



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 02:25 PM EDT

PDB ID : 2R9G
Title : Crystal structure of the C-terminal fragment of AAA ATPase from *Enterococcus faecium*
Authors : Ramagopal, U.A.; Patskovsky, Y.; Bonanno, J.B.; Shi, W.; Toro, R.; Meyer, A.J.; Rutter, M.; Wu, B.; Groshong, C.; Gheyi, T.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-09-12
Resolution : 2.09 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
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)

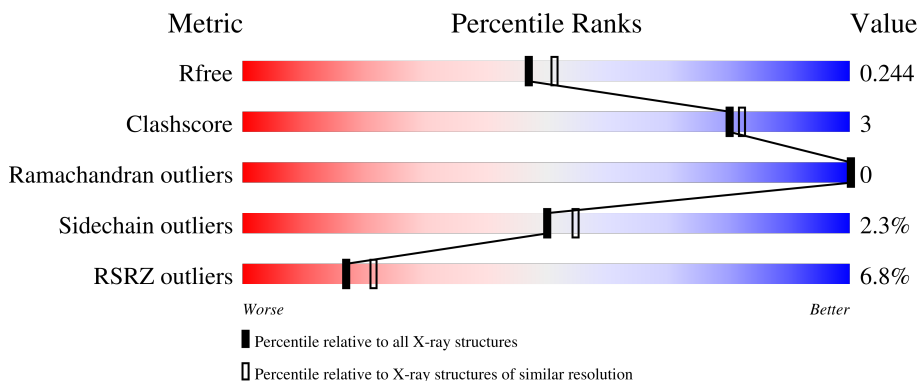
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


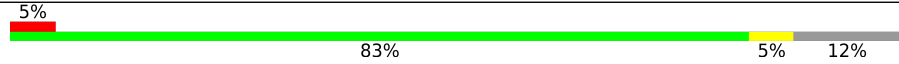
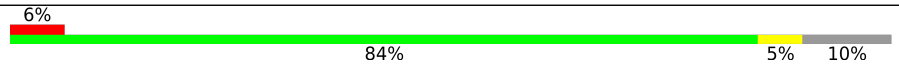

The reported resolution of this entry is 2.09 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	204	 5% 81% 6% 12%
1	B	204	 5% 83% 5% 12%
1	C	204	 6% 84% 5% 10%
1	D	204	 7% 81% 7% 12%

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Mol	Chain	Length	Quality of chain	
1	E	204	5%	83% 12%
1	F	204	6%	83% 5% 12%
1	G	204	4%	82% 5% 12%
1	H	204	3%	81% 6% 12%
1	I	204	4%	80% 7% 13%
1	J	204	9%	84% 5% 11%
1	K	204	8%	82% 6% 12%
1	L	204	6%	86% 5% 8%
1	M	204	7%	78% 7% 12%
1	N	204	6%	83% 12%
1	O	204	7%	80% 7% 12%
1	P	204	7%	84% 7% 8%

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	ACT	F	703	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24661 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 AAA ATPase, central region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	180	1433	908	253	267	5	0	3	0
1	B	180	1472	930	263	274	5	0	9	0
1	C	183	1469	930	260	274	5	0	6	0
1	D	180	1466	925	263	274	4	0	8	0
1	E	179	1463	926	262	270	5	0	9	0
1	F	180	1441	913	255	269	4	0	5	0
1	G	179	1465	930	259	271	5	0	9	0
1	H	179	1433	905	255	269	4	0	4	0
1	I	178	1430	908	252	266	4	0	4	0
1	J	181	1438	909	255	270	4	0	3	0
1	K	180	1440	911	255	269	5	0	4	0
1	L	188	1503	951	268	280	4	0	5	0
1	M	179	1443	915	254	270	4	0	6	0
1	N	180	1429	904	254	267	4	0	2	0
1	O	180	1437	910	256	267	4	0	4	0
1	P	187	1489	940	266	279	4	0	3	0

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	MET	-	expression tag	UNP Q3XY27
A	228	SER	-	expression tag	UNP Q3XY27
A	229	LEU	-	expression tag	UNP Q3XY27
A	423	GLU	-	expression tag	UNP Q3XY27
A	424	GLY	-	expression tag	UNP Q3XY27
A	425	HIS	-	expression tag	UNP Q3XY27
A	426	HIS	-	expression tag	UNP Q3XY27
A	427	HIS	-	expression tag	UNP Q3XY27
A	428	HIS	-	expression tag	UNP Q3XY27
A	429	HIS	-	expression tag	UNP Q3XY27
A	430	HIS	-	expression tag	UNP Q3XY27
B	227	MET	-	expression tag	UNP Q3XY27
B	228	SER	-	expression tag	UNP Q3XY27
B	229	LEU	-	expression tag	UNP Q3XY27
B	423	GLU	-	expression tag	UNP Q3XY27
B	424	GLY	-	expression tag	UNP Q3XY27
B	425	HIS	-	expression tag	UNP Q3XY27
B	426	HIS	-	expression tag	UNP Q3XY27
B	427	HIS	-	expression tag	UNP Q3XY27
B	428	HIS	-	expression tag	UNP Q3XY27
B	429	HIS	-	expression tag	UNP Q3XY27
B	430	HIS	-	expression tag	UNP Q3XY27
C	227	MET	-	expression tag	UNP Q3XY27
C	228	SER	-	expression tag	UNP Q3XY27
C	229	LEU	-	expression tag	UNP Q3XY27
C	423	GLU	-	expression tag	UNP Q3XY27
C	424	GLY	-	expression tag	UNP Q3XY27
C	425	HIS	-	expression tag	UNP Q3XY27
C	426	HIS	-	expression tag	UNP Q3XY27
C	427	HIS	-	expression tag	UNP Q3XY27
C	428	HIS	-	expression tag	UNP Q3XY27
C	429	HIS	-	expression tag	UNP Q3XY27
C	430	HIS	-	expression tag	UNP Q3XY27
D	227	MET	-	expression tag	UNP Q3XY27
D	228	SER	-	expression tag	UNP Q3XY27
D	229	LEU	-	expression tag	UNP Q3XY27
D	423	GLU	-	expression tag	UNP Q3XY27
D	424	GLY	-	expression tag	UNP Q3XY27
D	425	HIS	-	expression tag	UNP Q3XY27
D	426	HIS	-	expression tag	UNP Q3XY27
D	427	HIS	-	expression tag	UNP Q3XY27
D	428	HIS	-	expression tag	UNP Q3XY27

