



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:11 PM GMT

PDB ID : 1XTM
Title : Crystal structure of the double mutant Y88H-P104H of a SOD-like protein from *Bacillus subtilis*.
Authors : Calderone, V.; Mangani, S.; Banci, L.; Benvenuti, M.; Bertini, I.; Fantoni, A.; Viezzoli, M.S.
Deposited on : 2004-10-22
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

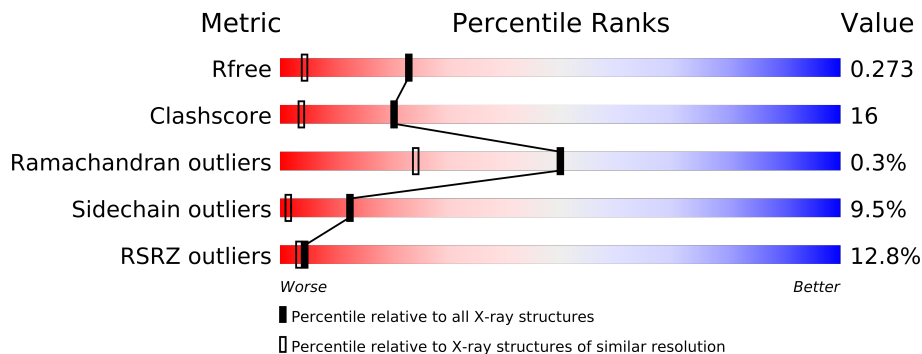
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.60 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	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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 ≥ 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	175	
1	B	175	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2507 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 Hypothetical superoxide dismutase-like protein yojM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	153	Total	C	N	O	S	0	0	0
			1140	705	206	225	4			
1	A	152	Total	C	N	O	S	0	0	0
			1134	702	205	223	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	88	HIS	TYR	ENGINEERED	UNP O31851
B	104	HIS	PRO	ENGINEERED	UNP O31851
A	88	HIS	TYR	ENGINEERED	UNP O31851
A	104	HIS	PRO	ENGINEERED	UNP O31851

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cu	0	0
			1	1		
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Zn	0	0
			4	4		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

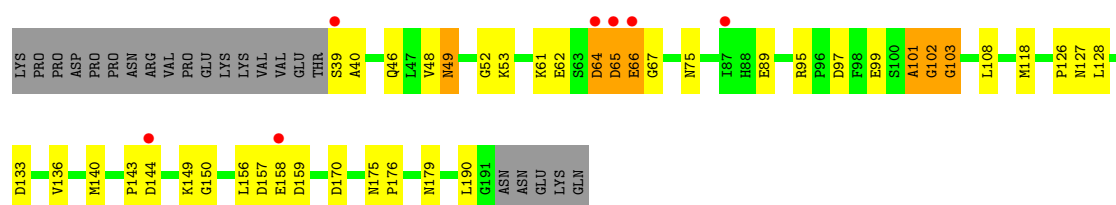
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	84	Total 84	O 84	0	0
4	B	142	Total 142	O 142	0	0

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.

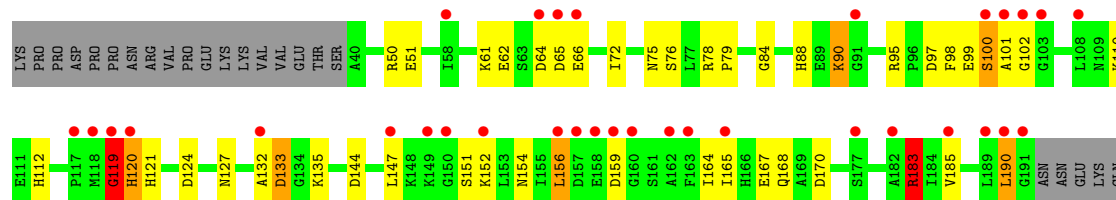
- Molecule 1: Hypothetical superoxide dismutase-like protein yojM

Chain B: 



