Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2016 – 06:17 PM EST

PDB ID	:	5LFQ
Title	:	Crystal Structure of the Bacterial Proteasome Activator Bpa of Mycobacterium tuberculosis (space group P3)
Authors	:	Bolten, M.; Delley, C.L.; Leibundgut, M.; Boehringer, D.; Ban, N.; Weber-Ban, E.
Deposited on	:	2016-07-04
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

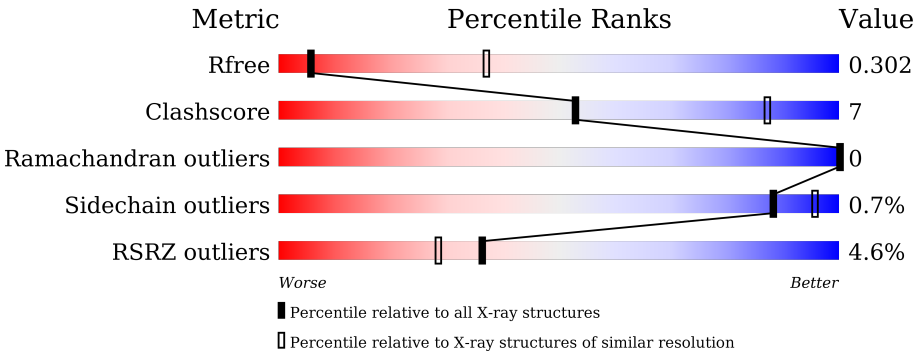
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.50 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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	131	2% 73% 14% 14%
1	B	131	7% 76% 10% 14%
1	C	131	4% 66% 20% 14%
1	D	131	3% 73% 14% 14%
1	E	131	2% 71% 15% 14%
1	F	131	5% 72% 15% 14%

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Mol	Chain	Length	Quality of chain
1	G	131	4% 66% 20% 14%
1	H	131	5% 69% 17% 14%
1	I	131	5% 65% 21% 14%
1	J	131	8% 76% 10% 14%
1	K	131	% 69% 17% 14%
1	L	131	5% 73% 13% 14%
1	M	131	2% 75% 11% 14%
1	N	131	3% 77% 9% 14%
1	O	131	2% 70% 16% 14%
1	P	131	6% 73% 14% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13856 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 Bacterial proteasome activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	B	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	C	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	D	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	E	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	F	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	G	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	H	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	I	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	J	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	K	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	L	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	M	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	N	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	O	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			
1	P	113	Total	C	N	O	Se	0	0	0
			866	542	155	167	2			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MSE	-	initiating methionine	UNP P9WKX3
A	30	HIS	-	expression tag	UNP P9WKX3
A	31	HIS	-	expression tag	UNP P9WKX3
A	32	HIS	-	expression tag	UNP P9WKX3
A	33	HIS	-	expression tag	UNP P9WKX3
A	34	HIS	-	expression tag	UNP P9WKX3
A	35	HIS	-	expression tag	UNP P9WKX3
B	29	MSE	-	initiating methionine	UNP P9WKX3
B	30	HIS	-	expression tag	UNP P9WKX3
B	31	HIS	-	expression tag	UNP P9WKX3
B	32	HIS	-	expression tag	UNP P9WKX3
B	33	HIS	-	expression tag	UNP P9WKX3
B	34	HIS	-	expression tag	UNP P9WKX3
B	35	HIS	-	expression tag	UNP P9WKX3
C	29	MSE	-	initiating methionine	UNP P9WKX3
C	30	HIS	-	expression tag	UNP P9WKX3
C	31	HIS	-	expression tag	UNP P9WKX3
C	32	HIS	-	expression tag	UNP P9WKX3
C	33	HIS	-	expression tag	UNP P9WKX3
C	34	HIS	-	expression tag	UNP P9WKX3
C	35	HIS	-	expression tag	UNP P9WKX3
D	29	MSE	-	initiating methionine	UNP P9WKX3
D	30	HIS	-	expression tag	UNP P9WKX3
D	31	HIS	-	expression tag	UNP P9WKX3
D	32	HIS	-	expression tag	UNP P9WKX3
D	33	HIS	-	expression tag	UNP P9WKX3
D	34	HIS	-	expression tag	UNP P9WKX3
D	35	HIS	-	expression tag	UNP P9WKX3
E	29	MSE	-	initiating methionine	UNP P9WKX3
E	30	HIS	-	expression tag	UNP P9WKX3
E	31	HIS	-	expression tag	UNP P9WKX3
E	32	HIS	-	expression tag	UNP P9WKX3
E	33	HIS	-	expression tag	UNP P9WKX3
E	34	HIS	-	expression tag	UNP P9WKX3
E	35	HIS	-	expression tag	UNP P9WKX3
F	29	MSE	-	initiating methionine	UNP P9WKX3
F	30	HIS	-	expression tag	UNP P9WKX3
F	31	HIS	-	expression tag	UNP P9WKX3
F	32	HIS	-	expression tag	UNP P9WKX3
F	33	HIS	-	expression tag	UNP P9WKX3
F	34	HIS	-	expression tag	UNP P9WKX3
F	35	HIS	-	expression tag	UNP P9WKX3

