



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:19 AM GMT

PDB ID : 2PVX  
Title : NMR and X-ray Analysis of Structural Additivity in Metal Binding Site-Swapped Hybrids of Rubredoxin  
Authors : Wang, L.; LeMaster, D.M.; Hernandez, G.; Li, H.  
Deposited on : 2007-05-10  
Resolution : 1.04 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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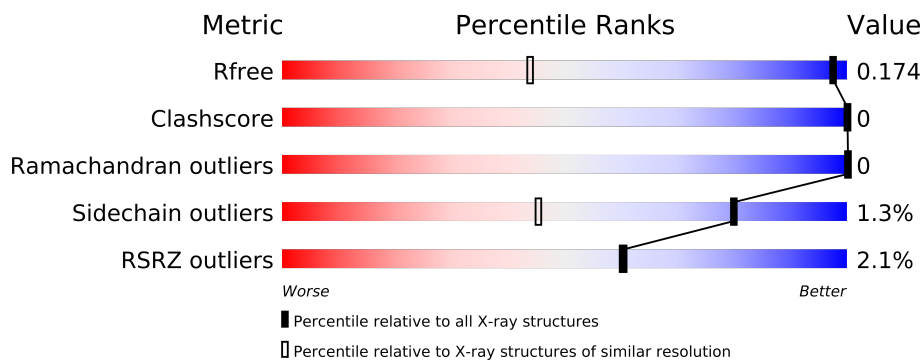
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.04 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	1106 (1.14-0.94)
Clashscore	79885	1011 (1.12-0.96)
Ramachandran outliers	78287	1151 (1.14-0.94)
Sidechain outliers	78261	1150 (1.14-0.94)
RSRZ outliers	66119	1106 (1.14-0.94)

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	54	
1	B	54	
1	C	54	
1	D	54	
1	E	54	
1	F	54	
1	G	54	
1	H	54	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7286 atoms, of which 3160 are hydrogens 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 Rubredoxin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	53	Total	C	H	N	O	S	0	5	0
			810	267	391	62	85	5			
1	B	54	Total	C	H	N	O	S	0	3	0
			819	270	391	64	89	5			
1	C	54	Total	C	H	N	O	S	0	6	0
			824	271	394	64	90	5			
1	D	54	Total	C	H	N	O	S	0	5	0
			808	267	385	63	88	5			
1	E	54	Total	C	H	N	O	S	0	8	0
			853	280	414	64	90	5			
1	F	54	Total	C	H	N	O	S	0	3	0
			835	275	400	64	91	5			
1	G	54	Total	C	H	N	O	S	0	1	0
			814	269	387	63	90	5			
1	H	54	Total	C	H	N	O	S	0	2	0
			829	273	398	64	89	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	LYS	ALA	ENGINEERED	UNP P24297
A	7	THR	LYS	ENGINEERED	UNP P24297
A	8	VAL	ILE	ENGINEERED	UNP P24297
A	41	LEU	ILE	ENGINEERED	UNP P24297
A	44	VAL	ALA	ENGINEERED	UNP P24297
A	45	GLY	PRO	ENGINEERED	UNP P24297
A	47	ASP	SER	ENGINEERED	UNP P24297
A	48	GLN	GLU	ENGINEERED	UNP P24297
B	102	LYS	ALA	ENGINEERED	UNP P24297
B	107	THR	LYS	ENGINEERED	UNP P24297
B	108	VAL	ILE	ENGINEERED	UNP P24297
B	141	LEU	ILE	ENGINEERED	UNP P24297
B	144	VAL	ALA	ENGINEERED	UNP P24297

