Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:32 pm BST

PDB ID	:	5OPW
Title	:	Crystal structure of the GroEL mutant A109C
Authors	:	Yan, X.; Shi, Q.; Bracher, A.; Milicic, G.; Singh, A.K.; Hartl, F.U.; Hayer-Hartl, M.
Deposited on	:	2017-08-10
Resolution	:	3.19 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 following versions of software and data (see references ⓘ) were used in the production of this report:

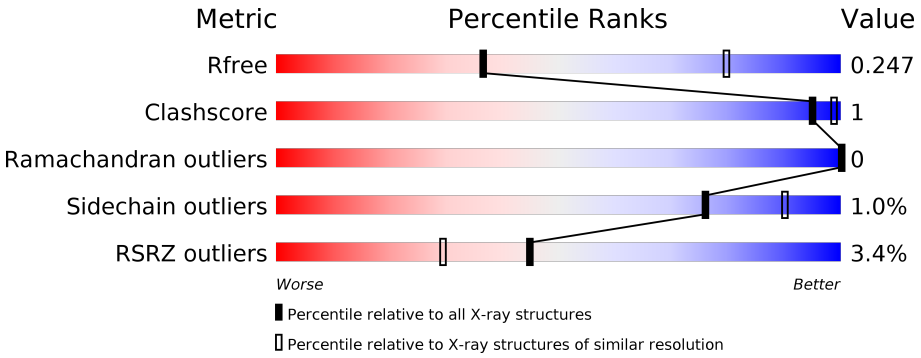
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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 <=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	547	2% 92%
1	B	547	% 92%
1	C	547	% 92%
1	D	547	3% 92%
1	E	547	5% 92%
1	F	547	2% 91%

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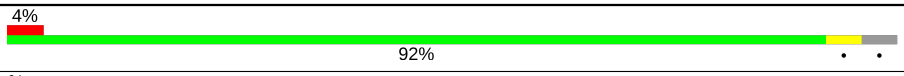
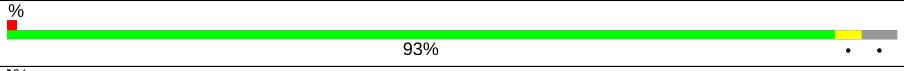
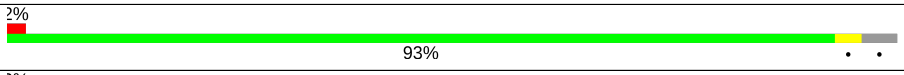
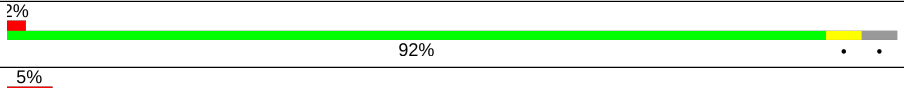
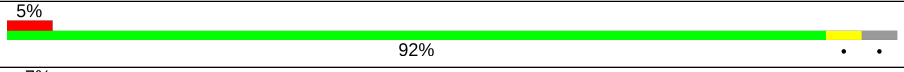
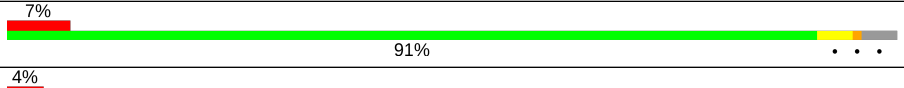
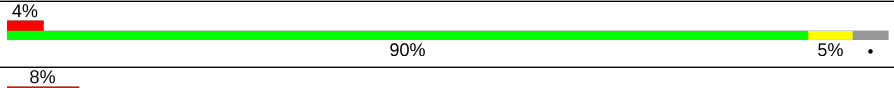
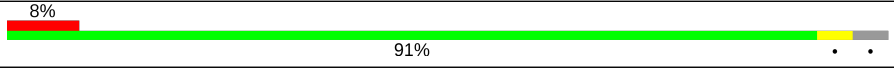
Mol	Chain	Length	Quality of chain
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 53984 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	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	773	21			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	CYS	ALA	engineered mutation	UNP P0A6F5

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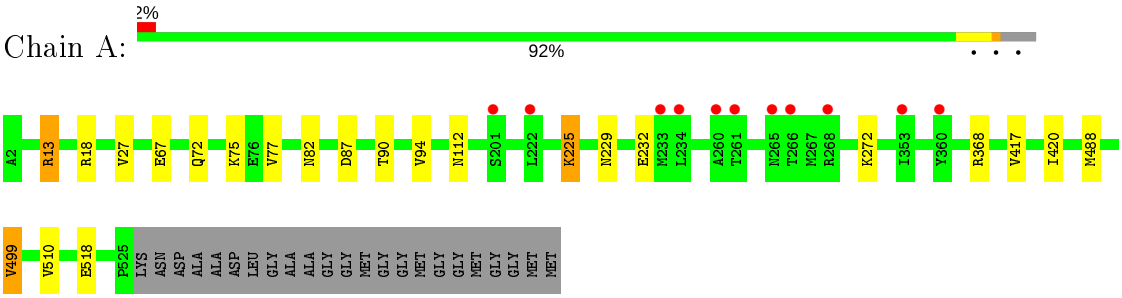
Chain	Residue	Modelled	Actual	Comment	Reference
B	109	CYS	ALA	engineered mutation	UNP P0A6F5
C	109	CYS	ALA	engineered mutation	UNP P0A6F5
D	109	CYS	ALA	engineered mutation	UNP P0A6F5
E	109	CYS	ALA	engineered mutation	UNP P0A6F5
F	109	CYS	ALA	engineered mutation	UNP P0A6F5
G	109	CYS	ALA	engineered mutation	UNP P0A6F5
H	109	CYS	ALA	engineered mutation	UNP P0A6F5
I	109	CYS	ALA	engineered mutation	UNP P0A6F5
J	109	CYS	ALA	engineered mutation	UNP P0A6F5
K	109	CYS	ALA	engineered mutation	UNP P0A6F5
L	109	CYS	ALA	engineered mutation	UNP P0A6F5
M	109	CYS	ALA	engineered mutation	UNP P0A6F5
N	109	CYS	ALA	engineered mutation	UNP P0A6F5

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 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.