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Chain	Residue	Modelled	Actual	Comment	Reference
D	429	HIS	-	expression tag	UNP Q3XY27
D	430	HIS	-	expression tag	UNP Q3XY27
E	227	MET	-	expression tag	UNP Q3XY27
E	228	SER	-	expression tag	UNP Q3XY27
E	229	LEU	-	expression tag	UNP Q3XY27
E	423	GLU	-	expression tag	UNP Q3XY27
E	424	GLY	-	expression tag	UNP Q3XY27
E	425	HIS	-	expression tag	UNP Q3XY27
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E	427	HIS	-	expression tag	UNP Q3XY27
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E	430	HIS	-	expression tag	UNP Q3XY27
F	227	MET	-	expression tag	UNP Q3XY27
F	228	SER	-	expression tag	UNP Q3XY27
F	229	LEU	-	expression tag	UNP Q3XY27
F	423	GLU	-	expression tag	UNP Q3XY27
F	424	GLY	-	expression tag	UNP Q3XY27
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F	428	HIS	-	expression tag	UNP Q3XY27
F	429	HIS	-	expression tag	UNP Q3XY27
F	430	HIS	-	expression tag	UNP Q3XY27
G	227	MET	-	expression tag	UNP Q3XY27
G	228	SER	-	expression tag	UNP Q3XY27
G	229	LEU	-	expression tag	UNP Q3XY27
G	423	GLU	-	expression tag	UNP Q3XY27
G	424	GLY	-	expression tag	UNP Q3XY27
G	425	HIS	-	expression tag	UNP Q3XY27
G	426	HIS	-	expression tag	UNP Q3XY27
G	427	HIS	-	expression tag	UNP Q3XY27
G	428	HIS	-	expression tag	UNP Q3XY27
G	429	HIS	-	expression tag	UNP Q3XY27
G	430	HIS	-	expression tag	UNP Q3XY27
H	227	MET	-	expression tag	UNP Q3XY27
H	228	SER	-	expression tag	UNP Q3XY27
H	229	LEU	-	expression tag	UNP Q3XY27
H	423	GLU	-	expression tag	UNP Q3XY27
H	424	GLY	-	expression tag	UNP Q3XY27
H	425	HIS	-	expression tag	UNP Q3XY27
H	426	HIS	-	expression tag	UNP Q3XY27

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Chain	Residue	Modelled	Actual	Comment	Reference
H	427	HIS	-	expression tag	UNP Q3XY27
H	428	HIS	-	expression tag	UNP Q3XY27
H	429	HIS	-	expression tag	UNP Q3XY27
H	430	HIS	-	expression tag	UNP Q3XY27
I	227	MET	-	expression tag	UNP Q3XY27
I	228	SER	-	expression tag	UNP Q3XY27
I	229	LEU	-	expression tag	UNP Q3XY27
I	423	GLU	-	expression tag	UNP Q3XY27
I	424	GLY	-	expression tag	UNP Q3XY27
I	425	HIS	-	expression tag	UNP Q3XY27
I	426	HIS	-	expression tag	UNP Q3XY27
I	427	HIS	-	expression tag	UNP Q3XY27
I	428	HIS	-	expression tag	UNP Q3XY27
I	429	HIS	-	expression tag	UNP Q3XY27
I	430	HIS	-	expression tag	UNP Q3XY27
J	227	MET	-	expression tag	UNP Q3XY27
J	228	SER	-	expression tag	UNP Q3XY27
J	229	LEU	-	expression tag	UNP Q3XY27
J	423	GLU	-	expression tag	UNP Q3XY27
J	424	GLY	-	expression tag	UNP Q3XY27
J	425	HIS	-	expression tag	UNP Q3XY27
J	426	HIS	-	expression tag	UNP Q3XY27
J	427	HIS	-	expression tag	UNP Q3XY27
J	428	HIS	-	expression tag	UNP Q3XY27
J	429	HIS	-	expression tag	UNP Q3XY27
J	430	HIS	-	expression tag	UNP Q3XY27
K	227	MET	-	expression tag	UNP Q3XY27
K	228	SER	-	expression tag	UNP Q3XY27
K	229	LEU	-	expression tag	UNP Q3XY27
K	423	GLU	-	expression tag	UNP Q3XY27
K	424	GLY	-	expression tag	UNP Q3XY27
K	425	HIS	-	expression tag	UNP Q3XY27
K	426	HIS	-	expression tag	UNP Q3XY27
K	427	HIS	-	expression tag	UNP Q3XY27
K	428	HIS	-	expression tag	UNP Q3XY27
K	429	HIS	-	expression tag	UNP Q3XY27
K	430	HIS	-	expression tag	UNP Q3XY27
L	227	MET	-	expression tag	UNP Q3XY27
L	228	SER	-	expression tag	UNP Q3XY27
L	229	LEU	-	expression tag	UNP Q3XY27
L	423	GLU	-	expression tag	UNP Q3XY27
L	424	GLY	-	expression tag	UNP Q3XY27

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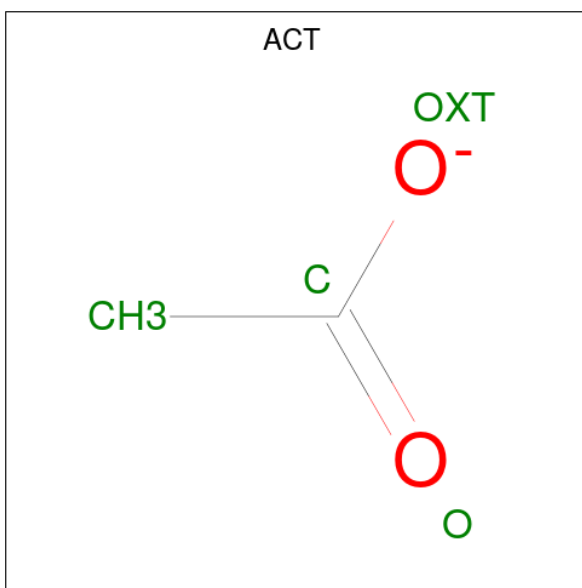
Chain	Residue	Modelled	Actual	Comment	Reference
L	425	HIS	-	expression tag	UNP Q3XY27
L	426	HIS	-	expression tag	UNP Q3XY27
L	427	HIS	-	expression tag	UNP Q3XY27
L	428	HIS	-	expression tag	UNP Q3XY27
L	429	HIS	-	expression tag	UNP Q3XY27
L	430	HIS	-	expression tag	UNP Q3XY27
M	227	MET	-	expression tag	UNP Q3XY27
M	228	SER	-	expression tag	UNP Q3XY27
M	229	LEU	-	expression tag	UNP Q3XY27
M	423	GLU	-	expression tag	UNP Q3XY27
M	424	GLY	-	expression tag	UNP Q3XY27
M	425	HIS	-	expression tag	UNP Q3XY27
M	426	HIS	-	expression tag	UNP Q3XY27
M	427	HIS	-	expression tag	UNP Q3XY27
M	428	HIS	-	expression tag	UNP Q3XY27
M	429	HIS	-	expression tag	UNP Q3XY27
M	430	HIS	-	expression tag	UNP Q3XY27
N	227	MET	-	expression tag	UNP Q3XY27
N	228	SER	-	expression tag	UNP Q3XY27
N	229	LEU	-	expression tag	UNP Q3XY27
N	423	GLU	-	expression tag	UNP Q3XY27
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N	425	HIS	-	expression tag	UNP Q3XY27
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N	427	HIS	-	expression tag	UNP Q3XY27
N	428	HIS	-	expression tag	UNP Q3XY27
N	429	HIS	-	expression tag	UNP Q3XY27
N	430	HIS	-	expression tag	UNP Q3XY27
O	227	MET	-	expression tag	UNP Q3XY27
O	228	SER	-	expression tag	UNP Q3XY27
O	229	LEU	-	expression tag	UNP Q3XY27
O	423	GLU	-	expression tag	UNP Q3XY27
O	424	GLY	-	expression tag	UNP Q3XY27
O	425	HIS	-	expression tag	UNP Q3XY27
O	426	HIS	-	expression tag	UNP Q3XY27
O	427	HIS	-	expression tag	UNP Q3XY27
O	428	HIS	-	expression tag	UNP Q3XY27
O	429	HIS	-	expression tag	UNP Q3XY27
O	430	HIS	-	expression tag	UNP Q3XY27
P	227	MET	-	expression tag	UNP Q3XY27
P	228	SER	-	expression tag	UNP Q3XY27
P	229	LEU	-	expression tag	UNP Q3XY27

