



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:23 AM GMT

PDB ID : 1G4B  
Title : CRYSTAL STRUCTURES OF THE HSLVU PEPTIDASE-ATPASE COM-  
PLEX REVEAL AN ATP-DEPENDENT PROTEOLYSIS MECHANISM  
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Deposited on : 2000-10-26  
Resolution : 7.00 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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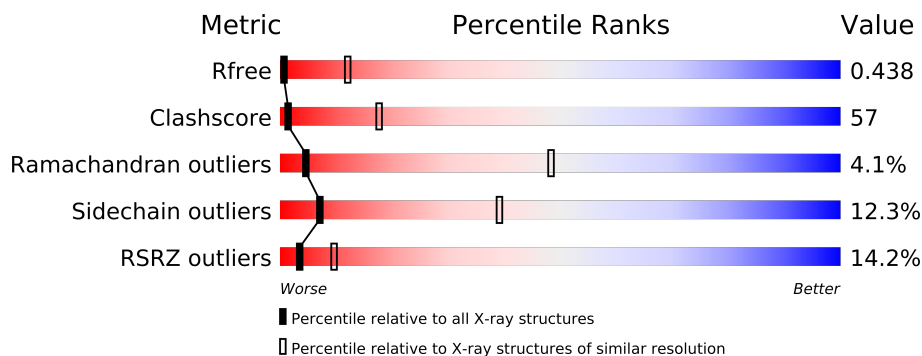
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 7.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1098 (10.00-3.50)
Clashscore	79885	1039 (10.00-3.52)
Ramachandran outliers	78287	1291 (9.50-3.50)
Sidechain outliers	78261	1265 (9.50-3.50)
RSRZ outliers	66119	1097 (10.00-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	E	443	
1	F	443	
1	K	443	
1	L	443	
2	M	175	
2	N	175	
2	O	175	
2	P	175	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17660 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUB-UNIT HSLU.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	F	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	K	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			
1	L	393	Total	C	N	O	S	0	0	0
			3096	1935	551	600	10			

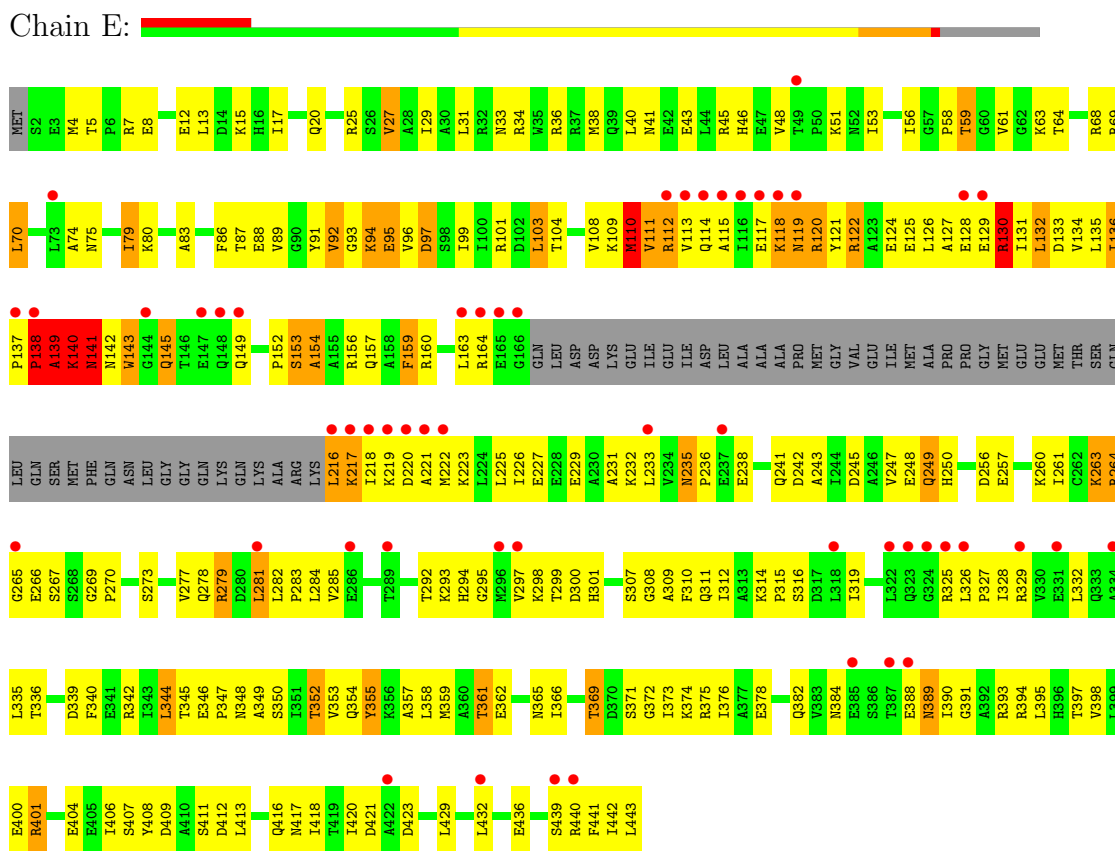
- Molecule 2 is a protein called ATP-DEPENDENT PROTEASE HSLV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	N	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	O	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			
2	P	173	Total	C	N	O	S	0	0	0
			1319	828	235	252	4			

