



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:12 am GMT

PDB ID : 5D7G  
Title : Structure of human ATG5 E122D-ATG16L1 complex at 3.0 Angstroms  
Authors : Qiu, Y.; Schulman, B.A.  
Deposited on : 2015-08-13  
Resolution : 3.00 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

<http://wwpdb.org/validation/2016/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  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28683  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : trunk28683

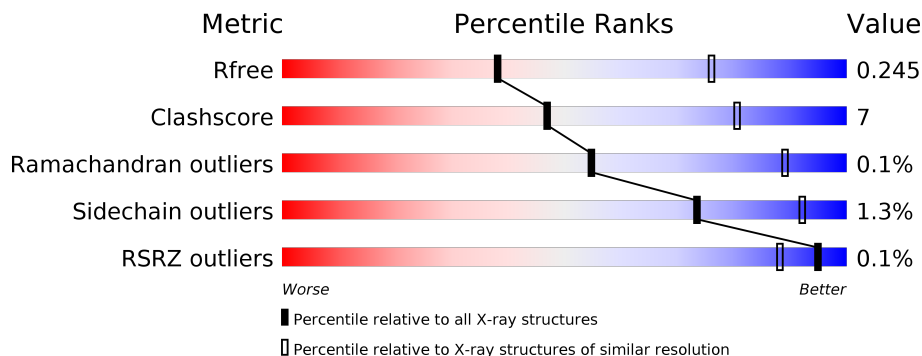
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.



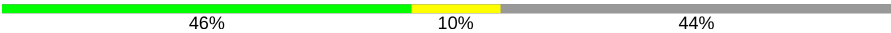
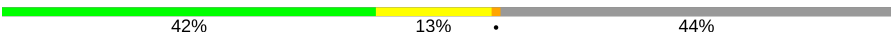
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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. 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	280	<div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	C	280	<div> <div>81%</div> <div>13%</div> <div>6%</div> </div>
1	E	280	<div> <div>76%</div> <div>16%</div> <div>7%</div> </div>
1	G	280	<div> <div>71%</div> <div>20%</div> <div>9%</div> </div>
2	B	71	<div> <div>46%</div> <div>8%</div> <div>45%</div> </div>
2	D	71	<div> <div>51%</div> <div>6%</div> <div>44%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	71	 46% 10% 44%
2	H	71	 42% 13% 44%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9417 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 Autophagy protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2033	1330	331	360	12			
1	C	263	Total	C	N	O	S	0	0	0
			2060	1342	341	365	12			
1	E	260	Total	C	N	O	S	0	0	0
			2052	1334	336	370	12			
1	G	256	Total	C	N	O	S	0	0	0
			2011	1313	329	357	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9H1Y0
A	-3	ALA	-	expression tag	UNP Q9H1Y0
A	-2	MET	-	expression tag	UNP Q9H1Y0
A	-1	GLY	-	expression tag	UNP Q9H1Y0
A	0	SER	-	expression tag	UNP Q9H1Y0
A	122	ASP	GLU	engineered mutation	UNP Q9H1Y0
C	-4	GLY	-	expression tag	UNP Q9H1Y0
C	-3	ALA	-	expression tag	UNP Q9H1Y0
C	-2	MET	-	expression tag	UNP Q9H1Y0
C	-1	GLY	-	expression tag	UNP Q9H1Y0
C	0	SER	-	expression tag	UNP Q9H1Y0
C	122	ASP	GLU	engineered mutation	UNP Q9H1Y0
E	-4	GLY	-	expression tag	UNP Q9H1Y0
E	-3	ALA	-	expression tag	UNP Q9H1Y0
E	-2	MET	-	expression tag	UNP Q9H1Y0
E	-1	GLY	-	expression tag	UNP Q9H1Y0
E	0	SER	-	expression tag	UNP Q9H1Y0
E	122	ASP	GLU	engineered mutation	UNP Q9H1Y0
G	-4	GLY	-	expression tag	UNP Q9H1Y0
G	-3	ALA	-	expression tag	UNP Q9H1Y0
G	-2	MET	-	expression tag	UNP Q9H1Y0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	GLY	-	expression tag	UNP Q9H1Y0
G	0	SER	-	expression tag	UNP Q9H1Y0
G	122	ASP	GLU	engineered mutation	UNP Q9H1Y0

- Molecule 2 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	39	Total	C	N	O	0	0	0
			295	186	58	51			
2	D	40	Total	C	N	O	0	0	0
			333	209	64	60			
2	F	40	Total	C	N	O	0	0	0
			321	199	65	57			
2	H	40	Total	C	N	O	0	0	0
			311	198	55	58			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q676U5
B	0	SER	-	expression tag	UNP Q676U5
D	-1	GLY	-	expression tag	UNP Q676U5
D	0	SER	-	expression tag	UNP Q676U5
F	-1	GLY	-	expression tag	UNP Q676U5
F	0	SER	-	expression tag	UNP Q676U5
H	-1	GLY	-	expression tag	UNP Q676U5
H	0	SER	-	expression tag	UNP Q676U5