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Chain	Residue	Modelled	Actual	Comment	Reference
P	423	GLU	-	expression tag	UNP Q3XY27
P	424	GLY	-	expression tag	UNP Q3XY27
P	425	HIS	-	expression tag	UNP Q3XY27
P	426	HIS	-	expression tag	UNP Q3XY27
P	427	HIS	-	expression tag	UNP Q3XY27
P	428	HIS	-	expression tag	UNP Q3XY27
P	429	HIS	-	expression tag	UNP Q3XY27
P	430	HIS	-	expression tag	UNP Q3XY27

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



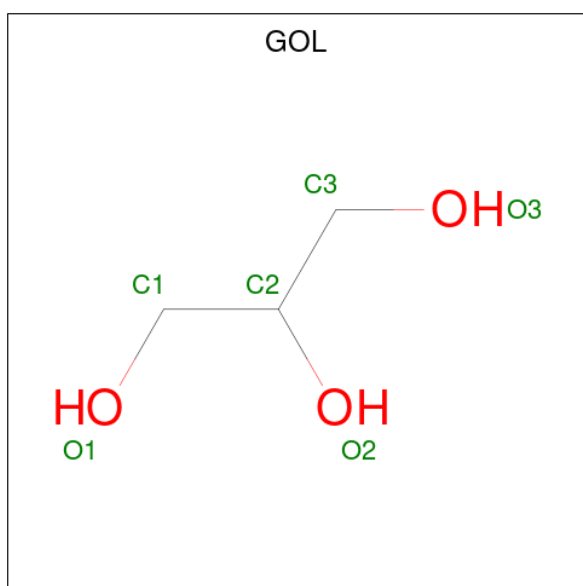
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	K	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total C O 4 2 2	0	0
2	L	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	O	1	Total C O 4 2 2	0	0
2	P	1	Total C O 4 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total C O 6 3 3	0	0
3	H	1	Total C O 6 3 3	0	0
3	J	1	Total C O 6 3 3	0	0
3	P	1	Total C O 6 3 3	0	0

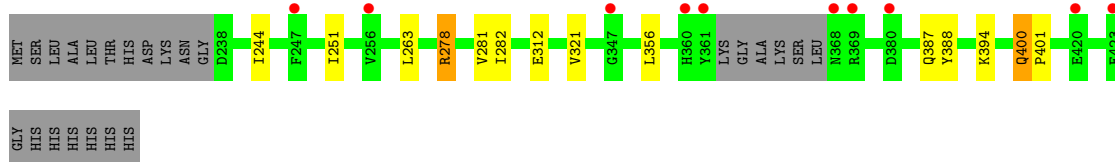
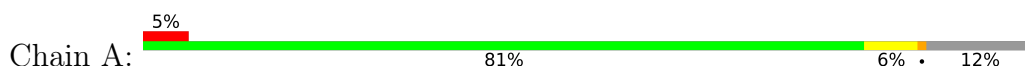
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	99	Total O 99 99	0	0
4	C	82	Total O 82 82	0	0
4	D	83	Total O 83 83	0	0
4	E	103	Total O 103 103	0	0
4	F	89	Total O 89 89	0	0
4	G	85	Total O 85 85	0	0
4	H	79	Total O 79 79	0	0
4	I	76	Total O 76 76	0	0
4	J	78	Total O 78 78	0	0
4	K	94	Total O 94 94	0	0
4	L	80	Total O 80 80	0	0
4	M	66	Total O 66 66	0	0
4	N	69	Total O 69 69	0	0
4	O	85	Total O 85 85	0	0
4	P	80	Total O 80 80	0	0

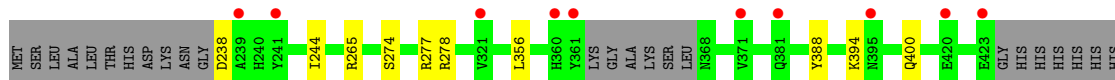
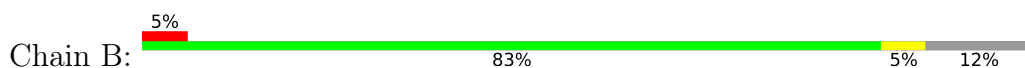
3 Residue-property plots [i](#)

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.

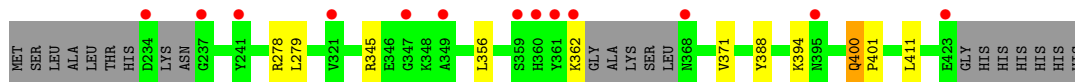
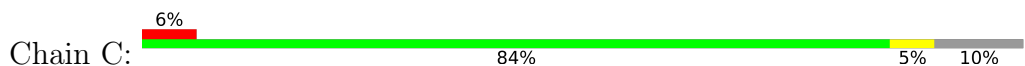
- Molecule 1: AAA ATPase, central region



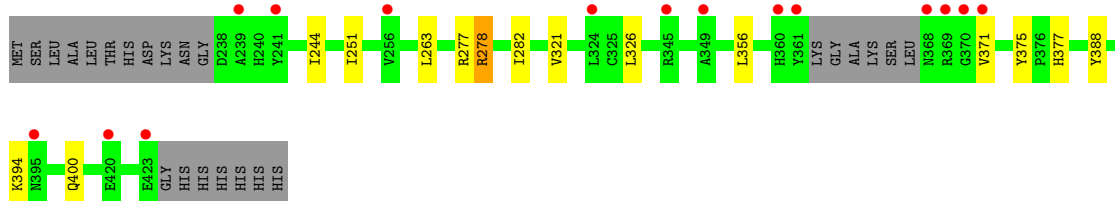
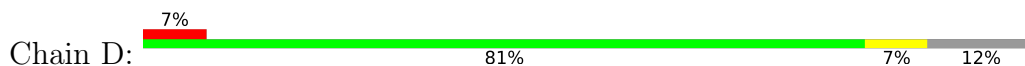
- Molecule 1: AAA ATPase, central region



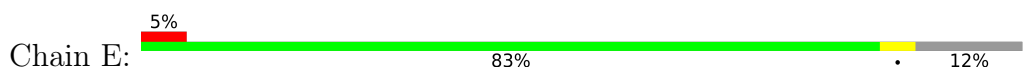
- Molecule 1: AAA ATPase, central region

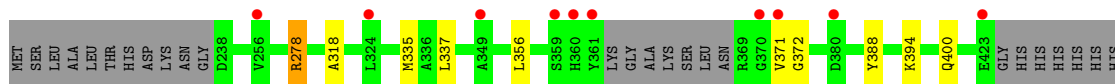


- Molecule 1: AAA ATPase, central region

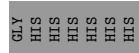
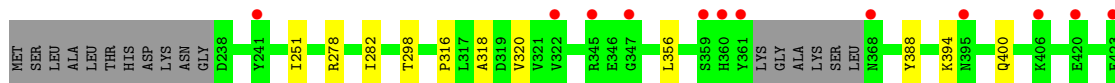
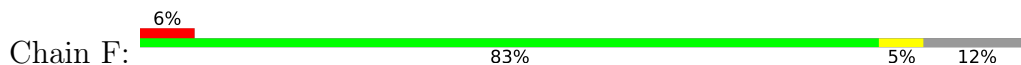


