



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 1, 2026 – 12:52 AM UTC

PDB ID : 4EED / pdb\_00004eed  
Title : CorA coiled-coil mutant under Mg<sup>2+</sup> presence  
Authors : Pfoh, R.; Pai, E.F.  
Deposited on : 2012-03-28  
Resolution : 3.92 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

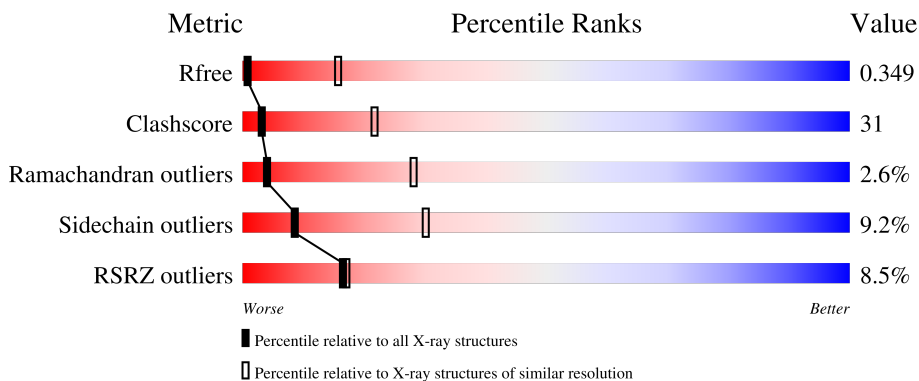
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.92 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))
$R_{free}$	180053	1033 (4.10-3.74)
Clashscore	190562	1070 (4.10-3.74)
Ramachandran outliers	187476	1017 (4.10-3.74)
Sidechain outliers	187428	1010 (4.10-3.74)
RSRZ outliers	180081	1033 (4.10-3.74)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	330	 10% 44% 44% 6% • 5%
1	B	330	 5% 47% 44% • • 5%
1	C	330	 10% 47% 42% 6% • 5%
1	D	330	 8% 42% 45% 7% • 5%
1	E	330	 7% 45% 42% 8% 5%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12979 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 Magnesium transport protein CorA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2593	1688	418	478	9	0	0	0
1	B	314	2593	1688	418	478	9	0	0	0
1	C	314	2593	1688	418	478	9	0	0	0
1	D	314	2593	1688	418	478	9	0	0	0
1	E	314	2593	1688	418	478	9	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q9WZ31
A	23	SER	-	expression tag	UNP Q9WZ31
A	24	HIS	-	expression tag	UNP Q9WZ31
A	25	MET	-	expression tag	UNP Q9WZ31
A	222	ALA	ARG	engineered mutation	UNP Q9WZ31
A	223	ALA	LYS	engineered mutation	UNP Q9WZ31
B	22	GLY	-	expression tag	UNP Q9WZ31
B	23	SER	-	expression tag	UNP Q9WZ31
B	24	HIS	-	expression tag	UNP Q9WZ31
B	25	MET	-	expression tag	UNP Q9WZ31
B	222	ALA	ARG	engineered mutation	UNP Q9WZ31
B	223	ALA	LYS	engineered mutation	UNP Q9WZ31
C	22	GLY	-	expression tag	UNP Q9WZ31
C	23	SER	-	expression tag	UNP Q9WZ31
C	24	HIS	-	expression tag	UNP Q9WZ31
C	25	MET	-	expression tag	UNP Q9WZ31
C	222	ALA	ARG	engineered mutation	UNP Q9WZ31
C	223	ALA	LYS	engineered mutation	UNP Q9WZ31
D	22	GLY	-	expression tag	UNP Q9WZ31

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Chain	Residue	Modelled	Actual	Comment	Reference
D	23	SER	-	expression tag	UNP Q9WZ31
D	24	HIS	-	expression tag	UNP Q9WZ31
D	25	MET	-	expression tag	UNP Q9WZ31
D	222	ALA	ARG	engineered mutation	UNP Q9WZ31
D	223	ALA	LYS	engineered mutation	UNP Q9WZ31
E	22	GLY	-	expression tag	UNP Q9WZ31
E	23	SER	-	expression tag	UNP Q9WZ31
E	24	HIS	-	expression tag	UNP Q9WZ31
E	25	MET	-	expression tag	UNP Q9WZ31
E	222	ALA	ARG	engineered mutation	UNP Q9WZ31
E	223	ALA	LYS	engineered mutation	UNP Q9WZ31

