



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:18 AM GMT

PDB ID : 3B9B  
Title : Structure of the E2 beryllium fluoride complex of the SERCA Ca<sup>2+</sup>-ATPase  
Authors : Olesen, C.; Picard, M.; Winther, A.M.L.; Morth, J.P.; Moller, J.V.; Nissen, P.  
Deposited on : 2007-11-04  
Resolution : 2.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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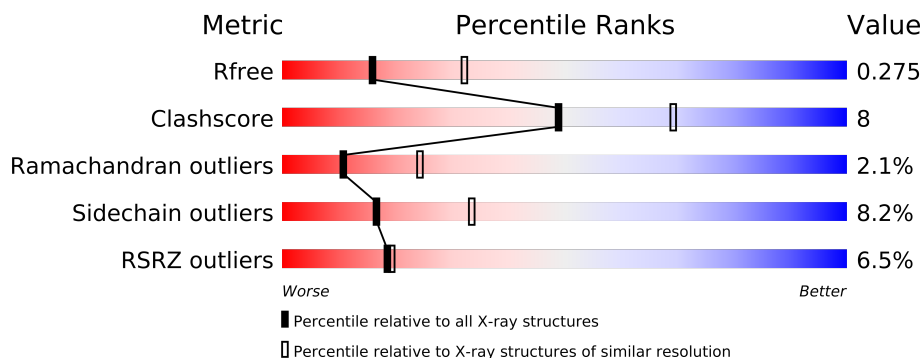
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.65 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	994	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	NA	A	995	-	X
3	MG	A	997	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 7743 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sarcoplasmic/endoplasmicreticulum calcium ATPase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	994	Total	C	N	O	S	1	0	0
			7671	4876	1287	1451	57			

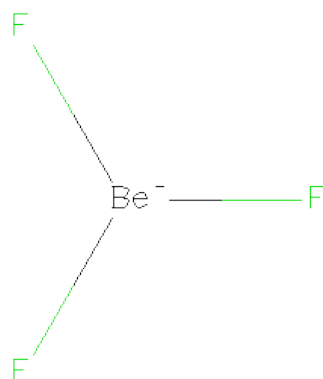
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Be	F	0	0
			4	1	3		

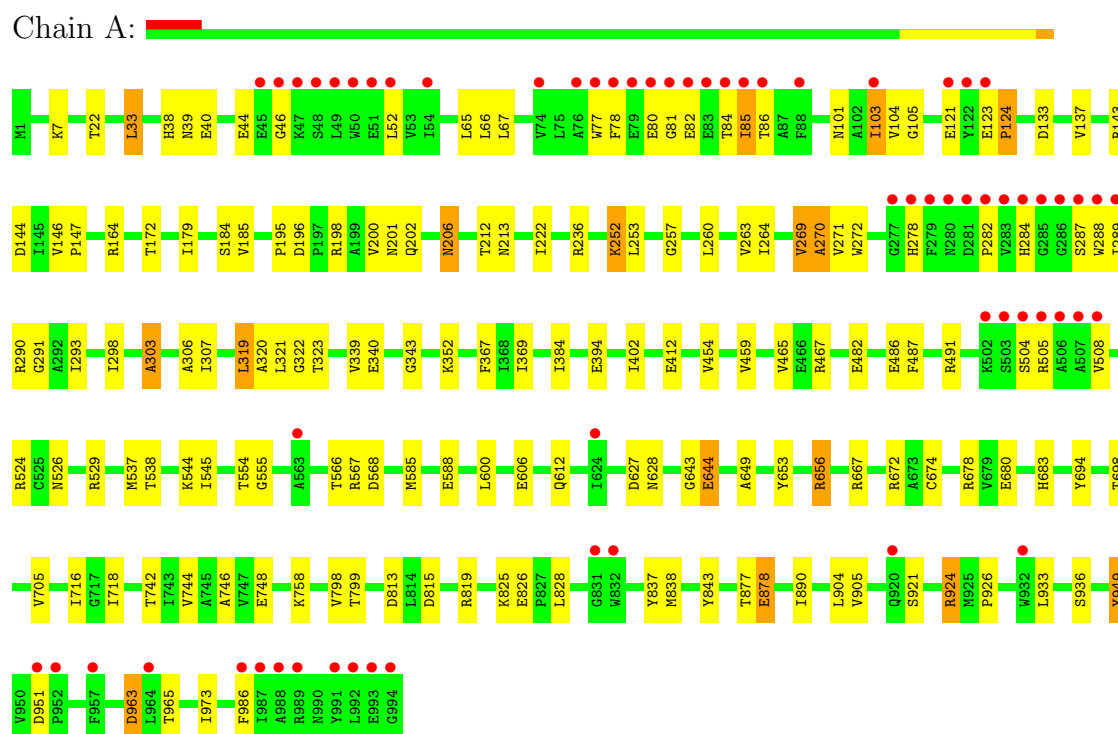
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		

