



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2022 – 08:10 PM JST

PDB ID : 7V9R
Title : Crystal Structure of the heptameric EcHsp60
Authors : Lai, M.C.; Lin, S.M.
Deposited on : 2021-08-26
Resolution : 3.50 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>.

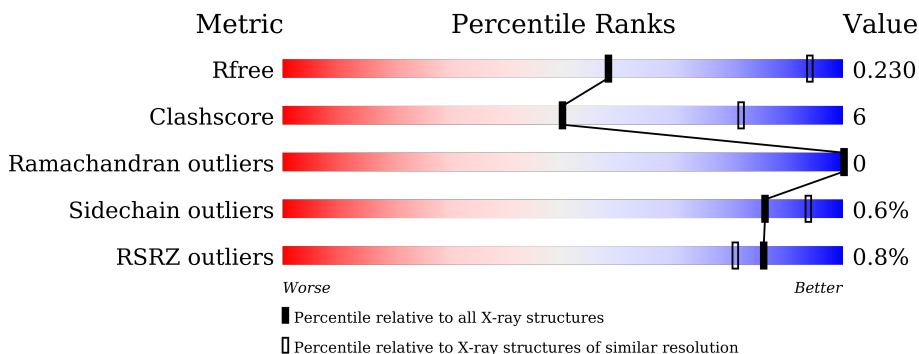
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
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)	:	2.30

i

X-RAY DIFFRACTION

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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	573	<div><div></div><div></div><div></div></div> 78%13%9%
1	B	573	<div><div></div><div></div><div></div></div> 75%16%9%
1	C	573	<div><div></div><div></div><div></div></div> 79%11%10%
1	D	573	<div><div></div><div></div><div></div></div> 76%14%10%
1	E	573	<div><div></div><div></div><div></div></div> 76%15%10%
1	F	573	<div><div></div><div></div><div></div></div> 79%12%9%

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Mol	Chain	Length	Quality of chain
1	G	573	<div><div>%</div><div><div></div></div><div>78%13%8%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26003 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	521	Total	C	N	O	S	0	0	0
			3766	2353	651	749	13			
1	B	520	Total	C	N	O	S	0	0	0
			3778	2364	655	746	13			
1	C	516	Total	C	N	O	S	0	0	0
			3676	2302	635	727	12			
1	D	514	Total	C	N	O	S	0	0	0
			3630	2280	625	712	13			
1	E	517	Total	C	N	O	S	0	0	0
			3705	2318	641	733	13			
1	F	522	Total	C	N	O	S	0	0	0
			3697	2314	638	732	13			
1	G	525	Total	C	N	O	S	0	0	0
			3751	2347	645	746	13			

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	VAL	MET	engineered mutation	UNP A0A097BVP4
A	553	ASP	-	expression tag	UNP A0A097BVP4
A	554	ILE	-	expression tag	UNP A0A097BVP4
A	555	HIS	-	expression tag	UNP A0A097BVP4
A	556	MET	-	expression tag	UNP A0A097BVP4
A	557	PHE	-	expression tag	UNP A0A097BVP4
A	558	ARG	-	expression tag	UNP A0A097BVP4
A	559	LEU	-	expression tag	UNP A0A097BVP4
A	560	PRO	-	expression tag	UNP A0A097BVP4
A	561	THR	-	expression tag	UNP A0A097BVP4
A	562	GLY	-	expression tag	UNP A0A097BVP4
A	563	MET	-	expression tag	UNP A0A097BVP4
A	564	GLY	-	expression tag	UNP A0A097BVP4
A	565	PHE	-	expression tag	UNP A0A097BVP4
A	566	LEU	-	expression tag	UNP A0A097BVP4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	567	GLU	-	expression tag	UNP A0A097BVP4
A	568	HIS	-	expression tag	UNP A0A097BVP4
A	569	HIS	-	expression tag	UNP A0A097BVP4
A	570	HIS	-	expression tag	UNP A0A097BVP4
A	571	HIS	-	expression tag	UNP A0A097BVP4
A	572	HIS	-	expression tag	UNP A0A097BVP4
A	573	HIS	-	expression tag	UNP A0A097BVP4
B	330	VAL	MET	engineered mutation	UNP A0A097BVP4
B	553	ASP	-	expression tag	UNP A0A097BVP4
B	554	ILE	-	expression tag	UNP A0A097BVP4
B	555	HIS	-	expression tag	UNP A0A097BVP4
B	556	MET	-	expression tag	UNP A0A097BVP4
B	557	PHE	-	expression tag	UNP A0A097BVP4
B	558	ARG	-	expression tag	UNP A0A097BVP4
B	559	LEU	-	expression tag	UNP A0A097BVP4
B	560	PRO	-	expression tag	UNP A0A097BVP4
B	561	THR	-	expression tag	UNP A0A097BVP4
B	562	GLY	-	expression tag	UNP A0A097BVP4
B	563	MET	-	expression tag	UNP A0A097BVP4
B	564	GLY	-	expression tag	UNP A0A097BVP4
B	565	PHE	-	expression tag	UNP A0A097BVP4
B	566	LEU	-	expression tag	UNP A0A097BVP4
B	567	GLU	-	expression tag	UNP A0A097BVP4
B	568	HIS	-	expression tag	UNP A0A097BVP4
B	569	HIS	-	expression tag	UNP A0A097BVP4
B	570	HIS	-	expression tag	UNP A0A097BVP4
B	571	HIS	-	expression tag	UNP A0A097BVP4
B	572	HIS	-	expression tag	UNP A0A097BVP4
B	573	HIS	-	expression tag	UNP A0A097BVP4
C	330	VAL	MET	engineered mutation	UNP A0A097BVP4
C	553	ASP	-	expression tag	UNP A0A097BVP4
C	554	ILE	-	expression tag	UNP A0A097BVP4
C	555	HIS	-	expression tag	UNP A0A097BVP4
C	556	MET	-	expression tag	UNP A0A097BVP4
C	557	PHE	-	expression tag	UNP A0A097BVP4
C	558	ARG	-	expression tag	UNP A0A097BVP4
C	559	LEU	-	expression tag	UNP A0A097BVP4
C	560	PRO	-	expression tag	UNP A0A097BVP4
C	561	THR	-	expression tag	UNP A0A097BVP4
C	562	GLY	-	expression tag	UNP A0A097BVP4
C	563	MET	-	expression tag	UNP A0A097BVP4
C	564	GLY	-	expression tag	UNP A0A097BVP4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	565	PHE	-	expression tag	UNP A0A097BVP4
C	566	LEU	-	expression tag	UNP A0A097BVP4
C	567	GLU	-	expression tag	UNP A0A097BVP4
C	568	HIS	-	expression tag	UNP A0A097BVP4
C	569	HIS	-	expression tag	UNP A0A097BVP4
C	570	HIS	-	expression tag	UNP A0A097BVP4
C	571	HIS	-	expression tag	UNP A0A097BVP4
C	572	HIS	-	expression tag	UNP A0A097BVP4
C	573	HIS	-	expression tag	UNP A0A097BVP4
D	330	VAL	MET	engineered mutation	UNP A0A097BVP4
D	553	ASP	-	expression tag	UNP A0A097BVP4
D	554	ILE	-	expression tag	UNP A0A097BVP4
D	555	HIS	-	expression tag	UNP A0A097BVP4
D	556	MET	-	expression tag	UNP A0A097BVP4
D	557	PHE	-	expression tag	UNP A0A097BVP4
D	558	ARG	-	expression tag	UNP A0A097BVP4
D	559	LEU	-	expression tag	UNP A0A097BVP4
D	560	PRO	-	expression tag	UNP A0A097BVP4
D	561	THR	-	expression tag	UNP A0A097BVP4
D	562	GLY	-	expression tag	UNP A0A097BVP4
D	563	MET	-	expression tag	UNP A0A097BVP4
D	564	GLY	-	expression tag	UNP A0A097BVP4
D	565	PHE	-	expression tag	UNP A0A097BVP4
D	566	LEU	-	expression tag	UNP A0A097BVP4
D	567	GLU	-	expression tag	UNP A0A097BVP4
D	568	HIS	-	expression tag	UNP A0A097BVP4
D	569	HIS	-	expression tag	UNP A0A097BVP4
D	570	HIS	-	expression tag	UNP A0A097BVP4
D	571	HIS	-	expression tag	UNP A0A097BVP4
D	572	HIS	-	expression tag	UNP A0A097BVP4
D	573	HIS	-	expression tag	UNP A0A097BVP4
E	330	VAL	MET	engineered mutation	UNP A0A097BVP4
E	553	ASP	-	expression tag	UNP A0A097BVP4
E	554	ILE	-	expression tag	UNP A0A097BVP4
E	555	HIS	-	expression tag	UNP A0A097BVP4
E	556	MET	-	expression tag	UNP A0A097BVP4
E	557	PHE	-	expression tag	UNP A0A097BVP4
E	558	ARG	-	expression tag	UNP A0A097BVP4
E	559	LEU	-	expression tag	UNP A0A097BVP4
E	560	PRO	-	expression tag	UNP A0A097BVP4
E	561	THR	-	expression tag	UNP A0A097BVP4
E	562	GLY	-	expression tag	UNP A0A097BVP4