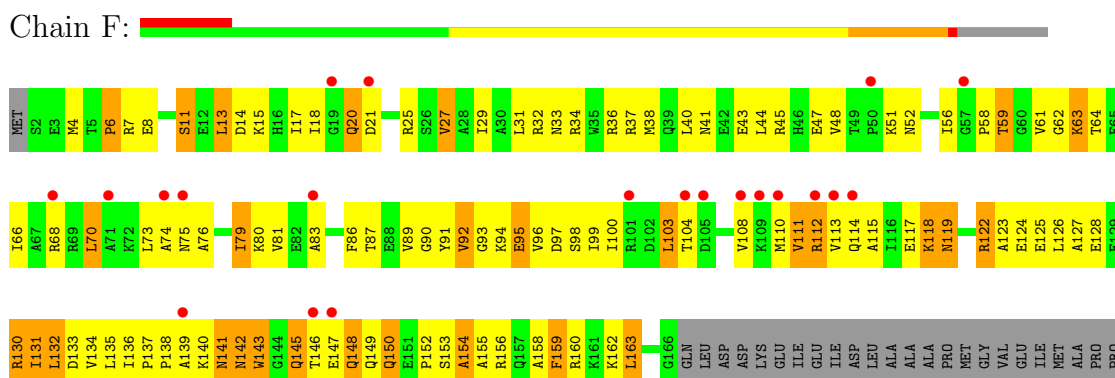
### 3 Residue-property plots

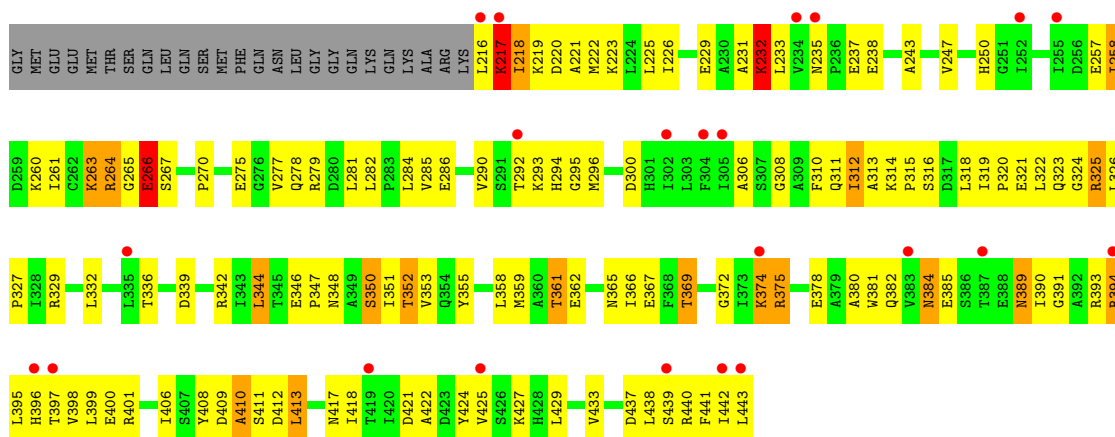
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU