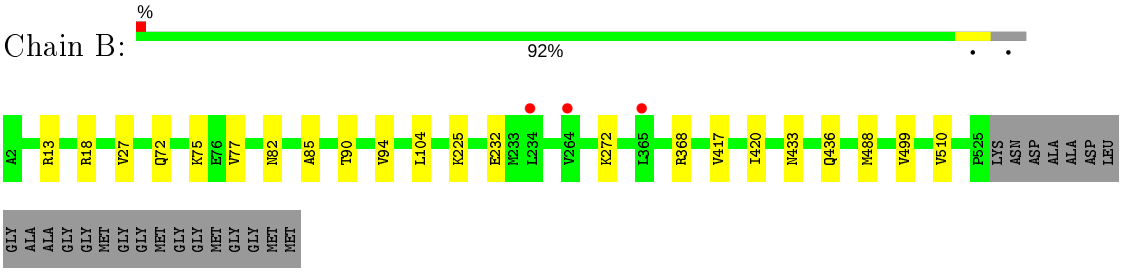
- Molecule 1: 60 kDa chaperonin

Chain A:



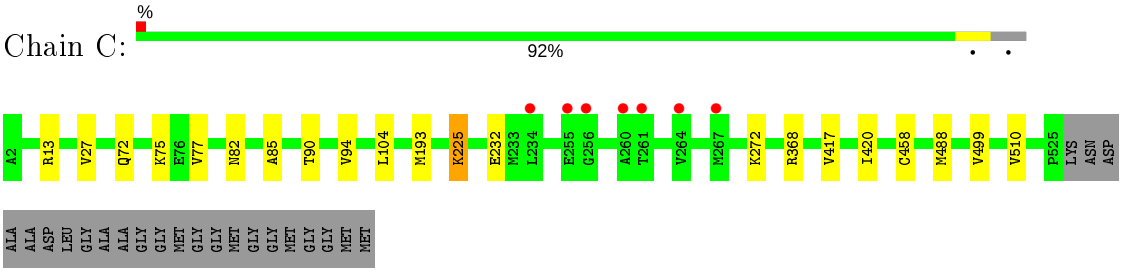
- Molecule 1: 60 kDa chaperonin

Chain B:



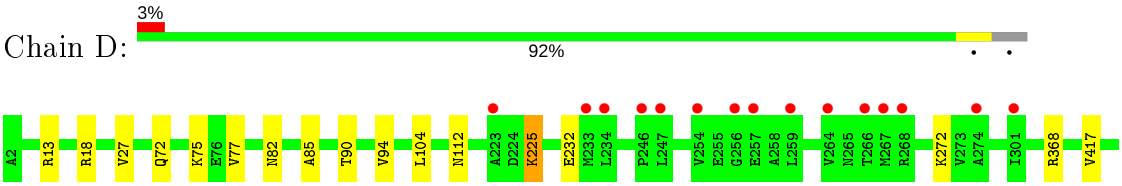
- Molecule 1: 60 kDa chaperonin

Chain C:



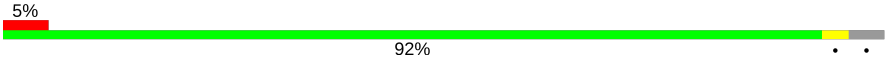
- Molecule 1: 60 kDa chaperonin

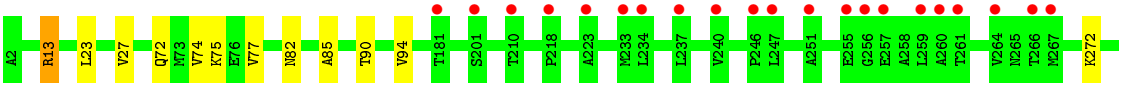
Chain D:

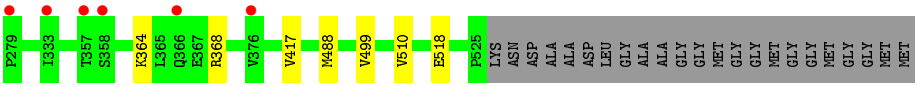


• Molecule 1: 60 kDa chaperonin

Chain E:

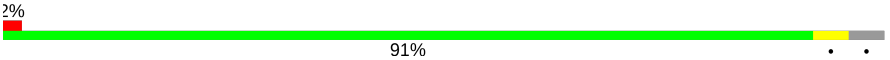


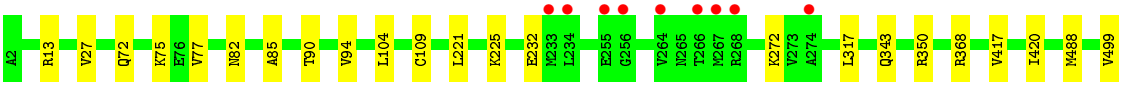




• Molecule 1: 60 kDa chaperonin

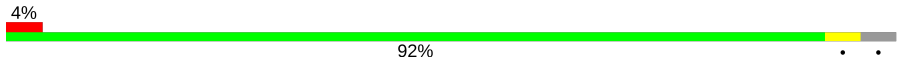
Chain F:

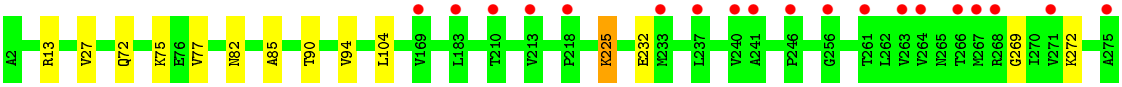


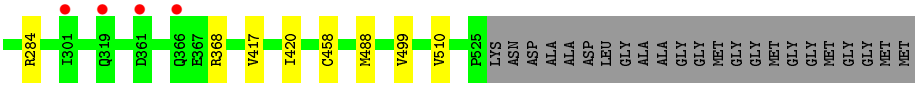


• Molecule 1: 60 kDa chaperonin

Chain G:

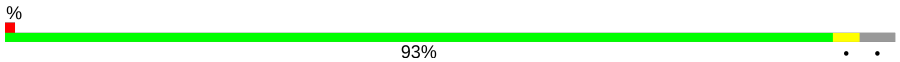


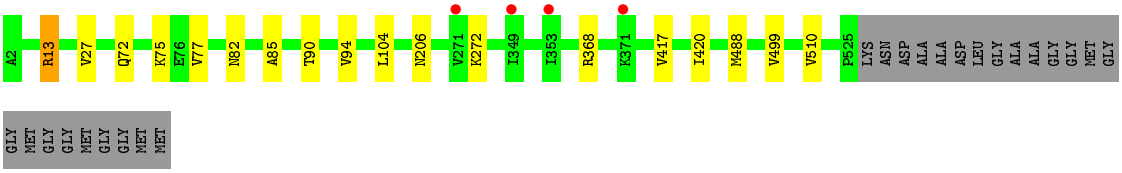




• Molecule 1: 60 kDa chaperonin

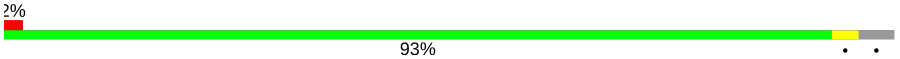
Chain H:

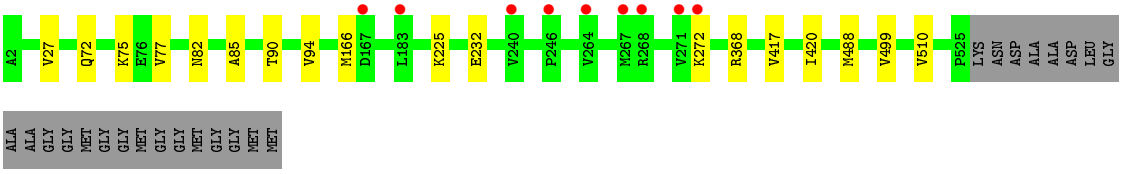




• Molecule 1: 60 kDa chaperonin

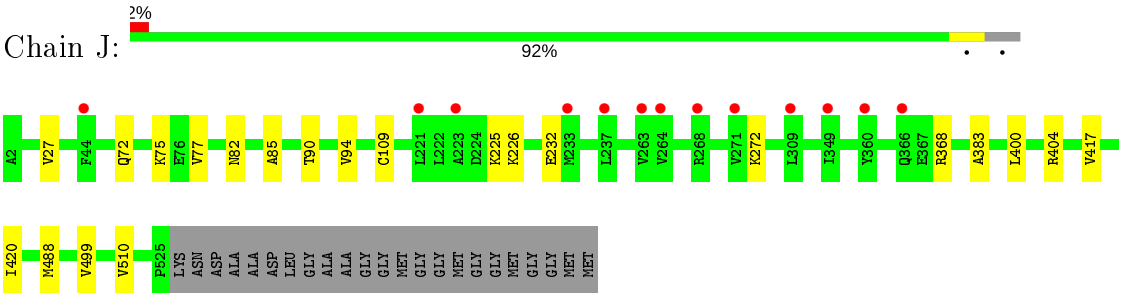
Chain I:





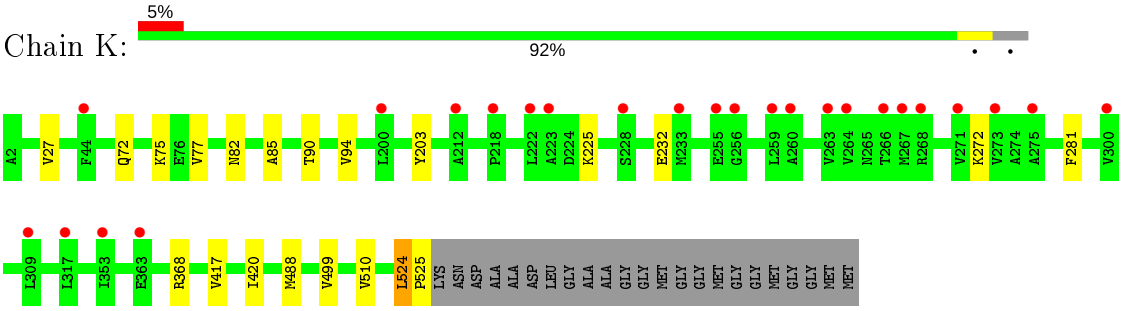
- Molecule 1: 60 kDa chaperonin

Chain J:



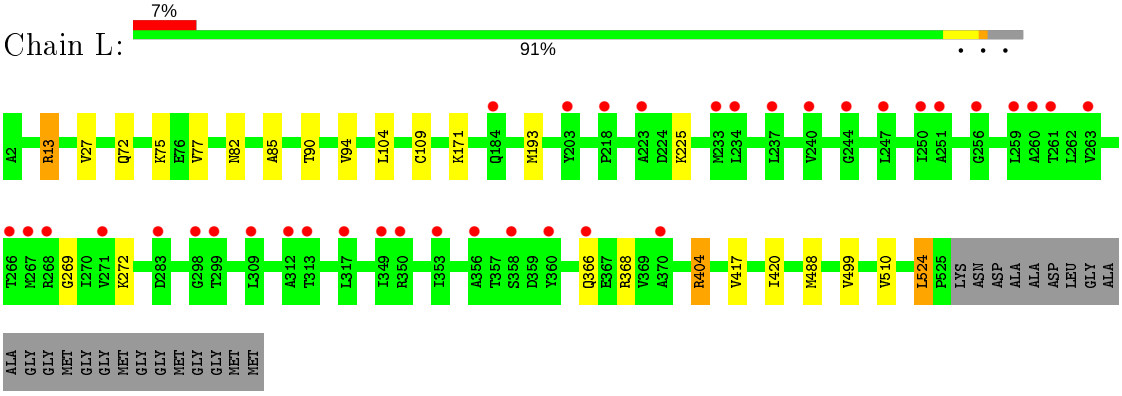
- Molecule 1: 60 kDa chaperonin

Chain K:



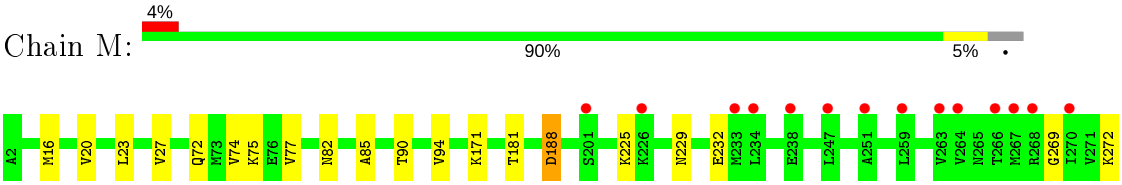
- Molecule 1: 60 kDa chaperonin

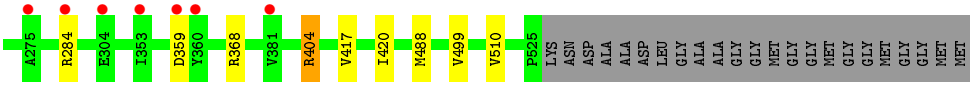
Chain L:



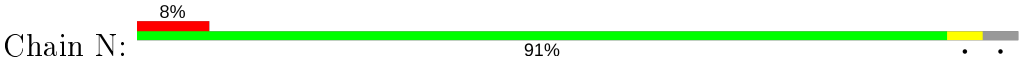
- Molecule 1: 60 kDa chaperonin

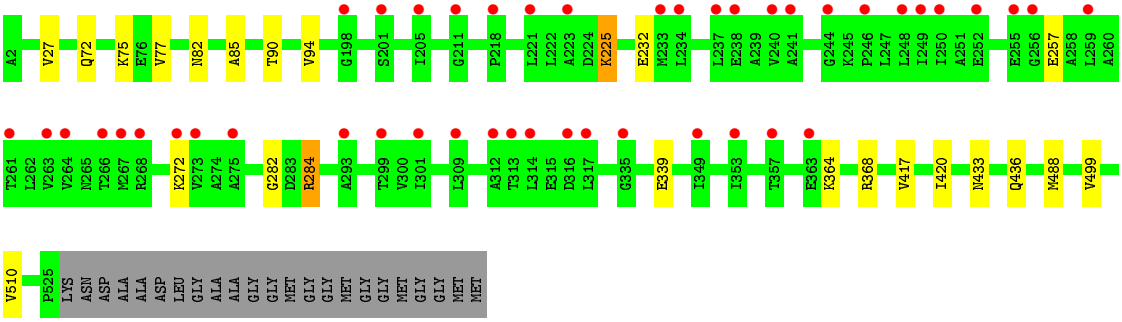
Chain M:





- Molecule 1: 60 kDa chaperonin





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	135.69Å 262.05Å 149.21Å 90.00° 100.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.19 49.35 – 3.19	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-3.19) 99.5 (49.35-3.19)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.245 , 0.252 0.240 , 0.247	Depositor DCC
R_{free} test set	8289 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	63.9	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 21.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	53984	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.27	0/3884	0.53	6/5244 (0.1%)
1	B	0.26	0/3884	0.47	1/5244 (0.0%)
1	C	0.26	0/3884	0.48	2/5244 (0.0%)
1	D	0.27	0/3884	0.47	1/5244 (0.0%)
1	E	0.26	0/3884	0.52	5/5244 (0.1%)
1	F	0.31	1/3884 (0.0%)	0.54	5/5244 (0.1%)
1	G	0.27	0/3884	0.50	4/5244 (0.1%)
1	H	0.26	0/3884	0.51	4/5244 (0.1%)
1	I	0.26	0/3884	0.46	1/5244 (0.0%)
1	J	0.27	0/3884	0.47	2/5244 (0.0%)
1	K	0.28	0/3884	0.51	4/5244 (0.1%)
1	L	0.29	0/3884	0.55	8/5244 (0.2%)
1	M	0.28	0/3884	0.51	4/5244 (0.1%)
1	N	0.33	3/3884 (0.1%)	0.86	5/5244 (0.1%)
All	All	0.28	4/54376 (0.0%)	0.54	52/73416 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	232	GLU	CD-OE2	-7.81	1.17	1.25
1	N	368	ARG	CZ-NH1	-7.81	1.22	1.33
1	N	368	ARG	CD-NE	-6.64	1.35	1.46
1	N	368	ARG	CZ-NH2	5.59	1.40	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	368	ARG	NE-CZ-NH1	-37.00	101.80	120.30
1	N	368	ARG	NE-CZ-NH2	34.39	137.50	120.30
1	E	13	ARG	NE-CZ-NH2	-12.79	113.90	120.30
1	H	13	ARG	NE-CZ-NH2	-12.69	113.95	120.30
1	L	13	ARG	NE-CZ-NH2	-12.65	113.98	120.30
1	A	13	ARG	NE-CZ-NH2	-12.55	114.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	350	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	N	284	ARG	NE-CZ-NH1	10.56	125.58	120.30
1	K	203	TYR	CB-CG-CD2	-9.34	115.40	121.00
1	K	203	TYR	CB-CG-CD1	9.08	126.45	121.00
1	C	193	MET	CG-SD-CE	-8.65	86.36	100.20
1	M	284	ARG	NE-CZ-NH2	8.24	124.42	120.30
1	M	404	ARG	CG-CD-NE	-8.13	94.73	111.80
1	N	284	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	G	284	ARG	NE-CZ-NH1	7.71	124.16	120.30
1	F	232	GLU	CG-CD-OE2	-7.59	103.11	118.30
1	A	499	VAL	CA-CB-CG2	7.45	122.08	110.90
1	F	232	GLU	CG-CD-OE1	7.01	132.32	118.30
1	E	13	ARG	NE-CZ-NH1	7.01	123.80	120.30
1	F	350	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	13	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	L	404	ARG	CG-CD-NE	-6.77	97.59	111.80
1	G	284	ARG	CD-NE-CZ	6.72	133.01	123.60
1	G	284	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	499	VAL	CB-CA-C	-6.51	99.04	111.40
1	H	13	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	L	193	MET	N-CA-CB	6.39	122.09	110.60
1	L	13	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	N	284	ARG	CD-NE-CZ	6.09	132.13	123.60
1	M	284	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	E	368	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	J	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	F	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	L	368	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	G	368	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	H	368	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	368	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	368	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	K	368	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	D	368	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	I	368	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	J	272	LYS	CB-CG-CD	5.71	126.45	111.60
1	M	368	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	L	225	LYS	CB-CA-C	-5.68	99.04	110.40
1	A	368	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	K	524	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	13	ARG	CD-NE-CZ	5.26	130.96	123.60
1	E	364	LYS	N-CA-CB	5.25	120.06	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	13	ARG	CD-NE-CZ	5.23	130.92	123.60
1	L	13	ARG	CD-NE-CZ	5.21	130.90	123.60
1	H	13	ARG	CD-NE-CZ	5.12	130.77	123.60
1	L	524	LEU	CA-CB-CG	5.07	126.96	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3975	13	0
1	B	3856	0	3975	9	0
1	C	3856	0	3975	10	0
1	D	3856	0	3975	11	0
1	E	3856	0	3975	7	0
1	F	3856	0	3975	8	0
1	G	3856	0	3975	10	0
1	H	3856	0	3975	8	0
1	I	3856	0	3975	7	1
1	J	3856	0	3975	10	0
1	K	3856	0	3975	10	0
1	L	3856	0	3975	9	0
1	M	3856	0	3975	18	1
1	N	3856	0	3975	14	0
All	All	53984	0	55650	136	1

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 1.

