



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:26 AM GMT

PDB ID : 2SCP
Title : STRUCTURE OF A SARCOPLASMIC CALCIUM-BINDING PROTEIN
FROM NEREIS DIVERSICOLOR REFINED AT 2.0 ANGSTROMS RES-
OLUTION
Authors : Cook, W.J.; Vijay-Kumar, S.
Deposited on : 1991-08-22
Resolution : 2.00 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>

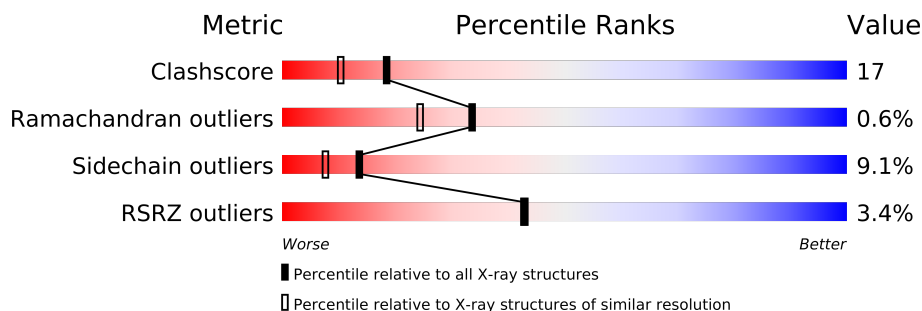
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

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	174	
1	B	174	

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	CA	A	190	-	X
2	CA	A	191	-	X
2	CA	A	192	-	X
2	CA	B	193	-	X
2	CA	B	194	-	X
2	CA	B	195	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2955 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 CALCIUM-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1368	868	218	272	10			
1	B	174	Total	C	N	O	S	0	0	0
			1368	868	218	272	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is water.

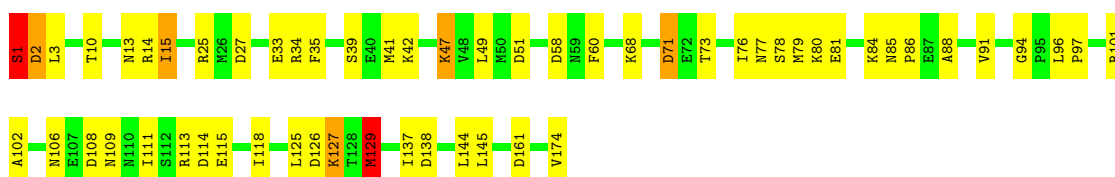
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total	O	0	0
			124	124		
3	B	89	Total	O	0	0
			89	89		

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.

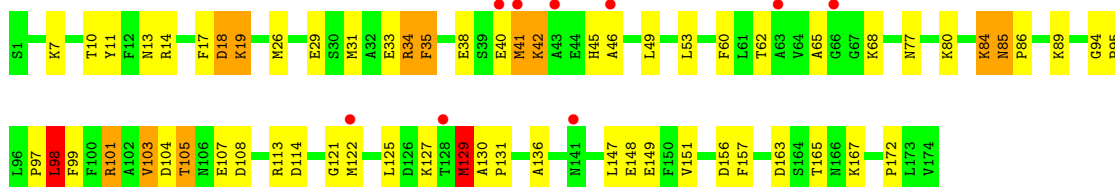
• Molecule 1: SARCOPLASMIC CALCIUM-BINDING PROTEIN

Chain A: 



• Molecule 1: SARCOPLASMIC CALCIUM-BINDING PROTEIN

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.60Å 56.00Å 65.80Å 90.00° 92.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 5.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 88.5 (5.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.68 , 94.8	EDS
Estimated twinning fraction	0.042 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 17863 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2955	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