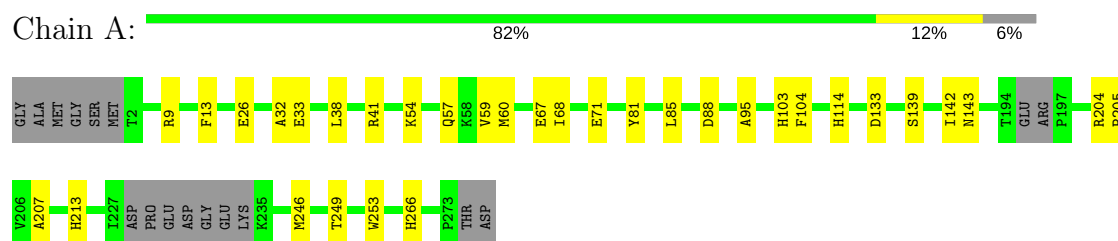
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	O	0	0
			1	1		

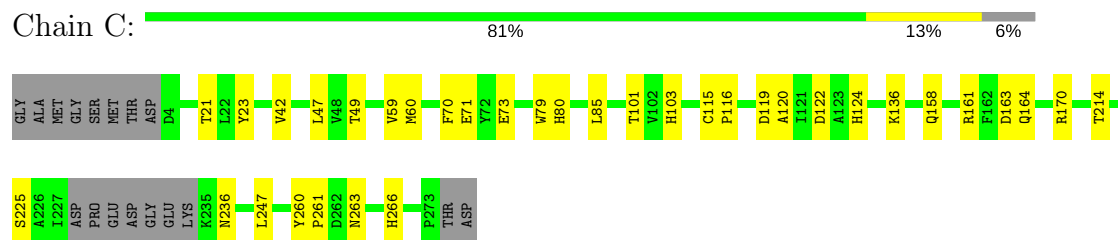
### 3 Residue-property plots [i](#)

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.

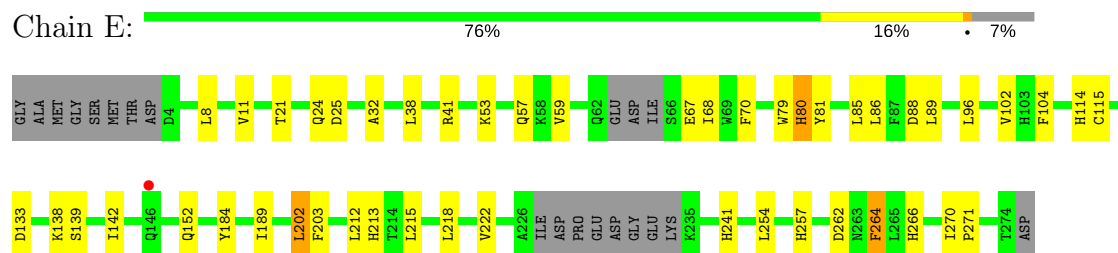
#### • Molecule 1: Autophagy protein 5



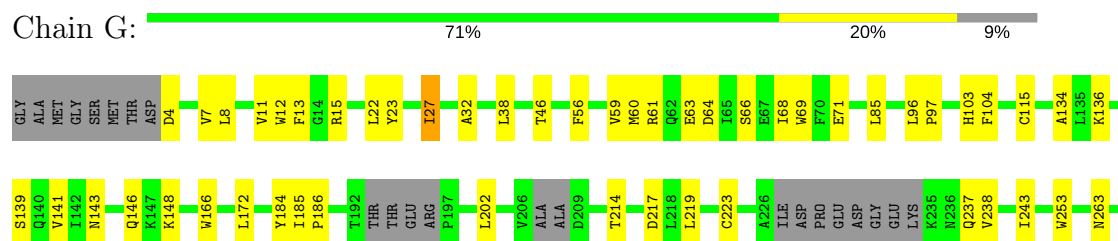
#### • Molecule 1: Autophagy protein 5



#### • Molecule 1: Autophagy protein 5



#### • Molecule 1: Autophagy protein 5



H266	H267	S268	I269	I270	P271	Q272	P273	THR	ASP
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● Molecule 2: Autophagy-related protein 16-1

Chain B: 

GLY	SER	MET	SER	SER	SER	GLY	LEU	ARG	ALA	ALA	ASP	F10	H13	H16	R26	Q30	E33	L43	L48	HIS	SER	VAL	LEU	GLN	LYS	LEU	GLN	ALA	GLU	LYS	HIS	VAL	PRO	ASN	ARG	HIS	GLU	ILE
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● Molecule 2: Autophagy-related protein 16-1

Chain D: 

GLY	SER	MET	SER	SER	GLY	LEU	ARG	ALA	ALA	ASP	F10	R15	E19	R23	R26	H49	SER	VAL	LEU	ALA	GLN	LYS	LEU	GLN	GLU	LYS	HIS	ASP	VAL	PRO	ASN	ARG	HIS	GLU	ILE
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● Molecule 2: Autophagy-related protein 16-1

Chain F: 