### 3 Residue-property plots

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.

- Molecule 1: Sarcoplasmic/endoplasmicreticulum calcium ATPase 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.60Å 114.60Å 229.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.35 – 2.65 29.35 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.35-2.65) 99.3 (29.35-2.65)	Depositor EDS
$R_{merge}$	0.27	Depositor
$R_{sym}$	0.27	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.64Å)	Xtriage
Refinement program	phenix.refine	Depositor
R, $R_{free}$	0.214 , 0.271 0.214 , 0.275	Depositor DCC
$R_{free}$ test set	1347 reflections (3.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.7	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 44779 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7743	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.35	0/7812	0.56	1/10592 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	N-CA-C	-5.70	95.60	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7671	0	0	59	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	4	0	0	0	0
5	A	65	0	0	0	0
All	All	7743	0	0	59	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 8.

All (59) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:282:PRO:CG	1:A:284:HIS:CD2	2.77	0.68
1:A:77:TRP:CD1	1:A:78:PHE:CD2	2.85	0.64
1:A:491:ARG:NH1	1:A:588:GLU:OE1	2.34	0.59
1:A:33:LEU:CD1	1:A:38:HIS:CD2	2.86	0.59
1:A:486:GLU:O	1:A:491:ARG:NH2	2.37	0.57
1:A:123:GLU:CG	1:A:124:PRO:CD	2.83	0.56
1:A:653:TYR:OH	1:A:672:ARG:NH1	2.38	0.56
1:A:200:VAL:CG1	1:A:201:ASN:N	2.70	0.55
1:A:287:SER:O	1:A:288:TRP:CD1	2.61	0.54
1:A:491:ARG:NH1	1:A:588:GLU:CD	2.62	0.53
1:A:80:GLU:O	1:A:82:GLU:N	2.42	0.52
1:A:82:GLU:O	1:A:82:GLU:CG	2.59	0.51
1:A:287:SER:O	1:A:288:TRP:CG	2.63	0.51
1:A:504:SER:O	1:A:505:ARG:CG	2.59	0.51
1:A:38:HIS:O	1:A:40:GLU:N	2.43	0.50
1:A:287:SER:C	1:A:288:TRP:CD1	2.86	0.49
1:A:742:THR:O	1:A:746:ALA:N	2.45	0.49
1:A:837:TYR:CD1	1:A:837:TYR:C	2.86	0.49
1:A:269:VAL:O	1:A:270:ALA:C	2.51	0.48
1:A:269:VAL:O	1:A:272:TRP:N	2.46	0.48
1:A:319:LEU:O	1:A:322:GLY:N	2.47	0.47
1:A:554:THR:CG2	1:A:555:GLY:N	2.78	0.47
1:A:278:HIS:CG	1:A:278:HIS:O	2.68	0.47