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: CA

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	1.00	1/1396 (0.1%)	1.44	14/1880 (0.7%)
1	B	0.94	0/1396	1.47	13/1880 (0.7%)
All	All	0.97	1/2792 (0.0%)	1.46	27/3760 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	174	VAL	C-O	6.04	1.34	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	B	114	ASP	CB-CG-OD1	8.31	125.78	118.30
1	B	18	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	A	129	MET	CA-CB-CG	7.78	126.53	113.30
1	B	113	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	174	VAL	CA-C-O	-7.62	104.09	120.10
1	A	71	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	34	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	25	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	51	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	113	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	156	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	15	ILE	CA-CB-CG2	6.56	124.02	110.90
1	B	149	GLU	OE1-CD-OE2	-6.49	115.52	123.30
1	A	34	ARG	CD-NE-CZ	6.32	132.44	123.60
1	B	101	ARG	NE-CZ-NH2	6.31	123.46	120.30
1	B	148	GLU	CG-CD-OE1	6.29	130.88	118.30
1	A	1	SER	N-CA-CB	-6.21	101.19	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	LEU	CA-CB-CG	6.20	129.56	115.30
1	A	34	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	138	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	113	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	47	LYS	N-CA-CB	5.90	121.22	110.60
1	B	129	MET	CA-CB-CG	5.71	123.01	113.30
1	B	11	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	A	115	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	B	108	ASP	CB-CG-OD1	5.19	122.97	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	1368	0	1310	35	0
1	B	1368	0	1310	56	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	124	0	0	7	0
3	B	89	0	0	2	0
All	All	2955	0	2620	90	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 17.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:129:MET:HB3	3:A:316:HOH:O	1.59	1.01
1:B:121:GLY:HA3	1:B:127:LYS:NZ	1.76	0.99
1:B:136:ALA:HB1	1:B:165:THR:HG22	1.46	0.97
1:B:86:PRO:O	1:B:89:LYS:HG3	1.64	0.95
1:B:45:HIS:CD2	1:B:105:THR:HG23	2.06	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:35:PHE:CD2	1:B:49:LEU:HD11	2.11	0.85
1:B:41:MET:HB3	1:B:105:THR:CG2	2.08	0.84
1:B:42:LYS:HE3	1:B:45:HIS:HB2	1.61	0.82
1:B:41:MET:HB3	1:B:105:THR:HG22	1.63	0.80
1:A:13:ASN:HD22	1:A:14:ARG:HE	1.27	0.80
1:B:99:PHE:O	1:B:103:VAL:HG12	1.83	0.79
1:A:78:SER:HA	1:A:81:GLU:OE1	1.82	0.79
1:B:121:GLY:HA3	1:B:127:LYS:HZ1	1.48	0.77
1:B:18:ASP:O	1:B:19:LYS:HB2	1.84	0.77
1:B:29:GLU:O	1:B:33:GLU:HG3	1.88	0.74
1:A:49:LEU:HD12	1:A:102:ALA:HB1	1.72	0.72
1:B:136:ALA:CB	1:B:165:THR:HG22	2.22	0.69
1:B:42:LYS:O	1:B:42:LYS:HD2	1.92	0.69
1:B:34:ARG:O	1:B:38:GLU:HG2	1.94	0.67
1:A:114:ASP:O	1:A:118:ILE:HD13	1.96	0.66
1:A:13:ASN:ND2	1:A:14:ARG:HE	1.92	0.66
1:A:129:MET:SD	3:A:316:HOH:O	2.53	0.65
1:B:26:MET:HG3	3:B:274:HOH:O	1.97	0.65
1:A:27:ASP:HB3	3:A:198:HOH:O	1.99	0.62
1:B:41:MET:CB	1:B:105:THR:HG22	2.30	0.62
1:B:85:ASN:H	1:B:85:ASN:ND2	1.98	0.60
1:B:41:MET:CB	1:B:105:THR:CG2	2.81	0.59
1:B:77:ASN:ND2	1:B:80:LYS:NZ	2.51	0.59
1:B:13:ASN:HD22	1:B:14:ARG:HE	1.51	0.58
1:A:88:ALA:O	1:A:91:VAL:HG13	2.04	0.58
1:B:41:MET:HB3	1:B:105:THR:HG21	1.85	0.58
1:B:163:ASP:CG	1:B:167:LYS:HZ2	2.07	0.58
1:A:49:LEU:CD1	1:A:102:ALA:HB1	2.33	0.57
1:B:41:MET:HE3	1:B:46:ALA:N	2.18	0.57
1:B:121:GLY:CA	1:B:127:LYS:NZ	2.61	0.57
1:B:121:GLY:HA3	1:B:127:LYS:HZ3	1.67	0.56
1:B:94:GLY:O	1:B:97:PRO:HD2	2.06	0.56
1:B:136:ALA:HB1	1:B:165:THR:CG2	2.28	0.56
1:B:35:PHE:O	1:B:35:PHE:HD1	1.90	0.55
1:B:84:LYS:O	1:B:86:PRO:HD3	2.06	0.55
1:B:77:ASN:HD22	1:B:80:LYS:NZ	2.05	0.54
1:A:94:GLY:O	1:A:97:PRO:HD2	2.08	0.54
1:B:65:ALA:O	1:B:68:LYS:HD3	2.08	0.53
1:B:77:ASN:ND2	1:B:80:LYS:HZ3	2.07	0.53
1:B:17:PHE:HZ	1:B:34:ARG:HD3	1.74	0.52
1:A:76:ILE:O	1:A:80:LYS:HB2	2.08	0.52
1:B:45:HIS:CD2	1:B:105:THR:CG2	2.85	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:ASP:HB3	1:A:129:MET:SD	2.49	0.52
1:B:31:MET:HG3	1:B:122:MET:SD	2.50	0.52
1:A:42:LYS:HD2	1:A:106:ASN:HA	1.92	0.51
1:A:118:ILE:HD12	1:A:127:LYS:NZ	2.25	0.51
1:A:126:ASP:O	1:A:129:MET:HG2	2.10	0.50
1:B:7:LYS:HE3	1:B:157:PHE:O	2.10	0.50
1:A:108:ASP:O	1:A:109:ASN:HB2	2.11	0.50
1:A:27:ASP:C	3:A:198:HOH:O	2.49	0.50
1:A:71:ASP:OD1	1:A:73:THR:N	2.45	0.50
1:A:60:PHE:CE1	1:A:94:GLY:HA3	2.47	0.49
1:A:1:SER:HB2	3:A:261:HOH:O	2.13	0.48
1:B:136:ALA:CB	1:B:165:THR:CG2	2.88	0.48
1:A:161:ASP:HB3	3:A:243:HOH:O	2.13	0.48
1:B:163:ASP:OD2	1:B:167:LYS:NZ	2.47	0.48
1:B:42:LYS:C	1:B:42:LYS:HD2	2.31	0.48
1:B:130:ALA:HB3	1:B:131:PRO:HD3	1.97	0.46
1:A:85:ASN:HA	1:A:86:PRO:HD2	1.80	0.45
1:A:1:SER:N	3:A:311:HOH:O	2.48	0.45
1:B:94:GLY:N	1:B:95:PRO:CD	2.80	0.45
1:B:60:PHE:CE1	1:B:94:GLY:HA3	2.52	0.44
1:A:77:ASN:O	1:A:81:GLU:HG3	2.17	0.44
1:B:41:MET:CG	1:B:105:THR:HG21	2.48	0.44
1:B:95:PRO:O	1:B:98:LEU:HB2	2.18	0.44
1:A:111:ILE:HB	1:A:145:LEU:HB2	2.00	0.44
1:A:81:GLU:O	1:A:84:LYS:HB2	2.18	0.44
1:A:13:ASN:HD22	1:A:14:ARG:NE	2.05	0.44
1:B:13:ASN:HB2	3:B:218:HOH:O	2.17	0.44
1:A:10:THR:O	1:A:14:ARG:HG2	2.18	0.43
1:B:147:LEU:O	1:B:151:VAL:HG13	2.19	0.42
1:B:42:LYS:HE3	1:B:45:HIS:CB	2.43	0.42
1:B:31:MET:CG	1:B:122:MET:CE	2.98	0.42
1:B:85:ASN:N	1:B:85:ASN:ND2	2.66	0.42
1:B:41:MET:CB	1:B:105:THR:HG21	2.47	0.42
1:B:45:HIS:HD2	1:B:105:THR:HG23	1.77	0.42
1:A:137:ILE:HG22	1:A:145:LEU:HD22	2.02	0.41
1:A:79:MET:HB3	1:A:79:MET:HE2	1.95	0.41
1:B:10:THR:O	1:B:14:ARG:HG2	2.20	0.41
1:A:96:LEU:N	1:A:97:PRO:CD	2.83	0.41
1:A:58:ASP:O	1:B:101:ARG:NE	2.54	0.41
1:A:39:SER:HB3	1:A:41:MET:HE3	2.03	0.41
1:A:118:ILE:HD12	1:A:127:LYS:HZ3	1.85	0.40
1:B:35:PHE:HB2	1:B:122:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:MET:HG3	1:B:172:PRO:HG2	2.02	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	172/174 (99%)	167 (97%)	4 (2%)	1 (1%)	33	24
1	B	172/174 (99%)	164 (95%)	7 (4%)	1 (1%)	33	24
All	All	344/348 (99%)	331 (96%)	11 (3%)	2 (1%)	33	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	107	GLU
1	A	2	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	148/148 (100%)	135 (91%)	13 (9%)	14	8
1	B	148/148 (100%)	134 (90%)	14 (10%)	12	7
All	All	296/296 (100%)	269 (91%)	27 (9%)	14	8