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Chain	Residue	Modelled	Actual	Comment	Reference
G	29	MSE	-	initiating methionine	UNP P9WKX3
G	30	HIS	-	expression tag	UNP P9WKX3
G	31	HIS	-	expression tag	UNP P9WKX3
G	32	HIS	-	expression tag	UNP P9WKX3
G	33	HIS	-	expression tag	UNP P9WKX3
G	34	HIS	-	expression tag	UNP P9WKX3
G	35	HIS	-	expression tag	UNP P9WKX3
H	29	MSE	-	initiating methionine	UNP P9WKX3
H	30	HIS	-	expression tag	UNP P9WKX3
H	31	HIS	-	expression tag	UNP P9WKX3
H	32	HIS	-	expression tag	UNP P9WKX3
H	33	HIS	-	expression tag	UNP P9WKX3
H	34	HIS	-	expression tag	UNP P9WKX3
H	35	HIS	-	expression tag	UNP P9WKX3
I	29	MSE	-	initiating methionine	UNP P9WKX3
I	30	HIS	-	expression tag	UNP P9WKX3
I	31	HIS	-	expression tag	UNP P9WKX3
I	32	HIS	-	expression tag	UNP P9WKX3
I	33	HIS	-	expression tag	UNP P9WKX3
I	34	HIS	-	expression tag	UNP P9WKX3
I	35	HIS	-	expression tag	UNP P9WKX3
J	29	MSE	-	initiating methionine	UNP P9WKX3
J	30	HIS	-	expression tag	UNP P9WKX3
J	31	HIS	-	expression tag	UNP P9WKX3
J	32	HIS	-	expression tag	UNP P9WKX3
J	33	HIS	-	expression tag	UNP P9WKX3
J	34	HIS	-	expression tag	UNP P9WKX3
J	35	HIS	-	expression tag	UNP P9WKX3
K	29	MSE	-	initiating methionine	UNP P9WKX3
K	30	HIS	-	expression tag	UNP P9WKX3
K	31	HIS	-	expression tag	UNP P9WKX3
K	32	HIS	-	expression tag	UNP P9WKX3
K	33	HIS	-	expression tag	UNP P9WKX3
K	34	HIS	-	expression tag	UNP P9WKX3
K	35	HIS	-	expression tag	UNP P9WKX3
L	29	MSE	-	initiating methionine	UNP P9WKX3
L	30	HIS	-	expression tag	UNP P9WKX3
L	31	HIS	-	expression tag	UNP P9WKX3
L	32	HIS	-	expression tag	UNP P9WKX3
L	33	HIS	-	expression tag	UNP P9WKX3
L	34	HIS	-	expression tag	UNP P9WKX3
L	35	HIS	-	expression tag	UNP P9WKX3

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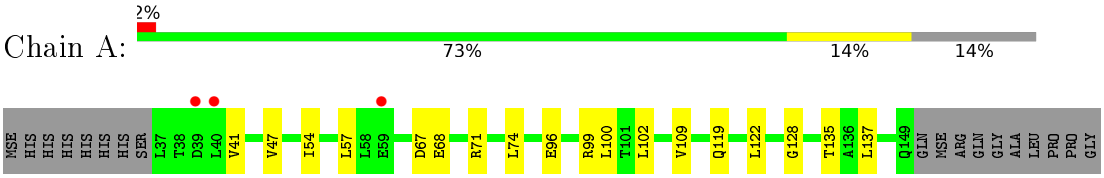
Chain	Residue	Modelled	Actual	Comment	Reference
M	29	MSE	-	initiating methionine	UNP P9WKX3
M	30	HIS	-	expression tag	UNP P9WKX3
M	31	HIS	-	expression tag	UNP P9WKX3
M	32	HIS	-	expression tag	UNP P9WKX3
M	33	HIS	-	expression tag	UNP P9WKX3
M	34	HIS	-	expression tag	UNP P9WKX3
M	35	HIS	-	expression tag	UNP P9WKX3
N	29	MSE	-	initiating methionine	UNP P9WKX3
N	30	HIS	-	expression tag	UNP P9WKX3
N	31	HIS	-	expression tag	UNP P9WKX3
N	32	HIS	-	expression tag	UNP P9WKX3
N	33	HIS	-	expression tag	UNP P9WKX3
N	34	HIS	-	expression tag	UNP P9WKX3
N	35	HIS	-	expression tag	UNP P9WKX3
O	29	MSE	-	initiating methionine	UNP P9WKX3
O	30	HIS	-	expression tag	UNP P9WKX3
O	31	HIS	-	expression tag	UNP P9WKX3
O	32	HIS	-	expression tag	UNP P9WKX3
O	33	HIS	-	expression tag	UNP P9WKX3
O	34	HIS	-	expression tag	UNP P9WKX3
O	35	HIS	-	expression tag	UNP P9WKX3
P	29	MSE	-	initiating methionine	UNP P9WKX3
P	30	HIS	-	expression tag	UNP P9WKX3
P	31	HIS	-	expression tag	UNP P9WKX3
P	32	HIS	-	expression tag	UNP P9WKX3
P	33	HIS	-	expression tag	UNP P9WKX3
P	34	HIS	-	expression tag	UNP P9WKX3
P	35	HIS	-	expression tag	UNP P9WKX3

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

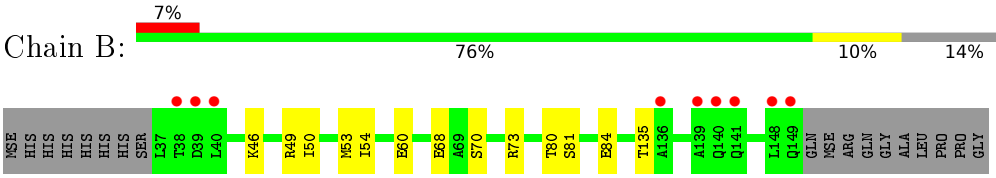
- Molecule 1: Bacterial proteasome activator

Chain A:



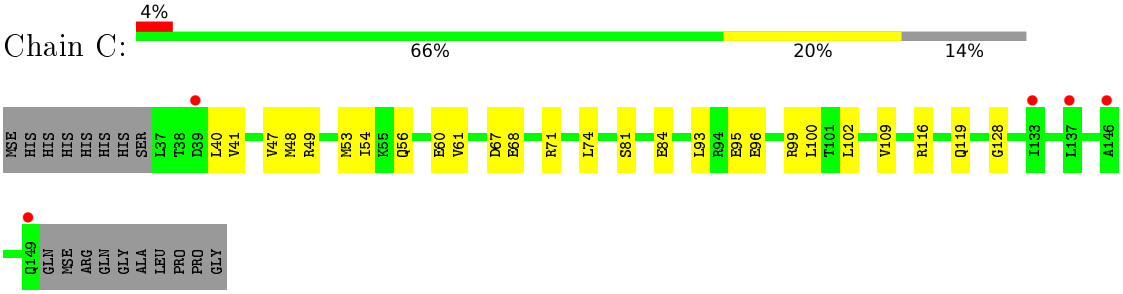
- Molecule 1: Bacterial proteasome activator

