wwPDB X-ray Structure Validation Summary Report (i)

May 6, 2020 – 04:10 PM EDT

PDB ID	:	6OWW
Title	:	Crystal structure of a Human Cardiac Calsequestrin Filament Complexed with Ytterbium
Deposited on	:	2019-05-12
Resolution	:	3.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

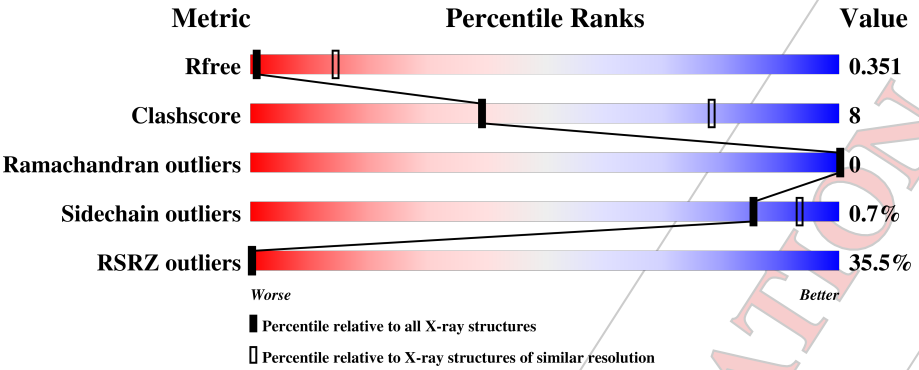
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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}	111664	1018 (4.08-3.60)
Clashscore	122126	1087 (4.08-3.60)
Ramachandran outliers	120053	1050 (4.08-3.60)
Sidechain outliers	120020	1044 (4.08-3.60)
RSRZ outliers	108989	1002 (4.10-3.58)

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 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 <=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	387	36% 65% 19% 15%
1	B	387	26% 68% 17% 15%
1	C	387	28% 67% 17% • 15%
1	D	387	32% 71% 14% 15%
1	E	387	30% 66% 19% 15%

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Mol	Chain	Length	Quality of chain
1	F	387	27% 70% 15% 15%
1	G	387	26% 68% 17% 15%
1	H	387	36% 64% 21% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	410	-	-	-	X
3	SO4	F	408	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21808 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 Calsequestrin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	B	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	C	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	D	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	E	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	F	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	G	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			
1	H	329	Total	C	N	O	S	0	0	0
			2715	1771	416	522	6			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	expression tag	UNP O14958
A	14	HIS	-	expression tag	UNP O14958
A	15	MET	-	expression tag	UNP O14958
A	16	ALA	-	expression tag	UNP O14958
A	17	SER	-	expression tag	UNP O14958
B	13	GLY	-	expression tag	UNP O14958
B	14	HIS	-	expression tag	UNP O14958
B	15	MET	-	expression tag	UNP O14958
B	16	ALA	-	expression tag	UNP O14958
B	17	SER	-	expression tag	UNP O14958
C	13	GLY	-	expression tag	UNP O14958
C	14	HIS	-	expression tag	UNP O14958
C	15	MET	-	expression tag	UNP O14958

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Chain	Residue	Modelled	Actual	Comment	Reference
C	16	ALA	-	expression tag	UNP O14958
C	17	SER	-	expression tag	UNP O14958
D	13	GLY	-	expression tag	UNP O14958
D	14	HIS	-	expression tag	UNP O14958
D	15	MET	-	expression tag	UNP O14958
D	16	ALA	-	expression tag	UNP O14958
D	17	SER	-	expression tag	UNP O14958
E	13	GLY	-	expression tag	UNP O14958
E	14	HIS	-	expression tag	UNP O14958
E	15	MET	-	expression tag	UNP O14958
E	16	ALA	-	expression tag	UNP O14958
E	17	SER	-	expression tag	UNP O14958
F	13	GLY	-	expression tag	UNP O14958
F	14	HIS	-	expression tag	UNP O14958
F	15	MET	-	expression tag	UNP O14958
F	16	ALA	-	expression tag	UNP O14958
F	17	SER	-	expression tag	UNP O14958
G	13	GLY	-	expression tag	UNP O14958
G	14	HIS	-	expression tag	UNP O14958
G	15	MET	-	expression tag	UNP O14958
G	16	ALA	-	expression tag	UNP O14958
G	17	SER	-	expression tag	UNP O14958
H	13	GLY	-	expression tag	UNP O14958
H	14	HIS	-	expression tag	UNP O14958
H	15	MET	-	expression tag	UNP O14958
H	16	ALA	-	expression tag	UNP O14958
H	17	SER	-	expression tag	UNP O14958