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Chain	Residue	Modelled	Actual	Comment	Reference
E	563	MET	-	expression tag	UNP A0A097BVP4
E	564	GLY	-	expression tag	UNP A0A097BVP4
E	565	PHE	-	expression tag	UNP A0A097BVP4
E	566	LEU	-	expression tag	UNP A0A097BVP4
E	567	GLU	-	expression tag	UNP A0A097BVP4
E	568	HIS	-	expression tag	UNP A0A097BVP4
E	569	HIS	-	expression tag	UNP A0A097BVP4
E	570	HIS	-	expression tag	UNP A0A097BVP4
E	571	HIS	-	expression tag	UNP A0A097BVP4
E	572	HIS	-	expression tag	UNP A0A097BVP4
E	573	HIS	-	expression tag	UNP A0A097BVP4
F	330	VAL	MET	engineered mutation	UNP A0A097BVP4
F	553	ASP	-	expression tag	UNP A0A097BVP4
F	554	ILE	-	expression tag	UNP A0A097BVP4
F	555	HIS	-	expression tag	UNP A0A097BVP4
F	556	MET	-	expression tag	UNP A0A097BVP4
F	557	PHE	-	expression tag	UNP A0A097BVP4
F	558	ARG	-	expression tag	UNP A0A097BVP4
F	559	LEU	-	expression tag	UNP A0A097BVP4
F	560	PRO	-	expression tag	UNP A0A097BVP4
F	561	THR	-	expression tag	UNP A0A097BVP4
F	562	GLY	-	expression tag	UNP A0A097BVP4
F	563	MET	-	expression tag	UNP A0A097BVP4
F	564	GLY	-	expression tag	UNP A0A097BVP4
F	565	PHE	-	expression tag	UNP A0A097BVP4
F	566	LEU	-	expression tag	UNP A0A097BVP4
F	567	GLU	-	expression tag	UNP A0A097BVP4
F	568	HIS	-	expression tag	UNP A0A097BVP4
F	569	HIS	-	expression tag	UNP A0A097BVP4
F	570	HIS	-	expression tag	UNP A0A097BVP4
F	571	HIS	-	expression tag	UNP A0A097BVP4
F	572	HIS	-	expression tag	UNP A0A097BVP4
F	573	HIS	-	expression tag	UNP A0A097BVP4
G	330	VAL	MET	engineered mutation	UNP A0A097BVP4
G	553	ASP	-	expression tag	UNP A0A097BVP4
G	554	ILE	-	expression tag	UNP A0A097BVP4
G	555	HIS	-	expression tag	UNP A0A097BVP4
G	556	MET	-	expression tag	UNP A0A097BVP4
G	557	PHE	-	expression tag	UNP A0A097BVP4
G	558	ARG	-	expression tag	UNP A0A097BVP4
G	559	LEU	-	expression tag	UNP A0A097BVP4
G	560	PRO	-	expression tag	UNP A0A097BVP4

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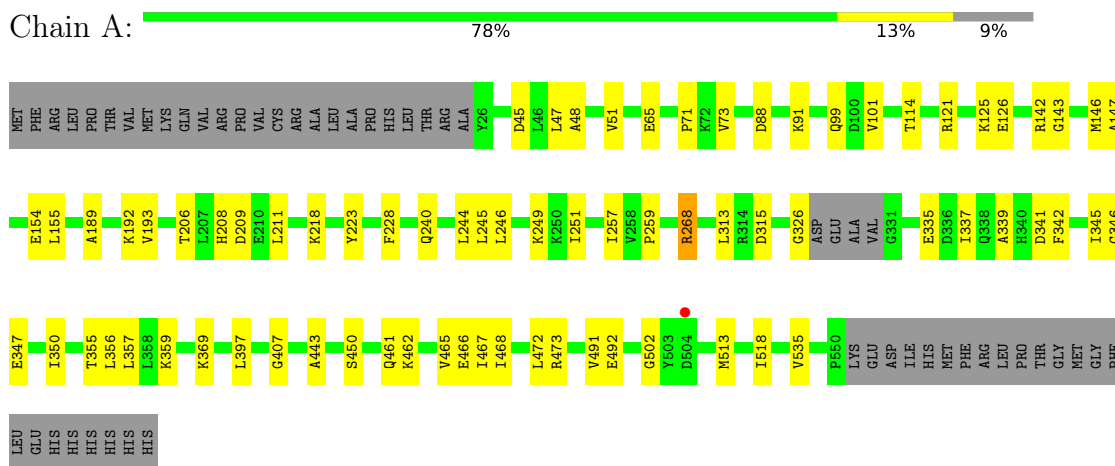
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Chain	Residue	Modelled	Actual	Comment	Reference
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G	562	GLY	-	expression tag	UNP A0A097BVP4
G	563	MET	-	expression tag	UNP A0A097BVP4
G	564	GLY	-	expression tag	UNP A0A097BVP4
G	565	PHE	-	expression tag	UNP A0A097BVP4
G	566	LEU	-	expression tag	UNP A0A097BVP4
G	567	GLU	-	expression tag	UNP A0A097BVP4
G	568	HIS	-	expression tag	UNP A0A097BVP4
G	569	HIS	-	expression tag	UNP A0A097BVP4
G	570	HIS	-	expression tag	UNP A0A097BVP4
G	571	HIS	-	expression tag	UNP A0A097BVP4
G	572	HIS	-	expression tag	UNP A0A097BVP4
G	573	HIS	-	expression tag	UNP A0A097BVP4