- Molecule 1: AAA ATPase, central region

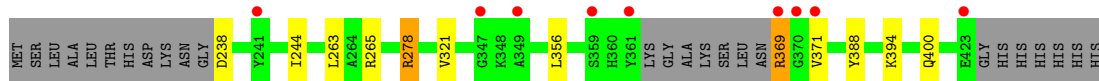
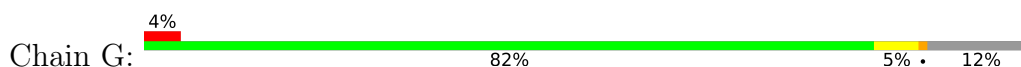




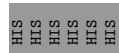
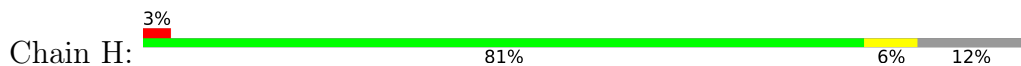
• Molecule 1: AAA ATPase, central region



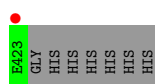
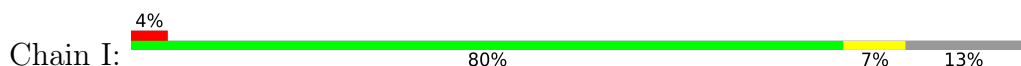
• Molecule 1: AAA ATPase, central region



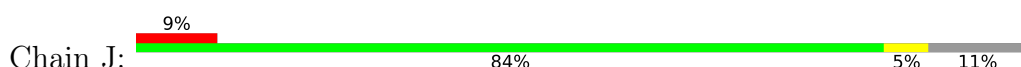
• Molecule 1: AAA ATPase, central region



• Molecule 1: AAA ATPase, central region

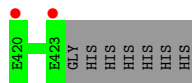
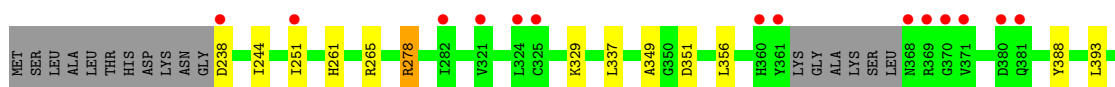
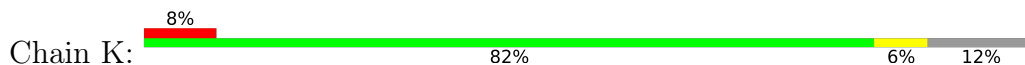


• Molecule 1: AAA ATPase, central region

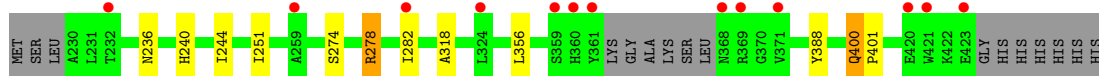
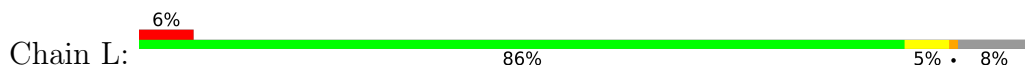




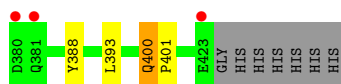
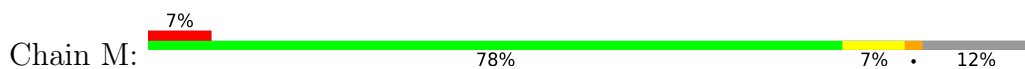
• Molecule 1: AAA ATPase, central region



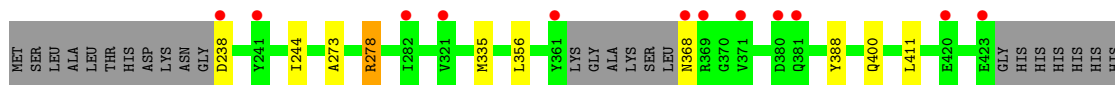
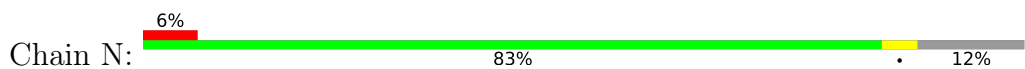
• Molecule 1: AAA ATPase, central region



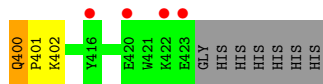
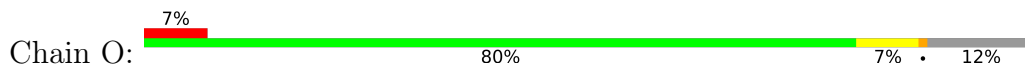
• Molecule 1: AAA ATPase, central region




• Molecule 1: AAA ATPase, central region

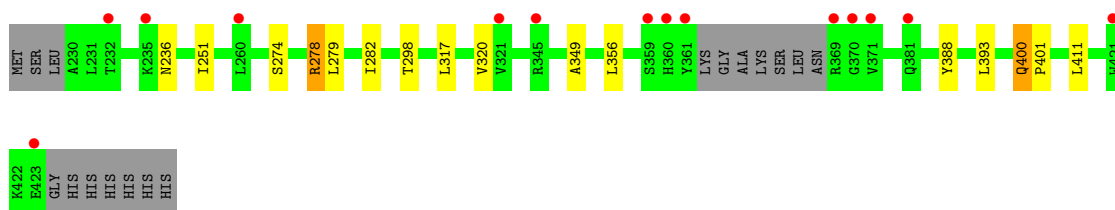


• Molecule 1: AAA ATPase, central region



- Molecule 1: AAA ATPase, central region

Chain P:  7% 84% 7% 8%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	82.78Å 103.39Å 103.37Å 90.01° 88.69° 86.05°	Depositor
Resolution (Å)	20.00 – 2.09 26.93 – 2.09	Depositor EDS
% Data completeness (in resolution range)	87.1 (20.00-2.09) 87.1 (26.93-2.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.3.0034	Depositor
R, R_{free}	0.197 , 0.248 0.198 , 0.244	Depositor DCC
R_{free} test set	5308 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtrriage
Anisotropy	0.345	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	24661	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1029e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL

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	0.38	0/1473	0.57	0/1996
1	B	0.40	0/1515	0.58	0/2051
1	C	0.38	0/1518	0.57	0/2053
1	D	0.46	0/1506	0.62	0/2039
1	E	0.39	0/1509	0.58	0/2041
1	F	0.39	0/1488	0.57	0/2018
1	G	0.44	0/1512	0.59	0/2047
1	H	0.45	0/1464	0.59	0/1984
1	I	0.37	0/1471	0.57	0/1993
1	J	0.38	0/1478	0.57	0/2002
1	K	0.40	0/1480	0.60	0/2004
1	L	0.39	0/1551	0.56	0/2101
1	M	0.37	0/1493	0.56	0/2023
1	N	0.38	0/1466	0.57	0/1986
1	O	0.49	0/1480	0.61	0/2004
1	P	0.38	0/1533	0.58	0/2077
All	All	0.41	0/23937	0.58	0/32419

