



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 02:39 PM GMT

PDB ID : 3A8G  
Title : Crystal structure of Nitrile Hydratase mutant S113A complexed with Trimethylacetone nitrile  
Authors : Yamanaka, Y.; Hashimoto, K.; Ohtaki, A.; Noguchi, K.; Yohda, M.; Odaka, M.  
Deposited on : 2009-10-06  
Resolution : 1.11 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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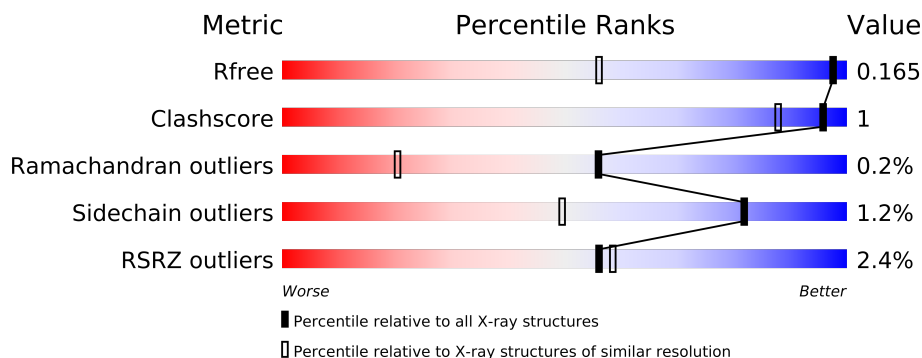
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.11 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	1225 (1.20-1.04)
Clashscore	79885	1354 (1.20-1.04)
Ramachandran outliers	78287	1287 (1.20-1.04)
Sidechain outliers	78261	1285 (1.20-1.04)
RSRZ outliers	66119	1225 (1.20-1.04)

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	207	
2	B	212	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NO	A	207	-	X
6	TAN	B	213	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 3706 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 Nitrile hydratase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	4	0
			1565	997	261	301	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	SER	ENGINEERED	UNP P13448

- Molecule 2 is a protein called Nitrile hydratase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	7	0
			1682	1067	286	318	11			

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		

- Molecule 4 is NITRIC OXIDE (three-letter code: NO) (formula: NO).

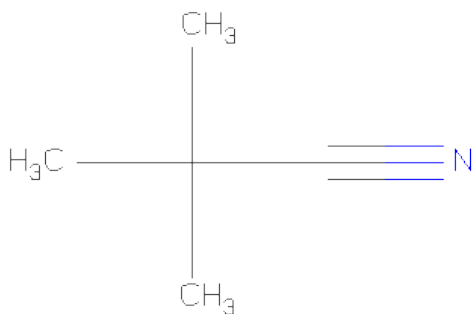


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			2	1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Mg	0	0
			3	3		

- Molecule 6 is 2,2-DIMETHYLPROPANENITRILE (three-letter code: TAN) (formula: C<sub>5</sub>H<sub>9</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			6	5	1		

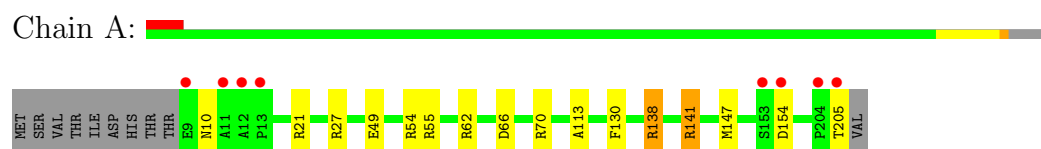
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	205	Total	O	0	0
			205	205		
7	B	242	Total	O	0	0
			242	242		

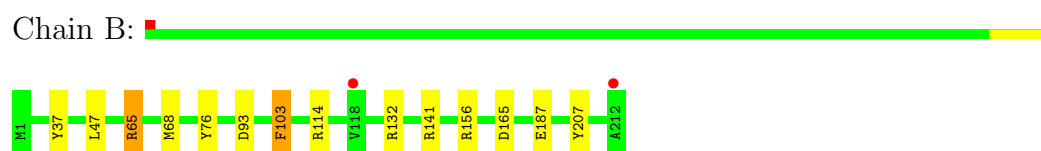
### 3 Residue-property plots

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 ( $RSRZ > 2$ ). 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: Nitrile hydratase subunit alpha



- Molecule 2: Nitrile hydratase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.41 Å   60.27 Å   81.81 Å 90.00°   124.92°   90.00°	Depositor
Resolution (Å)	19.01 – 1.11 19.01 – 1.11	Depositor EDS
% Data completeness (in resolution range)	89.2 (19.01-1.11) 89.9 (19.01-1.11)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 1.11 Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.143   ,   0.169 0.140   ,   0.165	Depositor DCC
$R_{free}$ test set	8169 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	8.7	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.49 , 63.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 169431 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.46% 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: MG, NO, CSD, CSO, FE, TAN

