



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 PM GMT

PDB ID : 4RQZ  
Title : re-refinement of Isoz, Crystal Structure of DegS protease in complex with an activating peptide  
Authors : Sauer, R.T.; Grant, R.A.  
Deposited on : 2014-11-05  
Resolution : 2.40 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.

---

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

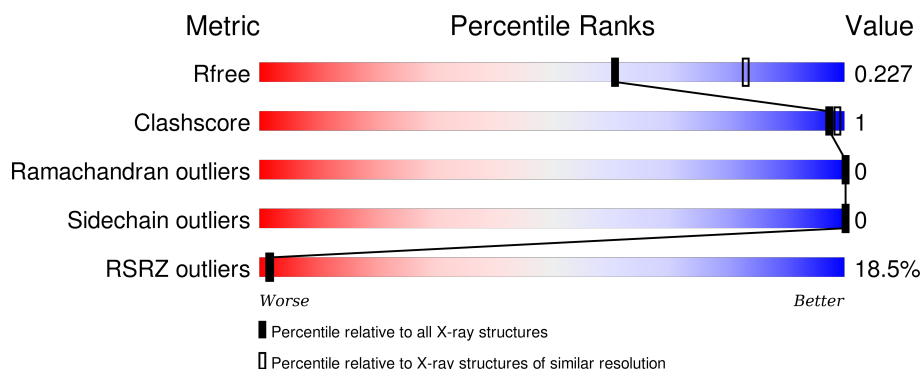
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	314	<div> <div>13%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>
1	B	314	<div> <div>16%</div> <div> <div></div> <div>85%</div> <div>13%</div> </div> </div>
1	C	314	<div> <div>17%</div> <div> <div></div> <div>82%</div> <div>14%</div> </div> </div>
2	D	10	<div> <div>30%</div> <div> <div></div> <div>30%</div> <div>70%</div> </div> </div>
2	E	10	<div> <div>30%</div> <div> <div></div> <div>30%</div> <div>10%</div> <div>60%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	10	<div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>20%30%70%</div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12205 atoms, of which 5952 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 Protease degS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	272	Total	C	H	N	O	S	0	1	0
			3904	1232	1937	352	378	5			
1	B	274	Total	C	H	N	O	S	0	0	0
			3952	1247	1980	346	374	5			
1	C	271	Total	C	H	N	O	S	0	0	0
			3918	1235	1958	348	372	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	MET	-	EXPRESSION TAG	UNP H9UXC8
B	42	MET	-	EXPRESSION TAG	UNP H9UXC8
C	42	MET	-	EXPRESSION TAG	UNP H9UXC8

- Molecule 2 is a protein called activating peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	3	Total	C	H	N	O	0	0	0
			58	23	25	4	6			
2	E	4	Total	C	H	N	O	0	0	0
			74	28	34	5	7			
2	F	3	Total	C	H	N	O	0	0	0
			44	17	18	4	5			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	117	Total	O	0	0
			117	117		
3	B	64	Total	O	0	0
			64	64		

*Continued on next page...*

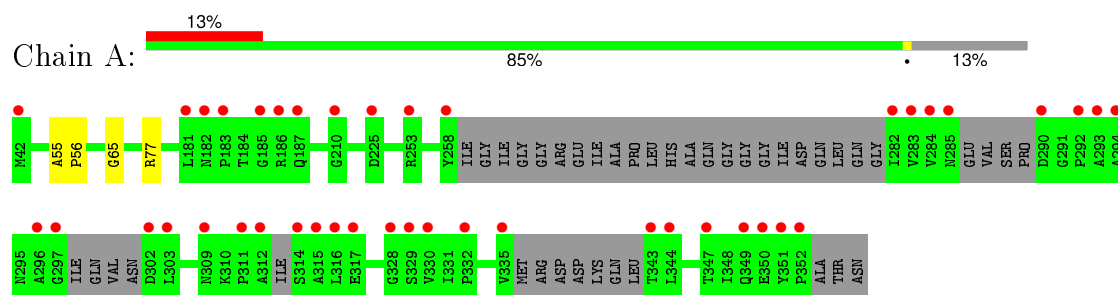
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	74	Total	O	0	0
			74	74		