1:A:949:TYR:N	1:A:949:TYR:CD1	2.82	0.47
1:A:84:THR:O	1:A:86:THR:N	2.48	0.47
1:A:269:VAL:O	1:A:271:VAL:N	2.47	0.46
1:A:986:PHE:C	1:A:986:PHE:CD2	2.89	0.46
1:A:491:ARG:NH1	1:A:588:GLU:OE2	2.50	0.45
1:A:843:TYR:OH	1:A:973:ILE:O	2.33	0.45
1:A:529:ARG:NH2	1:A:568:ASP:OD1	2.50	0.45
1:A:252:LYS:NZ	1:A:826:GLU:O	2.50	0.45
1:A:643:GLY:O	1:A:644:GLU:C	2.56	0.44
1:A:526:ASN:O	1:A:537:MET:N	2.50	0.44
1:A:290:ARG:NH1	1:A:291:GLY:O	2.52	0.43
1:A:198:ARG:CD	1:A:656:ARG:NH2	2.82	0.43
1:A:667:ARG:NH1	1:A:694:TYR:CE2	2.88	0.42
1:A:184:SER:OG	1:A:627:ASP:OD2	2.38	0.42
1:A:933:LEU:O	1:A:936:SER:OG	2.38	0.42
1:A:877:THR:CG2	1:A:878:GLU:N	2.83	0.42
1:A:412:GLU:OE1	1:A:529:ARG:CD	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:ILE:C	1:A:105:GLY:N	2.74	0.41
1:A:195:PRO:O	1:A:196:ASP:C	2.58	0.41
1:A:289:ILE:CG2	1:A:290:ARG:N	2.84	0.41
1:A:798:VAL:O	1:A:799:THR:C	2.59	0.41
1:A:146:VAL:C	1:A:147:PRO:O	2.57	0.41
1:A:963:ASP:OD2	1:A:963:ASP:C	2.57	0.41
1:A:303:ALA:O	1:A:306:ALA:N	2.54	0.41
1:A:78:PHE:C	1:A:78:PHE:CD1	2.94	0.41
1:A:253:LEU:O	1:A:257:GLY:N	2.54	0.41
1:A:264:ILE:CD1	1:A:307:ILE:CD1	2.99	0.41
1:A:206:ASN:N	1:A:206:ASN:ND2	2.69	0.41
1:A:340:GLU:O	1:A:343:GLY:N	2.54	0.41
1:A:924:ARG:O	1:A:926:PRO:CD	2.69	0.41
1:A:367:PHE:CD2	1:A:367:PHE:C	2.94	0.41
1:A:680:GLU:N	1:A:683:HIS:ND1	2.70	0.40
1:A:352:LYS:NZ	1:A:627:ASP:OD2	2.55	0.40
1:A:44:GLU:C	1:A:46:GLY:N	2.74	0.40
1:A:319:LEU:O	1:A:321:LEU:N	2.55	0.40
1:A:319:LEU:O	1:A:320:ALA:C	2.58	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	992/994 (100%)	895 (90%)	76 (8%)	21 (2%)	11 24

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	124	PRO
1	A	270	ALA
1	A	508	VAL

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Mol	Chain	Res	Type
1	A	649	ALA
1	A	924	ARG
1	A	951	ASP
1	A	81	GLY
1	A	85	ILE
1	A	269	VAL
1	A	487	PHE
1	A	644	GLU
1	A	905	VAL
1	A	293	ILE
1	A	921	SER
1	A	133	ASP
1	A	303	ALA
1	A	758	LYS
1	A	878	GLU
1	A	904	LEU
1	A	319	LEU

### 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	840/840 (100%)	771 (92%)	69 (8%)	17	33

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	22	THR
1	A	33	LEU
1	A	52	LEU
1	A	65	LEU
1	A	66	LEU
1	A	67	LEU
1	A	85	ILE
1	A	101	ASN
1	A	103	ILE
1	A	104	VAL

