



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:05 pm BST

PDB ID : 5X6V  
Title : Crystal structure of human heteroheptameric complex  
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Deposited on : 2017-02-23  
Resolution : 2.02 Å(reported)

This is a wwPDB X-ray Structure 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

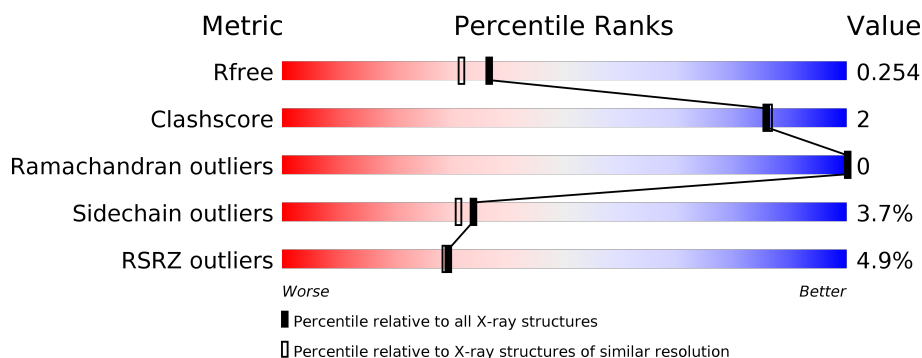
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 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	127	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
2	B	125	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
3	C	91	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>
4	D	99	<div> <div>10%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>14%</div> </div> </div>
5	E	123	<div> <div>10%</div> <div> <div></div> <div>80%</div> <div>7%</div> <div>•</div> <div>12%</div> </div> </div>
6	F	135	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	G	139	<div><div><div>%</div><div><div></div></div><div>88%</div><div>7%</div><div>5%</div></div></div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6417 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 Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			939	604	158	176	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP Q9UHA4
A	-1	GLY	-	expression tag	UNP Q9UHA4
A	0	SER	-	expression tag	UNP Q9UHA4
A	1	SER	-	expression tag	UNP Q9UHA4

- Molecule 2 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	1	0
			950	596	163	183	8			

- Molecule 3 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	2	0
			676	413	116	139	8			

- Molecule 4 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	85	Total	C	N	O	S	0	0	0
			647	407	116	123	1			

- Molecule 5 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	108	Total	C	N	O	S	0	0	0
			846	536	144	164	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	39	GLY	-	expression tag	UNP Q6IAA8
E	40	ALA	-	expression tag	UNP Q6IAA8
E	41	ALA	-	expression tag	UNP Q6IAA8
E	98	ASP	SER	engineered mutation	UNP Q6IAA8

- Molecule 6 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	118	Total	C	N	O	S	0	0	0
			956	610	167	173	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	179	MET	-	expression tag	UNP Q7L523
F	180	ALA	-	expression tag	UNP Q7L523
F	181	ASP	-	expression tag	UNP Q7L523
F	182	LEU	-	expression tag	UNP Q7L523

- Molecule 7 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	132	Total	C	N	O	S	0	1	0
			1050	677	162	203	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	237	MET	-	expression tag	UNP Q99K70

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Na	0	0
			1	1		

- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	G	1	Total	C	O	0	0
			4	2	2		

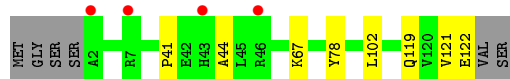
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	50	Total	O	0	0
			50	50		
10	B	70	Total	O	0	0
			70	70		
10	C	50	Total	O	0	0
			50	50		
10	D	19	Total	O	0	0
			19	19		
10	E	66	Total	O	0	0
			66	66		
10	F	25	Total	O	0	0
			25	25		
10	G	68	Total	O	0	0
			68	68		

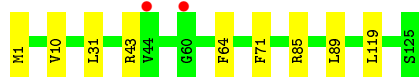
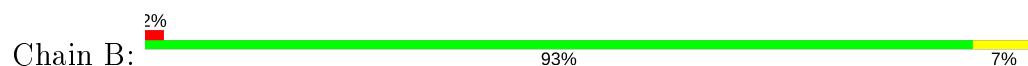
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

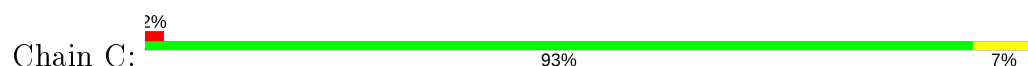
- Molecule 1: Regulator complex protein LAMTOR3



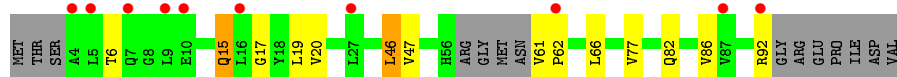
- Molecule 2: Regulator complex protein LAMTOR2



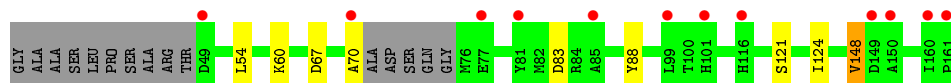
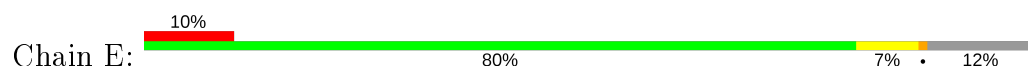
- Molecule 3: Regulator complex protein LAMTOR5