Chain B:



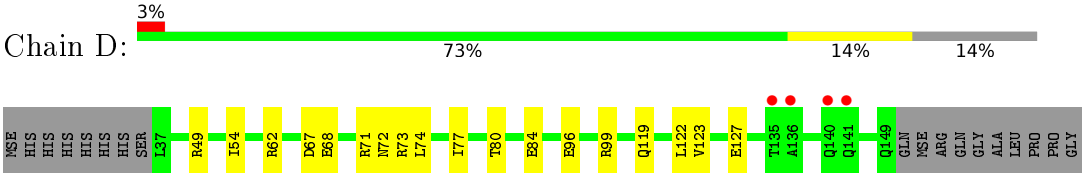
- Molecule 1: Bacterial proteasome activator

Chain C:



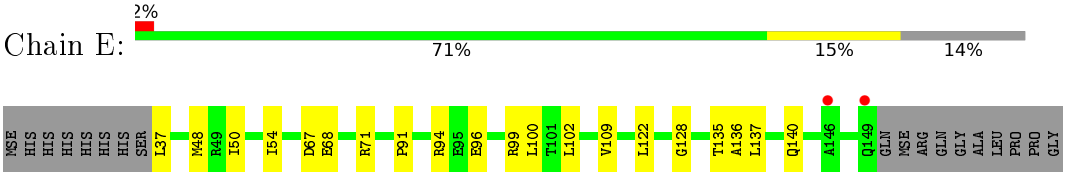
- Molecule 1: Bacterial proteasome activator

Chain D:



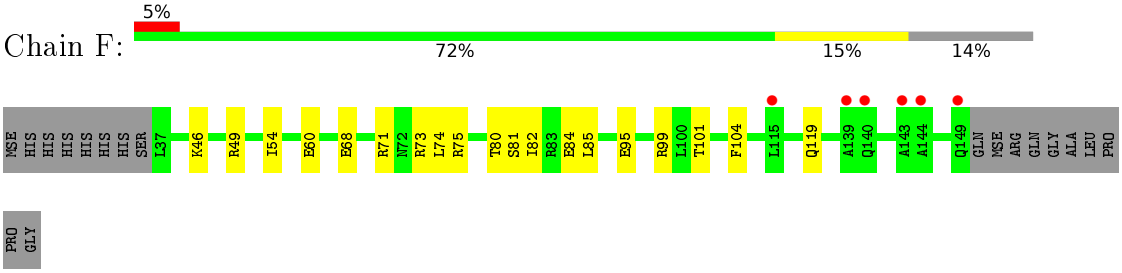
- Molecule 1: Bacterial proteasome activator

Chain E:



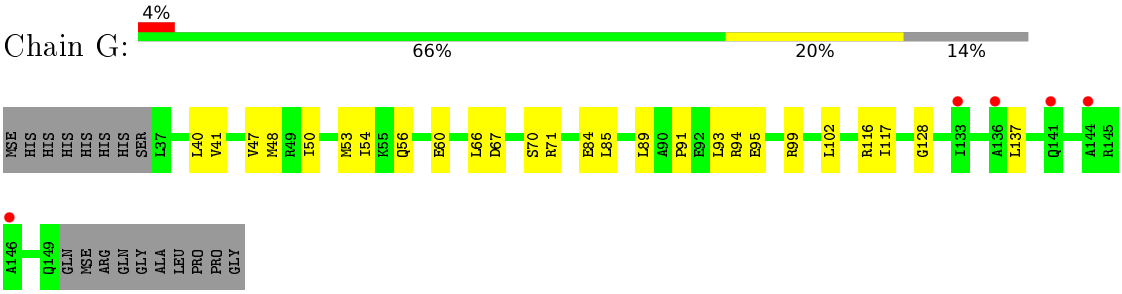
• Molecule 1: Bacterial proteasome activator

Chain F:



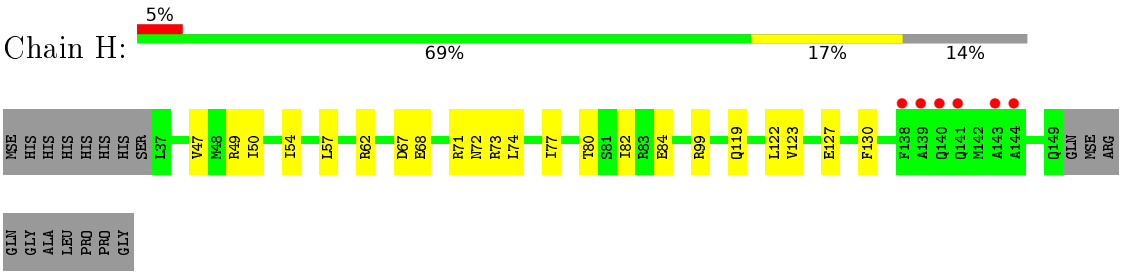
• Molecule 1: Bacterial proteasome activator

Chain G:



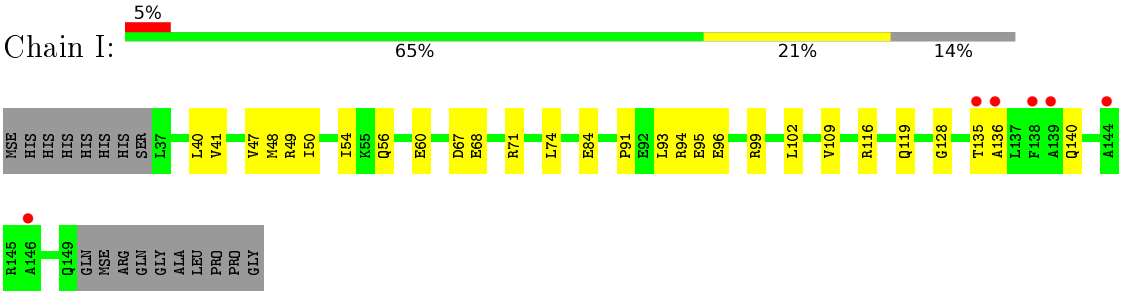
• Molecule 1: Bacterial proteasome activator

