wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 01:57 AM JST

PDB ID	:	6IU1
Title	:	Peroxiredoxin from Pyrococcus horikoshii 0Cys mutant)
Authors	:	Nakamura, T.; Himiyama, T.
Deposited on	:	2018-11-27
Resolution	:	2.89 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

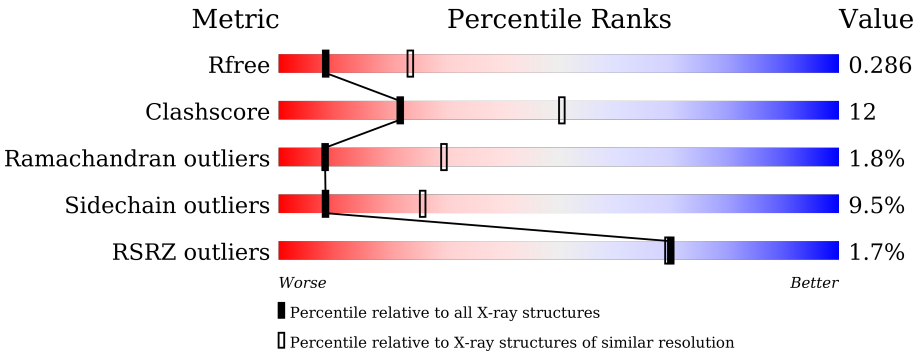
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.89 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 of 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	216	3% 59% 35%
1	B	216	4% 61% 31% 6%
1	C	216	3% 59% 31% 8%
1	D	216	2% 71% 25%
1	E	216	70% 25%
1	F	216	% 68% 26% 5%

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Mol	Chain	Length	Quality of chain
1	G	216	71% 22% 5%
1	H	216	65% 31%
1	I	216	72% 23%
1	J	216	70% 26%
1	K	216	3% 69% 27%
1	L	216	69% 25% 5%
1	M	216	71% 25%
1	N	216	2% 66% 29%
1	O	216	2% 70% 25%
1	P	216	3% 66% 28% 5%
1	Q	216	69% 26%
1	R	216	71% 25%
1	S	216	67% 28%
1	T	216	70% 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34738 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 Peroxiredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	B	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	C	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	D	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	E	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	F	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	G	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	H	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	I	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	J	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	K	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	L	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	M	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	N	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	O	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	P	215	Total	C	N	O	S	0	0	0
			1740	1138	283	316	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	R	215	Total	C	N	O	S	0	0	0
			1740	1138	283	316	3			
1	S	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			
1	T	214	Total	C	N	O	S	0	0	0
			1732	1133	282	315	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	SER	CYS	engineered mutation	UNP O58966
A	205	SER	CYS	engineered mutation	UNP O58966
A	211	SER	CYS	engineered mutation	UNP O58966
B	46	SER	CYS	engineered mutation	UNP O58966
B	205	SER	CYS	engineered mutation	UNP O58966
B	211	SER	CYS	engineered mutation	UNP O58966
C	46	SER	CYS	engineered mutation	UNP O58966
C	205	SER	CYS	engineered mutation	UNP O58966
C	211	SER	CYS	engineered mutation	UNP O58966
D	46	SER	CYS	engineered mutation	UNP O58966
D	205	SER	CYS	engineered mutation	UNP O58966
D	211	SER	CYS	engineered mutation	UNP O58966
E	46	SER	CYS	engineered mutation	UNP O58966
E	205	SER	CYS	engineered mutation	UNP O58966
E	211	SER	CYS	engineered mutation	UNP O58966
F	46	SER	CYS	engineered mutation	UNP O58966
F	205	SER	CYS	engineered mutation	UNP O58966
F	211	SER	CYS	engineered mutation	UNP O58966
G	46	SER	CYS	engineered mutation	UNP O58966
G	205	SER	CYS	engineered mutation	UNP O58966
G	211	SER	CYS	engineered mutation	UNP O58966
H	46	SER	CYS	engineered mutation	UNP O58966
H	205	SER	CYS	engineered mutation	UNP O58966
H	211	SER	CYS	engineered mutation	UNP O58966
I	46	SER	CYS	engineered mutation	UNP O58966
I	205	SER	CYS	engineered mutation	UNP O58966
I	211	SER	CYS	engineered mutation	UNP O58966
J	46	SER	CYS	engineered mutation	UNP O58966
J	205	SER	CYS	engineered mutation	UNP O58966
J	211	SER	CYS	engineered mutation	UNP O58966
K	46	SER	CYS	engineered mutation	UNP O58966