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

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	1433	0	1409	7	0
1	B	1472	0	1450	5	0
1	C	1469	0	1449	6	0
1	D	1466	0	1439	9	0
1	E	1463	0	1449	5	0
1	F	1441	0	1417	7	0
1	G	1465	0	1447	13	0
1	H	1433	0	1396	8	0
1	I	1430	0	1404	6	0
1	J	1438	0	1409	5	0
1	K	1440	0	1415	8	0
1	L	1503	0	1481	21	0
1	M	1443	0	1419	13	0
1	N	1429	0	1402	4	0
1	O	1437	0	1419	10	0
1	P	1489	0	1464	10	0
2	B	4	0	3	1	0
2	C	8	0	6	0	0
2	E	8	0	6	0	0
2	F	4	0	3	2	0
2	K	4	0	3	0	0
2	L	8	0	6	1	0
2	O	8	0	6	0	0
2	P	4	0	3	1	0
3	E	6	0	8	0	0
3	H	6	0	8	0	0
3	J	6	0	8	1	0
3	P	6	0	8	0	0
4	A	90	0	0	0	0
4	B	99	0	0	0	0
4	C	82	0	0	1	0
4	D	83	0	0	0	0
4	E	103	0	0	0	0
4	F	89	0	0	0	0
4	G	85	0	0	0	0
4	H	79	0	0	0	0
4	I	76	0	0	0	0
4	J	78	0	0	0	0
4	K	94	0	0	0	0
4	L	80	0	0	0	0
4	M	66	0	0	0	0
4	N	69	0	0	0	0
4	O	85	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	80	0	0	0	0
All	All	24661	0	22937	125	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 3.

