72	0
2	SO4	B	601	5/5	0.80	0.33	24,30,35,36	5
3	CA	O	601	1/1	0.81	0.09	73,73,73,73	0
2	SO4	C	601	5/5	0.81	0.27	41,46,67,74	5
2	SO4	E	601	5/5	0.81	0.29	43,47,62,63	5
2	SO4	M	602	5/5	0.81	0.28	54,55,71,77	5
4	MG	V	601	1/1	0.81	0.37	61,61,61,61	0
2	SO4	D	601	5/5	0.82	0.31	33,44,50,50	5
2	SO4	J	601	5/5	0.83	0.29	33,42,51,52	5
2	SO4	G	601	5/5	0.83	0.29	36,48,56,57	5
3	CA	K	602	1/1	0.83	0.07	82,82,82,82	0
2	SO4	Y	601	5/5	0.83	0.27	34,41,58,58	5
3	CA	Z	602	1/1	0.84	0.11	92,92,92,92	0
2	SO4	b	601	5/5	0.84	0.41	62,84,95,96	0
4	MG	H	601	1/1	0.85	0.18	51,51,51,51	0
2	SO4	F	601	5/5	0.86	0.26	25,34,38,38	5
4	MG	T	601	1/1	0.86	0.17	58,58,58,58	0
2	SO4	N	601	5/5	0.86	0.28	41,47,51,54	5
3	CA	J	602	1/1	0.87	0.13	72,72,72,72	0
2	SO4	a	601	5/5	0.88	0.21	50,53,63,69	5
2	SO4	R	602	5/5	0.89	0.29	23,33,34,34	5
3	CA	M	603	1/1	0.90	0.18	78,78,78,78	0
3	CA	G	602	1/1	0.91	0.14	76,76,76,76	0
3	CA	A	602	1/1	0.91	0.09	72,72,72,72	0
3	CA	a	602	1/1	0.92	0.06	78,78,78,78	0
3	CA	F	602	1/1	0.92	0.07	77,77,77,77	0
3	CA	R	603	1/1	0.95	0.06	64,64,64,64	0
3	CA	T	603	1/1	0.95	0.18	69,69,69,69	0
3	CA	I	601	1/1	0.95	0.09	79,79,79,79	0
3	CA	U	602	1/1	0.96	0.11	62,62,62,62	0
3	CA	V	603	1/1	0.97	0.09	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.