Chain H:



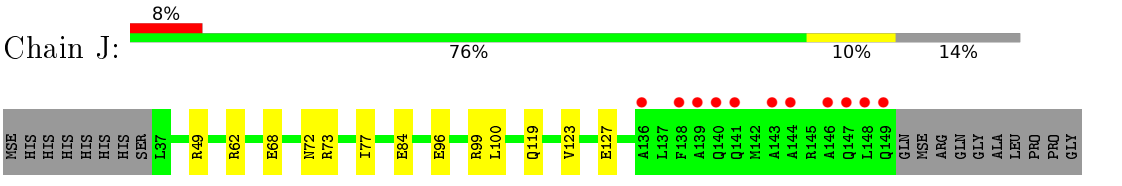
• Molecule 1: Bacterial proteasome activator

Chain I:



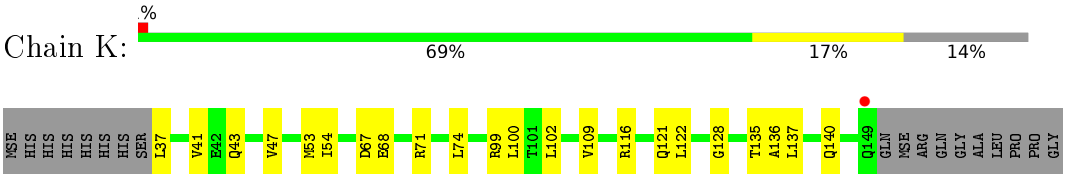
• Molecule 1: Bacterial proteasome activator

Chain J:



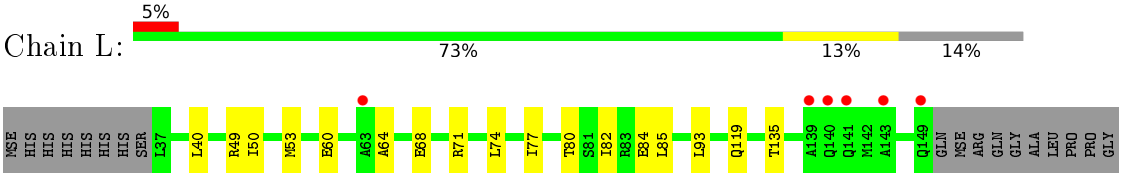
• Molecule 1: Bacterial proteasome activator

Chain K:



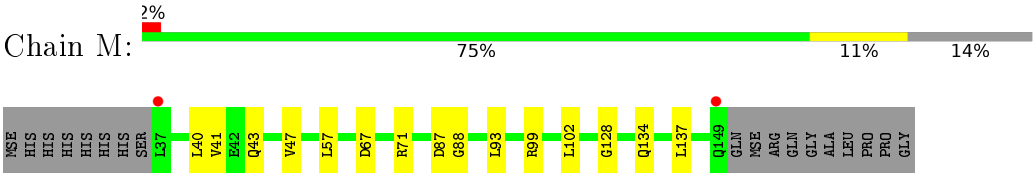
• Molecule 1: Bacterial proteasome activator

Chain L:



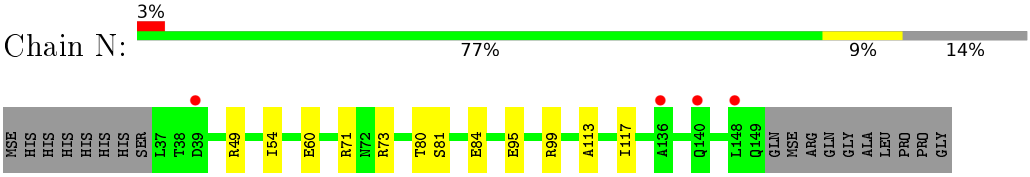
• Molecule 1: Bacterial proteasome activator

Chain M:



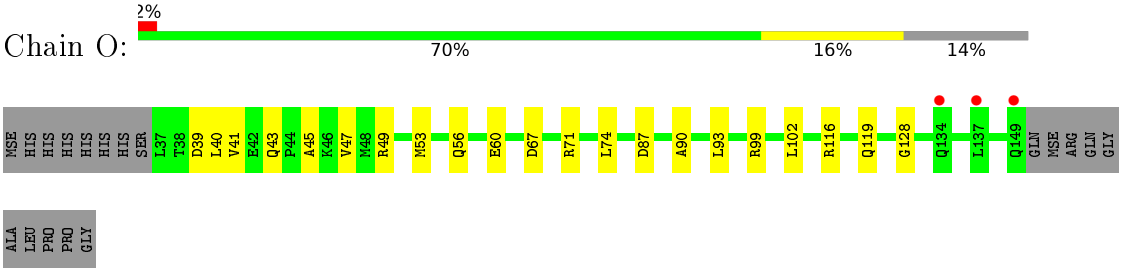
• Molecule 1: Bacterial proteasome activator

Chain N:



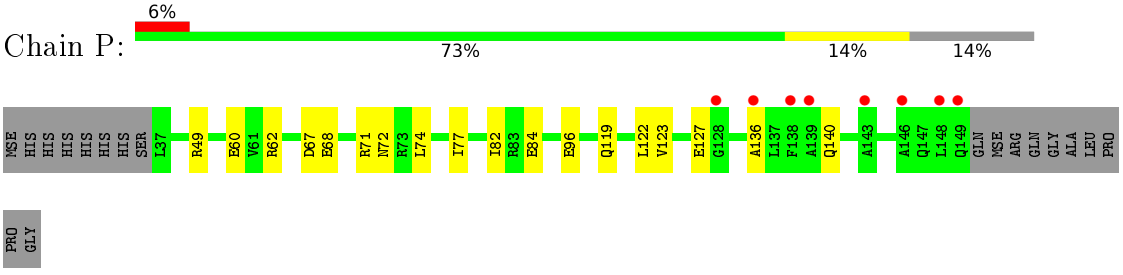
• Molecule 1: Bacterial proteasome activator