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Chain	Residue	Modelled	Actual	Comment	Reference
B	145	GLY	PRO	ENGINEERED	UNP P24297
B	147	ASP	SER	ENGINEERED	UNP P24297
B	148	GLN	GLU	ENGINEERED	UNP P24297
C	202	LYS	ALA	ENGINEERED	UNP P24297
C	207	THR	LYS	ENGINEERED	UNP P24297
C	208	VAL	ILE	ENGINEERED	UNP P24297
C	241	LEU	ILE	ENGINEERED	UNP P24297
C	244	VAL	ALA	ENGINEERED	UNP P24297
C	245	GLY	PRO	ENGINEERED	UNP P24297
C	247	ASP	SER	ENGINEERED	UNP P24297
C	248	GLN	GLU	ENGINEERED	UNP P24297
D	302	LYS	ALA	ENGINEERED	UNP P24297
D	307	THR	LYS	ENGINEERED	UNP P24297
D	308	VAL	ILE	ENGINEERED	UNP P24297
D	341	LEU	ILE	ENGINEERED	UNP P24297
D	344	VAL	ALA	ENGINEERED	UNP P24297
D	345	GLY	PRO	ENGINEERED	UNP P24297
D	347	ASP	SER	ENGINEERED	UNP P24297
D	348	GLN	GLU	ENGINEERED	UNP P24297
E	402	LYS	ALA	ENGINEERED	UNP P24297
E	407	THR	LYS	ENGINEERED	UNP P24297
E	408	VAL	ILE	ENGINEERED	UNP P24297
E	441	LEU	ILE	ENGINEERED	UNP P24297
E	444	VAL	ALA	ENGINEERED	UNP P24297
E	445	GLY	PRO	ENGINEERED	UNP P24297
E	447	ASP	SER	ENGINEERED	UNP P24297
E	448	GLN	GLU	ENGINEERED	UNP P24297
F	502	LYS	ALA	ENGINEERED	UNP P24297
F	507	THR	LYS	ENGINEERED	UNP P24297
F	508	VAL	ILE	ENGINEERED	UNP P24297
F	541	LEU	ILE	ENGINEERED	UNP P24297
F	544	VAL	ALA	ENGINEERED	UNP P24297
F	545	GLY	PRO	ENGINEERED	UNP P24297
F	547	ASP	SER	ENGINEERED	UNP P24297
F	548	GLN	GLU	ENGINEERED	UNP P24297
G	602	LYS	ALA	ENGINEERED	UNP P24297
G	607	THR	LYS	ENGINEERED	UNP P24297
G	608	VAL	ILE	ENGINEERED	UNP P24297
G	641	LEU	ILE	ENGINEERED	UNP P24297
G	644	VAL	ALA	ENGINEERED	UNP P24297
G	645	GLY	PRO	ENGINEERED	UNP P24297
G	647	ASP	SER	ENGINEERED	UNP P24297

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Chain	Residue	Modelled	Actual	Comment	Reference
G	648	GLN	GLU	ENGINEERED	UNP P24297
H	702	LYS	ALA	ENGINEERED	UNP P24297
H	707	THR	LYS	ENGINEERED	UNP P24297
H	708	VAL	ILE	ENGINEERED	UNP P24297
H	741	LEU	ILE	ENGINEERED	UNP P24297
H	744	VAL	ALA	ENGINEERED	UNP P24297
H	745	GLY	PRO	ENGINEERED	UNP P24297
H	747	ASP	SER	ENGINEERED	UNP P24297
H	748	GLN	GLU	ENGINEERED	UNP P24297

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	H	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	80	Total	O	0	2
			82	82		
3	B	77	Total	O	0	2
			79	79		
3	C	87	Total	O	0	2
			89	89		
3	D	74	Total	O	0	0
			74	74		
3	E	76	Total	O	0	3
			79	79		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	90	Total 93	O 93	0	4
3	G	76	Total 80	O 80	0	6
3	H	103	Total 110	O 110	0	7

### 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: Rubredoxin

Chain A: 



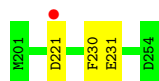
- Molecule 1: Rubredoxin

Chain B: 



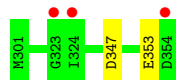
- Molecule 1: Rubredoxin

Chain C: 



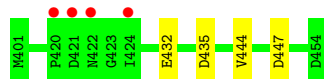
- Molecule 1: Rubredoxin

Chain D: 



- Molecule 1: Rubredoxin

Chain E: 



- Molecule 1: Rubredoxin

Chain F: 



- Molecule 1: Rubredoxin

Chain G: 



- Molecule 1: Rubredoxin

Chain H: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.26Å 45.84Å 95.08Å 90.00° 98.43° 90.00°	Depositor
Resolution (Å)	10.00 – 1.04 27.87 – 1.00	Depositor EDS
% Data completeness (in resolution range)	95.4 (10.00-1.04) 85.8 (27.87-1.00)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.60 (at 1.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.139 , 0.180 0.140 , 0.174	Depositor DCC
$R_{free}$ test set	8909 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	10.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 196658 reflections	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7286	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.21 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.1384e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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:  
ZN

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	0.76	0/438	1.12	2/595 (0.3%)
1	B	0.72	0/443	1.20	2/599 (0.3%)
1	C	0.72	0/449	1.26	2/608 (0.3%)
1	D	0.74	0/434	1.38	2/587 (0.3%)
1	E	0.75	0/466	1.35	4/630 (0.6%)
1	F	0.76	0/458	1.32	4/620 (0.6%)
1	G	0.82	0/442	1.24	2/598 (0.3%)
1	H	0.82	0/450	1.06	2/609 (0.3%)
All	All	0.76	0/3580	1.24	20/4846 (0.4%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	353[A]	GLU	CA-CB-CG	10.43	136.34	113.40
1	F	536	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	H	711	TYR	CG-CD2-CE2	7.69	127.45	121.30
1	E	447[A]	ASP	CB-CG-OD2	7.59	125.13	118.30
1	E	447[B]	ASP	CB-CG-OD2	7.59	125.13	118.30
1	F	521	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	C	230	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	A	47	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	F	547[A]	ASP	CB-CG-OD1	6.08	123.77	118.30
1	F	547[B]	ASP	CB-CG-OD1	6.08	123.77	118.30
1	E	432	GLU	OE1-CD-OE2	6.04	130.55	123.30
1	A	36	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	B	153	GLU	CA-CB-CG	-5.79	100.65	113.40
1	E	435	ASP	O-C-N	-5.67	113.63	122.70
1	D	347	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	G	614	ASP	CB-CG-OD2	-5.53	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	611	TYR	CG-CD1-CE1	5.36	125.59	121.30
1	C	231[A]	GLU	OE1-CD-OE2	5.17	129.51	123.30
1	H	736	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	B	121	ASP	CB-CG-OD1	-5.07	113.73	118.30