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Chain	Residue	Modelled	Actual	Comment	Reference
K	205	SER	CYS	engineered mutation	UNP O58966
K	211	SER	CYS	engineered mutation	UNP O58966
L	46	SER	CYS	engineered mutation	UNP O58966
L	205	SER	CYS	engineered mutation	UNP O58966
L	211	SER	CYS	engineered mutation	UNP O58966
M	46	SER	CYS	engineered mutation	UNP O58966
M	205	SER	CYS	engineered mutation	UNP O58966
M	211	SER	CYS	engineered mutation	UNP O58966
N	46	SER	CYS	engineered mutation	UNP O58966
N	205	SER	CYS	engineered mutation	UNP O58966
N	211	SER	CYS	engineered mutation	UNP O58966
O	46	SER	CYS	engineered mutation	UNP O58966
O	205	SER	CYS	engineered mutation	UNP O58966
O	211	SER	CYS	engineered mutation	UNP O58966
P	46	SER	CYS	engineered mutation	UNP O58966
P	205	SER	CYS	engineered mutation	UNP O58966
P	211	SER	CYS	engineered mutation	UNP O58966
Q	46	SER	CYS	engineered mutation	UNP O58966
Q	205	SER	CYS	engineered mutation	UNP O58966
Q	211	SER	CYS	engineered mutation	UNP O58966
R	46	SER	CYS	engineered mutation	UNP O58966
R	205	SER	CYS	engineered mutation	UNP O58966
R	211	SER	CYS	engineered mutation	UNP O58966
S	46	SER	CYS	engineered mutation	UNP O58966
S	205	SER	CYS	engineered mutation	UNP O58966
S	211	SER	CYS	engineered mutation	UNP O58966
T	46	SER	CYS	engineered mutation	UNP O58966
T	205	SER	CYS	engineered mutation	UNP O58966
T	211	SER	CYS	engineered mutation	UNP O58966

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	5	Total O 5 5	0	0
2	C	1	Total O 1 1	0	0
2	D	2	Total O 2 2	0	0
2	E	5	Total O 5 5	0	0

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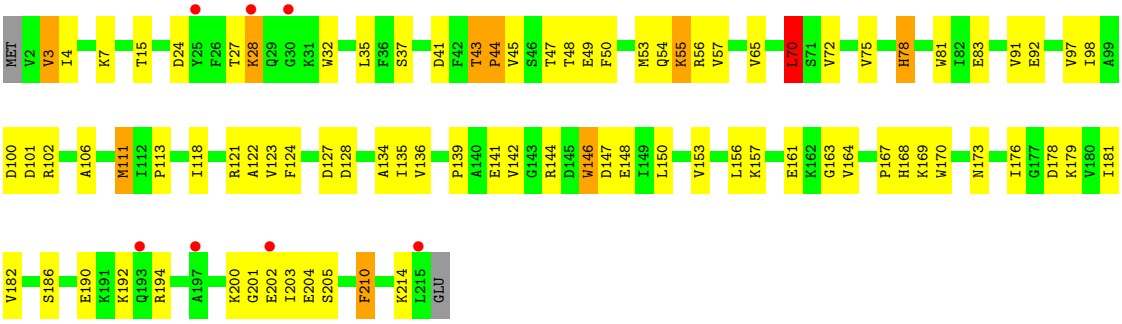
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	5	Total O 5 5	0	0
2	G	6	Total O 6 6	0	0
2	H	4	Total O 4 4	0	0
2	I	3	Total O 3 3	0	0
2	J	5	Total O 5 5	0	0
2	K	3	Total O 3 3	0	0
2	L	2	Total O 2 2	0	0
2	M	3	Total O 3 3	0	0
2	N	3	Total O 3 3	0	0
2	O	4	Total O 4 4	0	0
2	P	5	Total O 5 5	0	0
2	Q	6	Total O 6 6	0	0
2	R	5	Total O 5 5	0	0
2	S	10	Total O 10 10	0	0
2	T	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