Chain O:



• Molecule 1: Bacterial proteasome activator

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	100.85Å 100.85Å 207.43Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.35 – 3.50 49.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	80.7 (45.35-3.50) 72.6 (49.00-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.301 0.240 , 0.302	Depositor DCC
R_{free} test set	1772 reflections (7.85%)	DCC
Wilson B-factor (Å^2)	87.5	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 55.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.349 for -h,-k,l 0.389 for h,-h-k,-l 0.358 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13856	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.40 % 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 7.4983e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.29	0/874	0.47	0/1181
1	B	0.29	0/874	0.46	0/1181
1	C	0.29	0/874	0.45	0/1181
1	D	0.30	0/874	0.47	0/1181
1	E	0.28	0/874	0.45	0/1181
1	F	0.30	0/874	0.46	0/1181
1	G	0.29	0/874	0.47	0/1181
1	H	0.31	0/874	0.47	0/1181
1	I	0.28	0/874	0.45	0/1181
1	J	0.30	0/874	0.46	0/1181
1	K	0.29	0/874	0.46	0/1181
1	L	0.29	0/874	0.46	0/1181
1	M	0.28	0/874	0.44	0/1181
1	N	0.28	0/874	0.45	0/1181
1	O	0.30	0/874	0.47	0/1181
1	P	0.30	0/874	0.49	0/1181
All	All	0.29	0/13984	0.46	0/18896

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	866	0	856	14	0
1	B	866	0	856	10	0
1	C	866	0	856	21	0
1	D	866	0	856	17	0
1	E	866	0	856	14	0
1	F	866	0	856	15	0
1	G	866	0	856	19	0
1	H	866	0	856	21	0
1	I	866	0	856	22	0
1	J	866	0	856	12	0
1	K	866	0	856	15	0
1	L	866	0	856	12	0
1	M	866	0	856	11	0
1	N	866	0	856	10	0
1	O	866	0	856	18	0
1	P	866	0	856	16	0
All	All	13856	0	13696	181	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 7.