All (136) 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:A:229:ASN:OD1	1:G:269:GLY:O	1.83	0.95
1:L:171:LYS:O	1:L:404:ARG:NH1	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:171:LYS:O	1:M:404:ARG:NH2	2.07	0.86
1:J:225:LYS:HG2	1:J:226:LYS:N	1.92	0.85
1:M:20:VAL:HG13	1:M:74:VAL:HG21	1.67	0.74
1:A:18:ARG:HB2	1:A:18:ARG:HH11	1.53	0.74
1:E:13:ARG:NH2	1:E:518:GLU:OE2	2.21	0.73
1:A:13:ARG:NH2	1:A:518:GLU:OE2	2.21	0.72
1:M:188:ASP:OD1	1:M:188:ASP:N	2.25	0.70
1:N:284:ARG:HE	1:N:364:LYS:HB3	1.58	0.69
1:K:524:LEU:HG	1:K:525:PRO:HD2	1.81	0.62
1:J:400:LEU:O	1:J:404:ARG:HG2	2.00	0.61
1:M:269:GLY:O	1:N:257:GLU:HG3	2.00	0.60
1:L:269:GLY:O	1:M:229:ASN:OD1	2.18	0.60
1:C:85:ALA:HB1	1:C:499:VAL:HG12	1.86	0.58
1:F:85:ALA:HB1	1:F:499:VAL:HG12	1.86	0.58
1:K:85:ALA:HB1	1:K:499:VAL:HG12	1.86	0.58
1:E:85:ALA:HB1	1:E:499:VAL:HG12	1.86	0.58
1:N:85:ALA:HB1	1:N:499:VAL:HG12	1.86	0.58
1:D:85:ALA:HB1	1:D:499:VAL:HG12	1.86	0.58
1:G:85:ALA:HB1	1:G:499:VAL:HG12	1.86	0.58
1:H:85:ALA:HB1	1:H:499:VAL:HG12	1.86	0.58
1:I:85:ALA:HB1	1:I:499:VAL:HG12	1.86	0.58
1:L:85:ALA:HB1	1:L:499:VAL:HG12	1.86	0.58
1:J:85:ALA:HB1	1:J:499:VAL:HG12	1.86	0.58
1:B:85:ALA:HB1	1:B:499:VAL:HG12	1.86	0.57
1:M:85:ALA:HB1	1:M:499:VAL:HG12	1.86	0.57
1:D:453:GLN:O	1:D:457:ASN:OD1	2.25	0.54
1:J:225:LYS:NZ	1:J:232:GLU:OE1	2.40	0.54
1:N:225:LYS:NZ	1:N:232:GLU:OE1	2.41	0.53
1:D:225:LYS:NZ	1:D:232:GLU:OE1	2.41	0.53
1:N:284:ARG:CZ	1:N:364:LYS:HD2	2.39	0.52
1:E:72:GLN:OE1	1:E:75:LYS:HE2	2.10	0.52
1:I:225:LYS:NZ	1:I:232:GLU:OE1	2.39	0.52
1:I:72:GLN:OE1	1:I:75:LYS:HE2	2.10	0.52
1:A:225:LYS:NZ	1:A:232:GLU:OE1	2.41	0.52
1:F:72:GLN:OE1	1:F:75:LYS:HE2	2.10	0.52
1:G:72:GLN:OE1	1:G:75:LYS:HE2	2.10	0.52
1:H:72:GLN:OE1	1:H:75:LYS:HE2	2.10	0.52
1:C:225:LYS:NZ	1:C:232:GLU:OE1	2.41	0.51
1:M:225:LYS:NZ	1:M:232:GLU:OE1	2.39	0.51
1:J:72:GLN:OE1	1:J:75:LYS:HE2	2.10	0.51
1:N:72:GLN:OE1	1:N:75:LYS:HE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASN:ND2	1:B:436:GLN:OE1	2.44	0.51
1:L:72:GLN:OE1	1:L:75:LYS:HE2	2.10	0.51
1:M:72:GLN:OE1	1:M:75:LYS:HE2	2.10	0.51
1:F:221:LEU:HA	1:F:317:LEU:HD23	1.93	0.51
1:E:23:LEU:HD23	1:E:74:VAL:CG2	2.41	0.51
1:A:72:GLN:OE1	1:A:75:LYS:HE2	2.10	0.51
1:H:206:ASN:HD22	1:H:272:LYS:NZ	2.09	0.51
1:K:72:GLN:OE1	1:K:75:LYS:HE2	2.10	0.51
1:N:433:ASN:ND2	1:N:436:GLN:OE1	2.44	0.51
1:B:72:GLN:OE1	1:B:75:LYS:HE2	2.10	0.50
1:D:72:GLN:OE1	1:D:75:LYS:HE2	2.12	0.50
1:N:77:VAL:HG21	1:N:510:VAL:HB	1.94	0.49
1:D:77:VAL:HG21	1:D:510:VAL:HB	1.94	0.49
1:F:77:VAL:HG21	1:F:510:VAL:HB	1.94	0.49
1:L:77:VAL:HG21	1:L:510:VAL:HB	1.94	0.49
1:E:77:VAL:HG21	1:E:510:VAL:HB	1.94	0.49
1:H:77:VAL:HG21	1:H:510:VAL:HB	1.95	0.49
1:G:77:VAL:HG21	1:G:510:VAL:HB	1.95	0.49
1:K:77:VAL:HG21	1:K:510:VAL:HB	1.95	0.49
1:M:77:VAL:HG21	1:M:510:VAL:HB	1.95	0.49
1:A:77:VAL:HG21	1:A:510:VAL:HB	1.94	0.49
1:B:77:VAL:HG21	1:B:510:VAL:HB	1.94	0.49
1:C:72:GLN:OE1	1:C:75:LYS:HE2	2.12	0.49
1:C:77:VAL:HG21	1:C:510:VAL:HB	1.94	0.49
1:J:77:VAL:HG21	1:J:510:VAL:HB	1.95	0.49
1:C:72:GLN:OE1	1:C:72:GLN:HA	2.13	0.49
1:G:225:LYS:NZ	1:G:232:GLU:OE1	2.41	0.49
1:I:77:VAL:HG21	1:I:510:VAL:HB	1.95	0.49
1:M:23:LEU:HD23	1:M:74:VAL:CG2	2.41	0.49
1:D:72:GLN:OE1	1:D:72:GLN:HA	2.13	0.48
1:M:16:MET:O	1:M:20:VAL:HG23	2.14	0.48
1:C:458:CYS:O	1:D:112:ASN:ND2	2.44	0.48
1:H:13:ARG:HD2	1:H:104:LEU:HD22	1.95	0.48
1:B:225:LYS:NZ	1:B:232:GLU:OE1	2.44	0.47
1:K:225:LYS:NZ	1:K:232:GLU:OE1	2.44	0.47
1:L:13:ARG:HD2	1:L:104:LEU:HD22	1.95	0.47
1:A:87:ASP:O	1:A:499:VAL:HG13	2.16	0.45
1:M:20:VAL:CG1	1:M:74:VAL:HG11	2.47	0.45
1:F:27:VAL:HG12	1:F:90:THR:HG23	1.99	0.45
1:E:27:VAL:HG12	1:E:90:THR:HG23	1.99	0.44
1:I:27:VAL:HG12	1:I:90:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:VAL:HG12	1:J:90:THR:HG23	1.99	0.44
1:K:27:VAL:HG12	1:K:90:THR:HG23	1.99	0.44
1:G:27:VAL:HG12	1:G:90:THR:HG23	1.99	0.44
1:H:27:VAL:HG12	1:H:90:THR:HG23	1.99	0.44
1:L:27:VAL:HG12	1:L:90:THR:HG23	1.99	0.44
1:B:27:VAL:HG12	1:B:90:THR:HG23	1.99	0.44
1:A:417:VAL:HG21	1:A:488:MET:HG3	1.99	0.44
1:M:20:VAL:HG11	1:M:74:VAL:HG11	2.00	0.44
1:A:27:VAL:HG12	1:A:90:THR:HG23	1.99	0.44
1:D:417:VAL:HG21	1:D:488:MET:HG3	1.99	0.44
1:C:27:VAL:HG12	1:C:90:THR:HG23	1.99	0.43
1:M:417:VAL:HG21	1:M:488:MET:HG3	1.99	0.43
1:N:27:VAL:HG12	1:N:90:THR:HG23	1.99	0.43
1:E:417:VAL:HG21	1:E:488:MET:HG3	2.00	0.43
1:F:417:VAL:HG21	1:F:488:MET:HG3	1.99	0.43
1:I:417:VAL:HG21	1:I:488:MET:HG3	1.99	0.43
1:M:27:VAL:HG12	1:M:90:THR:HG23	1.99	0.43
1:B:417:VAL:HG21	1:B:488:MET:HG3	2.00	0.43
1:H:417:VAL:HG21	1:H:488:MET:HG3	1.99	0.43
1:L:417:VAL:HG21	1:L:488:MET:HG3	1.99	0.43
1:D:27:VAL:HG12	1:D:90:THR:HG23	1.99	0.43
1:G:417:VAL:HG21	1:G:488:MET:HG3	1.99	0.43
1:J:417:VAL:HG21	1:J:488:MET:HG3	1.99	0.43
1:K:524:LEU:CG	1:K:525:PRO:HD2	2.48	0.43
1:C:417:VAL:HG21	1:C:488:MET:HG3	1.99	0.43
1:K:417:VAL:HG21	1:K:488:MET:HG3	2.00	0.42
1:N:417:VAL:HG21	1:N:488:MET:HG3	2.00	0.42
1:M:181:THR:HA	1:N:282:GLY:CA	2.49	0.42
1:J:383:ALA:O	1:K:281:PHE:HZ	2.02	0.42
1:B:13:ARG:HD2	1:B:104:LEU:HD22	2.02	0.42
1:G:13:ARG:HD2	1:G:104:LEU:HD22	2.02	0.42
1:C:13:ARG:HD2	1:C:104:LEU:HD22	2.02	0.41
1:A:112:ASN:ND2	1:G:458:CYS:O	2.49	0.41
1:D:13:ARG:HD2	1:D:104:LEU:HD22	2.02	0.41
1:C:417:VAL:HA	1:C:420:ILE:HG22	2.03	0.41
1:D:417:VAL:HA	1:D:420:ILE:HG22	2.03	0.41
1:F:417:VAL:HA	1:F:420:ILE:HG22	2.03	0.41
1:B:417:VAL:HA	1:B:420:ILE:HG22	2.03	0.41
1:G:417:VAL:HA	1:G:420:ILE:HG22	2.03	0.41
1:J:417:VAL:HA	1:J:420:ILE:HG22	2.03	0.41
1:K:417:VAL:HA	1:K:420:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:417:VAL:HA	1:M:420:ILE:HG22	2.03	0.41
1:N:417:VAL:HA	1:N:420:ILE:HG22	2.03	0.41
1:L:417:VAL:HA	1:L:420:ILE:HG22	2.03	0.41
1:F:13:ARG:HD2	1:F:104:LEU:HD22	2.02	0.41
1:I:417:VAL:HA	1:I:420:ILE:HG22	2.03	0.41
1:M:181:THR:HA	1:N:282:GLY:HA3	2.03	0.41
1:A:18:ARG:CD	1:A:67:GLU:OE2	2.69	0.40
1:A:417:VAL:HA	1:A:420:ILE:HG22	2.03	0.40
1:A:18:ARG:HB2	1:A:18:ARG:NH1	2.26	0.40
1:H:417:VAL:HA	1:H:420:ILE:HG22	2.03	0.40
1:N:284:ARG:NE	1:N:364:LYS:HB3	2.32	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:MET:O	1:M:359:ASP:OD2[1_455]	2.09	0.11