- Molecule 2 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	8	Total Yb 8 8	0	0
2	D	8	Total Yb 8 8	0	0
2	E	9	Total Yb 9 9	0	0
2	H	6	Total Yb 6 6	0	0
2	B	7	Total Yb 7 7	0	0

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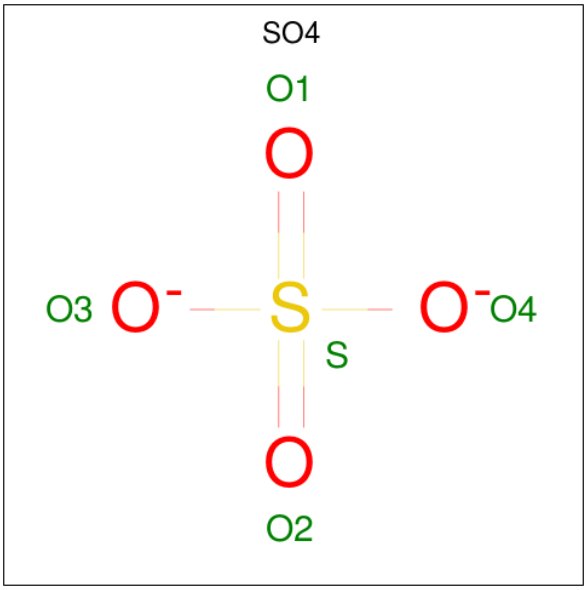
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	9	Total Yb 9 9	0	0
2	A	9	Total Yb 9 9	0	0
2	F	7	Total Yb 7 7	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



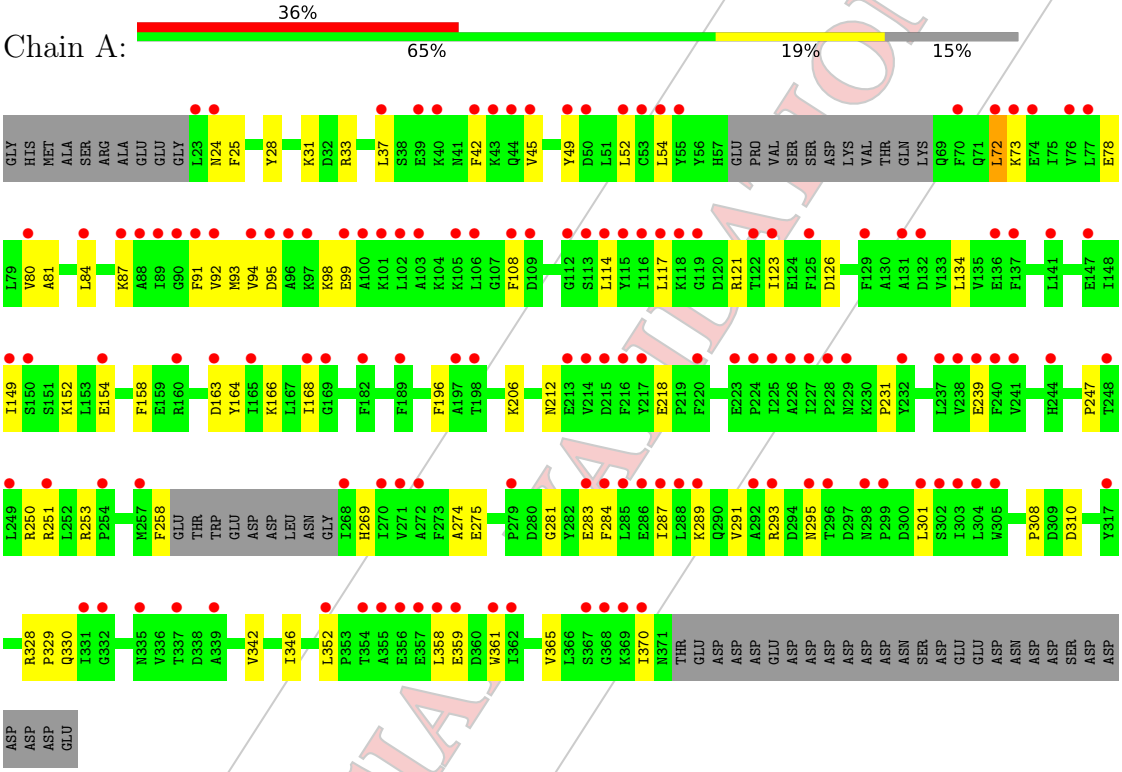
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