- Molecule 1: Hypothetical superoxide dismutase-like protein yojM

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	52.46Å 104.35Å 58.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.60 – 1.60 25.60 – 1.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.60-1.60) 99.5 (25.60-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.253 , 0.266 0.261 , 0.273	Depositor DCC
R_{free} test set	3317 reflections (8.33%)	DCC
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 81899 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2507	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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, CU

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	1.11	2/1158 (0.2%)	1.08	10/1563 (0.6%)
1	B	0.93	2/1164 (0.2%)	1.06	7/1571 (0.4%)
All	All	1.03	4/2322 (0.2%)	1.07	17/3134 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	GLY	C-N	-25.11	0.76	1.34
1	A	120	HIS	C-N	19.14	1.78	1.34
1	B	143	PRO	C-N	13.94	1.66	1.34
1	B	144	ASP	C-N	7.17	1.50	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLY	O-C-N	-11.82	103.78	122.70
1	A	120	HIS	CA-C-N	-10.75	93.55	117.20
1	A	119	GLY	C-N-CA	10.40	147.71	121.70
1	A	120	HIS	CA-C-O	9.39	139.82	120.10
1	B	102	GLY	N-CA-C	-8.86	90.94	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLY	CA-C-N	8.80	136.56	117.20
1	A	124	ASP	CB-CG-OD2	7.40	124.96	118.30
1	B	103	GLY	N-CA-C	-7.05	95.46	113.10
1	B	101	ALA	N-CA-C	6.80	129.37	111.00
1	A	190	LEU	CA-CB-CG	6.56	130.39	115.30
1	A	65	ASP	CB-CG-OD2	6.42	124.07	118.30
1	B	157	ASP	CB-CG-OD2	6.24	123.92	118.30
1	B	158	GLU	C-N-CA	5.70	135.96	121.70
1	A	144	ASP	CB-CG-OD2	5.31	123.08	118.30
1	A	183	ARG	CB-CA-C	5.31	121.02	110.40
1	B	144	ASP	CB-CA-C	5.30	121.01	110.40
1	B	64	ASP	CB-CG-OD2	5.16	122.95	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLY	Peptide
1	A	132	ALA	Peptide
1	B	101	ALA	Peptide
1	B	102	GLY	Peptide
1	B	190	LEU	Peptide

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	1134	0	1074	47	0
1	B	1140	0	1081	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
4	A	84	0	0	7	0
4	B	142	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2507	0	2155	70	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 16.

