



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 AM GMT

PDB ID : 2RHE  
Title : STRUCTURE OF A NOVEL BENCE-JONES PROTEIN (RHE) FRAGMENT AT 1.6 ANGSTROMS RESOLUTION  
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Deposited on : 1983-06-13  
Resolution : 1.60 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](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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

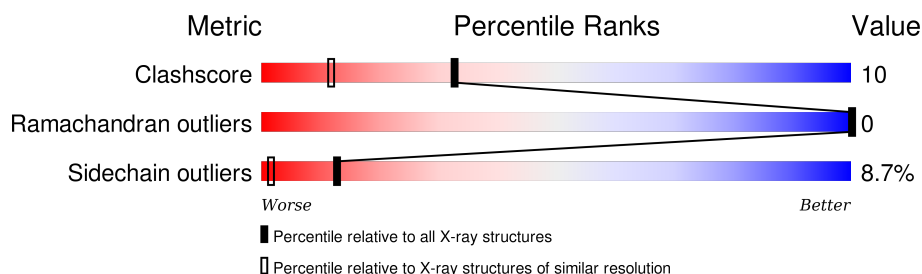
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	114	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1019 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 BENCE-JONES PROTEIN RHE (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			833	519	135	177	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	THR	SER	CONFLICT	PIR S25752
A	26	ALA	SER	CONFLICT	PIR S25752
A	27	THR	SER	CONFLICT	PIR S25752
A	28	ASP	ASN	CONFLICT	PIR S25752
A	33	SER	THR	CONFLICT	PIR S25752
A	35	ILE	ASN	CONFLICT	PIR S25752
A	40	VAL	LEU	CONFLICT	PIR S25752
A	43	LYS	THR	CONFLICT	PIR S25752
A	51	TYR	ARG	CONFLICT	PIR S25752
A	53	ASP	ASN	CONFLICT	PIR S25752
A	54	LEU	GLN	CONFLICT	PIR S25752
A	55	LEU	ARG	CONFLICT	PIR S25752
A	60	SER	PRO	CONFLICT	PIR S25752
A	65	ALA	GLY	CONFLICT	PIR S25752
A	80	GLU	GLN	CONFLICT	PIR S25752
A	93	ASN	ASP	CONFLICT	PIR S25752
A	97	ASP	ASN	CONFLICT	PIR S25752
A	98	GLU	GLY	CONFLICT	PIR S25752
A	99	PRO	VAL	CONFLICT	PIR S25752
A	100	GLY	VAL	CONFLICT	PIR S25752

- Molecule 2 is water.

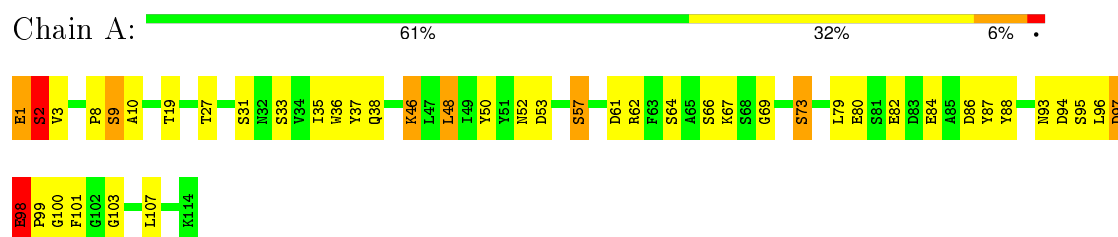
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	186	Total	O	0	0
			186	186		

### 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 ( $\text{RSRZ} > 2$ ). 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.

Note EDS was not executed.

- Molecule 1: BENICE-JONES PROTEIN RHE (LIGHT CHAIN)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.63Å 52.22Å 42.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-1.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1019	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

## 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	1.31	6/851 (0.7%)	2.34	51/1159 (4.4%)

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	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	SER	CA-CB	7.83	1.64	1.52
1	A	9	SER	CA-CB	7.65	1.64	1.52
1	A	84	GLU	CD-OE1	-5.92	1.19	1.25
1	A	66	SER	CB-OG	-5.67	1.34	1.42
1	A	98	GLU	CD-OE2	5.33	1.31	1.25
1	A	57	SER	CB-OG	-5.30	1.35	1.42