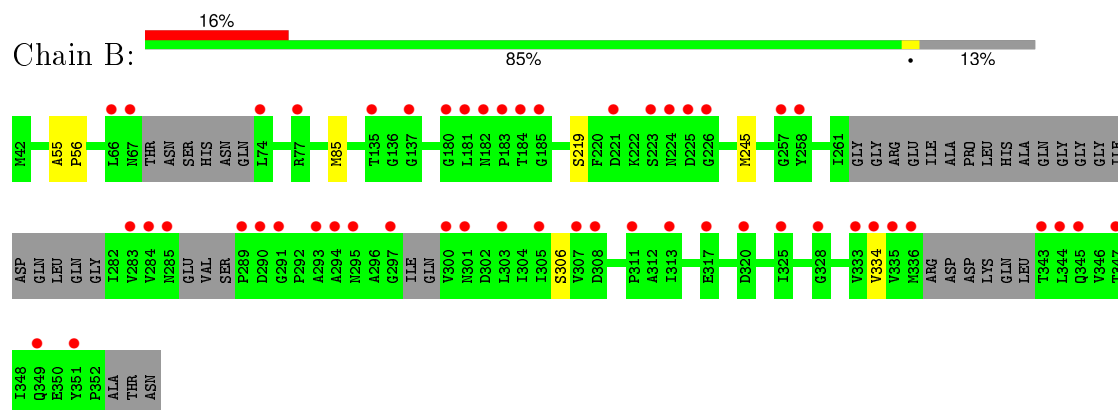
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

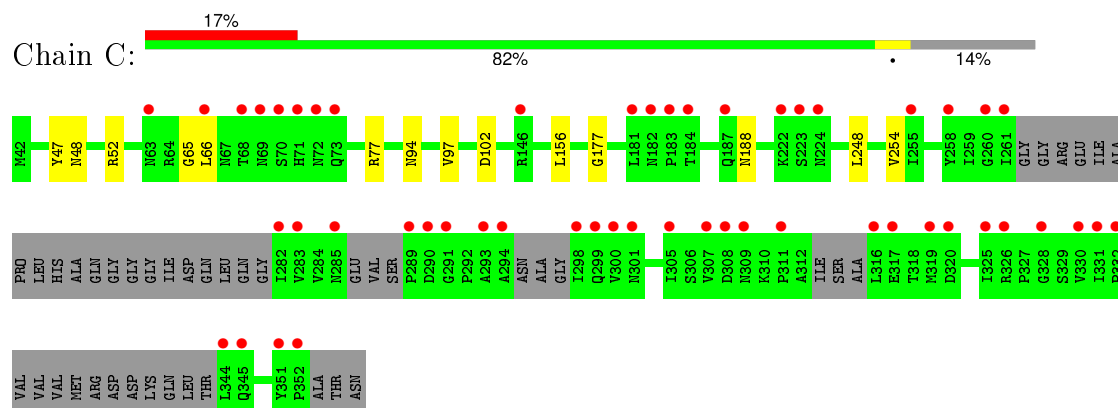
#### • Molecule 1: Protease degS



#### • Molecule 1: Protease degS



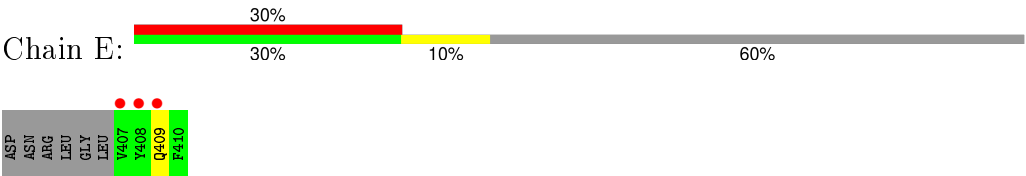
#### • Molecule 1: Protease degS



● Molecule 2: activating peptide



● Molecule 2: activating peptide



● Molecule 2: activating peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.98Å 142.71Å 41.17Å 90.00° 89.24° 90.00°	Depositor
Resolution (Å)	14.94 – 2.40 14.94 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.9 (14.94-2.40) 91.0 (14.94-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, $R_{free}$	0.196 , 0.226 0.195 , 0.227	Depositor DCC
$R_{free}$ test set	2134 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 76.3	EDS
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42042 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.12% 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	0.50	0/1993	0.63	0/2716
1	B	0.44	0/1995	0.57	0/2718
1	C	0.45	0/1982	0.58	0/2698
2	D	0.31	0/34	0.52	0/43
2	E	0.39	0/41	0.54	0/53
2	F	0.30	0/26	0.30	0/32
All	All	0.46	0/6071	0.59	0/8260

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	1967	1937	1937	2	0
1	B	1972	1980	1980	4	0
1	C	1960	1958	1958	7	0
2	D	33	25	25	0	0
2	E	40	34	34	1	0
2	F	26	18	18	0	0
3	A	117	0	0	0	0
3	B	64	0	0	1	0
3	C	74	0	0	0	0
All	All	6253	5952	5952	14	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 1.