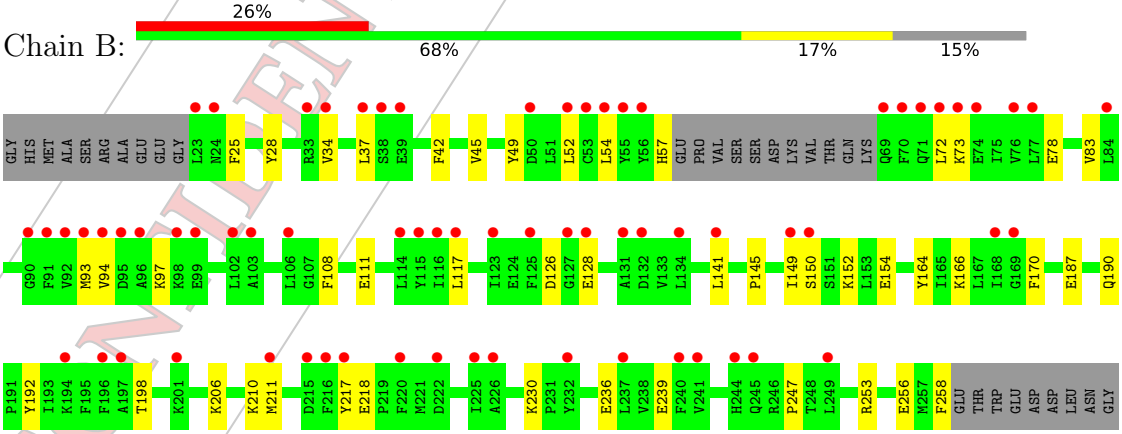
• Molecule 1: Calsequestrin-2

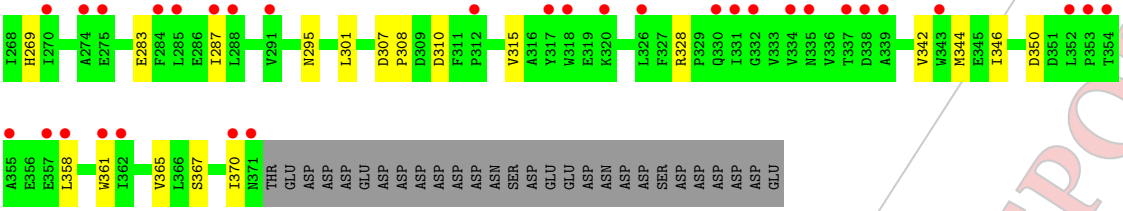
Chain A:



• Molecule 1: Calsequestrin-2

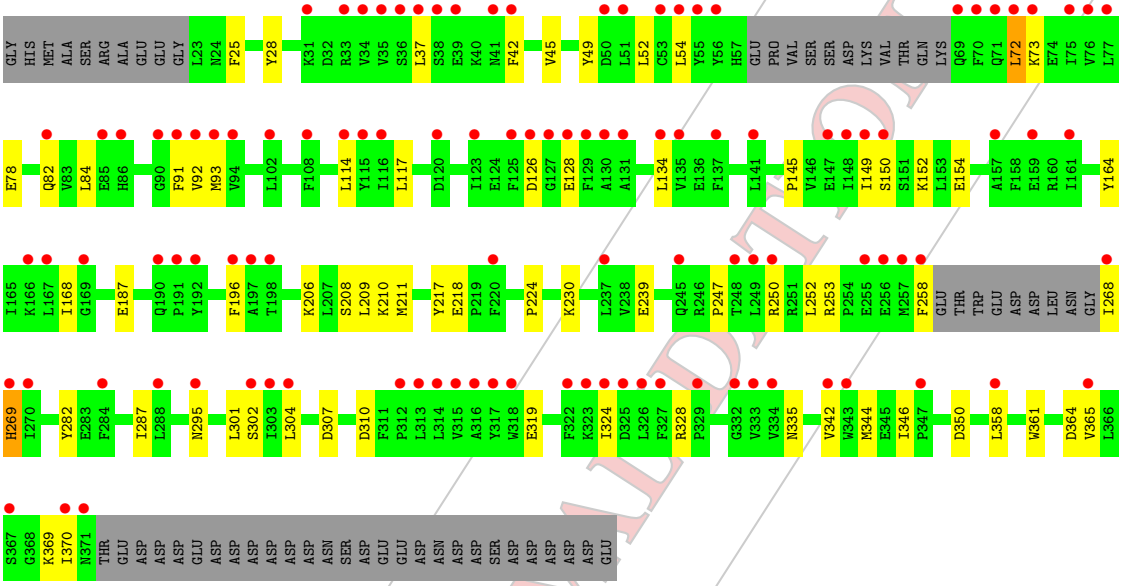
Chain B:





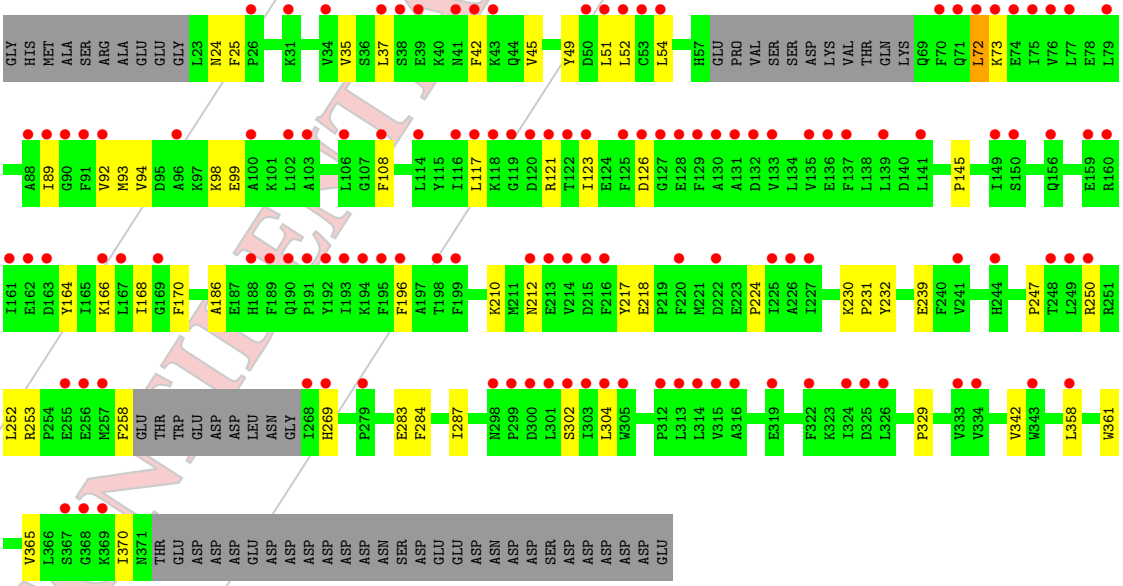
• Molecule 1: Calsequestrin-2

Chain C:



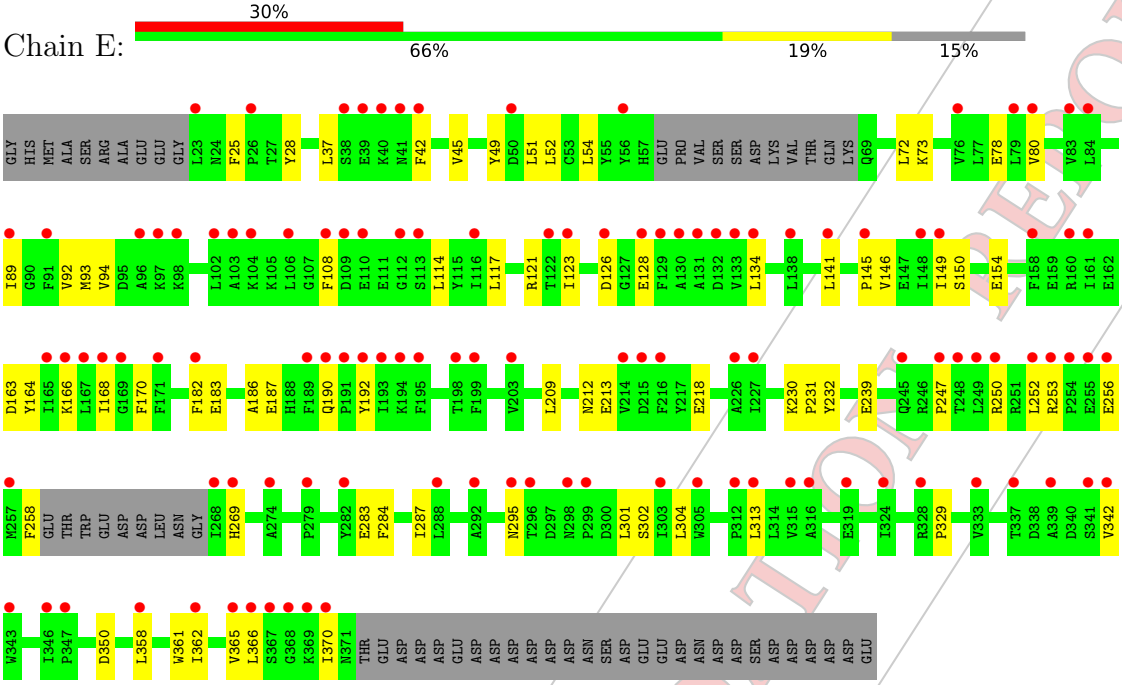
• Molecule 1: Calsequestrin-2

Chain D:



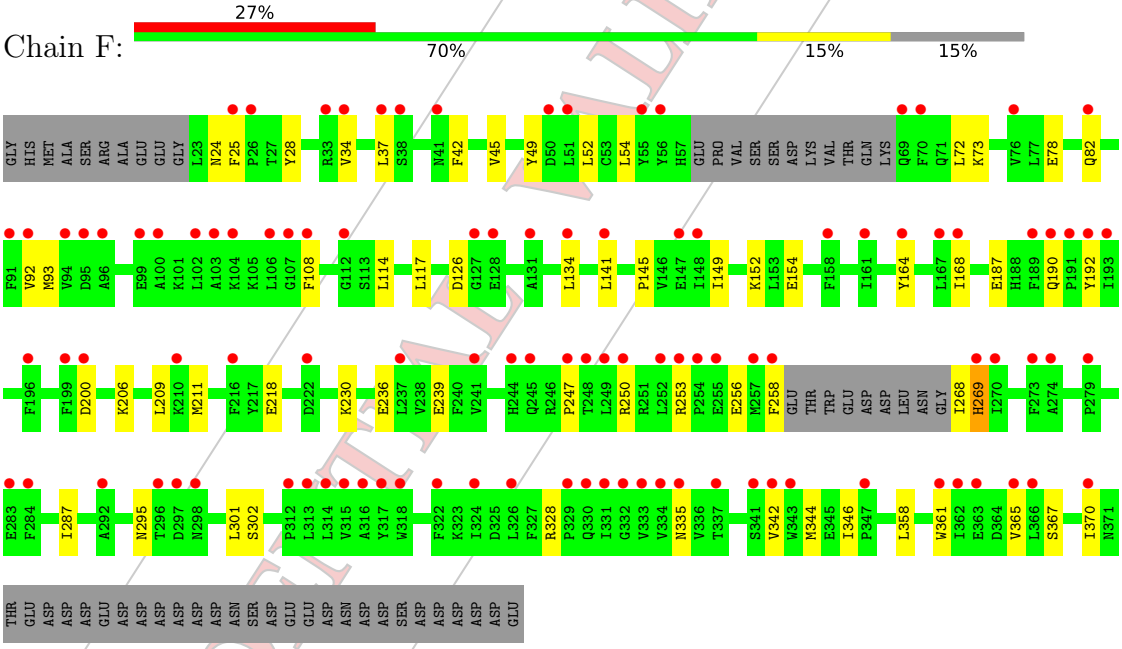
• Molecule 1: Calsequestrin-2

Chain E:



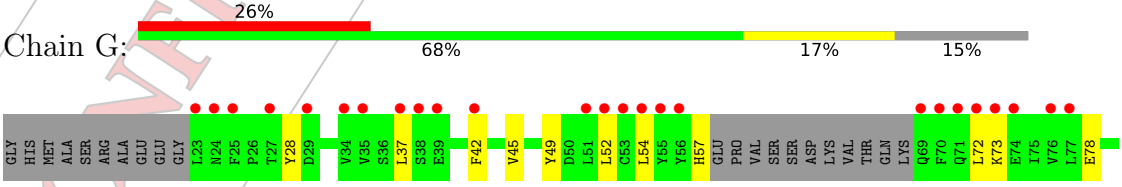
• Molecule 1: Calsequestrin-2

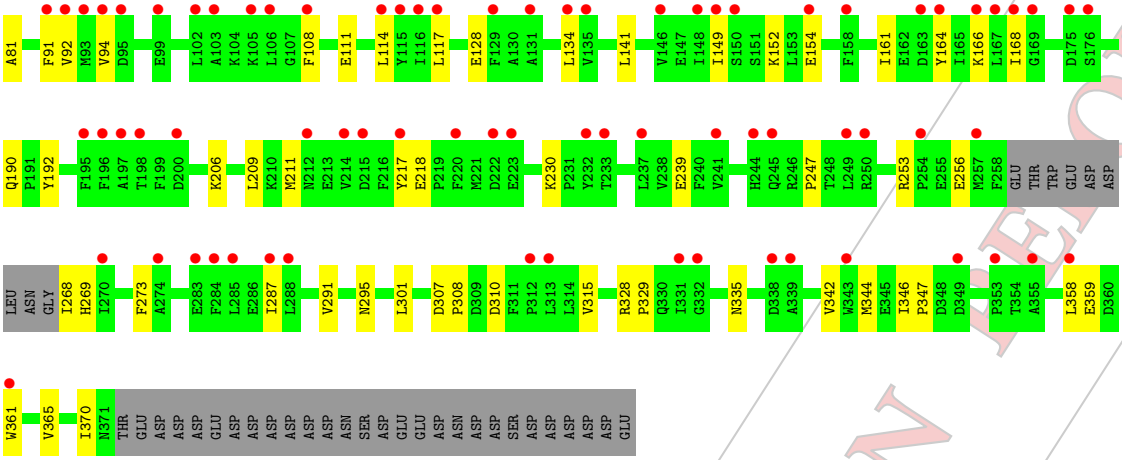
Chain F:



• Molecule 1: Calsequestrin-2

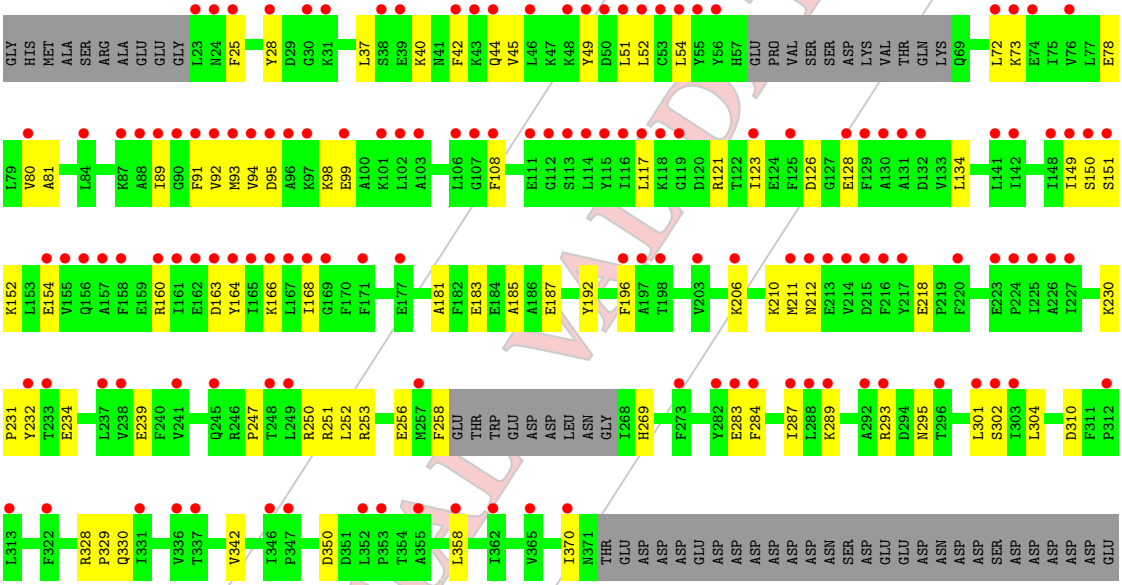
Chain G:





- Molecule 1: Calsequestrin-2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	85.83Å 86.02Å 214.34Å 90.00° 89.91° 90.00°	Depositor
Resolution (Å)	214.34 – 3.84 214.34 – 3.84	Depositor EDS
% Data completeness (in resolution range)	98.4 (214.34-3.84) 98.0 (214.34-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.290 , 0.340 0.296 , 0.351	Depositor DCC
R_{free} test set	1440 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	79.7	Xtriage
Anisotropy	0.919	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 81.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.21$	Xtriage
Estimated twinning fraction	0.266 for k,h,-l 0.266 for -k,-h,-l 0.266 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	21808	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YB, SO4