All (70) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:HIS:C	1:A:121:HIS:N	1.78	1.37
1:A:119:GLY:O	1:A:120:HIS:N	1.57	1.26
1:A:119:GLY:C	1:A:120:HIS:CA	2.14	1.15
1:A:119:GLY:CA	1:A:120:HIS:N	2.15	1.09
1:A:183:ARG:HG3	4:A:540:HOH:O	1.56	1.04
1:A:101:ALA:HB1	1:A:102:GLY:HA2	1.46	0.97
1:A:99:GLU:O	1:A:101:ALA:HA	1.65	0.96
1:A:120:HIS:CA	1:A:121:HIS:N	2.41	0.83
1:A:95:ARG:HG3	4:A:544:HOH:O	1.80	0.81
1:A:119:GLY:C	1:A:120:HIS:N	0.76	0.81
1:A:97:ASP:OD2	1:A:99:GLU:HG3	1.88	0.74
1:A:127:ASN:HD21	1:A:170:ASP:CB	2.00	0.73
1:A:154:ASN:ND2	1:A:156:LEU:O	2.22	0.72
1:A:51:GLU:HB3	4:A:577:HOH:O	1.93	0.69
1:A:127:ASN:HD21	1:A:170:ASP:HB3	1.59	0.66
1:A:102:GLY:O	1:A:183:ARG:NH1	2.28	0.66
1:A:133:ASP:HB3	1:A:135:LYS:H	1.61	0.66
1:B:118:MET:HA	1:B:118:MET:CE	2.26	0.65
1:A:167:GLU:HG3	1:A:168:GLN:HG3	1.81	0.63
1:B:66:GLU:HG2	1:B:67:GLY:N	2.14	0.62
1:A:154:ASN:CG	1:A:156:LEU:O	2.39	0.61
1:B:127:ASN:HD21	1:B:170:ASP:HB3	1.65	0.61
1:A:97:ASP:OD2	1:A:99:GLU:CG	2.48	0.60
1:B:49:ASN:HD22	1:B:49:ASN:C	2.06	0.59
1:A:120:HIS:HA	1:A:121:HIS:N	2.15	0.59
1:B:62:GLU:HG2	4:B:525:HOH:O	2.04	0.58
1:B:118:MET:HE2	1:B:118:MET:HA	1.84	0.57
1:B:65:ASP:OD2	1:B:66:GLU:HB2	2.04	0.57
1:A:101:ALA:HB1	1:A:102:GLY:CA	2.29	0.57
1:A:164:ILE:HG21	1:A:183:ARG:HB3	1.87	0.56
1:A:88:HIS:CG	1:A:164:ILE:HD13	2.41	0.56
1:B:39:SER:O	1:B:40:ALA:HB3	2.08	0.54
1:A:90:LYS:HD3	1:A:159:ASP:OD2	2.07	0.54
1:A:151:SER:HB3	1:A:154:ASN:HB2	1.89	0.53
1:B:66:GLU:HG2	1:B:67:GLY:H	1.72	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:127:ASN:HD21	1:A:170:ASP:H	1.55	0.53
1:A:110:LYS:NZ	4:A:582:HOH:O	2.41	0.52
1:A:84:GLY:HA2	1:A:127:ASN:HD22	1.76	0.51
1:A:51:GLU:CB	4:A:577:HOH:O	2.55	0.51
1:A:127:ASN:ND2	1:A:170:ASP:H	2.08	0.50
1:A:98:PHE:C	1:A:100:SER:H	2.14	0.50
1:A:62:GLU:CG	1:A:147:LEU:HD12	2.41	0.49
1:A:112:HIS:HB2	1:A:121:HIS:CE1	2.47	0.49
1:A:95:ARG:N	4:A:544:HOH:O	2.46	0.49
1:A:99:GLU:C	1:A:101:ALA:HA	2.32	0.49
1:A:50:ARG:NH1	4:A:533:HOH:O	2.22	0.48
1:A:101:ALA:CB	1:A:102:GLY:HA2	2.30	0.46
1:B:150:GLY:HA2	4:B:638:HOH:O	2.15	0.46
1:A:90:LYS:HB2	1:A:101:ALA:HB3	1.97	0.46
1:B:126:PRO:HD2	1:B:140:MET:SD	2.56	0.46
1:B:89:GLU:HG2	1:B:103:GLY:H	1.80	0.46
1:B:97:ASP:OD1	1:B:99:GLU:OE1	2.33	0.46
1:B:48:VAL:HG22	4:B:543:HOH:O	2.17	0.44
1:A:88:HIS:CD2	1:A:164:ILE:HD13	2.53	0.44
1:B:64:ASP:HA	1:B:65:ASP:OD1	2.18	0.43
1:A:62:GLU:HG3	1:A:147:LEU:HD12	2.01	0.43
1:B:66:GLU:CG	1:B:67:GLY:N	2.78	0.43
1:B:89:GLU:CD	1:B:103:GLY:H	2.21	0.43
1:A:165:ILE:HB	1:A:185:VAL:HB	2.01	0.43
1:B:127:ASN:HD21	1:B:170:ASP:CB	2.30	0.42
1:B:49:ASN:ND2	1:B:53:LYS:H	2.17	0.42
1:B:39:SER:O	1:B:40:ALA:CB	2.67	0.42
1:A:78:ARG:HA	1:A:79:PRO:HD3	1.87	0.42
1:A:98:PHE:C	1:A:100:SER:N	2.73	0.41
1:A:72:ILE:HD11	1:A:165:ILE:HD11	2.03	0.41
1:B:128:LEU:HD22	1:B:136:VAL:HG21	2.03	0.41
1:A:127:ASN:ND2	1:A:170:ASP:HB3	2.31	0.41
1:B:52:GLY:HA2	1:B:95:ARG:HD3	2.03	0.41
1:B:175:ASN:HA	1:B:176:PRO:HA	1.79	0.40
1:A:127:ASN:HD21	1:A:170:ASP:HB2	1.81	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	150/175 (86%)	136 (91%)	13 (9%)	1 (1%)	30	9
1	B	151/175 (86%)	141 (93%)	10 (7%)	0	100	100
All	All	301/350 (86%)	277 (92%)	23 (8%)	1 (0%)	50	24