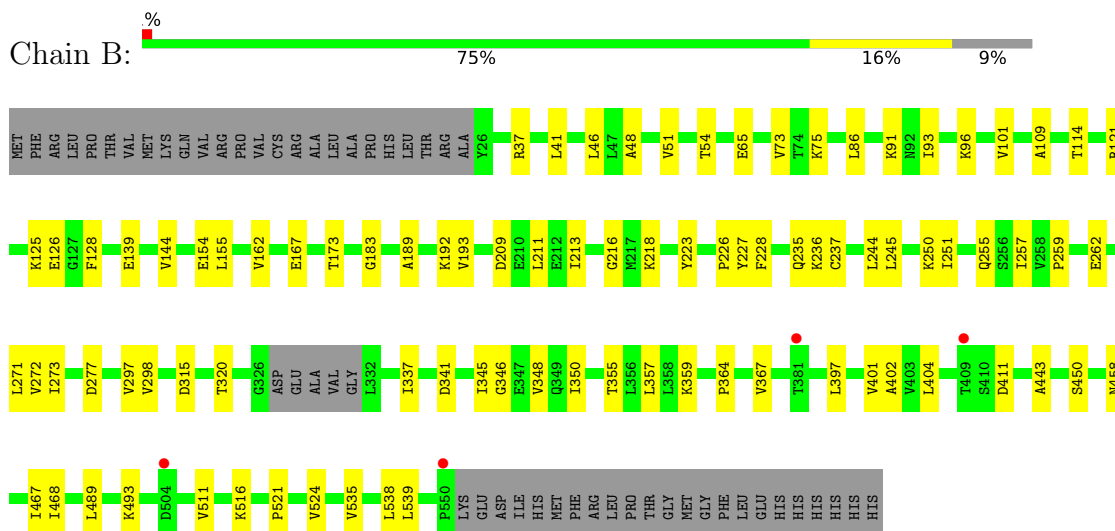
3 Residue-property plots [i](#)

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.

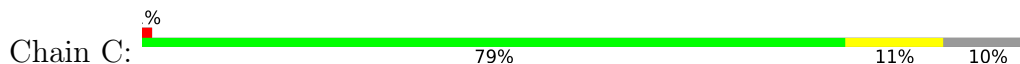
- Molecule 1: 60 kDa chaperonin

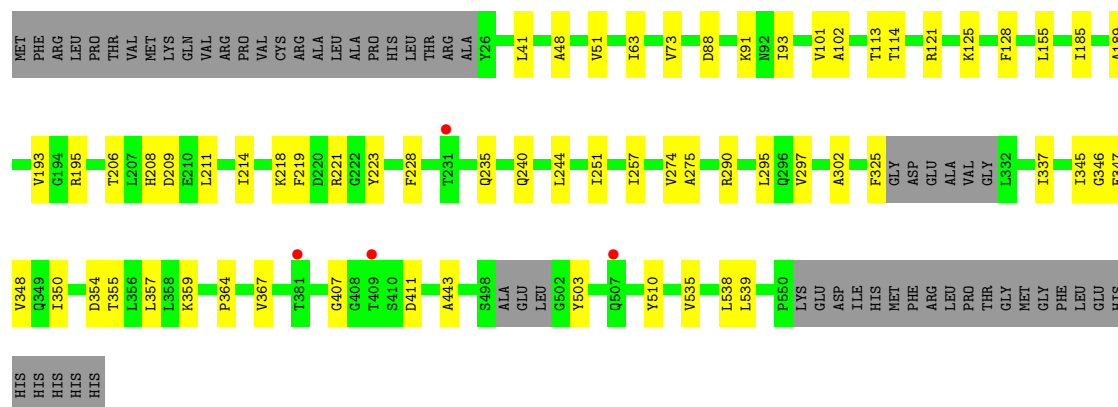


- Molecule 1: 60 kDa chaperonin

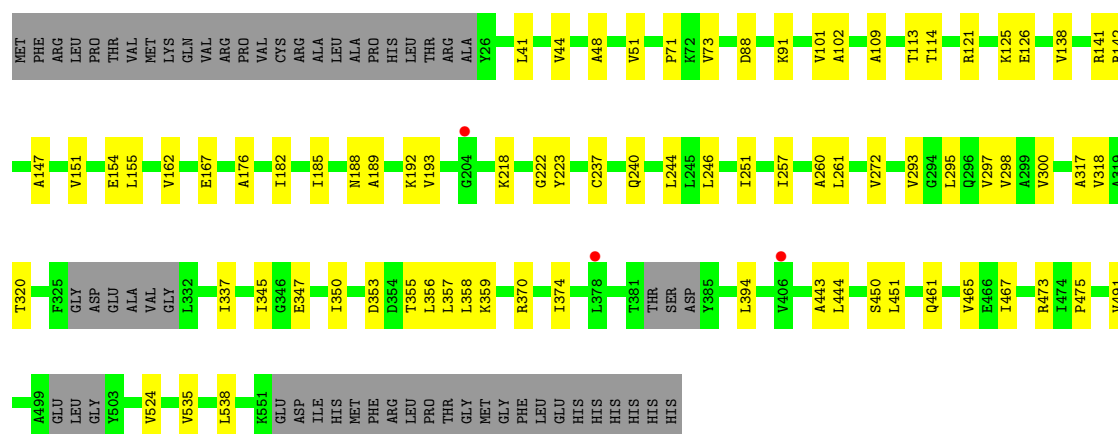
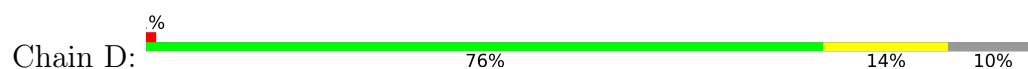