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	B	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	C	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	D	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	E	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	F	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	G	522/547 (95%)	516 (99%)	6 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	I	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	J	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	K	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	L	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	M	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
1	N	522/547 (95%)	516 (99%)	6 (1%)	0	100	100
All	All	7308/7658 (95%)	7224 (99%)	84 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	405/415 (98%)	401 (99%)	4 (1%)	76	90
1	B	405/415 (98%)	401 (99%)	4 (1%)	76	90
1	C	405/415 (98%)	401 (99%)	4 (1%)	76	90
1	D	405/415 (98%)	400 (99%)	5 (1%)	71	88
1	E	405/415 (98%)	402 (99%)	3 (1%)	84	94
1	F	405/415 (98%)	399 (98%)	6 (2%)	65	85
1	G	405/415 (98%)	401 (99%)	4 (1%)	76	90
1	H	405/415 (98%)	403 (100%)	2 (0%)	88	95
1	I	405/415 (98%)	402 (99%)	3 (1%)	84	94
1	J	405/415 (98%)	402 (99%)	3 (1%)	84	94
1	K	405/415 (98%)	402 (99%)	3 (1%)	84	94
1	L	405/415 (98%)	399 (98%)	6 (2%)	65	85
1	M	405/415 (98%)	401 (99%)	4 (1%)	76	90
1	N	405/415 (98%)	400 (99%)	5 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5670/5810 (98%)	5614 (99%)	56 (1%)	76 90