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	0.38	0/2779	0.56	1/3758 (0.0%)
1	B	0.40	0/2779	0.57	0/3758
1	C	0.40	0/2779	0.58	1/3758 (0.0%)
1	D	0.39	0/2779	0.57	1/3758 (0.0%)
1	E	0.40	0/2779	0.56	0/3758
1	F	0.40	0/2779	0.58	0/3758
1	G	0.40	0/2779	0.56	0/3758
1	H	0.39	0/2779	0.57	0/3758
All	All	0.40	0/22232	0.57	3/30064 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	LEU	CA-CB-CG	5.98	129.05	115.30
1	D	72	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	72	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2715	0	2653	49	0
1	B	2715	0	2653	45	0
1	C	2715	0	2653	49	0
1	D	2715	0	2653	37	0
1	E	2715	0	2653	48	0
1	F	2715	0	2653	42	0
1	G	2715	0	2653	41	0
1	H	2715	0	2653	53	0
2	A	9	0	0	0	0
2	B	7	0	0	0	0
2	C	9	0	0	0	0
2	D	8	0	0	0	0
2	E	9	0	0	0	0
2	F	7	0	0	0	0
2	G	8	0	0	0	0
2	H	6	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
All	All	21808	0	21224	346	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 8.

The worst 5 of 346 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:C:211:MET:O	1:C:230:LYS:NZ	2.19	0.76
1:F:211:MET:O	1:F:230:LYS:NZ	2.19	0.73
1:H:342:VAL:HG11	1:H:370:ILE:HG23	1.70	0.71
1:C:164:TYR:HD2	1:C:253:ARG:HH22	1.38	0.71
1:A:152:LYS:HB3	1:A:206:LYS:HE3	1.73	0.69

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	323/387 (84%)	309 (96%)	14 (4%)	0	100	100
1	B	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	C	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	D	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	E	323/387 (84%)	309 (96%)	14 (4%)	0	100	100
1	F	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	G	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
1	H	323/387 (84%)	310 (96%)	13 (4%)	0	100	100
All	All	2584/3096 (84%)	2478 (96%)	106 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	B	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	C	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	D	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	E	297/351 (85%)	295 (99%)	2 (1%)	85	93
1	F	297/351 (85%)	295 (99%)	2 (1%)	85	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	297/351 (85%)	295 (99%)	2 (1%)	85 93
1	H	297/351 (85%)	295 (99%)	2 (1%)	85 93
All	All	2376/2808 (85%)	2360 (99%)	16 (1%)	85 93

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	269	HIS
1	E	239	GLU
1	G	239	GLU
1	D	239	GLU
1	G	269	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	57	HIS
1	F	188	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 68 ligands modelled in this entry, 63 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
3	SO4	B	408	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	H	407	-	4,4,4	0.16	0	6,6,6	0.19	0
3	SO4	D	409	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	F	408	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	A	410	2	4,4,4	0.15	0	6,6,6	0.15	0

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

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^{th} 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	329/387 (85%)	2.15	139 (42%)	0 0	69, 99, 134, 141	0
1	B	329/387 (85%)	1.46	101 (30%)	0 0	54, 89, 137, 152	0
1	C	329/387 (85%)	1.53	110 (33%)	0 0	51, 87, 132, 154	0
1	D	329/387 (85%)	1.79	125 (37%)	0 0	57, 99, 133, 146	0
1	E	329/387 (85%)	1.64	116 (35%)	0 0	56, 97, 137, 148	0
1	F	329/387 (85%)	1.43	105 (31%)	0 0	48, 91, 133, 160	0
1	G	329/387 (85%)	1.40	99 (30%)	0 0	50, 92, 132, 156	0
1	H	329/387 (85%)	2.01	139 (42%)	0 0	61, 96, 133, 143	0
All	All	2632/3096 (85%)	1.68	934 (35%)	0 0	48, 94, 135, 160	0

The worst 5 of 934 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ALA	13.0
1	H	115	TYR	11.6
1	H	150	SER	10.5
1	D	257	MET	10.4
1	A	96	ALA	10.4