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	2	ASP
1	A	3	LEU
1	A	15	ILE
1	A	33	GLU
1	A	35	PHE
1	A	47	LYS
1	A	68	LYS
1	A	101	ARG
1	A	125	LEU
1	A	127	LYS
1	A	129	MET
1	A	144	LEU
1	B	19	LYS
1	B	35	PHE
1	B	40	GLU
1	B	41	MET
1	B	42	LYS
1	B	53	LEU
1	B	62	THR
1	B	84	LYS
1	B	85	ASN
1	B	98	LEU
1	B	103	VAL
1	B	105	THR
1	B	125	LEU
1	B	129	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	109	ASN
1	A	110	ASN
1	B	13	ASN
1	B	45	HIS
1	B	77	ASN
1	B	85	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 6 ligands modelled in this entry, 6 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	174/174 (100%)	-0.31	0 100 100	8, 16, 30, 34	0
1	B	174/174 (100%)	0.23	9 (5%) 26 26	11, 26, 31, 32	0
All	All	348/348 (100%)	-0.04	9 (2%) 43 53	8, 20, 31, 34	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	GLU	3.8
1	B	128	THR	2.8
1	B	141	ASN	2.6
1	B	43	ALA	2.6
1	B	66	GLY	2.4
1	B	63	ALA	2.4
1	B	41	MET	2.2
1	B	46	ALA	2.2
1	B	122	MET	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
2	CA	B	193	1/1	0.22	5.10	2,2,2,2	0
2	CA	A	192	1/1	0.17	5.01	2,2,2,2	0
2	CA	A	190	1/1	0.20	4.65	2,2,2,2	0
2	CA	B	194	1/1	0.23	3.09	9,9,9,9	0
2	CA	A	191	1/1	0.15	2.29	2,2,2,2	0
2	CA	B	195	1/1	0.28	2.19	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.