- Molecule 1: 60 kDa chaperonin

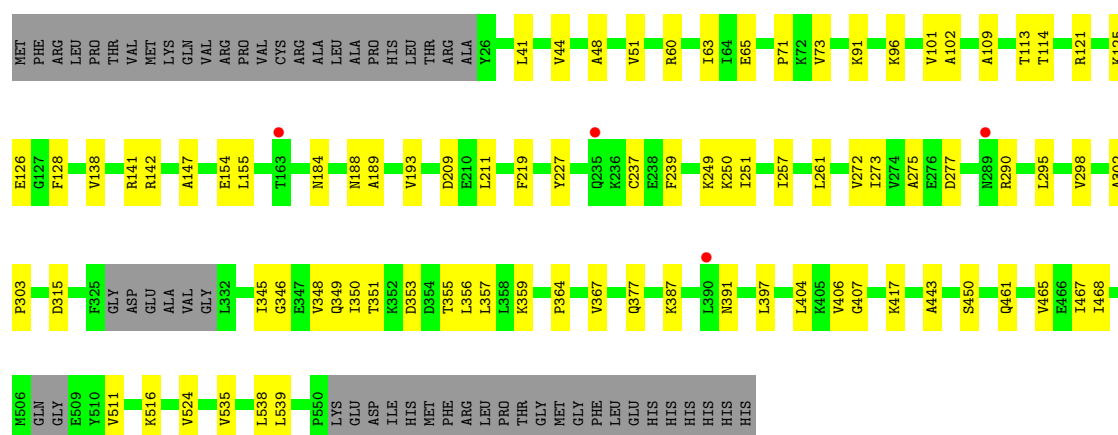
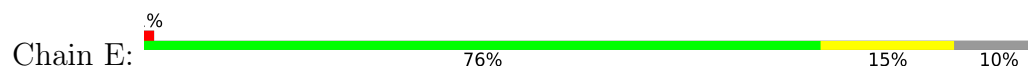




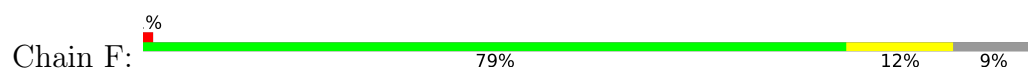
• Molecule 1: 60 kDa chaperonin

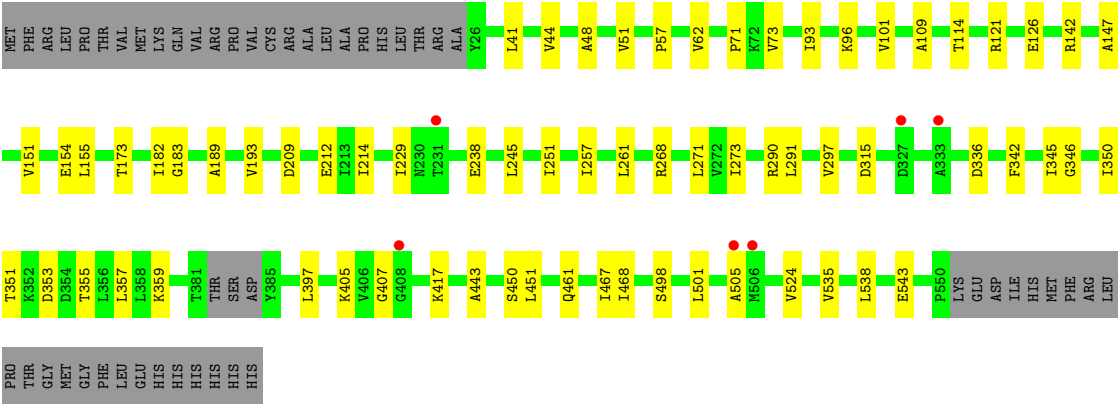


• Molecule 1: 60 kDa chaperonin

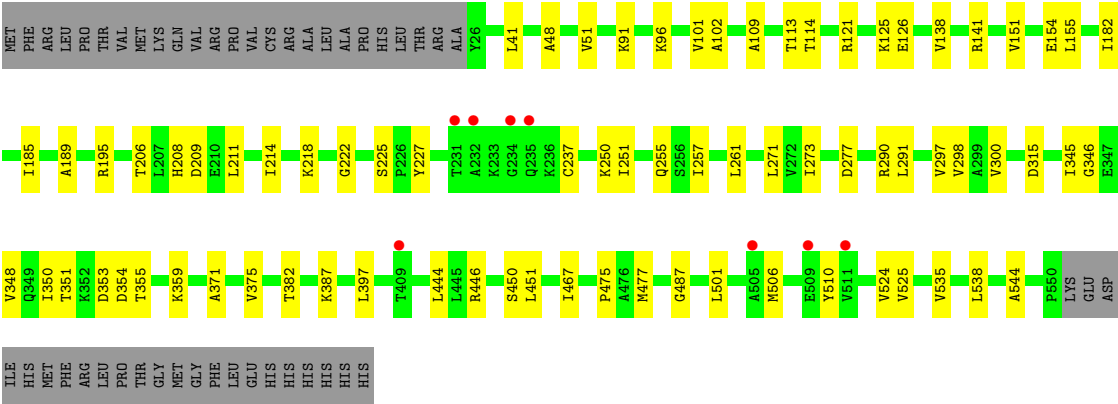
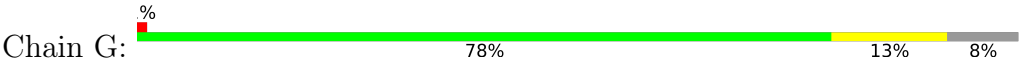


• Molecule 1: 60 kDa chaperonin





• Molecule 1: 60 kDa chaperonin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.06Å 140.97Å 240.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 3.50 29.79 – 3.48	Depositor EDS
% Data completeness (in resolution range)	85.7 (29.79-3.50) 81.9 (29.79-3.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.184 , 0.230 0.184 , 0.230	Depositor DCC
R_{free} test set	2002 reflections (3.81%)	wwPDB-VP
Wilson B-factor (Å ²)	111.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26003	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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](#)

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	0.25	0/3797	0.47	0/5147
1	B	0.25	0/3810	0.46	0/5162
1	C	0.24	0/3706	0.46	0/5032
1	D	0.24	0/3660	0.45	0/4976
1	E	0.25	0/3736	0.46	0/5074
1	F	0.24	0/3727	0.45	0/5067
1	G	0.24	0/3783	0.45	0/5139
All	All	0.25	0/26219	0.46	0/35597

There are no bond length outliers.

There are no bond angle outliers.

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	3766	0	3816	46	0
1	B	3778	0	3856	53	0
1	C	3676	0	3683	37	0
1	D	3630	0	3625	45	0
1	E	3705	0	3718	51	0
1	F	3697	0	3698	43	0
1	G	3751	0	3767	45	0
All	All	26003	0	26163	300	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 6.