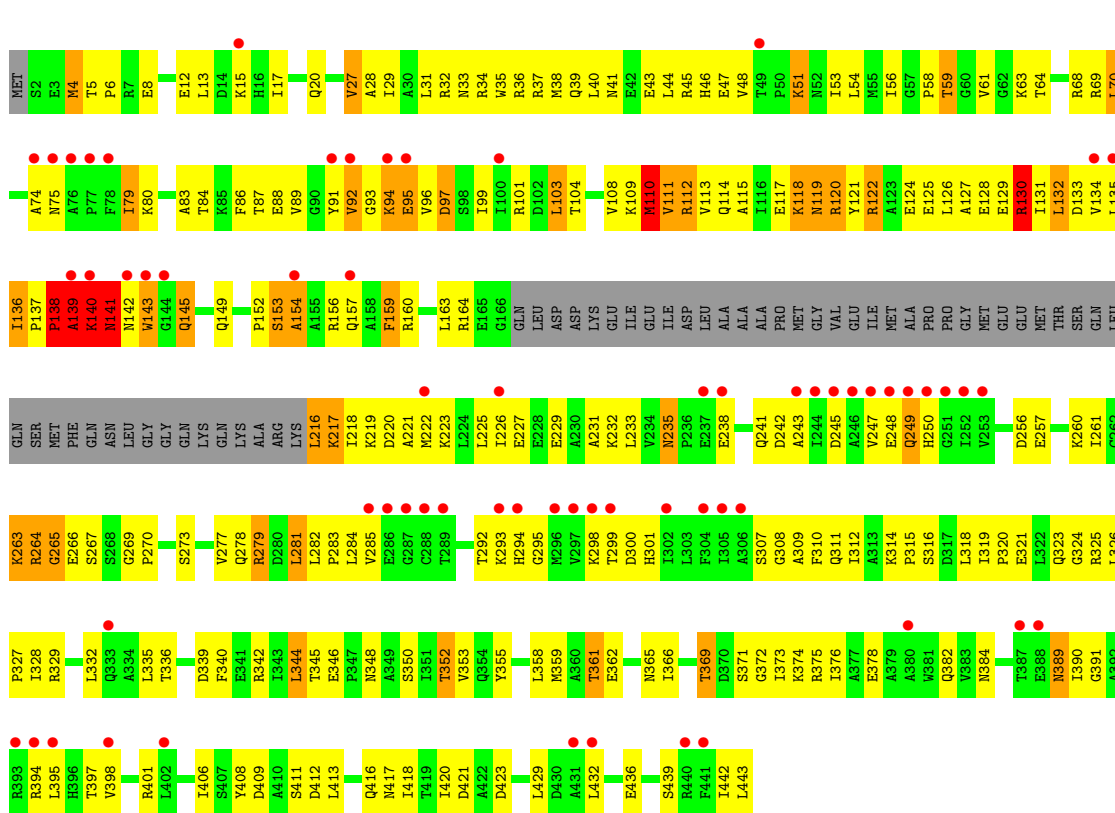
#### • Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU





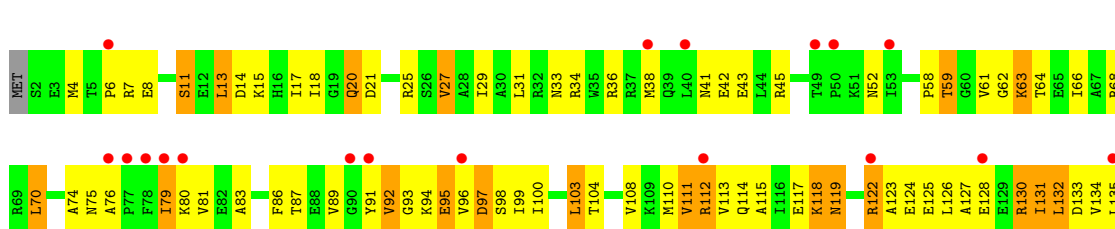
• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