All (125) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:369[B]:ARG:HH11	1:G:369[B]:ARG:HG3	1.05	1.15
1:G:369[B]:ARG:HG3	1:G:369[B]:ARG:NH1	1.75	0.93
1:L:240[B]:HIS:NE2	1:L:244[B]:ILE:HD11	1.85	0.92
1:G:369[B]:ARG:HH11	1:G:369[B]:ARG:CG	1.90	0.85
1:G:371[A]:VAL:HG22	1:G:371[A]:VAL:O	1.79	0.82
1:L:244[A]:ILE:HG23	1:L:278[A]:ARG:CD	2.12	0.80
1:H:371[A]:VAL:HG13	1:H:372[A]:GLY:O	1.87	0.74
1:B:244:ILE:HD12	1:B:278[A]:ARG:HG3	1.71	0.73
1:L:244[B]:ILE:HG22	1:L:278[B]:ARG:NH2	2.03	0.73
1:G:371[A]:VAL:O	1:G:371[A]:VAL:CG2	2.37	0.73
1:F:298[B]:THR:HG22	1:F:320[B]:VAL:HG21	1.73	0.71
1:L:244[B]:ILE:CG2	1:L:278[B]:ARG:NH2	2.54	0.70
1:I:349:ALA:HA	1:I:393:LEU:HD11	1.74	0.69
1:O:244:ILE:HD12	1:O:278[B]:ARG:HG3	1.74	0.69
1:L:244[A]:ILE:CG2	1:L:278[A]:ARG:CD	2.70	0.68
1:L:244[A]:ILE:CG2	1:L:278[A]:ARG:HD3	2.23	0.67
1:D:371[A]:VAL:HG22	1:D:371[A]:VAL:O	1.93	0.66
1:K:356:LEU:HD11	1:K:388:TYR:HA	1.80	0.64
1:F:298[B]:THR:HG22	1:F:320[B]:VAL:CG2	2.27	0.63
1:C:371:VAL:HG23	1:M:393:LEU:HD23	1.79	0.63
1:M:349:ALA:HA	1:M:393:LEU:HD11	1.80	0.62
1:L:244[A]:ILE:HG23	1:L:278[A]:ARG:HD2	1.80	0.61
1:G:244:ILE:HG23	1:G:278:ARG:HD2	1.83	0.60
1:L:244[B]:ILE:HG23	1:L:278[B]:ARG:HG2	1.83	0.60
1:D:244:ILE:HG23	1:D:278:ARG:HD3	1.84	0.60
1:D:356:LEU:HD11	1:D:388:TYR:HA	1.83	0.60
1:L:244[A]:ILE:CG2	1:L:278[A]:ARG:HD2	2.32	0.60
1:M:251:ILE:HD12	1:M:282:ILE:HD13	1.84	0.60
1:O:356:LEU:HD11	1:O:388:TYR:HA	1.84	0.60
1:M:356:LEU:HD11	1:M:388:TYR:HA	1.84	0.59
1:H:374:GLN:H	1:H:386:GLN:HE22	1.51	0.59
1:C:345:ARG:HD2	4:C:757:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:244[A]:ILE:HG23	1:L:278[A]:ARG:HD3	1.85	0.58
1:D:277[B]:ARG:HH11	1:I:273:ALA:HB3	1.68	0.58
1:L:356:LEU:HD11	1:L:388:TYR:HA	1.85	0.58
1:N:244:ILE:HG23	1:N:278:ARG:HD2	1.87	0.57
1:D:251:ILE:HD12	1:D:282:ILE:HD13	1.87	0.56
1:F:251:ILE:HD12	1:F:282:ILE:HD13	1.88	0.56
1:B:356:LEU:HD11	1:B:388:TYR:HA	1.88	0.56
1:K:238:ASP:HB2	1:K:265[B]:ARG:HH22	1.70	0.55
1:H:356:LEU:HD11	1:H:388:TYR:HA	1.88	0.55
1:B:277:ARG:NH1	2:B:1:ACT:O	2.40	0.55
1:P:349:ALA:HA	1:P:393:LEU:HD11	1.87	0.55
1:O:332:SER:HB3	1:O:402[B]:LYS:HG3	1.90	0.54
1:E:278[B]:ARG:HH21	1:E:278[B]:ARG:HA	1.73	0.53
1:P:356:LEU:HD11	1:P:388:TYR:HA	1.92	0.52
1:I:356:LEU:HD11	1:I:388:TYR:HA	1.91	0.52
1:E:356:LEU:HD11	1:E:388:TYR:HA	1.91	0.52
1:G:356:LEU:HD11	1:G:388:TYR:HA	1.92	0.52
1:E:337:LEU:HD22	1:F:318:ALA:HB2	1.90	0.51
1:N:411:LEU:HD22	1:O:326:LEU:HB2	1.92	0.51
1:E:371[A]:VAL:HG13	1:E:372[A]:GLY:O	2.11	0.51
1:L:278[A]:ARG:NH1	2:L:1:ACT:OXT	2.43	0.51
1:J:238:ASP:H	1:J:265:ARG:HH22	1.59	0.51
1:O:351:ASP:OD1	1:P:236:ASN:ND2	2.38	0.50
1:C:356:LEU:HD11	1:C:388:TYR:HA	1.93	0.50
1:L:240[B]:HIS:CD2	1:L:244[B]:ILE:HD11	2.46	0.50
1:L:251:ILE:HD12	1:L:282:ILE:HD13	1.94	0.50
1:D:371[A]:VAL:O	1:D:371[A]:VAL:CG2	2.59	0.50
1:F:356:LEU:HD11	1:F:388:TYR:HA	1.93	0.49
1:K:349:ALA:HA	1:K:393:LEU:HD11	1.93	0.49
1:M:244:ILE:HG23	1:M:278[A]:ARG:HD3	1.95	0.49
1:N:356:LEU:HD11	1:N:388:TYR:HA	1.95	0.48
1:I:251:ILE:HD12	1:I:282:ILE:HD13	1.96	0.48
1:F:316:PRO:O	1:F:320[B]:VAL:HG12	2.14	0.47
1:M:263:LEU:HD22	1:M:321:VAL:HG21	1.97	0.47
1:F:278[B]:ARG:NH2	2:F:703:ACT:O	2.48	0.47
1:O:261:HIS:CE1	1:O:265[A]:ARG:HD3	2.50	0.46
1:M:238:ASP:HB2	1:M:265:ARG:HH22	1.79	0.46
1:A:244[B]:ILE:HG23	1:A:278:ARG:HD2	1.98	0.46
1:P:274[B]:SER:OG	1:P:278[B]:ARG:NH1	2.48	0.46
1:K:251:ILE:O	1:K:329[B]:LYS:NZ	2.40	0.46
1:O:265[B]:ARG:NH1	4:O:789:HOH:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:HD11	1:A:388:TYR:HA	1.98	0.45
1:G:263:LEU:HD22	1:G:321:VAL:HG21	1.97	0.45
1:L:240[B]:HIS:CD2	1:L:244[B]:ILE:CD1	2.99	0.45
1:J:356:LEU:HD11	1:J:388:TYR:HA	1.98	0.45
1:J:263:LEU:HD22	1:J:321:VAL:HG21	1.98	0.45
1:J:277[B]:ARG:HE	3:J:1:GOL:H11	1.82	0.45
1:O:263:LEU:HD22	1:O:321:VAL:HG21	1.99	0.44
1:A:244[A]:ILE:HG23	1:A:278:ARG:HD2	1.98	0.44
1:L:244[B]:ILE:CG2	1:L:278[B]:ARG:HH21	2.30	0.44
1:G:369[B]:ARG:HA	1:G:369[B]:ARG:HD2	1.58	0.44
2:F:703:ACT:H1	1:N:273:ALA:HB3	1.99	0.44
1:L:240[B]:HIS:NE2	1:L:244[B]:ILE:CD1	2.71	0.43
1:I:411:LEU:HD22	1:J:326:LEU:HB2	2.00	0.43
1:H:244:ILE:HG23	1:H:278:ARG:CD	2.48	0.43
1:I:263:LEU:HD22	1:I:321:VAL:HG21	1.99	0.43
1:A:251:ILE:HD12	1:A:282:ILE:HD13	2.00	0.43
1:H:244:ILE:HG23	1:H:278:ARG:HD2	2.01	0.43
1:O:274:SER:O	1:O:278[B]:ARG:HG2	2.19	0.43
1:L:400:GLN:HA	1:L:401:PRO:HD2	1.90	0.42
1:B:274:SER:O	1:B:278[A]:ARG:HG2	2.20	0.42
1:D:263:LEU:HD22	1:D:321:VAL:HG21	2.01	0.42
1:M:278[B]:ARG:HA	1:M:278[B]:ARG:HD3	1.81	0.42
1:P:400:GLN:HA	1:P:401:PRO:HD2	1.89	0.42
1:H:263:LEU:HD22	1:H:321:VAL:HG21	2.02	0.42
1:A:400:GLN:HA	1:A:401:PRO:HD2	1.90	0.42
1:G:369[B]:ARG:NH2	1:H:242:ASP:OD2	2.51	0.42
1:B:238:ASP:HB2	1:B:265:ARG:HH22	1.84	0.42
1:C:279:LEU:HD12	1:C:279:LEU:HA	1.88	0.42
1:M:248:GLN:OE1	1:M:278[B]:ARG:NH2	2.53	0.42
1:P:251:ILE:HD12	1:P:282:ILE:HD13	2.02	0.42
1:G:369[B]:ARG:HD2	1:G:369[B]:ARG:N	2.25	0.42
1:D:375:TYR:CE2	1:D:377:HIS:HB2	2.55	0.41
1:E:318:ALA:HB2	1:H:337:LEU:HD22	2.01	0.41
1:P:279:LEU:HD12	1:P:317:LEU:HD22	2.01	0.41
1:G:369[B]:ARG:N	1:G:369[B]:ARG:CD	2.83	0.41
1:K:261:HIS:NE2	1:K:265[A]:ARG:HD2	2.35	0.41
1:C:400:GLN:HA	1:C:401:PRO:HD2	1.91	0.41
1:M:244:ILE:HD13	1:M:244:ILE:HA	1.97	0.41
1:A:263:LEU:HD22	1:A:321:VAL:HG21	2.03	0.41
1:C:411:LEU:HD22	1:D:326:LEU:HB2	2.03	0.41
1:M:400:GLN:HA	1:M:401:PRO:HD2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:244:ILE:HG23	1:K:278:ARG:HG2	2.01	0.41
1:K:337:LEU:HD22	1:L:318:ALA:HB2	2.03	0.41
1:K:351:ASP:OD1	1:L:236:ASN:ND2	2.54	0.41
1:O:400:GLN:HA	1:O:401:PRO:HD2	1.88	0.40
1:A:278:ARG:HH21	1:A:281:VAL:HG11	1.86	0.40
1:L:278[B]:ARG:HD2	1:L:278[B]:ARG:HA	1.87	0.40
1:G:238:ASP:HB3	1:G:265:ARG:HH22	1.85	0.40
1:M:271[B]:ASP:OD2	1:M:274[B]:SER:OG	2.33	0.40
1:P:278[B]:ARG:NH1	2:P:702:ACT:C	2.84	0.40
1:M:326:LEU:HB2	1:P:411:LEU:HD22	2.04	0.40
1:P:298[A]:THR:HG23	1:P:320:VAL:HG11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	179/204 (88%)	179 (100%)	0	0	100	100
1	B	184/204 (90%)	182 (99%)	2 (1%)	0	100	100
1	C	184/204 (90%)	183 (100%)	1 (0%)	0	100	100
1	D	183/204 (90%)	182 (100%)	1 (0%)	0	100	100
1	E	183/204 (90%)	183 (100%)	0	0	100	100
1	F	181/204 (89%)	181 (100%)	0	0	100	100
1	G	183/204 (90%)	182 (100%)	1 (0%)	0	100	100
1	H	178/204 (87%)	178 (100%)	0	0	100	100
1	I	178/204 (87%)	177 (99%)	1 (1%)	0	100	100
1	J	180/204 (88%)	180 (100%)	0	0	100	100
1	K	180/204 (88%)	178 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	189/204 (93%)	189 (100%)	0	0	100	100
1	M	181/204 (89%)	179 (99%)	2 (1%)	0	100	100
1	N	178/204 (87%)	178 (100%)	0	0	100	100
1	O	180/204 (88%)	179 (99%)	1 (1%)	0	100	100
1	P	187/204 (92%)	187 (100%)	0	0	100	100
All	All	2908/3264 (89%)	2897 (100%)	11 (0%)	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	146/162 (90%)	141 (97%)	5 (3%)	37	39
1	B	150/162 (93%)	148 (99%)	2 (1%)	69	75
1	C	151/162 (93%)	146 (97%)	5 (3%)	38	40
1	D	149/162 (92%)	146 (98%)	3 (2%)	55	60
1	E	149/162 (92%)	143 (96%)	6 (4%)	31	32
1	F	148/162 (91%)	146 (99%)	2 (1%)	67	73
1	G	149/162 (92%)	144 (97%)	5 (3%)	37	39
1	H	144/162 (89%)	141 (98%)	3 (2%)	53	59
1	I	145/162 (90%)	139 (96%)	6 (4%)	30	31
1	J	146/162 (90%)	144 (99%)	2 (1%)	67	73
1	K	147/162 (91%)	146 (99%)	1 (1%)	84	88
1	L	154/162 (95%)	149 (97%)	5 (3%)	39	41
1	M	148/162 (91%)	141 (95%)	7 (5%)	26	25
1	N	145/162 (90%)	140 (97%)	5 (3%)	37	39
1	O	146/162 (90%)	142 (97%)	4 (3%)	44	48
1	P	152/162 (94%)	148 (97%)	4 (3%)	46	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2369/2592 (91%)	2304 (97%)	65 (3%)	50 48