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	94	VAL
1	A	225	LYS
1	A	272	LYS
1	B	18	ARG
1	B	82	ASN
1	B	94	VAL
1	B	272	LYS
1	C	82	ASN
1	C	94	VAL
1	C	225	LYS
1	C	272	LYS
1	D	18	ARG
1	D	82	ASN
1	D	94	VAL
1	D	225	LYS
1	D	272	LYS
1	E	82	ASN
1	E	94	VAL
1	E	272	LYS
1	F	82	ASN
1	F	94	VAL
1	F	109	CYS
1	F	225	LYS
1	F	272	LYS
1	F	343	GLN
1	G	82	ASN
1	G	94	VAL
1	G	225	LYS
1	G	272	LYS
1	H	82	ASN
1	H	94	VAL
1	I	82	ASN
1	I	94	VAL
1	I	272	LYS
1	J	82	ASN
1	J	94	VAL

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Mol	Chain	Res	Type
1	J	109	CYS
1	K	82	ASN
1	K	94	VAL
1	K	272	LYS
1	L	82	ASN
1	L	94	VAL
1	L	109	CYS
1	L	272	LYS
1	L	366	GLN
1	L	524	LEU
1	M	82	ASN
1	M	94	VAL
1	M	188	ASP
1	M	272	LYS
1	N	82	ASN
1	N	94	VAL
1	N	225	LYS
1	N	272	LYS
1	N	339	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	453	GLN
1	B	37	ASN
1	B	453	GLN
1	C	453	GLN
1	E	37	ASN
1	E	453	GLN
1	F	37	ASN
1	G	453	GLN
1	G	457	ASN
1	H	453	GLN
1	H	457	ASN
1	J	453	GLN
1	J	457	ASN
1	K	453	GLN
1	K	457	ASN
1	M	453	GLN
1	N	453	GLN

5.3.3 RNA

There are no RNA molecules 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

There are no ligands in this entry.