All (300) 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:F:229:ILE:HG22	1:F:290:ARG:HH21	1.50	0.76
1:B:315:ASP:HB3	1:B:397:LEU:HD21	1.71	0.72
1:F:48:ALA:HB3	1:F:121:ARG:HD3	1.73	0.71
1:E:315:ASP:HB3	1:E:397:LEU:HD11	1.73	0.69
1:E:48:ALA:HB3	1:E:121:ARG:HD3	1.76	0.68
1:E:41:LEU:HD21	1:E:125:LYS:HD2	1.74	0.68
1:G:257:ILE:HD11	1:G:273:ILE:HD13	1.76	0.68
1:B:271:LEU:HB3	1:B:297:VAL:HG12	1.76	0.67
1:A:350:ILE:HG12	1:A:355:THR:HG23	1.77	0.67
1:D:48:ALA:HB3	1:D:121:ARG:HD3	1.78	0.66
1:A:71:PRO:HD3	1:B:96:LYS:HD2	1.78	0.65
1:B:245:LEU:HD23	1:B:273:ILE:HG12	1.79	0.65
1:D:318:VAL:HG21	1:D:370:ARG:HG3	1.79	0.65
1:A:268:ARG:NH1	1:B:255:GLN:OE1	2.28	0.64
1:C:290:ARG:HA	1:C:295:LEU:H	1.61	0.64
1:D:41:LEU:HD21	1:D:125:LYS:HD2	1.80	0.64
1:D:260:ALA:HB2	1:D:337:ILE:HD12	1.80	0.64
1:B:46:LEU:HD22	1:B:86:LEU:HD21	1.81	0.63
1:A:48:ALA:HB3	1:A:121:ARG:HD3	1.81	0.63
1:A:154:GLU:HG3	1:A:450:SER:HB2	1.82	0.62
1:G:237:CYS:SG	1:G:298:VAL:HG21	2.40	0.62
1:F:71:PRO:HD3	1:G:96:LYS:HD2	1.79	0.62
1:B:48:ALA:HB3	1:B:121:ARG:HD3	1.81	0.61
1:A:345:ILE:HD13	1:A:357:LEU:HD22	1.83	0.61
1:B:251:ILE:HG21	1:B:257:ILE:HD12	1.82	0.61
1:E:350:ILE:HG12	1:E:355:THR:HG23	1.82	0.61
1:C:325:PHE:HE2	1:C:337:ILE:HG23	1.65	0.61
1:A:51:VAL:HG12	1:A:114:THR:HG23	1.83	0.61
1:F:51:VAL:HG12	1:F:114:THR:HG23	1.82	0.60
1:G:315:ASP:HB3	1:G:397:LEU:HD11	1.84	0.60
1:E:511:VAL:HG21	1:E:516:LYS:HD2	1.83	0.60
1:A:346:GLY:HA3	1:A:359:LYS:HB2	1.83	0.59
1:A:143:GLY:HA2	1:A:146:MET:HE2	1.85	0.58
1:F:271:LEU:HB3	1:F:297:VAL:HG12	1.84	0.58
1:B:350:ILE:HG12	1:B:355:THR:HG23	1.86	0.58
1:D:162:VAL:HG13	1:D:167:GLU:HB3	1.85	0.58
1:B:346:GLY:HA3	1:B:359:LYS:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:ASP:HB3	1:F:397:LEU:HD21	1.87	0.57
1:F:498:SER:HB3	1:F:501:LEU:HB2	1.86	0.57
1:A:73:VAL:HG11	1:B:538:LEU:HD11	1.87	0.57
1:F:346:GLY:HA3	1:F:359:LYS:HB2	1.87	0.57
1:D:102:ALA:HB1	1:D:113:THR:HG23	1.85	0.57
1:D:51:VAL:HG12	1:D:114:THR:HG23	1.86	0.57
1:D:73:VAL:HG11	1:E:538:LEU:HD11	1.87	0.57
1:B:227:TYR:HB2	1:B:298:VAL:HG22	1.87	0.56
1:E:51:VAL:HG12	1:E:114:THR:HG23	1.86	0.56
1:E:126:GLU:HB3	1:E:467:ILE:HG12	1.87	0.56
1:E:138:VAL:HG12	1:E:141:ARG:HH22	1.69	0.56
1:A:473:ARG:NH1	1:A:492:GLU:OE2	2.38	0.56
1:D:350:ILE:HG12	1:D:355:THR:HG23	1.88	0.56
1:A:147:ALA:HB2	1:A:465:VAL:HG22	1.86	0.56
1:B:41:LEU:HD21	1:B:125:LYS:HD2	1.86	0.56
1:D:237:CYS:SG	1:D:298:VAL:HG21	2.45	0.56
1:B:73:VAL:HG11	1:C:538:LEU:HD11	1.87	0.56
1:E:227:TYR:HB3	1:E:298:VAL:HG22	1.88	0.56
1:F:101:VAL:HG21	1:F:535:VAL:HB	1.87	0.55
1:F:214:ILE:HD12	1:F:359:LYS:HE3	1.88	0.55
1:G:41:LEU:HD21	1:G:125:LYS:HD2	1.88	0.55
1:C:350:ILE:HG12	1:C:355:THR:HG23	1.89	0.55
1:E:261:LEU:HD12	1:E:295:LEU:HD21	1.89	0.55
1:C:63:ILE:HG12	1:C:73:VAL:HG22	1.89	0.54
1:E:71:PRO:HD3	1:F:96:LYS:HD2	1.87	0.54
1:B:250:LYS:HE3	1:B:277:ASP:HB3	1.89	0.54
1:C:346:GLY:HA3	1:C:359:LYS:HB2	1.89	0.54
1:B:257:ILE:HD11	1:B:273:ILE:HD13	1.89	0.54
1:C:48:ALA:HB3	1:C:121:ARG:HD3	1.90	0.54
1:A:240:GLN:HG2	1:A:347:GLU:HG2	1.89	0.54
1:C:51:VAL:HG12	1:C:114:THR:HG23	1.89	0.54
1:F:209:ASP:N	1:F:209:ASP:OD1	2.41	0.54
1:E:184:ASN:O	1:E:188:ASN:ND2	2.34	0.54
1:G:227:TYR:HB3	1:G:298:VAL:HG22	1.89	0.54
1:F:155:LEU:HD11	1:F:443:ALA:HB1	1.90	0.54
1:B:126:GLU:HB3	1:B:467:ILE:HG12	1.89	0.54
1:F:182:ILE:HD11	1:F:417:LYS:HE3	1.90	0.53
1:A:315:ASP:HB3	1:A:397:LEU:HD11	1.91	0.53
1:C:209:ASP:HB3	1:C:407:GLY:H	1.73	0.53
1:E:237:CYS:SG	1:E:298:VAL:HG21	2.48	0.53
1:G:251:ILE:HG21	1:G:257:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:LEU:HD23	1:D:246:LEU:HD11	1.90	0.53
1:C:240:GLN:HG2	1:C:347:GLU:HG2	1.91	0.53
1:B:173:THR:HG23	1:B:183:GLY:HA3	1.91	0.52
1:F:350:ILE:HG12	1:F:355:THR:HG23	1.91	0.52
1:G:501:LEU:HD21	1:G:510:TYR:HB3	1.91	0.52
1:E:250:LYS:HD2	1:E:277:ASP:HB3	1.91	0.52
1:C:218:LYS:HE2	1:C:354:ASP:HB2	1.92	0.52
1:F:345:ILE:HD12	1:F:357:LEU:HB3	1.92	0.52
1:D:293:VAL:HG23	1:D:295:LEU:HD23	1.91	0.52
1:E:351:THR:HG23	1:E:353:ASP:H	1.74	0.52
1:G:138:VAL:HG12	1:G:141:ARG:HH22	1.74	0.52
1:B:101:VAL:HG21	1:B:535:VAL:HB	1.91	0.51
1:F:73:VAL:HG11	1:G:538:LEU:HD11	1.91	0.51
1:D:374:ILE:HB	1:D:394:LEU:HD12	1.92	0.51
1:G:346:GLY:HA3	1:G:359:LYS:HB2	1.92	0.51
1:C:275:ALA:O	1:C:302:ALA:N	2.40	0.51
1:D:151:VAL:HG23	1:D:451:LEU:HD21	1.91	0.51
1:D:244:LEU:HD12	1:D:272:VAL:HB	1.92	0.51
1:G:51:VAL:HG12	1:G:114:THR:HG23	1.93	0.51
1:D:101:VAL:HG21	1:D:535:VAL:HB	1.92	0.51
1:E:65:GLU:HB2	1:F:93:ILE:HD11	1.93	0.51
1:E:209:ASP:OD1	1:E:209:ASP:N	2.42	0.51
1:C:503:TYR:H	1:C:510:TYR:HA	1.76	0.51
1:E:257:ILE:HD11	1:E:273:ILE:HD13	1.92	0.51
1:G:271:LEU:HB3	1:G:297:VAL:HG12	1.93	0.51
1:B:209:ASP:OD1	1:B:209:ASP:N	2.43	0.50
1:C:88:ASP:HB3	1:C:91:LYS:HD2	1.93	0.50