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	ARG
1	A	312	GLU
1	A	387	GLN
1	A	394	LYS
1	A	400	GLN
1	B	394	LYS
1	B	400	GLN
1	C	278[A]	ARG
1	C	278[B]	ARG
1	C	362	LYS
1	C	394	LYS
1	C	400	GLN
1	D	278	ARG
1	D	394	LYS
1	D	400	GLN
1	E	278[A]	ARG
1	E	278[B]	ARG
1	E	335[A]	MET
1	E	335[B]	MET
1	E	394	LYS
1	E	400	GLN
1	F	394	LYS
1	F	400	GLN
1	G	278	ARG
1	G	369[A]	ARG
1	G	369[B]	ARG
1	G	394	LYS
1	G	400	GLN
1	H	278	ARG
1	H	394	LYS
1	H	400	GLN
1	I	240	HIS
1	I	278[A]	ARG
1	I	278[B]	ARG
1	I	335	MET
1	I	394	LYS
1	I	400	GLN

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Mol	Chain	Res	Type
1	J	335	MET
1	J	400	GLN
1	K	278	ARG
1	L	274[A]	SER
1	L	274[B]	SER
1	L	278[A]	ARG
1	L	278[B]	ARG
1	L	400	GLN
1	M	238	ASP
1	M	271[A]	ASP
1	M	271[B]	ASP
1	M	278[A]	ARG
1	M	278[B]	ARG
1	M	369	ARG
1	M	400	GLN
1	N	238	ASP
1	N	278	ARG
1	N	335	MET
1	N	368	ASN
1	N	400	GLN
1	O	278[A]	ARG
1	O	278[B]	ARG
1	O	335	MET
1	O	400	GLN
1	P	278[A]	ARG
1	P	278[B]	ARG
1	P	278[C]	ARG
1	P	400	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	GLN
1	A	400	GLN
1	B	400	GLN
1	D	400	GLN
1	E	395	ASN
1	E	400	GLN
1	F	387	GLN
1	F	395	ASN
1	G	397	GLN
1	H	374	GLN