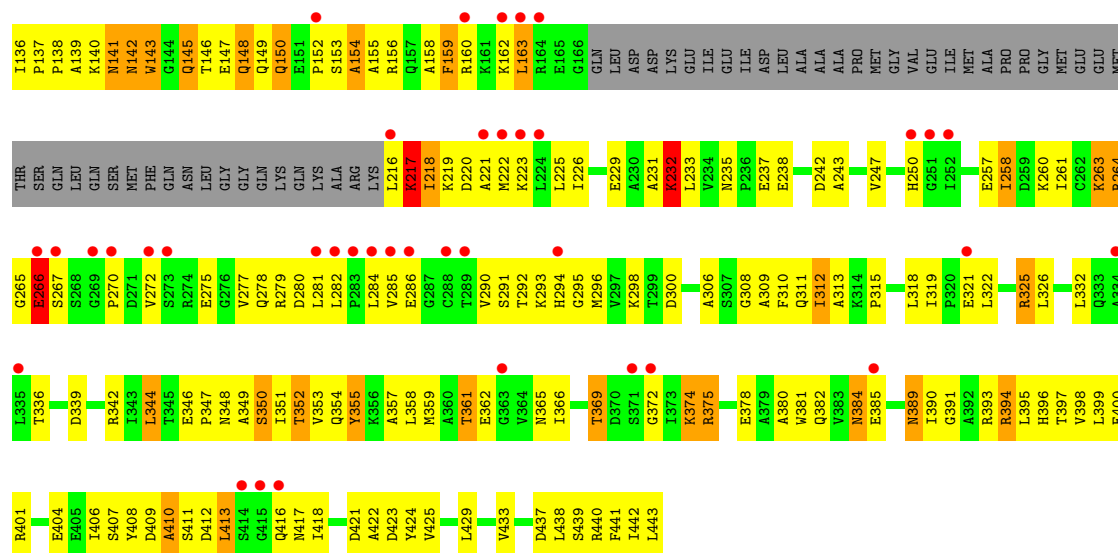
Chain K:



• Molecule 1: ATP-DEPENDENT HSL PROTEASE ATP-BINDING SUBUNIT HSLU

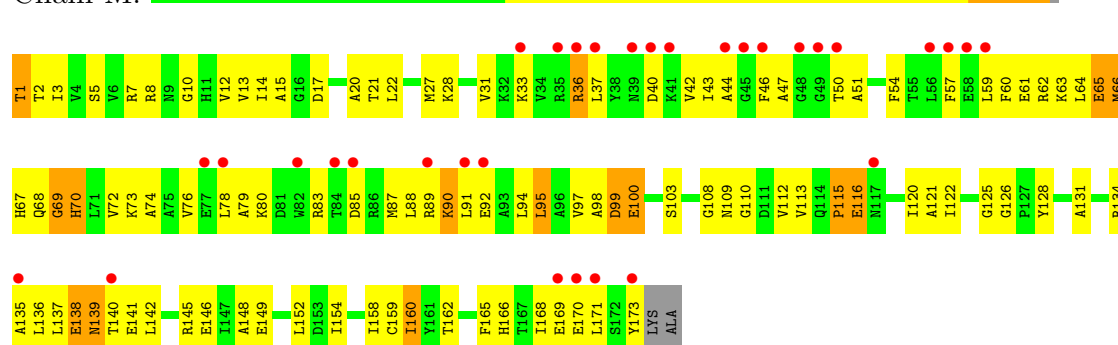
Chain L:





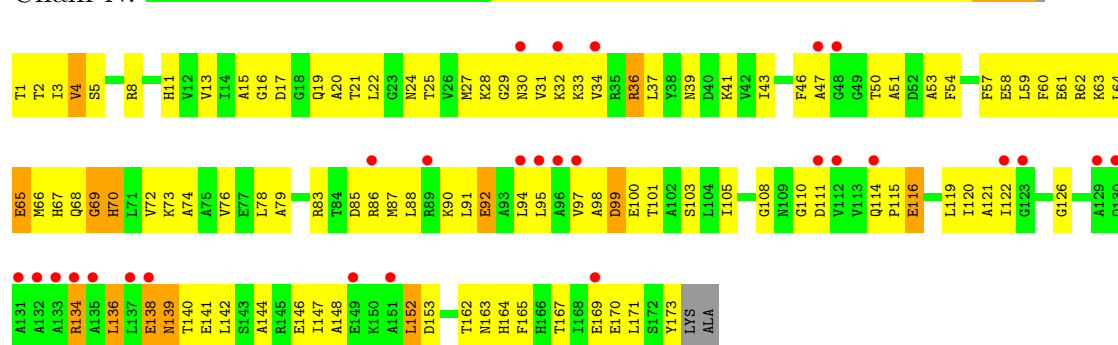
### • Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain M:



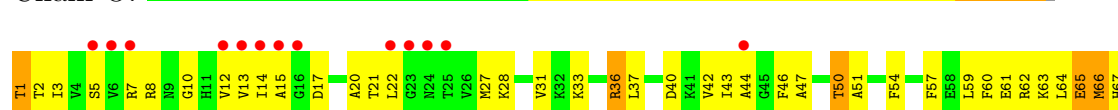
### • Molecule 2: ATP-DEPENDENT PROTEASE HSLV

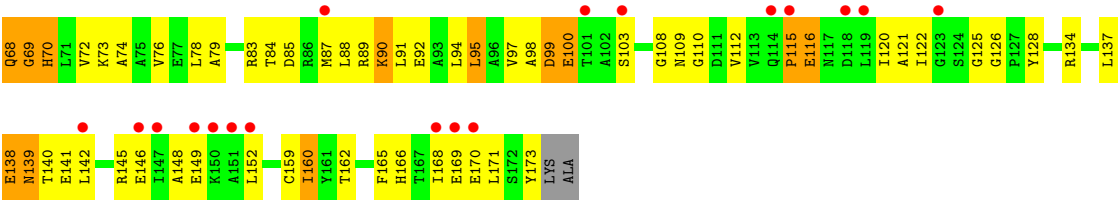
Chain N:



### • Molecule 2: ATP-DEPENDENT PROTEASE HSLV

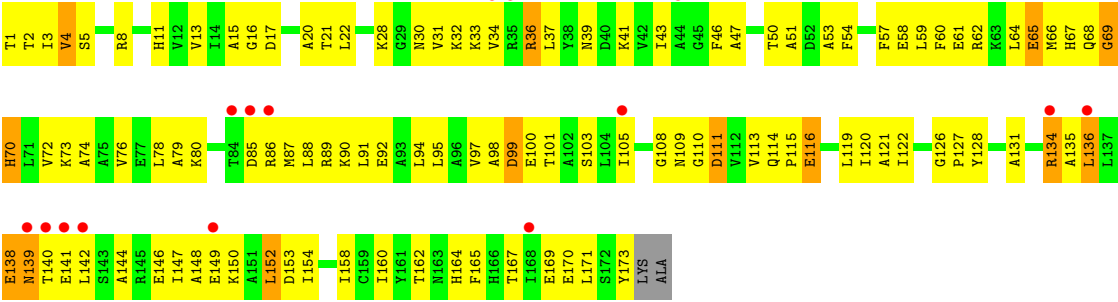
Chain O:





● Molecule 2: ATP-DEPENDENT PROTEASE HSLV

Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	173.38Å 173.38Å 254.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 7.00 82.06 – 7.00	Depositor EDS
% Data completeness (in resolution range)	66.0 (10.00-7.00) 81.1 (82.06-7.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 6.72Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.401 , 0.432 0.446 , 0.438	Depositor DCC
$R_{free}$ test set	560 reflections (9.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	101.1	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 118.1	EDS
Estimated twinning fraction	0.350 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 6405 reflections	Xtriage
$F_o, F_c$ correlation	0.32	EDS
Total number of atoms	17660	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 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	E	0.61	4/3135 (0.1%)	0.96	13/4228 (0.3%)
1	F	0.46	2/3135 (0.1%)	0.70	1/4228 (0.0%)
1	K	0.61	4/3135 (0.1%)	0.96	13/4228 (0.3%)
1	L	0.46	2/3135 (0.1%)	0.70	1/4228 (0.0%)
2	M	0.37	0/1336	0.65	0/1806
2	N	0.37	0/1336	0.65	0/1806
2	O	0.37	0/1336	0.65	0/1806
2	P	0.37	0/1336	0.65	0/1806
All	All	0.50	12/17884 (0.1%)	0.79	28/24136 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	K	0	2
All	All	0	4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	139	ALA	C-N	-17.84	0.93	1.34
1	K	139	ALA	C-N	-17.84	0.93	1.34
1	E	122	ARG	CB-CG	10.32	1.80	1.52
1	K	122	ARG	CB-CG	10.28	1.80	1.52
1	E	145	GLN	CG-CD	8.75	1.71	1.51

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ARG	CA-CB-CG	-18.01	73.78	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	122	ARG	CA-CB-CG	-18.00	73.80	113.40
1	K	141	ASN	CA-C-N	-16.91	80.01	117.20
1	E	141	ASN	CA-C-N	-16.89	80.04	117.20
1	K	145	GLN	CA-CB-CG	-12.09	86.80	113.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	139	ALA	Mainchain
1	E	141	ASN	Mainchain
1	K	139	ALA	Mainchain
1	K	141	ASN	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3096	0	3150	570	49
1	F	3096	0	3155	585	54
1	K	3096	0	3149	320	220
1	L	3096	0	3152	385	225
2	M	1319	0	1335	172	12
2	N	1319	0	1335	141	15
2	O	1319	0	1330	197	14
2	P	1319	0	1327	178	19
All	All	17660	0	17933	2026	305

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 57.