All (181) 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:I:116:ARG:NH1	1:N:60:GLU:OE1	2.18	0.77
1:C:60:GLU:OE2	1:D:62:ARG:NH2	2.20	0.75
1:L:60:GLU:OE1	1:O:116:ARG:NH1	2.22	0.72
1:A:99:ARG:NE	1:H:84:GLU:OE2	2.20	0.72
1:C:96:GLU:OE2	1:F:49:ARG:NH1	2.23	0.71
1:C:116:ARG:NH1	1:F:60:GLU:OE1	2.22	0.71
1:O:56:GLN:NE2	1:P:127:GLU:OE1	2.23	0.71
1:B:68:GLU:OE2	1:N:71:ARG:NH1	2.26	0.69
1:G:60:GLU:OE2	1:H:62:ARG:NH2	2.26	0.69
1:J:84:GLU:OE2	1:M:99:ARG:NE	2.25	0.68
1:C:84:GLU:OE2	1:D:99:ARG:NE	2.28	0.65
1:C:99:ARG:NE	1:F:84:GLU:OE2	2.28	0.64
1:D:84:GLU:OE2	1:E:99:ARG:NE	2.26	0.64
1:I:56:GLN:NE2	1:J:127:GLU:OE1	2.30	0.64
1:L:84:GLU:OE2	1:O:99:ARG:NE	2.27	0.63
1:O:40:LEU:HB3	1:O:93:LEU:HD11	1.82	0.62
1:I:99:ARG:NE	1:N:84:GLU:OE2	2.27	0.62
1:O:60:GLU:OE2	1:P:62:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:ARG:HG3	1:F:104:PHE:CD1	2.37	0.59
1:B:84:GLU:OE2	1:G:99:ARG:NE	2.30	0.59
1:K:99:ARG:NE	1:P:84:GLU:OE2	2.31	0.59
1:K:68:GLU:HG3	1:K:109:VAL:HG11	1.85	0.58
1:I:41:VAL:HG13	1:I:47:VAL:HG21	1.85	0.58
1:D:74:LEU:HD22	1:D:119:GLN:NE2	2.17	0.58
1:A:68:GLU:HG3	1:A:109:VAL:HG11	1.86	0.58
1:C:49:ARG:NH1	1:D:96:GLU:OE2	2.37	0.58
1:O:49:ARG:NH1	1:P:96:GLU:OE2	2.37	0.58
1:M:134:GLN:HA	1:M:137:LEU:HB2	1.84	0.57
1:K:54:ILE:HD13	1:K:122:LEU:HD23	1.87	0.57
1:O:41:VAL:HG13	1:O:47:VAL:HG21	1.85	0.57
1:G:40:LEU:HB3	1:G:93:LEU:HD11	1.87	0.57
1:C:40:LEU:HB3	1:C:93:LEU:HD11	1.87	0.57
1:P:74:LEU:HD22	1:P:119:GLN:NE2	2.20	0.56
1:H:74:LEU:HD22	1:H:119:GLN:NE2	2.20	0.56
1:I:60:GLU:OE2	1:J:62:ARG:NH2	2.38	0.56
1:C:68:GLU:HG3	1:C:109:VAL:HG11	1.87	0.56
1:D:74:LEU:HD22	1:D:119:GLN:HE22	1.71	0.56
1:L:74:LEU:HD22	1:L:119:GLN:HE22	1.71	0.55
1:N:54:ILE:HD11	1:N:81:SER:HB2	1.90	0.54
1:F:71:ARG:NH1	1:L:68:GLU:OE2	2.41	0.54
1:G:84:GLU:OE2	1:H:99:ARG:NE	2.37	0.53
1:K:128:GLY:HA3	1:P:49:ARG:HA	1.92	0.52
1:K:102:LEU:HD11	1:P:77:ILE:HG13	1.91	0.52
1:H:119:GLN:O	1:H:123:VAL:HG23	2.09	0.52
1:I:74:LEU:HD22	1:I:119:GLN:NE2	2.24	0.52
1:G:56:GLN:NE2	1:H:127:GLU:OE1	2.42	0.52
1:M:43:GLN:NE2	1:M:87:ASP:OD2	2.42	0.52
1:I:49:ARG:NH1	1:J:96:GLU:OE2	2.43	0.52
1:B:60:GLU:OE1	1:G:116:ARG:NH1	2.41	0.52
1:C:102:LEU:HD13	1:F:73:ARG:HG2	1.90	0.51
1:H:74:LEU:HD22	1:H:119:GLN:HE22	1.75	0.51
1:I:102:LEU:HD13	1:N:73:ARG:HG2	1.91	0.51
1:D:68:GLU:HG3	1:P:68:GLU:HG3	1.92	0.51
1:O:67:ASP:O	1:O:71:ARG:HG3	2.10	0.51
1:A:128:GLY:HA3	1:H:49:ARG:HA	1.92	0.51
1:K:67:ASP:O	1:K:71:ARG:HG3	2.10	0.51
1:C:41:VAL:HG13	1:C:47:VAL:HG21	1.92	0.51
1:B:50:ILE:HG23	1:B:53:MSE:HE2	1.93	0.51
1:D:80:THR:HG22	1:E:100:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:ARG:O	1:F:80:THR:HG21	2.11	0.50
1:B:73:ARG:HG2	1:G:102:LEU:HD13	1.92	0.50
1:I:84:GLU:OE2	1:J:99:ARG:NE	2.38	0.50
1:D:73:ARG:HG2	1:E:102:LEU:HD13	1.92	0.50
1:C:74:LEU:HD22	1:C:119:GLN:OE1	2.12	0.50
1:D:77:ILE:HG13	1:E:102:LEU:HD11	1.92	0.50
1:D:68:GLU:O	1:D:72:ASN:HB2	2.12	0.50
1:A:74:LEU:HD22	1:A:119:GLN:HE22	1.77	0.50
1:L:49:ARG:HA	1:O:128:GLY:HA3	1.95	0.49
1:C:100:LEU:HD21	1:F:84:GLU:HG3	1.94	0.49
1:E:54:ILE:HD13	1:E:122:LEU:HD23	1.94	0.49
1:I:74:LEU:HD22	1:I:119:GLN:HE22	1.78	0.49
1:M:41:VAL:HG13	1:M:47:VAL:HG21	1.95	0.49
1:D:119:GLN:O	1:D:123:VAL:HG23	2.13	0.48
1:E:67:ASP:O	1:E:71:ARG:HG3	2.13	0.48
1:I:68:GLU:HG3	1:I:109:VAL:HG11	1.94	0.48
1:J:119:GLN:O	1:J:123:VAL:HG23	2.13	0.48
1:O:74:LEU:HD22	1:O:119:GLN:NE2	2.29	0.48
1:I:128:GLY:HA3	1:N:49:ARG:HA	1.94	0.48
1:E:136:ALA:O	1:E:140:GLN:HG3	2.12	0.48
1:H:68:GLU:HG3	1:J:68:GLU:HG3	1.95	0.48
1:I:99:ARG:O	1:N:80:THR:HG21	2.14	0.48
1:A:41:VAL:HG13	1:A:47:VAL:HG21	1.96	0.48
1:F:82:ILE:HA	1:F:85:LEU:HB2	1.96	0.47
1:J:73:ARG:HG2	1:M:102:LEU:HD13	1.96	0.47
1:D:49:ARG:NH1	1:E:96:GLU:OE2	2.47	0.47
1:L:50:ILE:HG23	1:L:53:MSE:HE2	1.97	0.47
1:M:67:ASP:O	1:M:71:ARG:HG3	2.14	0.47
1:A:74:LEU:HD22	1:A:119:GLN:NE2	2.29	0.47
1:C:56:GLN:NE2	1:D:127:GLU:OE1	2.48	0.47
1:K:116:ARG:NH1	1:P:60:GLU:OE1	2.42	0.47
1:A:54:ILE:HD13	1:A:122:LEU:HD23	1.97	0.47
1:I:96:GLU:OE2	1:N:49:ARG:NH1	2.48	0.47
1:A:96:GLU:OE2	1:H:49:ARG:NH1	2.48	0.47
1:G:41:VAL:HG13	1:G:47:VAL:HG21	1.96	0.47
1:G:48:MSE:HE2	1:G:48:MSE:HB3	1.77	0.47
1:A:100:LEU:HD23	1:H:80:THR:HG22	1.96	0.47
1:H:50:ILE:O	1:H:54:ILE:HG13	2.15	0.46
1:G:53:MSE:HE2	1:G:53:MSE:HB3	1.91	0.46
1:K:41:VAL:HG13	1:K:47:VAL:HG21	1.97	0.46
1:K:100:LEU:O	1:K:121:GLN:NE2	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ILE:HD13	1:D:122:LEU:HD23	1.97	0.46
1:G:91:PRO:HA	1:G:94:ARG:HD2	1.97	0.45
1:N:113:ALA:O	1:N:117:ILE:HG12	2.16	0.45
1:I:48:MSE:HB3	1:I:48:MSE:HE2	1.84	0.45
1:C:48:MSE:HB3	1:C:48:MSE:HE2	1.93	0.45
1:P:82:ILE:HG12	1:P:122:LEU:HD21	1.99	0.45
1:P:74:LEU:HD22	1:P:119:GLN:HE22	1.81	0.45
1:H:67:ASP:O	1:H:71:ARG:HG3	2.17	0.45
1:P:119:GLN:O	1:P:123:VAL:HG23	2.17	0.44
1:I:84:GLU:HG3	1:J:100:LEU:HD21	1.98	0.44
1:C:53:MSE:HE2	1:C:53:MSE:HB3	1.79	0.44