1:E:387:LYS:O	1:E:391:ASN:ND2	2.44	0.50
1:F:268:ARG:NH1	1:G:255:GLN:OE1	2.44	0.50
1:G:48:ALA:HB3	1:G:121:ARG:HD3	1.92	0.50
1:B:193:VAL:HG11	1:B:402:ALA:HB2	1.94	0.50
1:E:349:GLN:HB2	1:E:356:LEU:HB3	1.93	0.50
1:E:406:VAL:HB	1:E:417:LYS:HD2	1.93	0.50
1:B:244:LEU:HD12	1:B:272:VAL:HB	1.92	0.50
1:E:128:PHE:HZ	1:E:539:LEU:HB3	1.76	0.50
1:F:251:ILE:HG21	1:F:257:ILE:HD12	1.93	0.49
1:B:51:VAL:HG12	1:B:114:THR:HG23	1.93	0.49
1:C:209:ASP:OD1	1:C:209:ASP:N	2.44	0.49
1:F:126:GLU:HB3	1:F:467:ILE:HG12	1.95	0.49
1:G:250:LYS:HE3	1:G:277:ASP:HB3	1.94	0.49
1:D:251:ILE:HG21	1:D:257:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:473:ARG:HD2	1:D:491:VAL:HG11	1.94	0.49
1:A:462:LYS:O	1:A:466:GLU:HG2	2.13	0.49
1:B:345:ILE:HG21	1:B:348:VAL:HB	1.93	0.49
1:A:101:VAL:HG21	1:A:535:VAL:HB	1.95	0.49
1:A:209:ASP:HB3	1:A:407:GLY:H	1.77	0.49
1:F:189:ALA:O	1:F:193:VAL:HG22	2.13	0.48
1:B:192:LYS:HD3	1:B:213:ILE:HD11	1.95	0.48
1:D:347:GLU:HB2	1:D:358:LEU:HB2	1.95	0.48
1:F:245:LEU:HB2	1:F:342:PHE:HE1	1.78	0.48
1:A:473:ARG:HD3	1:A:491:VAL:HG11	1.96	0.48
1:A:246:LEU:HB3	1:A:313:LEU:HD22	1.96	0.48
1:C:128:PHE:HZ	1:C:539:LEU:HB3	1.79	0.48
1:G:189:ALA:HB2	1:G:211:LEU:HD22	1.94	0.48
1:C:223:TYR:CZ	1:C:228:PHE:HE1	2.32	0.48
1:F:351:THR:HG23	1:F:353:ASP:H	1.78	0.48
1:D:176:ALA:HB1	1:D:182:ILE:HD11	1.95	0.48
1:A:189:ALA:O	1:A:193:VAL:HG22	2.14	0.48
1:C:189:ALA:O	1:C:193:VAL:HG22	2.14	0.48
1:C:295:LEU:HB3	1:C:297:VAL:HG22	1.95	0.48
1:A:155:LEU:HD11	1:A:443:ALA:HB1	1.95	0.47
1:E:345:ILE:HD12	1:E:357:LEU:HB3	1.96	0.47
1:C:41:LEU:HD21	1:C:125:LYS:HD2	1.96	0.47
1:D:88:ASP:HB3	1:D:91:LYS:HD2	1.96	0.47
1:B:189:ALA:O	1:B:193:VAL:HG22	2.14	0.47
1:C:73:VAL:HG11	1:D:538:LEU:HD11	1.95	0.47
1:A:337:ILE:HG23	1:A:341:ASP:HB2	1.96	0.47
1:B:223:TYR:CZ	1:B:228:PHE:HE1	2.32	0.47
1:D:138:VAL:HG12	1:D:141:ARG:HH22	1.79	0.47
1:A:223:TYR:CZ	1:A:228:PHE:HE1	2.32	0.47
1:B:244:LEU:HD22	1:B:320:THR:HG21	1.96	0.47
1:C:228:PHE:CE1	1:C:235:GLN:HB3	2.49	0.47
1:E:102:ALA:HB1	1:E:113:THR:HG23	1.97	0.47
1:D:261:LEU:HD22	1:D:297:VAL:HG21	1.97	0.47
1:B:337:ILE:HG23	1:B:341:ASP:HB2	1.95	0.47
1:C:345:ILE:HD12	1:C:357:LEU:HB3	1.96	0.47
1:F:261:LEU:HD22	1:F:297:VAL:HG11	1.97	0.47
1:G:155:LEU:HD21	1:G:525:VAL:HG13	1.97	0.47
1:A:218:LYS:HD3	1:A:356:LEU:HD13	1.96	0.46
1:C:155:LEU:HD11	1:C:443:ALA:HB1	1.97	0.46
1:E:73:VAL:HG11	1:F:538:LEU:HD11	1.98	0.46
1:E:345:ILE:HG21	1:E:348:VAL:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:HB3	1:A:342:PHE:CE1	2.50	0.46
1:D:444:LEU:HD12	1:D:475:PRO:HG3	1.97	0.46
1:A:143:GLY:HA2	1:A:146:MET:HB2	1.97	0.46
1:D:155:LEU:HD11	1:D:443:ALA:HB1	1.96	0.46
1:G:444:LEU:HD12	1:G:475:PRO:HG3	1.96	0.46
1:E:154:GLU:HG3	1:E:450:SER:CB	2.45	0.46
1:A:502:GLY:HA3	1:A:513:MET:SD	2.55	0.46
1:G:214:ILE:HD12	1:G:359:LYS:HE3	1.98	0.46
1:F:229:ILE:HD11	1:F:238:GLU:O	2.15	0.46
1:D:222:GLY:O	1:D:300:VAL:HG23	2.16	0.46
1:E:364:PRO:HA	1:E:367:VAL:HG22	1.97	0.46
1:C:206:THR:HG22	1:C:208:HIS:H	1.81	0.45
1:D:189:ALA:O	1:D:193:VAL:HG22	2.16	0.45
1:E:109:ALA:HB1	1:E:524:VAL:HG22	1.97	0.45
1:G:350:ILE:HG12	1:G:355:THR:HG23	1.98	0.45
1:B:154:GLU:HG3	1:B:450:SER:CB	2.47	0.45
1:D:126:GLU:HB3	1:D:467:ILE:HG12	1.97	0.45
1:E:147:ALA:HB1	1:E:468:ILE:HG21	1.98	0.45
1:A:244:LEU:HD22	1:A:345:ILE:HD11	1.98	0.45
1:A:126:GLU:HB3	1:A:467:ILE:HG12	1.98	0.45
1:A:251:ILE:HG21	1:A:257:ILE:HD12	1.98	0.45
1:F:212:GLU:OE2	1:F:405:LYS:NZ	2.49	0.45
1:F:62:VAL:HG22	1:G:544:ALA:HB3	1.99	0.45
1:B:237:CYS:SG	1:B:298:VAL:HG21	2.57	0.45
1:G:195:ARG:H	1:G:195:ARG:HG2	1.62	0.45
1:A:337:ILE:HG22	1:A:339:ALA:H	1.82	0.45
1:C:364:PRO:HA	1:C:367:VAL:HG22	1.98	0.45
1:D:240:GLN:HG3	1:D:347:GLU:HG2	1.99	0.45
1:E:147:ALA:HB2	1:E:465:VAL:HG22	1.99	0.45
1:G:151:VAL:HG23	1:G:451:LEU:HD21	1.99	0.45
1:E:346:GLY:HA3	1:E:359:LYS:HB2	1.98	0.45
1:E:142:ARG:O	1:E:461:GLN:HG2	2.17	0.44
1:G:477:MET:HG3	1:G:487:GLY:HA3	1.98	0.44
1:A:65:GLU:HB2	1:B:93:ILE:HD11	1.99	0.44
1:D:345:ILE:HD12	1:D:357:LEU:HB3	1.99	0.44
1:E:155:LEU:HD11	1:E:443:ALA:HB1	1.99	0.44
1:F:57:PRO:HG2	1:F:505:ALA:HB3	1.98	0.44
1:A:192:LYS:HD2	1:A:211:LEU:HD11	1.98	0.44
1:A:209:ASP:OD1	1:A:209:ASP:N	2.50	0.44
1:C:185:ILE:HG13	1:C:211:LEU:HD23	1.99	0.44
1:G:126:GLU:HB3	1:G:467:ILE:HG12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PRO:HG2	1:A:335:GLU:HB2	1.98	0.44
1:D:71:PRO:HD3	1:E:96:LYS:HD2	1.99	0.44
1:F:257:ILE:HD11	1:F:273:ILE:HD13	2.00	0.44
1:F:151:VAL:HG23	1:F:451:LEU:HD21	1.99	0.44
1:A:206:THR:HG22	1:A:208:HIS:H	1.83	0.44
1:B:139:GLU:HG3	1:B:458:ASN:HD21	1.81	0.44
1:G:382:THR:HA	1:G:387:LYS:HE2	2.00	0.44
1:D:91:LYS:HE2	1:D:91:LYS:HB3	1.70	0.44
1:B:211:LEU:HA	1:B:404:LEU:HA	2.00	0.43
1:B:493:LYS:HB3	1:B:493:LYS:HE2	1.77	0.43