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	524/547 (95%)	0.16	11 (2%)	63	49	35, 67, 147, 180	0
1	B	524/547 (95%)	0.10	3 (0%)	89	83	41, 76, 141, 161	0
1	C	524/547 (95%)	-0.01	7 (1%)	77	65	36, 62, 122, 154	0
1	D	524/547 (95%)	0.19	15 (2%)	51	36	34, 71, 146, 176	0
1	E	524/547 (95%)	0.27	27 (5%)	27	15	37, 83, 158, 189	0
1	F	524/547 (95%)	0.03	9 (1%)	70	57	37, 64, 133, 176	0
1	G	524/547 (95%)	0.23	23 (4%)	34	21	39, 80, 145, 177	0
1	H	524/547 (95%)	0.00	4 (0%)	86	78	41, 77, 125, 147	0
1	I	524/547 (95%)	0.10	9 (1%)	70	57	40, 74, 134, 162	0
1	J	524/547 (95%)	0.16	13 (2%)	57	43	45, 84, 137, 158	0
1	K	524/547 (95%)	0.32	25 (4%)	30	18	45, 98, 151, 166	0
1	L	524/547 (95%)	0.35	36 (6%)	16	9	47, 89, 170, 196	0
1	M	524/547 (95%)	0.21	21 (4%)	38	25	42, 79, 160, 199	0
1	N	524/547 (95%)	0.42	45 (8%)	10	5	45, 90, 181, 215	0
All	All	7336/7658 (95%)	0.18	248 (3%)	45	29	34, 74, 149, 215	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	THR	6.6
1	N	233	MET	6.4
1	E	233	MET	6.4
1	M	268	ARG	6.1
1	N	317	LEU	6.0
1	N	263	VAL	5.8
1	N	266	THR	5.6
1	N	268	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	L	233	MET	5.0
1	K	228	SER	4.9
1	L	260	ALA	4.7
1	N	237	LEU	4.7
1	N	261	THR	4.6
1	K	44	PHE	4.6
1	F	256	GLY	4.6
1	G	268	ARG	4.5
1	L	266	THR	4.5
1	N	240	VAL	4.4
1	G	266	THR	4.4
1	G	264	VAL	4.4
1	M	238	GLU	4.4
1	D	266	THR	4.2
1	L	360	TYR	4.2
1	K	263	VAL	4.1
1	L	268	ARG	4.0
1	L	218	PRO	4.0
1	D	246	PRO	4.0
1	E	237	LEU	4.0
1	L	299	THR	4.0
1	L	358	SER	3.9
1	E	259	LEU	3.9
1	N	264	VAL	3.9
1	K	223	ALA	3.9
1	G	267	MET	3.8
1	G	256	GLY	3.8
1	E	210	THR	3.8
1	E	240	VAL	3.8
1	K	266	THR	3.8
1	J	233	MET	3.7
1	E	234	LEU	3.7
1	N	223	ALA	3.7
1	E	266	THR	3.6
1	M	264	VAL	3.6
1	L	259	LEU	3.6
1	N	301	ILE	3.6
1	L	309	LEU	3.6
1	I	271	VAL	3.6
1	D	234	LEU	3.5
1	F	266	THR	3.5
1	L	237	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	255	GLU	3.5
1	N	353	ILE	3.4
1	N	316	ASP	3.4
1	L	223	ALA	3.4
1	L	353	ILE	3.4
1	N	256	GLY	3.4
1	N	255	GLU	3.4
1	L	240	VAL	3.3
1	E	256	GLY	3.3
1	E	246	PRO	3.3
1	L	250	ILE	3.3
1	E	181	THR	3.3
1	L	313	THR	3.3
1	L	261	THR	3.3
1	M	266	THR	3.3
1	K	218	PRO	3.3
1	N	267	MET	3.3
1	D	233	MET	3.2
1	L	251	ALA	3.2
1	L	349	ILE	3.1
1	E	223	ALA	3.1
1	A	268	ARG	3.1
1	E	251	ALA	3.1
1	I	268	ARG	3.1
1	N	314	LEU	3.1
1	L	312	ALA	3.0
1	N	218	PRO	3.0
1	N	312	ALA	2.9
1	M	275	ALA	2.9
1	K	200	LEU	2.9
1	L	298	GLY	2.9
1	A	353	ILE	2.9
1	E	267	MET	2.9
1	G	263	VAL	2.9
1	G	237	LEU	2.9
1	J	360	TYR	2.9
1	F	267	MET	2.9
1	J	263	VAL	2.9
1	K	222	LEU	2.9
1	L	317	LEU	2.9
1	J	309	LEU	2.9
1	G	240	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	167	ASP	2.8
1	L	256	GLY	2.8
1	A	233	MET	2.8
1	K	259	LEU	2.8
1	M	233	MET	2.8
1	G	183	LEU	2.8
1	H	349	ILE	2.8
1	A	234	LEU	2.8
1	D	247	LEU	2.8
1	N	234	LEU	2.8
1	A	201	SER	2.8
1	B	264	VAL	2.8
1	A	261	THR	2.8
1	N	313	THR	2.8
1	L	267	MET	2.8
1	M	284	ARG	2.7
1	M	226	LYS	2.7
1	B	365	LEU	2.7
1	L	244	GLY	2.7
1	L	366	GLN	2.7
1	G	210	THR	2.7
1	K	268	ARG	2.7
1	K	256	GLY	2.7
1	F	268	ARG	2.7
1	D	268	ARG	2.7
1	M	259	LEU	2.7
1	J	349	ILE	2.7
1	D	256	GLY	2.6
1	E	257	GLU	2.6
1	D	301	ILE	2.6
1	M	234	LEU	2.6
1	D	267	MET	2.6
1	J	264	VAL	2.6
1	N	335	GLY	2.6
1	E	358	SER	2.6
1	E	357	THR	2.6
1	N	246	PRO	2.6
1	L	263	VAL	2.6
1	C	234	LEU	2.6
1	M	359	ASP	2.6
1	N	241	ALA	2.6
1	I	267	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	353	ILE	2.6
1	C	256	GLY	2.6
1	F	255	GLU	2.5
1	G	169	VAL	2.5
1	I	240	VAL	2.5
1	I	264	VAL	2.5
1	N	238	GLU	2.5
1	J	271	VAL	2.5
1	K	264	VAL	2.5
1	N	211	GLY	2.5
1	N	221	LEU	2.5
1	N	309	LEU	2.5
1	M	251	ALA	2.5
1	N	349	ILE	2.5
1	A	260	ALA	2.5
1	L	356	ALA	2.5
1	F	233	MET	2.5
1	E	260	ALA	2.5
1	N	249	ILE	2.5
1	G	319	GLN	2.4
1	C	264	VAL	2.4
1	M	304	GLU	2.4
1	K	275	ALA	2.4
1	K	353	ILE	2.4
1	N	201	SER	2.4
1	J	366	GLN	2.4
1	G	246	PRO	2.4
1	M	267	MET	2.4
1	H	353	ILE	2.4
1	N	198	GLY	2.3
1	N	273	VAL	2.3
1	G	366	GLN	2.3
1	K	212	ALA	2.3
1	N	293	ALA	2.3
1	G	261	THR	2.3
1	K	260	ALA	2.3
1	I	246	PRO	2.3
1	L	370	ALA	2.3
1	K	300	VAL	2.3
1	J	268	ARG	2.3
1	K	233	MET	2.3
1	E	247	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	264	VAL	2.3
1	G	301	ILE	2.3
1	G	218	PRO	2.3
1	E	333	ILE	2.3
1	J	223	ALA	2.3
1	N	252	GLU	2.3
1	K	267	MET	2.3
1	N	244	GLY	2.2
1	L	247	LEU	2.2
1	M	247	LEU	2.2
1	L	271	VAL	2.2
1	F	234	LEU	2.2
1	J	237	LEU	2.2
1	L	234	LEU	2.2
1	M	270	ILE	2.2
1	D	223	ALA	2.2
1	N	275	ALA	2.2
1	M	263	VAL	2.2
1	K	363	GLU	2.2
1	B	234	LEU	2.2
1	N	259	LEU	2.2
1	M	381	VAL	2.2
1	N	248	LEU	2.2
1	G	241	ALA	2.2
1	H	371	LYS	2.2
1	A	222	LEU	2.2
1	K	317	LEU	2.2
1	D	254	VAL	2.2
1	K	273	VAL	2.2
1	N	250	ILE	2.2
1	J	221	LEU	2.2
1	L	184	GLN	2.2
1	N	357	THR	2.1
1	J	44	PHE	2.1
1	E	366	GLN	2.1
1	C	260	ALA	2.1
1	N	205	ILE	2.1
1	A	360	TYR	2.1
1	E	218	PRO	2.1
1	D	274	ALA	2.1
1	A	265	ASN	2.1
1	M	201	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	257	GLU	2.1
1	F	274	ALA	2.1
1	M	360	TYR	2.1
1	C	255	GLU	2.1
1	E	201	SER	2.1
1	D	264	VAL	2.1
1	N	272	LYS	2.1
1	C	261	THR	2.1
1	N	363	GLU	2.1
1	K	271	VAL	2.1
1	L	203	TYR	2.1
1	L	350	ARG	2.1
1	G	275	ALA	2.0
1	N	299	THR	2.0
1	K	309	LEU	2.0
1	I	272	LYS	2.0
1	H	271	VAL	2.0
1	E	261	THR	2.0
1	C	267	MET	2.0
1	E	255	GLU	2.0
1	G	361	ASP	2.0
1	G	213	VAL	2.0
1	E	264	VAL	2.0
1	L	283	ASP	2.0
1	E	279	PRO	2.0
1	G	233	MET	2.0
1	I	183	LEU	2.0
1	D	259	LEU	2.0
1	E	376	VAL	2.0
1	G	271	VAL	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.