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	GLU	CA-CB-CG	20.87	159.31	113.40
1	A	61	ASP	CB-CG-OD2	-13.57	106.09	118.30
1	A	97	ASP	CB-CG-OD1	-13.52	106.13	118.30
1	A	86	ASP	CB-CG-OD2	-11.70	107.77	118.30
1	A	62	ARG	CD-NE-CZ	11.56	139.78	123.60
1	A	46	LYS	CB-CG-CD	11.39	141.22	111.60
1	A	57	SER	N-CA-CB	10.44	126.15	110.50
1	A	53	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	2	SER	N-CA-CB	9.56	124.84	110.50
1	A	9	SER	CA-CB-OG	-9.11	86.62	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	ILE	CA-CB-CG2	8.50	127.91	110.90
1	A	94	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	57	SER	CA-CB-OG	-8.26	88.89	111.20
1	A	67	LYS	CG-CD-CE	7.86	135.47	111.90
1	A	69	GLY	CA-C-O	-7.64	106.85	120.60
1	A	73	SER	N-CA-CB	-6.88	100.18	110.50
1	A	10	ALA	N-CA-CB	6.85	119.69	110.10
1	A	80	GLU	OE1-CD-OE2	6.57	131.19	123.30
1	A	101	PHE	CB-CG-CD2	-6.52	116.24	120.80
1	A	88	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	A	2	SER	CA-CB-OG	6.27	128.12	111.20
1	A	64	SER	N-CA-CB	6.26	119.89	110.50
1	A	88	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	A	1	GLU	C-N-CA	6.23	137.27	121.70
1	A	94	ASP	OD1-CG-OD2	-6.21	111.51	123.30
1	A	37	TYR	CB-CG-CD2	-6.11	117.33	121.00
1	A	1	GLU	CA-C-O	5.96	132.63	120.10
1	A	86	ASP	OD1-CG-OD2	5.88	134.47	123.30
1	A	97	ASP	OD1-CG-OD2	5.81	134.34	123.30
1	A	87	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	A	3	VAL	CA-CB-CG1	5.75	119.52	110.90
1	A	84	GLU	CG-CD-OE1	5.74	129.77	118.30
1	A	62	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	52	ASN	CB-CG-OD1	-5.68	110.24	121.60
1	A	48	LEU	CB-CG-CD2	5.65	120.60	111.00
1	A	95	SER	CB-CA-C	5.62	120.79	110.10
1	A	82	GLU	CG-CD-OE2	-5.60	107.11	118.30
1	A	31	SER	N-CA-CB	-5.48	102.28	110.50
1	A	9	SER	CB-CA-C	-5.32	99.99	110.10
1	A	69	GLY	O-C-N	5.30	131.19	122.70
1	A	98	GLU	CB-CG-CD	5.27	128.44	114.20
1	A	98	GLU	CB-CA-C	5.23	120.86	110.40
1	A	61	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	84	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	A	57	SER	CB-CA-C	-5.18	100.26	110.10
1	A	87	TYR	CB-CG-CD1	5.16	124.09	121.00
1	A	36	TRP	CE2-CD2-CG	-5.14	103.19	107.30
1	A	8	PRO	N-CD-CG	-5.14	95.49	103.20
1	A	2	SER	O-C-N	5.13	130.91	122.70
1	A	3	VAL	CB-CA-C	5.06	121.01	111.40
1	A	48	LEU	CB-CG-CD1	-5.04	102.44	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	35	ILE	CB

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	833	0	800	17	0
2	A	186	0	0	7	0
All	All	1019	0	800	17	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 10.

All (17) 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:A:96:LEU:HD12	2:A:273:HOH:O	1.76	0.86
1:A:1:GLU:HG2	1:A:2:SER:H	1.56	0.70
1:A:1:GLU:HB2	1:A:103:GLY:HA2	1.78	0.64
1:A:93:ASN:HB3	2:A:273:HOH:O	2.00	0.61
1:A:98:GLU:HB3	2:A:150:HOH:O	2.00	0.60
1:A:1:GLU:CG	1:A:2:SER:H	2.15	0.57
1:A:1:GLU:CG	1:A:2:SER:N	2.69	0.55
1:A:27:THR:HG23	2:A:247:HOH:O	2.07	0.55
1:A:38:GLN:HG3	1:A:48:LEU:HD11	1.88	0.54
1:A:1:GLU:HG3	2:A:251:HOH:O	2.10	0.52
1:A:99:PRO:C	2:A:273:HOH:O	2.49	0.50
1:A:100:GLY:N	2:A:273:HOH:O	2.47	0.48
1:A:98:GLU:HB2	1:A:99:PRO:HD2	1.94	0.48
1:A:1:GLU:OE1	1:A:2:SER:HB3	2.13	0.47
1:A:19:THR:CG2	1:A:73:SER:OG	2.68	0.42
1:A:79:LEU:HD11	1:A:107:LEU:HD21	2.02	0.41
1:A:98:GLU:HB2	1:A:99:PRO:CD	2.51	0.40

There are no symmetry-related clashes.



## 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	A	112/114 (98%)	106 (95%)	6 (5%)	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	92/92 (100%)	84 (91%)	8 (9%)	13	1

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	9	SER
1	A	33	SER
1	A	46	LYS
1	A	50	TYR
1	A	57	SER
1	A	97	ASP
1	A	98	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.