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	ASP

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	120/143 (84%)	109 (91%)	11 (9%)	13	2
1	B	121/143 (85%)	109 (90%)	12 (10%)	11	1
All	All	241/286 (84%)	218 (90%)	23 (10%)	12	1

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	49	ASN
1	B	61	LYS
1	B	65	ASP
1	B	66	GLU
1	B	75	ASN
1	B	108	LEU
1	B	133	ASP

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Mol	Chain	Res	Type
1	B	149	LYS
1	B	156	LEU
1	B	159	ASP
1	B	179	ASN
1	A	61	LYS
1	A	64	ASP
1	A	66	GLU
1	A	75	ASN
1	A	76	SER
1	A	90	LYS
1	A	100	SER
1	A	152	LYS
1	A	156	LEU
1	A	183	ARG
1	A	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	49	ASN
1	B	75	ASN
1	B	127	ASN
1	A	75	ASN
1	A	127	ASN
1	A	179	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 7 ligands modelled in this entry, 7 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, 95th 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 ²)	Q<0.9
1	A	152/175 (86%)	1.36	33 (21%) 1 1	17, 32, 48, 51	0
1	B	153/175 (87%)	0.32	7 (4%) 31 30	11, 17, 30, 43	0
All	All	305/350 (87%)	0.84	40 (13%) 4 3	11, 25, 44, 51	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	ASP	7.3
1	B	64	ASP	5.9
1	A	64	ASP	5.8
1	A	108	LEU	5.8
1	B	65	ASP	4.8
1	B	39	SER	4.8
1	A	118	MET	4.7
1	A	191	GLY	4.7
1	A	150	GLY	4.1
1	A	101	ALA	4.0
1	A	190	LEU	3.7
1	A	156	LEU	3.7
1	A	149	LYS	3.7
1	A	162	ALA	3.4
1	A	158	GLU	3.4
1	A	120	HIS	3.3
1	A	102	GLY	3.3
1	A	182	ALA	3.2
1	A	66	GLU	3.1
1	A	100	SER	3.0
1	A	157	ASP	2.9
1	A	132	ALA	2.8
1	A	119	GLY	2.8
1	A	160	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	2.6
1	B	158	GLU	2.6
1	A	117	PRO	2.5
1	A	165	ILE	2.5
1	A	91	GLY	2.4
1	A	163	PHE	2.4
1	A	177	SER	2.3
1	A	189	LEU	2.3
1	A	185	VAL	2.2
1	B	66	GLU	2.2
1	A	152	LYS	2.2
1	A	159	ASP	2.1
1	B	87	ILE	2.1
1	A	58	ILE	2.1
1	A	147	LEU	2.1
1	B	144	ASP	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, 95th 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 ²)	Q<0.9
3	ZN	B	505	1/1	0.15	0.30	26,26,26,26	1
3	ZN	B	506	1/1	0.06	-1.28	21,21,21,21	1
3	ZN	B	501	1/1	0.04	-1.36	20,20,20,20	0
3	ZN	A	504	1/1	0.04	-3.17	33,33,33,33	1
3	ZN	B	502	1/1	0.04	-3.84	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CU	A	503	1/1	0.04	-8.31	41,41,41,41	0
2	CU	B	500	1/1	0.03	-10.55	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.