1:E:68:GLU:HG3	1:E:109:VAL:HG11	1.97	0.44
1:H:68:GLU:O	1:H:72:ASN:HB2	2.18	0.44
1:O:39:ASP:O	1:O:90:ALA:HB2	2.17	0.44
1:F:46:LYS:HE2	1:F:84:GLU:O	2.18	0.44
1:G:50:ILE:O	1:G:54:ILE:HG13	2.17	0.44
1:O:74:LEU:HD22	1:O:119:GLN:HE22	1.83	0.44
1:D:49:ARG:HA	1:E:128:GLY:HA3	2.00	0.44
1:I:50:ILE:O	1:I:54:ILE:HG13	2.18	0.44
1:F:68:GLU:OE2	1:L:71:ARG:NH1	2.51	0.44
1:A:102:LEU:HD11	1:H:77:ILE:HG13	1.99	0.44
1:F:54:ILE:HD11	1:F:81:SER:HB2	1.99	0.43
1:A:99:ARG:O	1:H:80:THR:HG21	2.18	0.43
1:B:54:ILE:HD11	1:B:81:SER:HB2	1.99	0.43
1:C:67:ASP:O	1:C:71:ARG:HG3	2.19	0.43
1:H:74:LEU:HA	1:H:74:LEU:HD23	1.89	0.43
1:P:67:ASP:O	1:P:71:ARG:HG3	2.19	0.43
1:P:68:GLU:O	1:P:72:ASN:HB2	2.18	0.43
1:B:46:LYS:HE2	1:B:84:GLU:O	2.19	0.43
1:B:49:ARG:HA	1:G:128:GLY:HA3	2.01	0.43
1:E:91:PRO:HA	1:E:94:ARG:HD2	2.00	0.43
1:C:128:GLY:HA3	1:F:49:ARG:HA	2.00	0.43
1:C:54:ILE:HD11	1:C:81:SER:HB2	2.00	0.43
1:M:57:LEU:HA	1:M:57:LEU:HD23	1.91	0.43
1:H:82:ILE:HG12	1:H:122:LEU:HD21	2.01	0.43
1:L:80:THR:HG21	1:O:99:ARG:O	2.19	0.42
1:I:95:GLU:O	1:I:99:ARG:N	2.45	0.42
1:K:37:LEU:HD12	1:K:37:LEU:HA	1.84	0.42
1:P:74:LEU:HA	1:P:74:LEU:HD23	1.89	0.42
1:L:40:LEU:HB3	1:L:93:LEU:HD11	2.01	0.42
1:G:85:LEU:O	1:G:89:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:68:GLU:O	1:J:72:ASN:HB2	2.19	0.42
1:A:67:ASP:O	1:A:71:ARG:HG3	2.19	0.42
1:L:82:ILE:HA	1:L:85:LEU:HB2	2.02	0.42
1:J:49:ARG:HA	1:M:128:GLY:HA3	2.02	0.42
1:L:64:ALA:HB3	1:O:116:ARG:NH2	2.35	0.42
1:A:102:LEU:HD13	1:H:73:ARG:HG2	2.02	0.42
1:C:95:GLU:O	1:C:99:ARG:HG3	2.19	0.42
1:G:67:ASP:O	1:G:71:ARG:HG3	2.20	0.42
1:K:43:GLN:O	1:K:47:VAL:HG23	2.20	0.42
1:O:53:MSE:HB3	1:O:53:MSE:HE2	1.87	0.42
1:E:50:ILE:O	1:E:54:ILE:HG13	2.19	0.42
1:F:74:LEU:HD22	1:F:119:GLN:OE1	2.20	0.42
1:M:40:LEU:HB3	1:M:93:LEU:HD11	2.02	0.41
1:P:136:ALA:O	1:P:140:GLN:HG3	2.20	0.41
1:K:137:LEU:HD23	1:K:137:LEU:HA	1.93	0.41
1:O:43:GLN:NE2	1:O:87:ASP:OD2	2.54	0.41
1:D:67:ASP:O	1:D:71:ARG:HG3	2.19	0.41
1:G:66:LEU:HB3	1:G:70:SER:OG	2.20	0.41
1:H:47:VAL:HG12	1:H:130:PHE:CZ	2.55	0.41
1:H:57:LEU:HA	1:H:57:LEU:HD23	1.92	0.41
1:I:136:ALA:O	1:I:140:GLN:HG3	2.20	0.41
1:I:91:PRO:HA	1:I:94:ARG:HD2	2.01	0.41
1:J:77:ILE:HG13	1:M:102:LEU:HD11	2.03	0.41
1:B:70:SER:HB3	1:G:117:ILE:HG13	2.03	0.41
1:G:95:GLU:O	1:G:99:ARG:HG3	2.20	0.41
1:B:80:THR:HG21	1:G:99:ARG:O	2.20	0.41
1:K:53:MSE:HE2	1:K:53:MSE:HB3	1.88	0.41
1:M:43:GLN:HG3	1:M:88:GLY:HA2	2.02	0.41
1:L:77:ILE:HD11	1:O:102:LEU:HD11	2.02	0.41
1:O:45:ALA:O	1:O:49:ARG:HB2	2.20	0.41
1:I:67:ASP:O	1:I:71:ARG:HG3	2.20	0.41
1:K:136:ALA:O	1:K:140:GLN:HG3	2.21	0.41
1:K:74:LEU:HD23	1:K:74:LEU:HA	1.84	0.41
1:A:57:LEU:HA	1:A:57:LEU:HD23	1.92	0.40
1:E:48:MSE:HE2	1:E:48:MSE:HB3	1.88	0.40
1:I:40:LEU:HB3	1:I:93:LEU:HD11	2.04	0.40
1:E:137:LEU:HD23	1:E:137:LEU:HA	1.91	0.40
1:C:61:VAL:HG22	1:C:74:LEU:HD11	2.04	0.40
1:F:95:GLU:O	1:F:99:ARG:HG3	2.21	0.40
1:N:95:GLU:O	1:N:99:ARG:HG3	2.22	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	111/131 (85%)	110 (99%)	1 (1%)	0	100	100
1	B	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	C	111/131 (85%)	110 (99%)	1 (1%)	0	100	100
1	D	111/131 (85%)	110 (99%)	1 (1%)	0	100	100
1	E	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	F	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	G	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	H	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	I	111/131 (85%)	110 (99%)	1 (1%)	0	100	100
1	J	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	K	111/131 (85%)	110 (99%)	1 (1%)	0	100	100
1	L	111/131 (85%)	108 (97%)	3 (3%)	0	100	100
1	M	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
1	N	111/131 (85%)	107 (96%)	4 (4%)	0	100	100
1	O	111/131 (85%)	108 (97%)	3 (3%)	0	100	100
1	P	111/131 (85%)	109 (98%)	2 (2%)	0	100	100
All	All	1776/2096 (85%)	1745 (98%)	31 (2%)	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	87/103 (84%)	85 (98%)	2 (2%)	58 85
1	B	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	C	87/103 (84%)	87 (100%)	0	100 100
1	D	87/103 (84%)	87 (100%)	0	100 100
1	E	87/103 (84%)	85 (98%)	2 (2%)	58 85
1	F	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	G	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	H	87/103 (84%)	87 (100%)	0	100 100
1	I	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	J	87/103 (84%)	87 (100%)	0	100 100
1	K	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	L	87/103 (84%)	86 (99%)	1 (1%)	80 92
1	M	87/103 (84%)	87 (100%)	0	100 100
1	N	87/103 (84%)	87 (100%)	0	100 100
1	O	87/103 (84%)	87 (100%)	0	100 100
1	P	87/103 (84%)	87 (100%)	0	100 100
All	All	1392/1648 (84%)	1382 (99%)	10 (1%)	88 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	THR
1	A	137	LEU
1	B	135	THR
1	E	37	LEU
1	E	135	THR
1	F	101	THR
1	G	137	LEU
1	I	135	THR
1	K	135	THR
1	L	135	THR