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Mol	Chain	Res	Type
1	H	386	GLN
1	H	387	GLN
1	H	400	GLN
1	J	400	GLN
1	M	240	HIS
1	N	368	ASN
1	P	387	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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	ACT	B	1	-	3,3,3	0.72	0	3,3,3	1.57	0
2	ACT	O	701	-	3,3,3	0.76	0	3,3,3	1.45	0
2	ACT	C	707	-	3,3,3	0.90	0	3,3,3	0.97	0
2	ACT	E	705	-	3,3,3	0.80	0	3,3,3	1.22	0
2	ACT	F	703	-	3,3,3	0.85	0	3,3,3	1.54	0
2	ACT	K	1	-	3,3,3	0.79	0	3,3,3	1.37	0
2	ACT	O	704	-	3,3,3	0.74	0	3,3,3	1.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	E	706	-	5,5,5	0.35	0	5,5,5	0.64	0
2	ACT	E	1	-	3,3,3	0.78	0	3,3,3	1.38	0
2	ACT	C	1	-	3,3,3	0.85	0	3,3,3	1.44	0
2	ACT	L	706	-	3,3,3	0.86	0	3,3,3	0.92	0
3	GOL	J	1	-	5,5,5	0.36	0	5,5,5	0.28	0
3	GOL	P	1	-	5,5,5	0.37	0	5,5,5	0.31	0
2	ACT	P	702	-	3,3,3	0.71	0	3,3,3	1.71	2 (66%)
2	ACT	L	1	-	3,3,3	0.77	0	3,3,3	1.56	0
3	GOL	H	1	-	5,5,5	0.38	0	5,5,5	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	H	1	-	-	4/4/4/4	-
3	GOL	P	1	-	-	1/4/4/4	-
3	GOL	J	1	-	-	2/4/4/4	-
3	GOL	E	706	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	702	ACT	OXT-C-O	-2.14	114.18	122.05
2	P	702	ACT	OXT-C-CH3	2.05	123.66	115.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	706	GOL	C1-C2-C3-O3
3	H	1	GOL	C1-C2-C3-O3
3	J	1	GOL	C1-C2-C3-O3
3	H	1	GOL	O1-C1-C2-C3
3	P	1	GOL	C1-C2-C3-O3
3	H	1	GOL	O2-C2-C3-O3
3	E	706	GOL	O2-C2-C3-O3
3	J	1	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	H	1	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	ACT	1	0
2	F	703	ACT	2	0
3	J	1	GOL	1	0
2	P	702	ACT	1	0
2	L	1	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	180/204 (88%)	0.08	10 (5%) 24 29	22, 31, 60, 84	0
1	B	180/204 (88%)	0.02	10 (5%) 24 29	16, 30, 61, 86	0
1	C	183/204 (89%)	0.31	13 (7%) 16 20	21, 32, 70, 100	0
1	D	180/204 (88%)	0.14	15 (8%) 11 14	20, 34, 64, 97	0
1	E	179/204 (87%)	0.05	10 (5%) 24 29	17, 30, 60, 93	0
1	F	180/204 (88%)	0.13	12 (6%) 17 22	20, 32, 67, 97	0
1	G	179/204 (87%)	0.14	9 (5%) 28 34	21, 33, 65, 96	0
1	H	179/204 (87%)	0.01	7 (3%) 39 45	20, 31, 57, 86	0
1	I	178/204 (87%)	0.22	9 (5%) 28 33	23, 34, 64, 97	0
1	J	181/204 (88%)	0.16	18 (9%) 7 9	18, 32, 60, 87	0
1	K	180/204 (88%)	0.13	16 (8%) 9 12	18, 31, 63, 90	0
1	L	188/204 (92%)	0.32	13 (6%) 16 21	21, 33, 69, 105	0
1	M	179/204 (87%)	0.26	15 (8%) 11 14	19, 35, 68, 99	0
1	N	180/204 (88%)	0.22	12 (6%) 17 22	21, 33, 63, 88	0
1	O	180/204 (88%)	0.15	14 (7%) 13 17	16, 30, 65, 87	0
1	P	187/204 (91%)	0.22	14 (7%) 14 18	17, 32, 64, 99	0
All	All	2893/3264 (88%)	0.16	197 (6%) 17 21	16, 32, 65, 105	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	361	TYR	11.2
1	M	361	TYR	10.7
1	I	361	TYR	10.5
1	D	361	TYR	8.5
1	K	371	VAL	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	361	TYR	7.8
1	I	371	VAL	6.9
1	P	361	TYR	6.7
1	F	361	TYR	6.7
1	P	371	VAL	6.7
1	F	360	HIS	6.5
1	L	371	VAL	6.4
1	M	371	VAL	6.3
1	K	368	ASN	6.2
1	L	368	ASN	5.9
1	P	360	HIS	5.8
1	C	368	ASN	5.8
1	C	360	HIS	5.4
1	O	371	VAL	5.4
1	L	361	TYR	5.1
1	J	360	HIS	5.0
1	J	361	TYR	4.9
1	L	369	ARG	4.9
1	N	368	ASN	4.9
1	L	360	HIS	4.8
1	E	360	HIS	4.5
1	H	360	HIS	4.5
1	A	360	HIS	4.4
1	M	359	SER	4.4
1	P	423	GLU	4.2
1	M	360	HIS	4.2
1	O	369	ARG	4.2
1	K	370	GLY	4.1
1	D	360	HIS	4.1
1	A	361	TYR	4.1
1	C	349	ALA	4.0
1	E	361	TYR	4.0
1	C	237	GLY	3.8
1	B	360	HIS	3.8
1	G	369[A]	ARG	3.8
1	L	423	GLU	3.7
1	P	369	ARG	3.7
1	A	368	ASN	3.6
1	G	349	ALA	3.6
1	M	423	GLU	3.6
1	N	420	GLU	3.6
1	N	369	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	237	GLY	3.3
1	I	360	HIS	3.3
1	O	360	HIS	3.2
1	N	321	VAL	3.2
1	C	234	ASP	3.2
1	J	423	GLU	3.2
1	M	260	LEU	3.2
1	H	361	TYR	3.1
1	E	371[A]	VAL	3.1
1	G	370[A]	GLY	3.1
1	F	368	ASN	3.1
1	D	369[A]	ARG	3.1
1	C	359	SER	3.1
1	K	321	VAL	3.1
1	L	420	GLU	3.1
1	N	380	ASP	3.1
1	C	423	GLU	3.0
1	E	370[A]	GLY	3.0
1	N	241	TYR	3.0
1	B	241	TYR	3.0
1	M	381	GLN	3.0
1	M	369	ARG	3.0
1	F	345	ARG	2.9
1	D	420	GLU	2.9
1	K	420	GLU	2.9
1	B	423	GLU	2.9
1	L	421	TRP	2.9
1	D	371[A]	VAL	2.9
1	N	282	ILE	2.9
1	M	241[A]	TYR	2.9
1	B	395	ASN	2.9
1	L	232	THR	2.9
1	B	371[A]	VAL	2.8
1	G	371[A]	VAL	2.8
1	J	371	VAL	2.8
1	P	370	GLY	2.8
1	K	423	GLU	2.8
1	G	359	SER	2.8
1	P	381	GLN	2.8
1	H	423	GLU	2.8
1	K	381	GLN	2.8
1	B	361	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	423	GLU	2.8
1	E	349	ALA	2.8
1	F	423	GLU	2.8
1	P	235	LYS	2.8
1	J	236	ASN	2.8
1	I	423	GLU	2.8
1	C	241	TYR	2.8
1	E	359	SER	2.8
1	K	282	ILE	2.7
1	C	362	LYS	2.7
1	N	361	TYR	2.7
1	F	420	GLU	2.7
1	A	347	GLY	2.7
1	D	368[A]	ASN	2.7
1	K	251	ILE	2.7
1	M	256	VAL	2.7
1	N	371	VAL	2.7
1	G	423	GLU	2.7
1	N	238	ASP	2.7
1	N	381	GLN	2.7
1	J	380[A]	ASP	2.6
1	M	370	GLY	2.6
1	O	423	GLU	2.6
1	O	416	TYR	2.6
1	D	239	ALA	2.6
1	F	347	GLY	2.6
1	I	421	TRP	2.6
1	D	423	GLU	2.6
1	D	256	VAL	2.5
1	C	395	ASN	2.5
1	D	345	ARG	2.5
1	K	238	ASP	2.5
1	M	321	VAL	2.5
1	F	241	TYR	2.5
1	D	349	ALA	2.5
1	J	321	VAL	2.5
1	O	259	ALA	2.5
1	L	324	LEU	2.4
1	L	359	SER	2.4
1	M	282	ILE	2.4
1	A	380	ASP	2.4
1	P	232	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	347	GLY	2.4
1	P	359	SER	2.4
1	I	238	ASP	2.4
1	J	238	ASP	2.4
1	K	380	ASP	2.4
1	J	251	ILE	2.4
1	G	241[A]	TYR	2.4
1	E	423	GLU	2.3
1	P	321	VAL	2.3
1	H	239	ALA	2.3
1	P	345	ARG	2.3
1	J	259	ALA	2.3
1	L	282	ILE	2.3
1	J	381	GLN	2.3
1	P	260	LEU	2.3
1	A	256	VAL	2.3
1	O	321	VAL	2.3
1	H	380	ASP	2.3
1	D	370[A]	GLY	2.3
1	E	256	VAL	2.3
1	O	361	TYR	2.2
1	O	238	ASP	2.2
1	C	321	VAL	2.2
1	A	420	GLU	2.2
1	A	423	GLU	2.2
1	O	420	GLU	2.2
1	J	358	ASP	2.2
1	I	420	GLU	2.2
1	B	239	ALA	2.2
1	K	325	CYS	2.2
1	K	369	ARG	2.2
1	B	321	VAL	2.2
1	F	359	SER	2.2
1	O	324	LEU	2.2
1	K	324	LEU	2.1
1	D	395	ASN	2.1
1	K	360	HIS	2.1
1	B	381	GLN	2.1
1	J	241	TYR	2.1
1	K	361	TYR	2.1
1	M	259	ALA	2.1
1	E	380	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	251	ILE	2.1
1	A	369	ARG	2.1
1	F	406	LYS	2.1
1	I	325	CYS	2.1
1	M	380	ASP	2.1
1	B	420	GLU	2.1
1	D	324	LEU	2.1
1	J	359	SER	2.1
1	J	247	PHE	2.1
1	J	318	ALA	2.1
1	L	259	ALA	2.1
1	H	251	ILE	2.1
1	D	241	TYR	2.1
1	O	422	LYS	2.1
1	E	324	LEU	2.0
1	J	322	VAL	2.0
1	A	247	PHE	2.0
1	O	346	GLU	2.0
1	F	395	ASN	2.0
1	G	347	GLY	2.0
1	P	421	TRP	2.0
1	F	322	VAL	2.0
1	H	347	GLY	2.0
1	I	321	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 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(\AA^2)	Q<0.9
3	GOL	J	1	6/6	0.71	0.21	63,76,79,79	0
3	GOL	E	706	6/6	0.82	0.17	49,57,62,65	0
3	GOL	H	1	6/6	0.83	0.19	59,65,67,69	0
2	ACT	P	702	4/4	0.88	0.19	44,50,51,54	0
3	GOL	P	1	6/6	0.90	0.10	46,56,58,62	0
2	ACT	L	1	4/4	0.92	0.18	47,47,49,53	0
2	ACT	C	707	4/4	0.92	0.21	28,31,37,43	0
2	ACT	E	1	4/4	0.93	0.13	44,48,48,49	0
2	ACT	C	1	4/4	0.94	0.19	44,48,50,50	0
2	ACT	B	1	4/4	0.95	0.13	47,47,47,51	0
2	ACT	L	706	4/4	0.95	0.11	25,31,32,35	0
2	ACT	O	701	4/4	0.95	0.15	47,48,50,51	0
2	ACT	E	705	4/4	0.95	0.18	40,42,43,48	0
2	ACT	F	703	4/4	0.96	0.12	40,43,45,48	0
2	ACT	O	704	4/4	0.97	0.09	33,34,36,40	0
2	ACT	K	1	4/4	0.98	0.11	36,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.