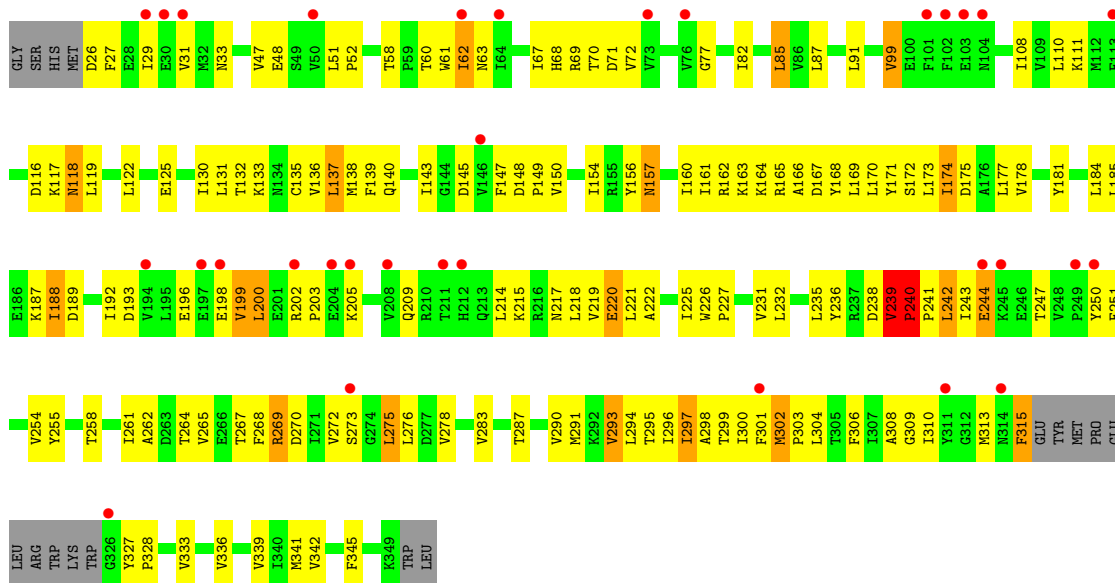
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Mg 4 4	0	0
2	B	3	Total Mg 3 3	0	0
2	C	2	Total Mg 2 2	0	0
2	D	3	Total Mg 3 3	0	0
2	E	2	Total Mg 2 2	0	0