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

Mol	Chain	Res	Type
1	L	119	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	110/131 (83%)	-0.08	3 (2%) 58 47	60, 91, 213, 265	0
1	B	110/131 (83%)	0.03	9 (8%) 14 12	56, 83, 234, 392	0
1	C	110/131 (83%)	0.08	5 (4%) 37 29	70, 99, 225, 350	0
1	D	110/131 (83%)	0.13	4 (3%) 46 37	61, 91, 229, 325	0
1	E	110/131 (83%)	-0.00	2 (1%) 71 62	77, 96, 195, 261	0
1	F	110/131 (83%)	0.12	6 (5%) 29 22	76, 94, 218, 406	0
1	G	110/131 (83%)	-0.02	5 (4%) 37 29	47, 91, 180, 315	0
1	H	110/131 (83%)	0.25	6 (5%) 29 22	41, 86, 241, 407	0
1	I	110/131 (83%)	0.11	6 (5%) 29 22	73, 99, 182, 348	0
1	J	110/131 (83%)	0.37	11 (10%) 9 9	59, 96, 229, 369	0
1	K	110/131 (83%)	-0.06	1 (0%) 85 78	55, 90, 203, 263	0
1	L	110/131 (83%)	0.10	6 (5%) 29 22	49, 86, 222, 410	0
1	M	110/131 (83%)	-0.05	2 (1%) 71 62	81, 102, 213, 305	0
1	N	110/131 (83%)	0.06	4 (3%) 46 37	74, 95, 202, 367	0
1	O	110/131 (83%)	-0.06	3 (2%) 58 47	47, 92, 199, 301	0
1	P	110/131 (83%)	0.09	8 (7%) 18 14	40, 87, 204, 439	0
All	All	1760/2096 (83%)	0.07	81 (4%) 36 28	40, 93, 225, 439	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	143	ALA	10.0
1	J	140	GLN	9.9
1	H	140	GLN	9.2
1	J	143	ALA	6.8
1	L	140	GLN	6.2

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Mol	Chain	Res	Type	RSRZ
1	C	149	GLN	6.2
1	J	139	ALA	5.8
1	J	141	GLN	5.5
1	H	139	ALA	5.4
1	J	149	GLN	5.0
1	F	139	ALA	4.9
1	D	140	GLN	4.9
1	D	141	GLN	4.8
1	N	140	GLN	4.7
1	F	144	ALA	4.6
1	B	140	GLN	4.5
1	J	144	ALA	4.5
1	I	135	THR	4.5
1	H	144	ALA	4.4
1	J	148	LEU	4.4
1	D	136	ALA	3.9
1	F	140	GLN	3.9
1	O	149	GLN	3.8
1	H	141	GLN	3.7
1	P	148	LEU	3.7
1	L	141	GLN	3.7
1	P	146	ALA	3.6
1	P	149	GLN	3.6
1	B	136	ALA	3.5
1	C	39	ASP	3.4
1	I	146	ALA	3.4
1	G	146	ALA	3.3
1	G	144	ALA	3.1
1	H	138	PHE	3.1
1	L	149	GLN	3.1
1	N	136	ALA	3.1
1	B	38	THR	3.1
1	O	134	GLN	2.9
1	M	149	GLN	2.9
1	F	149	GLN	2.9
1	J	138	PHE	2.8
1	L	139	ALA	2.7
1	B	141	GLN	2.7
1	B	149	GLN	2.7
1	J	146	ALA	2.7
1	A	39	ASP	2.7
1	F	143	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	141	GLN	2.6
1	B	148	LEU	2.6
1	P	128	GLY	2.6
1	K	149	GLN	2.6
1	J	136	ALA	2.5
1	B	39	ASP	2.4
1	E	146	ALA	2.4
1	P	136	ALA	2.4
1	I	136	ALA	2.4
1	L	63	ALA	2.4
1	N	39	ASP	2.4
1	I	144	ALA	2.3
1	G	133	ILE	2.3
1	A	40	LEU	2.3
1	D	135	THR	2.2
1	G	136	ALA	2.2
1	C	137	LEU	2.2
1	B	139	ALA	2.2
1	A	59	GLU	2.2
1	P	139	ALA	2.2
1	I	138	PHE	2.2
1	J	147	GLN	2.1
1	I	139	ALA	2.1
1	P	138	PHE	2.1
1	F	115	LEU	2.1
1	E	149	GLN	2.1
1	P	143	ALA	2.1
1	C	133	ILE	2.1
1	M	37	LEU	2.1
1	O	137	LEU	2.1
1	L	143	ALA	2.1
1	N	148	LEU	2.0
1	C	146	ALA	2.0
1	B	40	LEU	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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.