1:E:209:ASP:HB3	1:E:407:GLY:H	1.83	0.43
1:C:214:ILE:HD12	1:C:359:LYS:HE3	2.00	0.43
1:E:60:ARG:HG3	1:F:543:GLU:HG3	2.00	0.43
1:F:73:VAL:HG21	1:G:538:LEU:HD21	2.00	0.43
1:A:88:ASP:HB3	1:A:91:LYS:HD2	2.00	0.43
1:B:73:VAL:HG21	1:C:538:LEU:HD21	2.00	0.43
1:F:154:GLU:HG3	1:F:450:SER:CB	2.49	0.43
1:A:45:ASP:OD1	1:A:125:LYS:HE3	2.19	0.43
1:E:275:ALA:O	1:E:302:ALA:N	2.50	0.43
1:G:185:ILE:HG12	1:G:211:LEU:HD23	1.99	0.43
1:C:251:ILE:HG21	1:C:257:ILE:HD12	2.00	0.43
1:D:182:ILE:O	1:D:185:ILE:HG22	2.18	0.43
1:E:101:VAL:HG21	1:E:535:VAL:HB	2.00	0.43
1:E:219:PHE:CD1	1:E:303:PRO:HG3	2.54	0.43
1:G:446:ARG:HH21	1:G:501:LEU:N	2.16	0.43
1:A:142:ARG:O	1:A:461:GLN:HG2	2.19	0.43
1:B:109:ALA:HB1	1:B:524:VAL:HG22	2.00	0.43
1:E:272:VAL:HG21	1:E:348:VAL:HG11	2.00	0.43
1:G:290:ARG:HE	1:G:291:LEU:HD22	1.84	0.43
1:E:63:ILE:HG12	1:E:73:VAL:HG22	2.01	0.43
1:A:47:LEU:HD13	1:A:99:GLN:HE21	1.84	0.43
1:D:246:LEU:HD22	1:D:317:ALA:HB2	2.01	0.43
1:F:41:LEU:HA	1:F:44:VAL:HG22	2.01	0.43
1:F:147:ALA:HB3	1:F:468:ILE:HG21	2.00	0.43
1:G:261:LEU:HD22	1:G:297:VAL:HG11	2.01	0.43
1:A:249:LYS:HG3	1:A:326:GLY:HA2	2.00	0.42
1:B:259:PRO:HA	1:B:262:GLU:HG2	2.00	0.42
1:D:218:LYS:HB2	1:D:356:LEU:HD12	1.99	0.42
1:G:154:GLU:HG3	1:G:450:SER:CB	2.48	0.42
1:B:128:PHE:HZ	1:B:539:LEU:HB3	1.84	0.42
1:F:209:ASP:HB3	1:F:407:GLY:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:209:ASP:OD1	1:G:209:ASP:N	2.51	0.42
1:B:144:VAL:HG13	1:B:468:ILE:HD11	2.01	0.42
1:E:96:LYS:HB2	1:E:96:LYS:HE3	1.85	0.42
1:G:218:LYS:HE2	1:G:354:ASP:HB2	2.01	0.42
1:C:101:VAL:HG21	1:C:535:VAL:HB	2.01	0.42
1:C:244:LEU:HD11	1:C:274:VAL:HG23	2.01	0.42
1:G:101:VAL:HG21	1:G:535:VAL:HB	2.01	0.42
1:G:102:ALA:HB1	1:G:113:THR:HG23	2.01	0.42
1:G:371:ALA:O	1:G:375:VAL:HG23	2.20	0.42
1:A:91:LYS:HE2	1:A:91:LYS:HB3	1.74	0.42
1:B:226:PRO:HB3	1:B:228:PHE:CZ	2.55	0.42
1:G:206:THR:HG22	1:G:208:HIS:H	1.84	0.42
1:B:216:GLY:HA3	1:B:401:VAL:HG13	2.02	0.42
1:D:188:ASN:O	1:D:192:LYS:HG2	2.19	0.42
1:D:244:LEU:HD22	1:D:320:THR:HG21	2.01	0.42
1:E:41:LEU:HA	1:E:44:VAL:HG22	2.02	0.42
1:G:109:ALA:HB1	1:G:524:VAL:HG22	2.02	0.42
1:E:211:LEU:HA	1:E:404:LEU:HA	2.01	0.41
1:B:511:VAL:HB	1:B:516:LYS:HD3	2.02	0.41
1:G:345:ILE:HG21	1:G:348:VAL:HB	2.02	0.41
1:B:54:THR:HB	1:B:75:LYS:O	2.21	0.41
1:C:102:ALA:HB1	1:C:113:THR:HG23	2.02	0.41
1:E:251:ILE:HG21	1:E:257:ILE:HD12	2.01	0.41
1:G:351:THR:HG23	1:G:353:ASP:H	1.84	0.41
1:A:468:ILE:O	1:A:472:LEU:HG	2.21	0.41
1:B:37:ARG:HD2	1:B:128:PHE:CE1	2.55	0.41
1:D:142:ARG:O	1:D:461:GLN:HG2	2.20	0.41
1:E:91:LYS:HB3	1:E:91:LYS:HE2	1.80	0.41
1:F:96:LYS:HB2	1:F:96:LYS:HE3	1.90	0.41
1:B:489:LEU:HD12	1:B:489:LEU:HA	1.92	0.41
1:B:91:LYS:HB3	1:B:91:LYS:HE2	1.79	0.41
1:B:155:LEU:HD11	1:B:443:ALA:HB1	2.03	0.41
1:E:249:LYS:HB3	1:E:249:LYS:HE2	1.82	0.41
1:B:364:PRO:HA	1:B:367:VAL:HG22	2.01	0.41
1:D:41:LEU:HA	1:D:44:VAL:HG22	2.01	0.41
1:C:195:ARG:H	1:C:195:ARG:HG2	1.62	0.41
1:D:182:ILE:HA	1:D:185:ILE:HG22	2.02	0.41
1:E:189:ALA:O	1:E:193:VAL:HG22	2.20	0.41
1:F:109:ALA:HB1	1:F:524:VAL:HG22	2.03	0.41
1:A:337:ILE:HD12	1:A:337:ILE:H	1.85	0.41
1:B:65:GLU:HB2	1:C:93:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:VAL:HG13	1:B:167:GLU:HB3	2.03	0.41
1:B:521:PRO:HB2	1:B:524:VAL:HG23	2.02	0.41
1:D:73:VAL:HG21	1:E:538:LEU:HD21	2.02	0.41
1:D:109:ALA:HB1	1:D:524:VAL:HG22	2.02	0.41
1:F:142:ARG:O	1:F:461:GLN:HG2	2.21	0.41
1:F:173:THR:HG23	1:F:183:GLY:HA3	2.03	0.41
1:G:222:GLY:O	1:G:300:VAL:HG23	2.21	0.41
1:D:147:ALA:HB2	1:D:465:VAL:HG22	2.03	0.40
1:C:219:PHE:CD1	1:C:221:ARG:HB2	2.56	0.40
1:C:345:ILE:HG21	1:C:348:VAL:HB	2.02	0.40
1:D:154:GLU:HG3	1:D:450:SER:CB	2.51	0.40
1:B:345:ILE:HD12	1:B:357:LEU:HB3	2.02	0.40
1:F:290:ARG:HD3	1:F:291:LEU:HD22	2.02	0.40
1:G:182:ILE:O	1:G:185:ILE:HG22	2.22	0.40
1:A:369:LYS:HE2	1:A:369:LYS:HB3	1.84	0.40
1:G:91:LYS:HE2	1:G:91:LYS:HB3	1.73	0.40
1:A:513:MET:HB3	1:A:518:ILE:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/573 (90%)	506 (98%)	11 (2%)	0	100	100
1	B	516/573 (90%)	503 (98%)	13 (2%)	0	100	100
1	C	510/573 (89%)	500 (98%)	10 (2%)	0	100	100
1	D	506/573 (88%)	497 (98%)	9 (2%)	0	100	100
1	E	511/573 (89%)	497 (97%)	14 (3%)	0	100	100
1	F	518/573 (90%)	509 (98%)	9 (2%)	0	100	100
1	G	523/573 (91%)	513 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3601/4011 (90%)	3525 (98%)	76 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	389/461 (84%)	388 (100%)	1 (0%)	92	97
1	B	393/461 (85%)	389 (99%)	4 (1%)	76	88
1	C	371/461 (80%)	370 (100%)	1 (0%)	92	97
1	D	362/461 (78%)	359 (99%)	3 (1%)	81	91
1	E	377/461 (82%)	374 (99%)	3 (1%)	81	91
1	F	371/461 (80%)	370 (100%)	1 (0%)	92	97
1	G	381/461 (83%)	379 (100%)	2 (0%)	88	94
All	All	2644/3227 (82%)	2629 (99%)	15 (1%)	86	94