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Mol	Chain	Res	Type
1	A	137	VAL
1	A	143	ARG
1	A	144	ASP
1	A	164	ARG
1	A	172	THR
1	A	179	ILE
1	A	185	VAL
1	A	202	GLN
1	A	206	ASN
1	A	212	THR
1	A	213	ASN
1	A	222	ILE
1	A	236	ARG
1	A	252	LYS
1	A	260	LEU
1	A	263	VAL
1	A	298	ILE
1	A	323	THR
1	A	339	VAL
1	A	369	ILE
1	A	384	ILE
1	A	394	GLU
1	A	402	ILE
1	A	454	VAL
1	A	459	VAL
1	A	465	VAL
1	A	467	ARG
1	A	482	GLU
1	A	524	ARG
1	A	538	THR
1	A	544	LYS
1	A	545	ILE
1	A	566	THR
1	A	567	ARG
1	A	585	MET
1	A	600	LEU
1	A	606	GLU
1	A	612	GLN
1	A	628	ASN
1	A	656	ARG
1	A	674	CYS
1	A	678	ARG

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Mol	Chain	Res	Type
1	A	698	THR
1	A	705	VAL
1	A	716	ILE
1	A	718	ILE
1	A	744	VAL
1	A	748	GLU
1	A	813	ASP
1	A	815	ASP
1	A	819	ARG
1	A	825	LYS
1	A	828	LEU
1	A	838	MET
1	A	890	ILE
1	A	949	TYR
1	A	963	ASP
1	A	965	THR

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 chains 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 4 ligands modelled in this entry, 3 are 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	$\# Z  > 2$
4	BEF	A	998	1	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEF	A	998	1	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	994/994 (100%)	-0.00	64 (6%)	19 20	8, 49, 133, 318	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	VAL	16.0
1	A	505	ARG	13.5
1	A	78	PHE	12.9
1	A	48	SER	10.1
1	A	122	TYR	9.7
1	A	506	ALA	8.9
1	A	287	SER	8.8
1	A	994	GLY	8.6
1	A	504	SER	8.6
1	A	81	GLY	8.2
1	A	285	GLY	7.9
1	A	121	GLU	7.0
1	A	991	TYR	6.9
1	A	49	LEU	6.8
1	A	85	ILE	6.6
1	A	281	ASP	6.6
1	A	50	TRP	6.4
1	A	288	TRP	6.3
1	A	951	ASP	6.3
1	A	86	THR	6.2
1	A	280	ASN	6.2
1	A	80	GLU	6.1
1	A	84	THR	5.8
1	A	286	GLY	5.8
1	A	88	PHE	5.5
1	A	503	SER	5.5
1	A	79	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	279	PHE	5.3
1	A	83	GLU	5.2
1	A	74	VAL	5.1
1	A	993	GLU	4.9
1	A	77	TRP	4.7
1	A	123	GLU	4.3
1	A	508	VAL	4.2
1	A	987	ILE	4.2
1	A	278	HIS	4.1
1	A	284	HIS	4.1
1	A	988	ALA	3.9
1	A	52	LEU	3.8
1	A	289	ILE	3.6
1	A	831	GLY	3.5
1	A	82	GLU	3.1
1	A	282	PRO	3.0
1	A	964	LEU	3.0
1	A	952	PRO	3.0
1	A	502	LYS	3.0
1	A	47	LYS	2.8
1	A	992	LEU	2.6
1	A	277	GLY	2.6
1	A	920	GLN	2.5
1	A	832	TRP	2.4
1	A	76	ALA	2.4
1	A	932	TRP	2.4
1	A	45	GLU	2.2
1	A	51	GLU	2.2
1	A	624	ILE	2.2
1	A	563	ALA	2.2
1	A	957	PHE	2.2
1	A	46	GLY	2.1
1	A	54	ILE	2.1
1	A	103	ILE	2.1
1	A	989	ARG	2.1
1	A	986	PHE	2.0
1	A	507	ALA	2.0

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

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	A	995	1/1	0.72	8.47	69,69,69,69	0
3	MG	A	997	1/1	0.29	3.80	98,98,98,98	0
3	MG	A	996	1/1	0.17	1.02	13,13,13,13	0
4	BEF	A	998	4/4	0.18	0.56	30,35,37,45	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.