



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:47 AM GMT

PDB ID : 2BM8  
Title : CMCI-N160 APO-STRUCTURE  
Authors : Oster, L.M.; Lester, D.R.; Terwisscha Van Scheltinga, A.; Svenda, M.;  
Genereux, C.; Andersson, I.  
Deposited on : 2005-03-10  
Resolution : 2.50 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

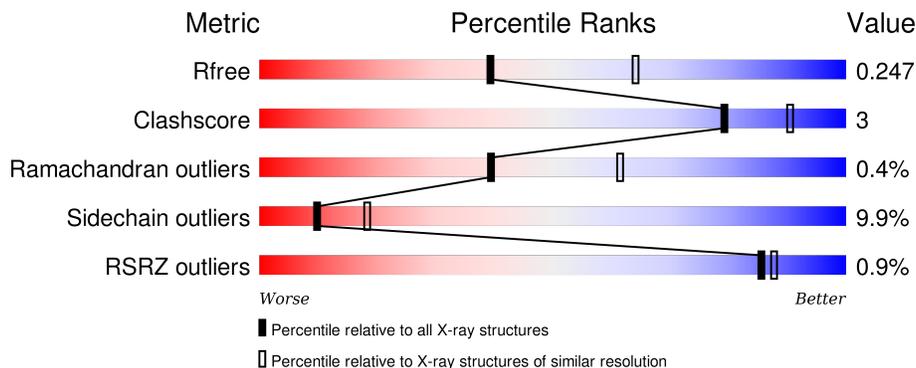
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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. 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	236	
1	B	236	
1	C	236	
1	D	236	
1	E	236	

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Mol	Chain	Length	Quality of chain
1	F	236	 <p>80% 17% ..</p>
1	G	236	 <p>82% 14% ..</p>
1	H	236	 <p>80% 17% ..</p>
1	I	236	 <p>82% 14% ..</p>
1	J	236	 <p>80% 17% ..</p>
1	K	236	 <p>79% 17% ..</p>
1	L	236	 <p>80% 19% .</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23710 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 CEPHALOSPORIN HYDROXYLASE CMCI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	232	1915	1219	331	353	12	6	0	0
1	B	233	1920	1222	332	354	12	0	0	0
1	C	232	1915	1219	331	353	12	0	0	0
1	D	232	1915	1219	331	353	12	0	0	0
1	E	233	1920	1222	332	354	12	6	0	0
1	F	233	1920	1222	332	354	12	0	0	0
1	G	232	1912	1218	330	352	12	0	0	0
1	H	233	1920	1222	332	354	12	0	0	0
1	I	232	1915	1219	331	353	12	0	0	0
1	J	232	1915	1219	331	353	12	0	0	0
1	K	231	1907	1215	329	351	12	0	0	0
1	L	233	1919	1222	332	353	12	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
A	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
A	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
B	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
B	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726

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Chain	Residue	Modelled	Actual	Comment	Reference
B	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
C	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
C	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
C	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
D	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
D	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
D	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
E	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
E	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
E	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
F	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
F	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
F	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
G	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
G	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
G	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
H	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
H	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
H	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
I	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
I	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
I	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
J	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
J	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
J	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
K	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
K	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
K	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726
L	10	GLN	LEU	ENGINEERED MUTATION	UNP O85726
L	160	ASN	ASP	ENGINEERED MUTATION	UNP O85726
L	200	PHE	LEU	ENGINEERED MUTATION	UNP O85726

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	51	Total O 51 51	0	0
2	B	66	Total O 66 66	0	0
2	C	60	Total O 60 60	0	0
2	D	42	Total O 42 42	0	0

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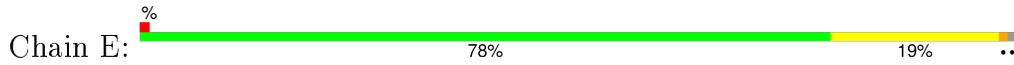
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
2	E	43	Total 43	O 43	0	0
2	F	60	Total 60	O 60	0	0
2	G	84	Total 84	O 84	0	0
2	H	74	Total 74	O 74	0	0
2	I	37	Total 37	O 37	0	0
2	J	65	Total 65	O 65	0	0
2	K	79	Total 79	O 79	0	0
2	L	56	Total 56	O 56	0	0