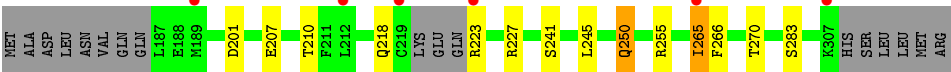
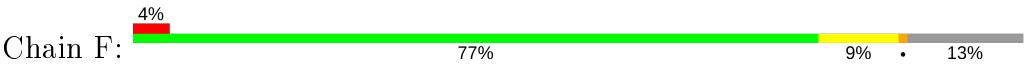
- Molecule 4: Regulator complex protein LAMTOR4



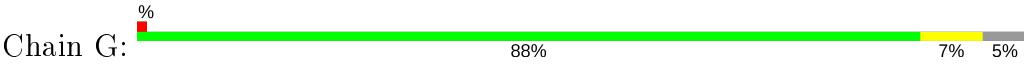
- Molecule 5: Regulator complex protein LAMTOR1



- Molecule 6: Ras-related GTP-binding protein A



● Molecule 7: Ras-related GTP-binding protein C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.10 Å 93.48 Å 125.45 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.36 – 2.02 74.96 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.36-2.02) 99.3 (74.96-2.02)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.02 Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.193 , 0.243 0.200 , 0.254	Depositor DCC
$R_{free}$ test set	2899 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.605	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 58.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.47	0/956	0.65	0/1297
2	B	0.51	0/961	0.66	0/1301
3	C	0.51	0/685	0.63	0/929
4	D	0.43	0/654	0.70	0/883
5	E	0.50	0/862	0.63	0/1172
6	F	0.49	0/972	0.71	0/1306
7	G	0.56	0/1070	0.66	0/1444
All	All	0.50	0/6160	0.66	0/8332

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	939	0	963	5	0
2	B	950	0	959	4	0
3	C	676	0	679	4	0
4	D	647	0	657	8	0
5	E	846	0	849	4	0
6	F	956	0	965	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1050	0	1054	5	0
8	C	1	0	0	0	0
9	G	4	0	3	0	0
10	A	50	0	0	0	0
10	B	70	0	0	0	0
10	C	50	0	0	0	0
10	D	19	0	0	0	0
10	E	66	0	0	0	0
10	F	25	0	0	0	0
10	G	68	0	0	0	0
All	All	6417	0	6129	27	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 2.

The worst 5 of 27 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)
4:D:46:LEU:HD13	4:D:66:LEU:HD21	1.75	0.69
1:A:102:LEU:HD22	3:C:47:VAL:HG21	1.75	0.68
4:D:19:LEU:HB2	4:D:86:VAL:HB	1.82	0.61
6:F:265:ILE:O	6:F:270:THR:O	2.18	0.61
7:G:287:MET:HG3	7:G:317:ILE:HD12	1.85	0.58

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	119/127 (94%)	118 (99%)	1 (1%)	0	100	100
2	B	124/125 (99%)	120 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	91/91 (100%)	91 (100%)	0	0	100	100
4	D	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
5	E	104/123 (85%)	98 (94%)	6 (6%)	0	100	100
6	F	114/135 (84%)	110 (96%)	4 (4%)	0	100	100
7	G	131/139 (94%)	131 (100%)	0	0	100	100
All	All	764/839 (91%)	746 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	105/110 (96%)	104 (99%)	1 (1%)	76	80
2	B	99/98 (101%)	96 (97%)	3 (3%)	41	40
3	C	79/77 (103%)	77 (98%)	2 (2%)	47	48
4	D	71/83 (86%)	66 (93%)	5 (7%)	15	10
5	E	95/104 (91%)	90 (95%)	5 (5%)	22	17
6	F	107/123 (87%)	100 (94%)	7 (6%)	17	11
7	G	121/127 (95%)	119 (98%)	2 (2%)	60	63
All	All	677/722 (94%)	652 (96%)	25 (4%)	34	31

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	54	LEU
5	E	83	ASP
7	G	301	LYS
5	E	60	LYS
5	E	121	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	15	GLN
6	F	218	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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
9	ACT	G	401	-	1,3,3	5.55	1 (100%)	0,3,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	401	ACT	CH3-C	5.55	1.55	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	A	121/127 (95%)	0.27	4 (3%) 46 46	36, 58, 91, 127	0
2	B	125/125 (100%)	0.21	2 (1%) 72 71	32, 46, 84, 102	0
3	C	91/91 (100%)	0.25	2 (2%) 62 61	30, 43, 74, 122	0
4	D	85/99 (85%)	0.64	10 (11%) 4 4	44, 69, 103, 130	0
5	E	108/123 (87%)	0.84	12 (11%) 5 5	32, 74, 117, 126	0
6	F	118/135 (87%)	0.48	6 (5%) 28 27	32, 63, 91, 133	0
7	G	132/139 (94%)	0.15	2 (1%) 73 73	30, 43, 82, 121	0
All	All	780/839 (92%)	0.39	38 (4%) 29 29	30, 55, 100, 133	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	99	LEU	6.6
7	G	369	GLY	6.5
5	E	161	PRO	6.4
4	D	7	GLN	4.7
3	C	91	SER	4.4

### 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](#)

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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
8	NA	C	101	1/1	0.91	0.08	52,52,52,52	0
9	ACT	G	401	4/4	0.98	0.15	32,37,40,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.