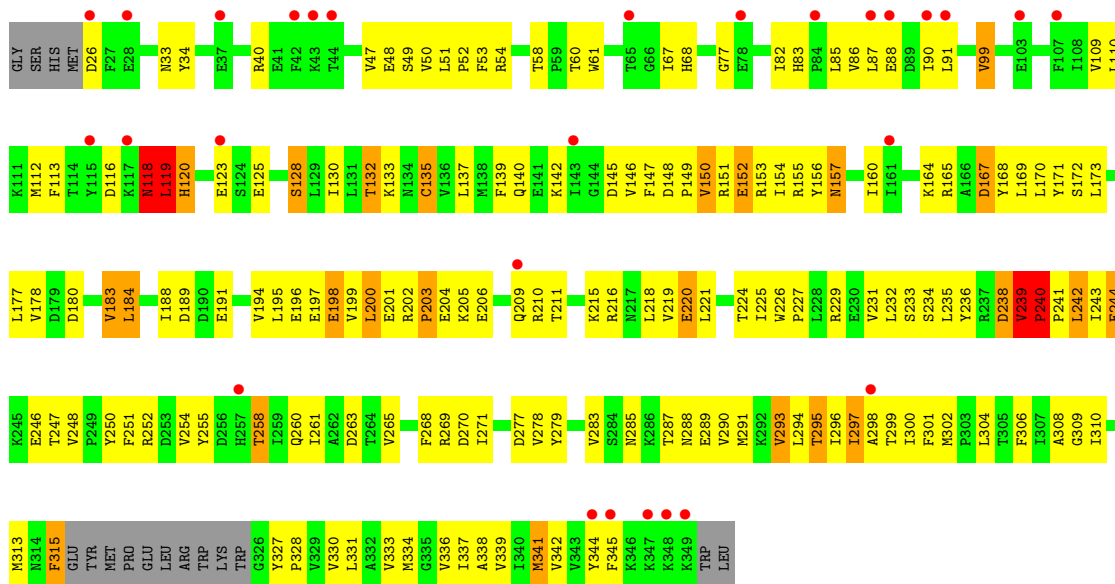




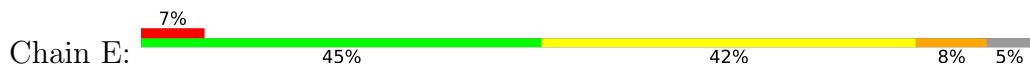
• Molecule 1: Magnesium transport protein CorA

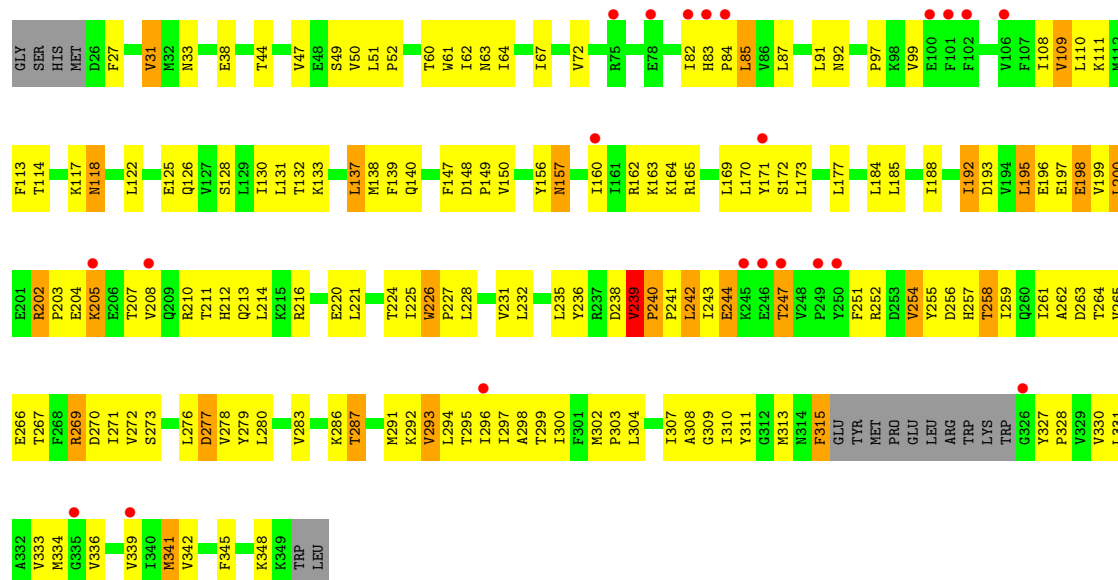


• Molecule 1: Magnesium transport protein CorA



• Molecule 1: Magnesium transport protein CorA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.70Å 132.50Å 179.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.92 48.79 – 3.92	Depositor EDS
% Data completeness (in resolution range)	82.1 (48.79-3.92) 81.9 (48.79-3.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.88Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.297 , 0.351 0.297 , 0.349	Depositor DCC
$R_{free}$ test set	1097 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	142.1	Xtrriage
Anisotropy	0.017	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 137.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	12979	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	145.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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](#)

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

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	0.73	2/2646 (0.1%)	0.88	3/3588 (0.1%)
1	B	0.70	1/2646 (0.0%)	0.85	1/3588 (0.0%)
1	C	0.71	1/2646 (0.0%)	0.86	3/3588 (0.1%)
1	D	0.78	3/2646 (0.1%)	0.90	2/3588 (0.1%)
1	E	0.73	0/2646	0.90	1/3588 (0.0%)
All	All	0.73	7/13230 (0.1%)	0.88	10/17940 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	ASP	CA-C	6.96	1.55	1.52
1	D	240	PRO	CA-C	5.95	1.57	1.52
1	C	143	ILE	CA-CB	5.63	1.59	1.54
1	D	271	ILE	CA-CB	-5.63	1.47	1.54
1	A	240	PRO	CA-C	5.31	1.57	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	VAL	CB-CA-C	-6.58	103.42	112.04
1	E	254	VAL	N-CA-C	-6.04	105.93	111.67
1	A	64	ILE	CB-CA-C	-5.75	105.32	112.45
1	B	272	VAL	CB-CA-C	-5.74	104.30	112.22
1	D	240	PRO	N-CA-C	5.35	117.23	110.70

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	2593	0	2630	193	0
1	B	2593	0	2630	165	0
1	C	2593	0	2630	172	0
1	D	2593	0	2630	178	0
1	E	2593	0	2630	176	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	2	0	0	0	0
All	All	12979	0	13150	816	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 31.