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 (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^{th} 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^2)	Q<0.9
2	YB	E	403	1/1	0.48	0.14	133,133,133,133	1
2	YB	E	407	1/1	0.53	0.16	115,115,115,115	1
2	YB	B	404	1/1	0.58	0.10	202,202,202,202	0
2	YB	B	402	1/1	0.59	0.10	124,124,124,124	1
3	SO4	A	410	5/5	0.68	0.61	119,129,144,148	0
2	YB	A	408	1/1	0.69	0.14	94,94,94,94	1
2	YB	F	404	1/1	0.71	0.17	129,129,129,129	1
2	YB	C	407	1/1	0.73	0.14	88,88,88,88	1
2	YB	H	402	1/1	0.73	0.08	165,165,165,165	1
2	YB	H	404	1/1	0.74	0.17	159,159,159,159	0
3	SO4	H	407	5/5	0.75	0.23	105,113,123,123	0
2	YB	G	407	1/1	0.75	0.17	100,100,100,100	1
2	YB	F	402	1/1	0.76	0.11	135,135,135,135	1
2	YB	A	407	1/1	0.76	0.15	105,105,105,105	1
2	YB	C	405	1/1	0.76	0.16	129,129,129,129	1
2	YB	G	403	1/1	0.77	0.19	111,111,111,111	1
2	YB	H	406	1/1	0.77	0.12	307,307,307,307	0
2	YB	A	404	1/1	0.78	0.07	149,149,149,149	1
2	YB	F	405	1/1	0.78	0.27	116,116,116,116	1
2	YB	E	408	1/1	0.78	0.17	120,120,120,120	1
3	SO4	F	408	5/5	0.78	0.53	112,121,124,127	0
2	YB	G	406	1/1	0.78	0.12	182,182,182,182	1
2	YB	D	408	1/1	0.79	0.17	347,347,347,347	1
2	YB	B	407	1/1	0.79	0.10	97,97,97,97	1
2	YB	F	403	1/1	0.80	0.05	184,184,184,184	0
2	YB	H	405	1/1	0.81	0.18	184,184,184,184	1
2	YB	E	405	1/1	0.81	0.09	170,170,170,170	0
2	YB	C	402	1/1	0.81	0.07	149,149,149,149	1
2	YB	H	403	1/1	0.81	0.13	130,130,130,130	1
2	YB	A	403	1/1	0.82	0.16	123,123,123,123	1
2	YB	G	408	1/1	0.82	0.31	169,169,169,169	1
2	YB	C	403	1/1	0.83	0.16	120,120,120,120	1
2	YB	A	402	1/1	0.84	0.11	134,134,134,134	1
2	YB	F	407	1/1	0.84	0.18	325,325,325,325	1
2	YB	B	401	1/1	0.85	0.14	127,127,127,127	0
2	YB	D	407	1/1	0.85	0.17	130,130,130,130	1
2	YB	A	406	1/1	0.85	0.14	115,115,115,115	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	YB	D	401	1/1	0.85	0.19	149,149,149,149	1
2	YB	E	409	1/1	0.85	0.26	116,116,116,116	1
2	YB	B	406	1/1	0.85	0.19	109,109,109,109	1
3	SO4	B	408	5/5	0.85	0.20	99,100,111,111	0
2	YB	E	402	1/1	0.86	0.08	148,148,148,148	1
2	YB	D	403	1/1	0.87	0.11	161,161,161,161	0
2	YB	B	405	1/1	0.87	0.12	123,123,123,123	1
3	SO4	D	409	5/5	0.87	0.17	100,107,113,117	0
2	YB	A	409	1/1	0.87	0.14	315,315,315,315	0
2	YB	G	401	1/1	0.87	0.13	165,165,165,165	0
2	YB	C	408	1/1	0.88	0.16	100,100,100,100	1
2	YB	D	404	1/1	0.88	0.11	166,166,166,166	1
2	YB	D	405	1/1	0.88	0.16	85,85,85,85	1
2	YB	E	401	1/1	0.90	0.11	153,153,153,153	1
2	YB	B	403	1/1	0.90	0.07	150,150,150,150	1
2	YB	A	405	1/1	0.91	0.22	92,92,92,92	1
2	YB	F	406	1/1	0.91	0.09	160,160,160,160	0
2	YB	C	401	1/1	0.91	0.13	142,142,142,142	0
2	YB	G	404	1/1	0.91	0.27	122,122,122,122	1
2	YB	E	406	1/1	0.92	0.09	94,94,94,94	1
2	YB	F	401	1/1	0.92	0.13	134,134,134,134	0
2	YB	G	405	1/1	0.93	0.17	129,129,129,129	1
2	YB	H	401	1/1	0.93	0.17	158,158,158,158	1
2	YB	G	402	1/1	0.93	0.09	162,162,162,162	0
2	YB	D	406	1/1	0.93	0.21	137,137,137,137	1
2	YB	C	406	1/1	0.93	0.07	130,130,130,130	1
2	YB	A	401	1/1	0.94	0.19	157,157,157,157	1
2	YB	E	404	1/1	0.94	0.06	92,92,92,92	1
2	YB	C	404	1/1	0.95	0.11	161,161,161,161	1
2	YB	D	402	1/1	0.96	0.19	115,115,115,115	1
2	YB	C	409	1/1	0.96	0.14	130,130,130,130	1

6.5 Other polymers (i)

There are no such residues in this entry.