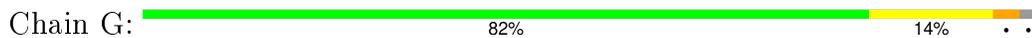
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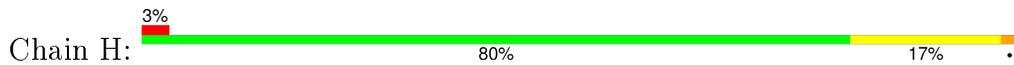
• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



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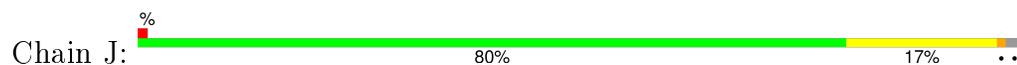


• Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI

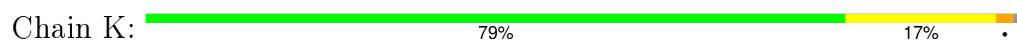




- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



- Molecule 1: CEPHALOSPORIN HYDROXYLASE CMCI



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.65Å 182.64Å 103.24Å 90.00° 91.05° 90.00°	Depositor
Resolution (Å)	95.35 – 2.50 93.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.35-2.50) 99.5 (93.64-2.50)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.82 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.192 , 0.245 0.195 , 0.247	Depositor DCC
$R_{free}$ test set	5962 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 13.8	EDS
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 118959 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23710	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	1/1970 (0.1%)	0.83	9/2679 (0.3%)
1	B	0.48	0/1975	0.88	12/2686 (0.4%)
1	C	0.48	0/1970	0.84	8/2679 (0.3%)
1	D	0.42	0/1970	0.82	9/2679 (0.3%)
1	E	0.47	0/1975	0.84	10/2686 (0.4%)
1	F	0.48	0/1975	0.83	9/2686 (0.3%)
1	G	0.53	0/1967	0.84	5/2675 (0.2%)
1	H	0.48	0/1975	0.87	11/2686 (0.4%)
1	I	0.45	0/1970	0.83	9/2679 (0.3%)
1	J	0.46	0/1970	0.85	11/2679 (0.4%)
1	K	0.50	0/1962	0.89	10/2668 (0.4%)
1	L	0.46	0/1974	0.83	6/2685 (0.2%)
All	All	0.48	1/23653 (0.0%)	0.84	109/32167 (0.3%)

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	B	0	1
1	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	ARG	CB-CG	7.78	1.73	1.52

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	47	ASP	CB-CG-OD2	8.01	125.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	47	ASP	CB-CG-OD2	7.18	124.76	118.30
1	L	68	ASP	CB-CG-OD2	7.16	124.75	118.30
1	H	47	ASP	CB-CG-OD2	7.15	124.74	118.30
1	B	47	ASP	CB-CG-OD2	7.13	124.72	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	148	LEU	Peptide
1	I	148	LEU	Peptide

## 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	1915	0	1816	19	0
1	B	1920	0	1821	19	0
1	C	1915	0	1816	12	0
1	D	1915	0	1816	15	0
1	E	1920	0	1821	18	0
1	F	1920	0	1821	17	0
1	G	1912	0	1815	16	0
1	H	1920	0	1821	15	0
1	I	1915	0	1816	11	0
1	J	1915	0	1816	13	0
1	K	1907	0	1810	14	0
1	L	1919	0	1821	16	0
2	A	51	0	0	0	0
2	B	66	0	0	0	0
2	C	60	0	0	2	0
2	D	42	0	0	1	0
2	E	43	0	0	1	0
2	F	60	0	0	1	0
2	G	84	0	0	1	0
2	H	74	0	0	0	0
2	I	37	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	65	0	0	0	0
2	K	79	0	0	0	0
2	L	56	0	0	0	0
All	All	23710	0	21810	156	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 3.