GLY	SER	MET	SER	SER	GLY	LEU	ARG	ALA	ALA	ASP	PHE	P11	H12	H13	H16	I17	Q20	Q28	E33	S50	VAL	LEU	ALA	GLN	LYS	LEU	GLN	ALA	GLU	LYS	HIS	ASP	VAL	PRO	ASN	ARG	HIS	GLU	ILE
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● Molecule 2: Autophagy-related protein 16-1

Chain H: 

GLY	SER	MET	SER	SER	GLY	LEU	ARG	ALA	ALA	ASP	F10	H13	K14	I17	L21	R24	D25	R29	E33	L48	H49	SER	VAL	LEU	ALA	GLN	LYS	LEU	GLN	ALA	GLU	LYS	HIS	ASP	VAL	PRO	ASN	ARG	HIS	GLU	ILE
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.11Å 84.48Å 151.85Å 90.00° 133.81° 90.00°	Depositor
Resolution (Å)	49.53 – 3.00 49.54 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.53-3.00) 92.5 (49.54-3.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.198 , 0.244 0.198 , 0.245	Depositor DCC
$R_{free}$ test set	1919 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	89.8	Xtriage
Anisotropy	0.620	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 63.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h+2*k,-h-l 0.015 for h,-k,-h-l 0.019 for -h-2*k,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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](#)

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	0.37	0/2098	0.51	0/2873
1	C	0.38	0/2126	0.50	0/2912
1	E	0.39	0/2117	0.52	0/2897
1	G	0.42	0/2075	0.50	0/2835
2	B	0.38	0/300	0.49	0/408
2	D	0.37	0/338	0.49	0/455
2	F	0.40	0/327	0.47	0/441
2	H	0.43	0/316	0.52	0/429
All	All	0.39	0/9697	0.51	0/13250

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	2033	0	1852	26	0
1	C	2060	0	1890	20	0
1	E	2052	0	1882	33	0
1	G	2011	0	1845	38	0
2	B	295	0	252	7	0
2	D	333	0	315	3	0
2	F	321	0	287	5	0
2	H	311	0	278	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
All	All	9417	0	8601	128	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.

The worst 5 of 128 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:71:GLU:OE1	1:G:103:HIS:HE1	1.50	0.93
1:E:85:LEU:HD13	1:E:266:HIS:HB3	1.63	0.81
2:H:24:ARG:NH1	2:H:25:ASP:OD1	2.21	0.73
1:G:71:GLU:OE1	1:G:103:HIS:CE1	2.41	0.70
1:G:243:ILE:HD13	2:H:21:LEU:HG	1.79	0.65

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	257/280 (92%)	248 (96%)	9 (4%)	0	100	100
1	C	259/280 (92%)	253 (98%)	6 (2%)	0	100	100
1	E	254/280 (91%)	246 (97%)	8 (3%)	0	100	100
1	G	248/280 (89%)	245 (99%)	2 (1%)	1 (0%)	38	78
2	B	37/71 (52%)	36 (97%)	1 (3%)	0	100	100
2	D	38/71 (54%)	38 (100%)	0	0	100	100
2	F	38/71 (54%)	38 (100%)	0	0	100	100
2	H	38/71 (54%)	38 (100%)	0	0	100	100
All	All	1169/1404 (83%)	1142 (98%)	26 (2%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	271	PRO

### 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	202/256 (79%)	202 (100%)	0	100	100
1	C	208/256 (81%)	205 (99%)	3 (1%)	71	91
1	E	211/256 (82%)	206 (98%)	5 (2%)	54	85
1	G	205/256 (80%)	202 (98%)	3 (2%)	70	91
2	B	24/64 (38%)	24 (100%)	0	100	100
2	D	33/64 (52%)	33 (100%)	0	100	100
2	F	30/64 (47%)	30 (100%)	0	100	100
2	H	29/64 (45%)	28 (97%)	1 (3%)	42	78
All	All	942/1280 (74%)	930 (99%)	12 (1%)	73	92

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	152	GLN
1	E	202	LEU
1	G	61	ARG
1	E	80	HIS
1	G	27	ILE

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

Mol	Chain	Res	Type
1	E	80	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	263/280 (93%)	-0.36	0 100 100	60, 89, 133, 159	0
1	C	263/280 (93%)	-0.48	0 100 100	55, 88, 127, 161	0
1	E	260/280 (92%)	-0.23	1 (0%) 92 77	57, 92, 145, 165	0
1	G	256/280 (91%)	-0.46	0 100 100	65, 91, 136, 160	0
2	B	39/71 (54%)	-0.61	0 100 100	68, 95, 127, 136	0
2	D	40/71 (56%)	-0.30	0 100 100	59, 94, 130, 133	0
2	F	40/71 (56%)	-0.41	0 100 100	62, 95, 155, 163	0
2	H	40/71 (56%)	-0.34	0 100 100	65, 93, 139, 149	0
All	All	1201/1404 (85%)	-0.39	1 (0%) 95 88	55, 91, 136, 165	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	146	GLN	2.3

### 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.