All (14) 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:B:219:SER:OG	3:B:463:HOH:O	2.04	0.74
1:B:85:MET:HG3	1:B:245:MET:SD	2.45	0.56
1:C:177:GLY:HA2	1:C:188:ASN:HB2	1.93	0.51
2:E:409:GLN:N	2:E:409:GLN:OE1	2.44	0.50
1:C:94:ASN:HB2	1:C:97:VAL:HG23	1.94	0.49
1:C:47:TYR:HB3	1:C:156:LEU:HD11	1.96	0.48
1:A:55:ALA:N	1:A:56:PRO:CD	2.77	0.47
1:C:66:LEU:N	1:C:102:ASP:OD2	2.48	0.47
1:B:55:ALA:N	1:B:56:PRO:CD	2.79	0.45
1:C:48:ASN:OD1	1:C:52:ARG:NH1	2.50	0.45
1:C:65:GLY:HA3	1:C:77:ARG:HD2	1.99	0.43
1:A:65:GLY:HA3	1:A:77:ARG:HD3	2.02	0.42
1:C:248:LEU:HD21	1:C:254:VAL:HG23	2.02	0.42
1:B:306:SER:HB3	1:B:334:VAL:HB	2.03	0.41

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	261/314 (83%)	257 (98%)	4 (2%)	0	100	100
1	B	262/314 (83%)	259 (99%)	3 (1%)	0	100	100
1	C	259/314 (82%)	254 (98%)	5 (2%)	0	100	100
2	D	1/10 (10%)	0	1 (100%)	0	100	100
2	E	2/10 (20%)	2 (100%)	0	0	100	100
2	F	1/10 (10%)	1 (100%)	0	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	786/972 (81%)	773 (98%)	13 (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	202/253 (80%)	202 (100%)	0	100	100
1	B	204/253 (81%)	204 (100%)	0	100	100
1	C	202/253 (80%)	202 (100%)	0	100	100
2	D	3/9 (33%)	3 (100%)	0	100	100
2	E	4/9 (44%)	4 (100%)	0	100	100
2	F	2/9 (22%)	2 (100%)	0	100	100
All	All	617/786 (78%)	617 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