The worst 5 of 156 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:162:HIS:HE1	1:A:186:GLU:O	1.60	0.83
1:A:105:ILE:HD11	1:B:105:ILE:CD1	2.12	0.80
1:D:58:TRP:HA	1:E:74:HIS:HE1	1.47	0.80
1:D:105:ILE:HG21	1:E:105:ILE:HD11	1.64	0.79
1:J:162:HIS:HE1	1:J:186:GLU:O	1.66	0.79

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	230/236 (98%)	217 (94%)	12 (5%)	1 (0%)	39 61
1	B	231/236 (98%)	218 (94%)	12 (5%)	1 (0%)	39 61
1	C	230/236 (98%)	217 (94%)	12 (5%)	1 (0%)	39 61
1	D	230/236 (98%)	218 (95%)	10 (4%)	2 (1%)	21 37
1	E	231/236 (98%)	217 (94%)	14 (6%)	0	100 100
1	F	231/236 (98%)	219 (95%)	11 (5%)	1 (0%)	39 61
1	G	230/236 (98%)	218 (95%)	11 (5%)	1 (0%)	39 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	231/236 (98%)	221 (96%)	8 (4%)	2 (1%)	21	37
1	I	230/236 (98%)	220 (96%)	10 (4%)	0	100	100
1	J	230/236 (98%)	218 (95%)	12 (5%)	0	100	100
1	K	229/236 (97%)	221 (96%)	7 (3%)	1 (0%)	39	61
1	L	231/236 (98%)	219 (95%)	11 (5%)	1 (0%)	39	61
All	All	2764/2832 (98%)	2623 (95%)	130 (5%)	11 (0%)	39	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	233	ALA
1	B	5	SER
1	D	141	ASP
1	K	208	ARG
1	A	53	PHE

### 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	204/207 (99%)	181 (89%)	23 (11%)	7	13
1	B	204/207 (99%)	186 (91%)	18 (9%)	12	23
1	C	204/207 (99%)	182 (89%)	22 (11%)	8	15
1	D	204/207 (99%)	184 (90%)	20 (10%)	10	19
1	E	204/207 (99%)	179 (88%)	25 (12%)	6	11
1	F	204/207 (99%)	186 (91%)	18 (9%)	12	23
1	G	203/207 (98%)	184 (91%)	19 (9%)	11	20
1	H	204/207 (99%)	186 (91%)	18 (9%)	12	23
1	I	204/207 (99%)	188 (92%)	16 (8%)	16	29
1	J	204/207 (99%)	182 (89%)	22 (11%)	8	15
1	K	203/207 (98%)	180 (89%)	23 (11%)	7	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	204/207 (99%)	185 (91%)	19 (9%)	11	21
All	All	2446/2484 (98%)	2203 (90%)	243 (10%)	10	18

5 of 243 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	14	LEU
1	G	92	ASN
1	L	6	ARG
1	F	80	LEU
1	F	194	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	7	GLN
1	G	153	HIS
1	K	160	ASN
1	G	131	ASN
1	G	160	ASN

### 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

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	232/236 (98%)	-0.26	2 (0%) 85 88	15, 23, 42, 45	1 (0%)
1	B	233/236 (98%)	-0.24	3 (1%) 79 82	10, 18, 38, 42	0
1	C	232/236 (98%)	-0.34	1 (0%) 93 93	8, 20, 33, 43	0
1	D	232/236 (98%)	-0.16	4 (1%) 73 76	11, 28, 49, 58	0
1	E	233/236 (98%)	-0.25	2 (0%) 85 88	19, 27, 39, 42	1 (0%)
1	F	233/236 (98%)	-0.33	2 (0%) 85 88	6, 17, 33, 42	0
1	G	232/236 (98%)	-0.36	1 (0%) 93 93	5, 13, 32, 37	0
1	H	233/236 (98%)	-0.21	6 (2%) 59 63	9, 19, 42, 47	0
1	I	232/236 (98%)	-0.21	1 (0%) 93 93	16, 26, 46, 49	0
1	J	232/236 (98%)	-0.31	2 (0%) 85 88	13, 21, 37, 40	0
1	K	231/236 (97%)	-0.31	1 (0%) 93 93	9, 15, 35, 41	0
1	L	233/236 (98%)	-0.32	1 (0%) 93 93	14, 20, 35, 45	0
All	All	2788/2832 (98%)	-0.27	26 (0%) 85 88	5, 21, 38, 58	2 (0%)

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	ALA	4.9
1	H	2	ASN	3.7
1	E	234	ALA	3.2
1	J	2	ASN	3.1
1	D	147	HIS	2.9

### 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

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.