The worst 5 of 2026 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:441:PHE:CD1	1:F:56:ILE:HD13	1.27	1.66
1:K:122:ARG:CB	1:K:122:ARG:CG	1.80	1.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:309:ALA:HB1	2:O:66:MET:CE	1.28	1.58
1:E:442:ILE:HA	1:F:329:ARG:CB	1.12	1.58
1:E:122:ARG:CB	1:E:122:ARG:CG	1.80	1.56

The worst 5 of 305 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:51:LYS:CG	1:L:400:GLU:OE1[3_665]	0.41	1.79
1:K:35:TRP:CE3	1:L:362:GLU:OE2[3_665]	0.55	1.65
1:K:47:GLU:O	1:L:354:GLN:OE1[3_665]	0.59	1.61
1:E:316:SER:CB	1:F:440:ARG:O[2_655]	0.62	1.58
1:K:315:PRO:CA	1:L:440:ARG:O[3_665]	0.66	1.54

## 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	E	389/443 (88%)	335 (86%)	40 (10%)	14 (4%)	5	52
1	F	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	3	43
1	K	389/443 (88%)	335 (86%)	40 (10%)	14 (4%)	5	52
1	L	389/443 (88%)	329 (85%)	41 (10%)	19 (5%)	3	43
2	M	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	4	44
2	N	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	7	58
2	O	171/175 (98%)	145 (85%)	18 (10%)	8 (5%)	4	44
2	P	171/175 (98%)	143 (84%)	23 (14%)	5 (3%)	7	58
All	All	2240/2472 (91%)	1904 (85%)	244 (11%)	92 (4%)	4	48

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	92	VAL

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Mol	Chain	Res	Type
1	E	140	LYS
1	E	154	ALA
1	E	300	ASP
1	F	92	VAL

### 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	E	336/377 (89%)	294 (88%)	42 (12%)	7	38
1	F	336/377 (89%)	287 (85%)	49 (15%)	5	30
1	K	336/377 (89%)	293 (87%)	43 (13%)	6	37
1	L	336/377 (89%)	288 (86%)	48 (14%)	5	31
2	M	135/136 (99%)	124 (92%)	11 (8%)	17	61
2	N	135/136 (99%)	121 (90%)	14 (10%)	10	48
2	O	135/136 (99%)	124 (92%)	11 (8%)	17	61
2	P	135/136 (99%)	121 (90%)	14 (10%)	10	48
All	All	1884/2052 (92%)	1652 (88%)	232 (12%)	7	39

5 of 232 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	103	LEU
1	K	375	ARG
2	O	138	GLU
1	K	119	ASN
1	K	232	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	75	ASN
1	K	389	ASN
2	O	70	HIS

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Mol	Chain	Res	Type
1	K	119	ASN
1	K	235	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	E	393/443 (88%)	0.90	53 (13%) 4 10	60, 60, 60, 60	0
1	F	393/443 (88%)	0.83	43 (10%) 6 14	60, 60, 60, 60	0
1	K	393/443 (88%)	1.03	64 (16%) 2 8	60, 60, 60, 60	0
1	L	393/443 (88%)	0.98	56 (14%) 3 9	60, 60, 60, 60	0
2	M	173/175 (98%)	1.05	32 (18%) 2 6	60, 60, 60, 60	0
2	N	173/175 (98%)	1.05	28 (16%) 2 8	60, 60, 60, 60	0
2	O	173/175 (98%)	1.13	31 (17%) 2 7	60, 60, 60, 60	0
2	P	173/175 (98%)	0.71	15 (8%) 10 19	60, 60, 60, 60	0
All	All	2264/2472 (91%)	0.95	322 (14%) 3 9	60, 60, 60, 60	0

The worst 5 of 322 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	8.8
1	F	443	LEU	7.5
1	L	288	CYS	7.3
1	L	289	THR	7.2
1	K	289	THR	6.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.