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	419	391	0	0	0
1	B	428	391	0	0	0
1	C	430	394	0	0	0
1	D	423	385	0	0	0
1	E	439	414	0	0	0
1	F	435	400	0	0	0
1	G	427	387	0	0	0
1	H	431	398	0	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	82	0	0	0	0
3	B	79	0	0	0	0
3	C	89	0	0	0	0
3	D	74	0	0	0	0
3	E	79	0	0	0	0
3	F	93	0	0	0	0
3	G	80	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	110	0	0	0	0
All	All	4126	3160	0	0	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 0.

There are no clashes within the asymmetric unit.

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	53/54 (98%)	53 (100%)	0	0	100	100
1	B	53/54 (98%)	53 (100%)	0	0	100	100
1	C	54/54 (100%)	54 (100%)	0	0	100	100
1	D	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
1	E	56/54 (104%)	55 (98%)	1 (2%)	0	100	100
1	F	55/54 (102%)	55 (100%)	0	0	100	100
1	G	53/54 (98%)	53 (100%)	0	0	100	100
1	H	54/54 (100%)	54 (100%)	0	0	100	100
All	All	430/432 (100%)	428 (100%)	2 (0%)	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	48/47 (102%)	46 (96%)	2 (4%)	40	6
1	B	48/47 (102%)	47 (98%)	1 (2%)	66	24
1	C	49/47 (104%)	48 (98%)	1 (2%)	68	27
1	D	47/47 (100%)	47 (100%)	0	100	100
1	E	51/47 (108%)	49 (96%)	2 (4%)	43	7
1	F	50/47 (106%)	48 (96%)	2 (4%)	42	7
1	G	48/47 (102%)	48 (100%)	0	100	100
1	H	49/47 (104%)	49 (100%)	0	100	100
All	All	390/376 (104%)	382 (98%)	8 (2%)	80	24

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44[A]	VAL
1	A	44[B]	VAL
1	B	131[A]	GLU
1	C	221[A]	ASP
1	E	444[A]	VAL
1	E	444[B]	VAL
1	F	544[A]	VAL
1	F	544[B]	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	48	GLN
1	F	522	ASN
1	G	622	ASN

### 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 8 ligands modelled in this entry, 8 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.

## 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	53/54 (98%)	-0.30	0 100 100	8, 13, 29, 39	0
1	B	54/54 (100%)	-0.23	1 (1%) 64 63	8, 14, 35, 55	1 (1%)
1	C	54/54 (100%)	-0.23	1 (1%) 64 63	9, 15, 30, 41	0
1	D	54/54 (100%)	0.05	3 (5%) 24 24	9, 18, 42, 50	2 (3%)
1	E	54/54 (100%)	-0.02	4 (7%) 14 15	10, 16, 38, 48	2 (3%)
1	F	54/54 (100%)	-0.51	0 100 100	8, 13, 21, 27	0
1	G	54/54 (100%)	-0.52	0 100 100	8, 13, 26, 33	0
1	H	54/54 (100%)	-0.64	0 100 100	8, 12, 15, 23	0
All	All	431/432 (99%)	-0.30	9 (2%) 60 60	8, 14, 33, 55	5 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	354[A]	ASP	4.7
1	E	420[A]	PRO	4.0
1	E	421[A]	ASP	4.0
1	E	424[A]	ILE	3.5
1	D	323	GLY	3.2
1	C	221[A]	ASP	3.1
1	D	324	ILE	2.9
1	B	154	ASP	2.9
1	E	422[A]	ASN	2.1

### 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	ZN	D	904	1/1	0.03	-0.77	10,10,10,10	0
2	ZN	A	901	1/1	0.04	-1.11	9,9,9,9	0
2	ZN	C	903	1/1	0.04	-1.20	10,10,10,10	0
2	ZN	H	908	1/1	0.02	-1.26	9,9,9,9	0
2	ZN	E	905	1/1	0.03	-1.29	12,12,12,12	0
2	ZN	B	902	1/1	0.04	-1.33	9,9,9,9	0
2	ZN	F	906	1/1	0.02	-1.42	11,11,11,11	0
2	ZN	G	907	1/1	0.02	-1.52	10,10,10,10	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.