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	0.77	1/1600 (0.1%)	1.39	22/2186 (1.0%)
2	B	0.74	0/1758	1.20	14/2388 (0.6%)
All	All	0.76	1/3358 (0.0%)	1.30	36/4574 (0.8%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ARG	CZ-NH1	9.02	1.44	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ARG	NE-CZ-NH1	16.08	128.34	120.30
1	A	70	ARG	NE-CZ-NH1	-14.86	112.87	120.30
1	A	54	ARG	NE-CZ-NH2	-13.09	113.76	120.30
1	A	141	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	138	ARG	NE-CZ-NH2	10.49	125.55	120.30
1	A	70	ARG	NE-CZ-NH2	9.78	125.19	120.30
1	A	21	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	A	54	ARG	CD-NE-CZ	8.95	136.13	123.60
2	B	37	TYR	CB-CG-CD2	-7.50	116.50	121.00
2	B	65[A]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
2	B	65[B]	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	A	66	ASP	CB-CG-OD2	7.00	124.60	118.30
1	A	21	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	55	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	27	ARG	CD-NE-CZ	6.16	132.23	123.60
1	A	147	MET	CG-SD-CE	-6.11	90.43	100.20
2	B	156	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	A	62	ARG	NE-CZ-NH2	-6.00	117.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLU	OE1-CD-OE2	-5.97	116.13	123.30
2	B	93	ASP	CB-CG-OD2	-5.87	113.02	118.30
2	B	141	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	141	ARG	NH1-CZ-NH2	-5.82	113.00	119.40
2	B	132	ARG	NE-CZ-NH2	-5.71	117.45	120.30
2	B	47	LEU	CB-CG-CD1	5.64	120.58	111.00
2	B	76	TYR	CB-CG-CD2	-5.55	117.67	121.00
2	B	187	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	A	54	ARG	CB-CG-CD	5.39	125.61	111.60
2	B	114	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	B	207	TYR	CB-CG-CD1	5.23	124.14	121.00
1	A	55	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	55	ARG	NH1-CZ-NH2	5.17	125.09	119.40
2	B	103	PHE	CB-CG-CD1	5.16	124.41	120.80
1	A	138	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
1	A	70	ARG	CD-NE-CZ	-5.08	116.48	123.60
2	B	37	TYR	CB-CG-CD1	5.07	124.04	121.00
1	A	130	PHE	CB-CG-CD1	5.01	124.30	120.80

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	1565	0	0	4	0
2	B	1682	0	0	1	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	B	3	0	0	0	0
6	B	6	0	0	0	0
7	A	205	0	0	2	0
7	B	242	0	0	0	0
All	All	3706	0	0	4	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 1.

All (4) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:138:ARG:NH2	7:A:329:HOH:O	2.47	0.46
1:A:141:ARG:NH2	7:A:424:HOH:O	2.47	0.46
1:A:10:ASN:OD1	2:B:65[B]:ARG:NE	2.51	0.44

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	197/207 (95%)	192 (98%)	4 (2%)	1 (0%)	38	9
2	B	217/212 (102%)	215 (99%)	2 (1%)	0	100	100
All	All	414/419 (99%)	407 (98%)	6 (1%)	1 (0%)	56	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ALA

### 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	164/170 (96%)	163 (99%)	1 (1%)	92	73
2	B	180/173 (104%)	176 (98%)	4 (2%)	64	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	344/343 (100%)	339 (98%)	5 (2%)	82	39

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	THR
2	B	68[A]	MET
2	B	68[B]	MET
2	B	103	PHE
2	B	165	ASP

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 ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	CSD	A	112	1,3	7,7,8	7.89	2 (28%)	6,8,10	2.26	3 (50%)
1	CSO	A	114	1,3	6,6,7	7.59	2 (33%)	3,6,8	1.96	1 (33%)

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
1	CSD	A	112	1,3	-	1/3/6/8	0/0/0/0
1	CSO	A	114	1,3	-	0/2/5/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	CSD	O-C	20.59	1.25	1.11
1	A	114	CSO	O-C	18.20	1.23	1.11
1	A	112	CSD	CA-C	3.26	1.54	1.48
1	A	114	CSO	CA-C	3.03	1.54	1.48

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	CSD	CA-CB-SG	3.45	115.75	110.82
1	A	114	CSO	CA-CB-SG	-3.11	107.47	113.01
1	A	112	CSD	C-CA-N	-2.94	110.89	113.83
1	A	112	CSD	OD2-SG-CB	2.23	106.40	97.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	112	CSD	CA-CB-SG-OD1

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	NO	A	207	3	0,1,1	0.00	-	0,0,0	0.00	-
6	TAN	B	213	-	5,5,5	0.86	0	7,7,7	2.88	4 (57%)

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	NO	A	207	3	-	0/0/0/0	0/0/0/0
6	TAN	B	213	-	-	0/3/3/3	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	213	TAN	C2-C-N	-4.48	155.02	176.44
6	B	213	TAN	C1-C2-C	4.25	116.61	108.41
6	B	213	TAN	C4-C2-C	3.17	114.52	108.41
6	B	213	TAN	C4-C2-C3	-2.58	97.83	109.54

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	197/207 (95%)	-0.08	8 (4%) 35 38	7, 12, 26, 48	0
2	B	212/212 (100%)	-0.19	2 (0%) 81 84	7, 12, 23, 45	0
All	All	409/419 (97%)	-0.14	10 (2%) 56 58	7, 12, 24, 48	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	212	ALA	8.1
1	A	205	THR	7.1
1	A	154[A]	ASP	4.1
2	B	118	VAL	4.1
1	A	153[A]	SER	2.9
1	A	12	ALA	2.5
1	A	9	GLU	2.4
1	A	11	ALA	2.4
1	A	204	PRO	2.3
1	A	13	PRO	2.1

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

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
1	CSO	A	114	7/8	0.05	-1.11	7,7,9,11	0
1	CSD	A	112	8/9	0.05	-1.11	6,6,7,8	0

### 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
6	TAN	B	213	6/6	0.14	8.62	19,24,28,43	0
4	NO	A	207	2/2	0.09	5.55	9,9,9,26	0
5	MG	B	302	1/1	0.05	0.62	9,9,9,9	1
5	MG	B	304	1/1	0.06	-0.51	16,16,16,16	1
5	MG	B	303	1/1	0.04	-1.59	15,15,15,15	1
3	FE	A	301	1/1	0.01	-8.00	6,6,6,6	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.