The worst 5 of 816 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:221:LEU:HG	1:B:225:ILE:HD11	1.27	1.17
1:C:294:LEU:HD22	1:D:294:LEU:HD11	1.11	1.05
1:E:221:LEU:HG	1:E:225:ILE:HD11	1.36	1.04
1:B:302:MET:HE3	1:C:301:PHE:HB2	1.39	1.04
1:B:302:MET:HE2	1:C:298:ALA:HA	1.40	1.02

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	310/330 (94%)	258 (83%)	44 (14%)	8 (3%)	4	28
1	B	310/330 (94%)	257 (83%)	44 (14%)	9 (3%)	3	26
1	C	310/330 (94%)	255 (82%)	49 (16%)	6 (2%)	6	33
1	D	310/330 (94%)	250 (81%)	48 (16%)	12 (4%)	2	22
1	E	310/330 (94%)	258 (83%)	47 (15%)	5 (2%)	7	36
All	All	1550/1650 (94%)	1278 (82%)	232 (15%)	40 (3%)	4	28

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	244	GLU
1	B	244	GLU
1	C	157	ASN
1	A	157	ASN

### 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	295/310 (95%)	268 (91%)	27 (9%)	8	30
1	B	295/310 (95%)	272 (92%)	23 (8%)	11	35
1	C	295/310 (95%)	269 (91%)	26 (9%)	9	32
1	D	295/310 (95%)	264 (90%)	31 (10%)	6	24
1	E	295/310 (95%)	266 (90%)	29 (10%)	7	27
All	All	1475/1550 (95%)	1339 (91%)	136 (9%)	8	30

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	162	ARG

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Mol	Chain	Res	Type
1	E	198	GLU
1	E	277	ASP
1	B	315	PHE
1	B	297	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	212	HIS
1	E	213	GLN
1	C	314	ASN
1	E	33	ASN
1	C	217	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

## 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	314/330 (95%)	0.41	33 (10%) 11 13	82, 149, 185, 198	0
1	B	314/330 (95%)	0.31	18 (5%) 29 24	83, 153, 195, 210	0
1	C	314/330 (95%)	0.43	32 (10%) 12 14	81, 151, 193, 207	0
1	D	314/330 (95%)	0.47	28 (8%) 15 16	80, 145, 179, 192	0
1	E	314/330 (95%)	0.29	22 (7%) 22 20	81, 145, 181, 193	0
All	All	1570/1650 (95%)	0.38	133 (8%) 16 17	80, 149, 188, 210	0

The worst 5 of 133 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	84	PRO	7.5
1	C	103	GLU	6.8
1	E	249	PRO	6.7
1	D	28	GLU	6.7
1	A	143	ILE	6.6

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	D	503	1/1	0.36	0.39	80,80,80,80	0
2	MG	E	502	1/1	0.78	0.14	56,56,56,56	0
2	MG	D	502	1/1	0.82	0.16	17,17,17,17	0
2	MG	A	401	1/1	0.82	0.08	75,75,75,75	0
2	MG	C	501	1/1	0.82	0.10	79,79,79,79	0
2	MG	B	502	1/1	0.86	0.22	58,58,58,58	0
2	MG	E	501	1/1	0.87	0.12	48,48,48,48	0
2	MG	A	402	1/1	0.87	0.09	45,45,45,45	0
2	MG	A	403	1/1	0.88	0.22	23,23,23,23	0
2	MG	A	404	1/1	0.89	0.09	88,88,88,88	0
2	MG	B	503	1/1	0.93	0.14	22,22,22,22	0
2	MG	C	502	1/1	0.94	0.08	47,47,47,47	0
2	MG	D	501	1/1	0.94	0.04	113,113,113,113	0
2	MG	B	501	1/1	0.96	0.03	90,90,90,90	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.