### 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

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	A	272/314 (86%)	0.62	42 (15%) 3 3	39, 60, 162, 193	0
1	B	274/314 (87%)	0.84	51 (18%) 2 1	41, 74, 166, 195	0
1	C	271/314 (86%)	0.82	52 (19%) 2 1	44, 73, 169, 196	0
2	D	3/10 (30%)	3.63	3 (100%) 0 0	141, 141, 151, 151	0
2	E	4/10 (40%)	5.62	3 (75%) 0 0	136, 150, 150, 154	0
2	F	3/10 (30%)	5.41	2 (66%) 0 0	158, 158, 158, 166	0
All	All	827/972 (85%)	0.81	153 (18%) 2 2	39, 70, 166, 196	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	408	TYR	10.6
2	F	408	TYR	10.1
1	C	289	PRO	9.8
1	B	301	ASN	8.8
1	B	300	VAL	8.6
2	E	407	VAL	8.4
1	A	294	ALA	7.9
1	A	290	ASP	7.4
1	B	290	ASP	7.4
1	B	66	LEU	7.3
1	A	328	GLY	7.1
1	C	283	VAL	7.0
1	A	349	GLN	6.9
1	C	309	ASN	6.7
1	B	313	ILE	6.7
1	C	181	LEU	6.6
1	C	68	THR	6.4
1	B	224	ASN	6.4
1	C	300	VAL	6.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	344	LEU	6.2
1	B	283	VAL	6.2
1	C	316	LEU	6.1
1	C	182	ASN	6.0
1	B	351	TYR	6.0
1	A	315	ALA	5.9
1	C	328	GLY	5.8
1	B	67	ASN	5.8
1	C	311	PRO	5.8
1	C	298	ILE	5.8
1	B	294	ALA	5.6
1	A	42	MET	5.6
1	A	258	TYR	5.4
1	C	345	GLN	5.4
1	A	329	SER	5.4
1	C	183	PRO	5.3
1	B	183	PRO	5.2
1	C	332	PRO	5.2
1	A	314	SER	5.2
1	A	293	ALA	5.2
1	A	285	ASN	5.2
1	B	311	PRO	5.1
1	C	282	ILE	5.1
1	B	223	SER	5.0
1	A	182	ASN	5.0
1	B	285	ASN	5.0
1	B	289	PRO	4.9
1	A	343	THR	4.9
1	C	261	ILE	4.9
1	C	305	ILE	4.7
1	B	221	ASP	4.7
2	D	408	TYR	4.7
1	B	349	GLN	4.7
1	B	291	GLY	4.7
1	B	135	THR	4.7
1	A	283	VAL	4.6
1	A	225	ASP	4.6
1	A	296	ALA	4.6
1	B	334	VAL	4.5
2	F	409	GLN	4.5
1	A	344	LEU	4.4
1	B	293	ALA	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	282	ILE	4.4
1	C	352	PRO	4.4
1	A	303	LEU	4.3
1	A	311	PRO	4.3
1	A	352	PRO	4.3
1	C	290	ASP	4.3
1	A	351	TYR	4.3
1	C	70	SER	4.2
1	A	330	VAL	4.1
1	A	181	LEU	4.1
1	B	226	GLY	4.1
1	C	260	GLY	4.1
1	C	317	GLU	4.1
1	B	303	LEU	4.0
1	C	294	ALA	3.9
1	C	72	ASN	3.9
1	A	347	THR	3.9
1	C	184	THR	3.8
1	B	317	GLU	3.8
1	B	225	ASP	3.7
1	A	335	VAL	3.7
1	A	284	VAL	3.7
1	C	330	VAL	3.6
1	C	66	LEU	3.6
1	B	297	GLY	3.5
1	B	284	VAL	3.5
1	C	258	TYR	3.5
1	B	335	VAL	3.5
1	A	332	PRO	3.5
1	B	182	ASN	3.4
2	D	409	GLN	3.4
1	C	325	ILE	3.4
1	A	297	GLY	3.4
1	B	308	ASP	3.4
1	B	184	THR	3.3
1	A	187	GLN	3.3
1	C	255	ILE	3.3
1	B	258	TYR	3.3
2	E	409	GLN	3.3
1	B	336	MET	3.2
1	C	69	ASN	3.2
1	B	345	GLN	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	301	ASN	3.2
1	B	77	ARG	3.0
1	C	299	GLN	2.9
1	C	71	HIS	2.8
1	C	291	GLY	2.8
1	C	320	ASP	2.8
2	D	410	PHE	2.8
1	B	181	LEU	2.8
1	B	347	THR	2.7
1	A	186	ARG	2.7
1	A	302	ASP	2.6
1	C	73	GLN	2.6
1	B	74	LEU	2.6
1	B	307	VAL	2.5
1	C	146	ARG	2.5
1	A	312	ALA	2.5
1	A	292	PRO	2.5
1	C	326	ARG	2.5
1	A	316	LEU	2.5
1	B	325	ILE	2.5
1	A	350	GLU	2.5
1	C	319	MET	2.5
1	C	187	GLN	2.4
1	A	185	GLY	2.4
1	C	222	LYS	2.4
1	B	343	THR	2.4
1	A	210	GLY	2.4
1	C	224	ASN	2.4
1	B	333	VAL	2.3
1	B	137	GLY	2.3
1	C	351	TYR	2.3
1	B	185	GLY	2.3
1	B	305	ILE	2.2
1	A	183	PRO	2.2
1	B	295	ASN	2.2
1	B	257	GLY	2.2
1	C	308	ASP	2.2
1	C	223	SER	2.2
1	C	331	ILE	2.2
1	C	285	ASN	2.1
1	B	344	LEU	2.1
1	B	320	ASP	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	180	GLY	2.1
1	C	307	VAL	2.1
1	A	253	ARG	2.1
1	B	328	GLY	2.1
1	C	293	ALA	2.0
1	A	317	GLU	2.0
1	A	309	ASN	2.0
1	C	63	ASN	2.0

## 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.