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	ARG
1	B	218	LYS
1	B	235	GLN
1	B	236	LYS
1	B	411	ASP
1	C	411	ASP
1	D	223	TYR
1	D	353	ASP
1	D	359	LYS
1	E	239	PHE
1	E	290	ARG
1	E	377	GLN
1	F	336	ASP

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Mol	Chain	Res	Type
1	G	225	SER
1	G	506	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	521/573 (90%)	-0.30	1 (0%)	95 93	63, 106, 158, 189	0
1	B	520/573 (90%)	-0.24	4 (0%)	86 81	61, 106, 156, 207	0
1	C	516/573 (90%)	-0.27	4 (0%)	86 81	66, 116, 162, 209	0
1	D	514/573 (89%)	-0.19	3 (0%)	89 86	69, 122, 173, 227	0
1	E	517/573 (90%)	-0.24	4 (0%)	86 81	66, 119, 170, 198	0
1	F	522/573 (91%)	-0.22	6 (1%)	80 75	64, 115, 165, 216	0
1	G	525/573 (91%)	-0.26	8 (1%)	73 68	61, 112, 165, 215	0
All	All	3635/4011 (90%)	-0.25	30 (0%)	86 81	61, 114, 165, 227	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	ASP	3.9
1	E	163	THR	3.4
1	E	390	LEU	2.9
1	G	235	GLN	2.9
1	F	506	MET	2.7
1	D	378	LEU	2.6
1	G	409	THR	2.6
1	F	408	GLY	2.6
1	D	406	VAL	2.6
1	D	204	GLY	2.6
1	F	231	THR	2.4
1	G	511	VAL	2.4
1	F	505	ALA	2.3
1	E	235	GLN	2.3
1	B	381	THR	2.2
1	B	504	ASP	2.2
1	G	234	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	509	GLU	2.2
1	C	231	THR	2.2
1	G	232	ALA	2.2
1	B	409	THR	2.2
1	C	409	THR	2.2
1	F	333	ALA	2.1
1	B	550	PRO	2.1
1	C	507	GLN	2.1
1	C	381	THR	2.1
1	F	327	ASP	2.1
1	G	505	ALA	2.1
1	E	289	ASN	2.0
1	G	231	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.