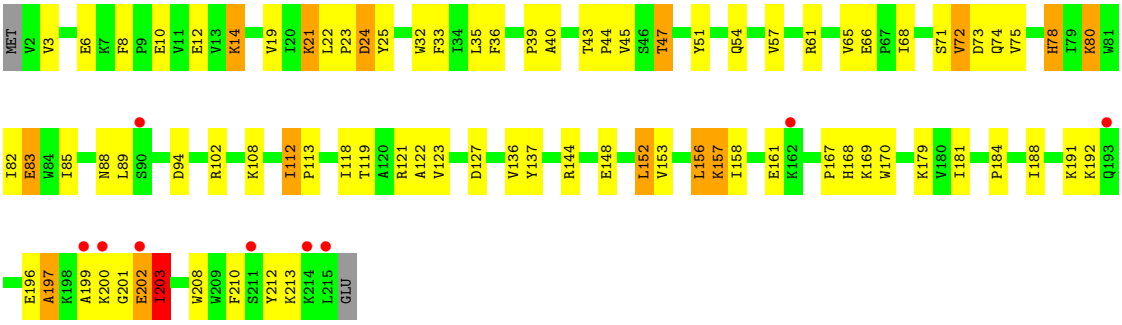
• Molecule 1: Peroxiredoxin

Chain A:



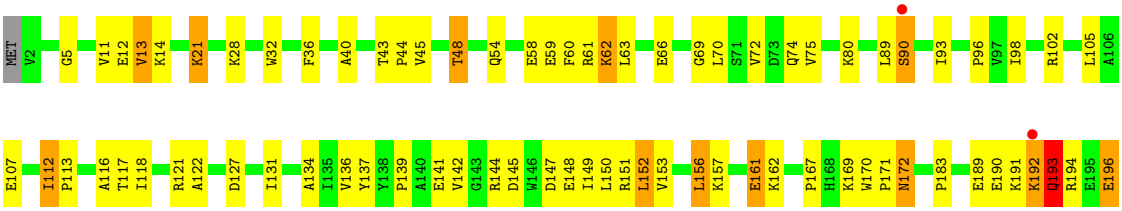
• Molecule 1: Peroxiredoxin

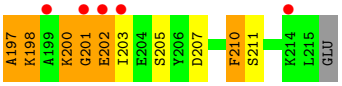
Chain B:



• Molecule 1: Peroxiredoxin

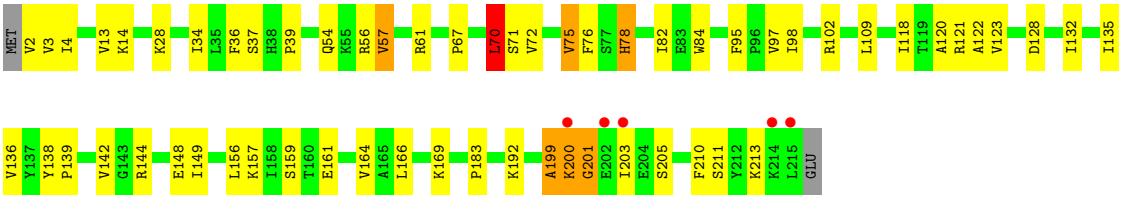
Chain C:





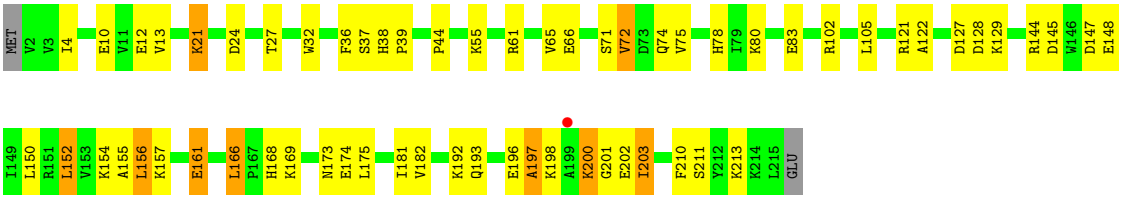
• Molecule 1: Peroxiredoxin

Chain D:



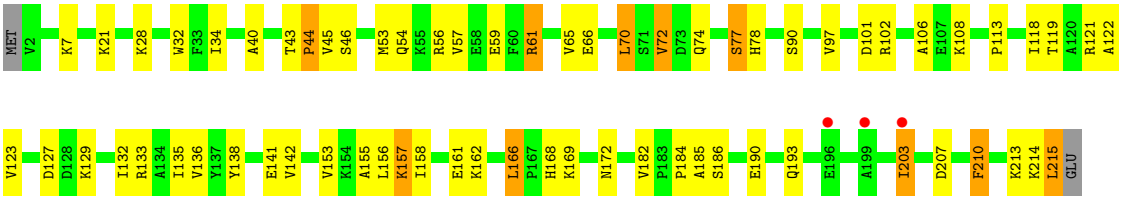
• Molecule 1: Peroxiredoxin

Chain E:



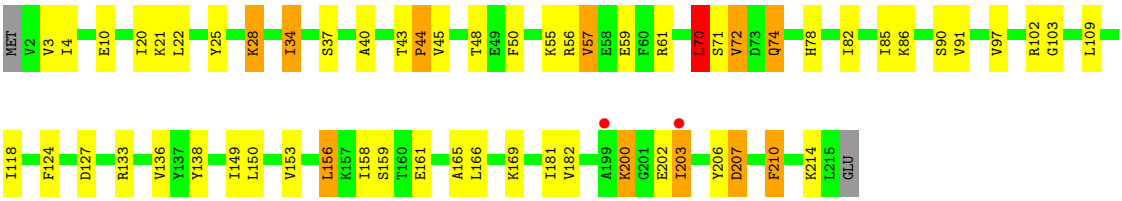
• Molecule 1: Peroxiredoxin

Chain F:



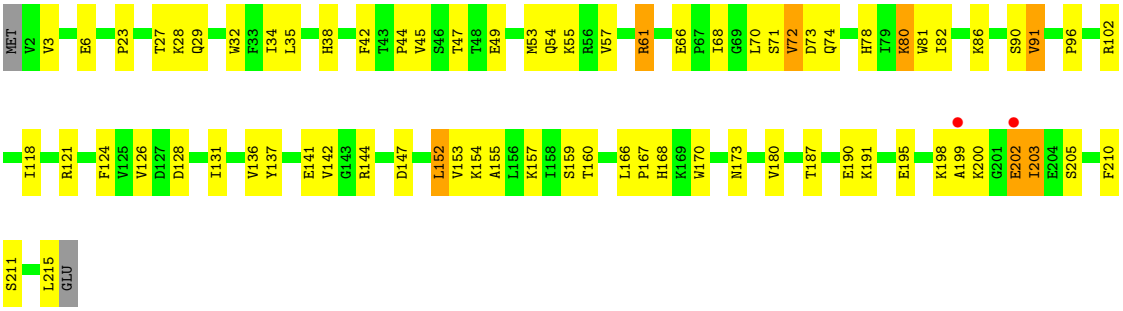
• Molecule 1: Peroxiredoxin

Chain G:



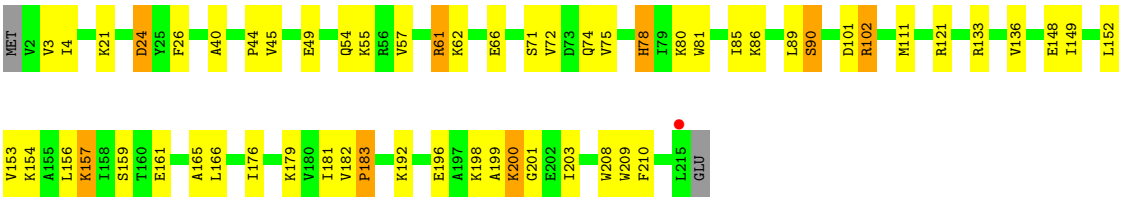
• Molecule 1: Peroxiredoxin

Chain H:



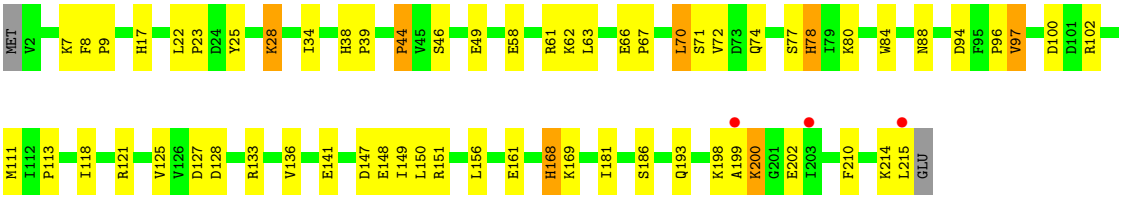
• Molecule 1: Peroxiredoxin

Chain I:



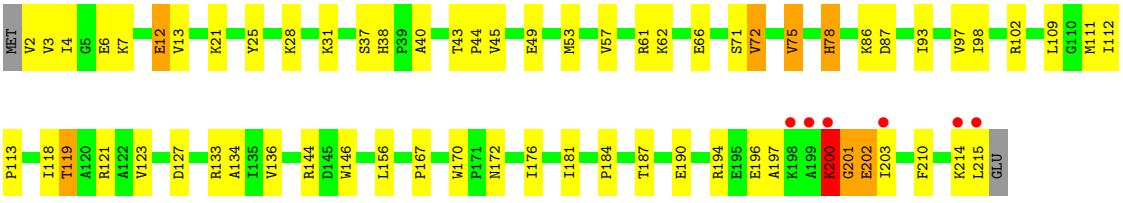
• Molecule 1: Peroxiredoxin

Chain J:



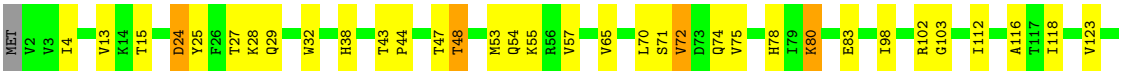
• Molecule 1: Peroxiredoxin

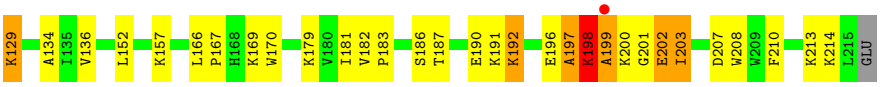
Chain K:



• Molecule 1: Peroxiredoxin

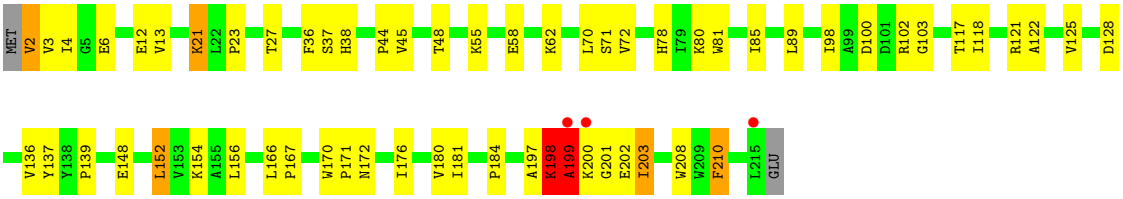
Chain L:





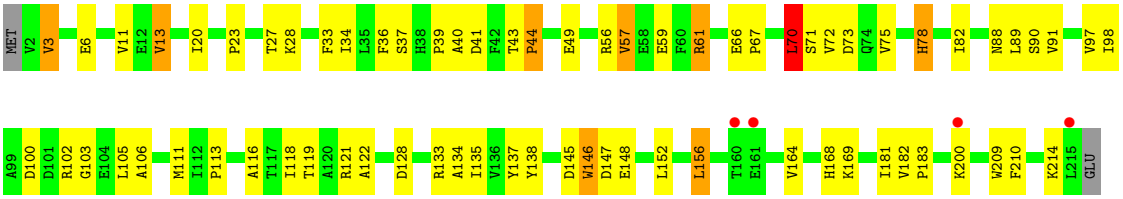
• Molecule 1: Peroxiredoxin

Chain M:



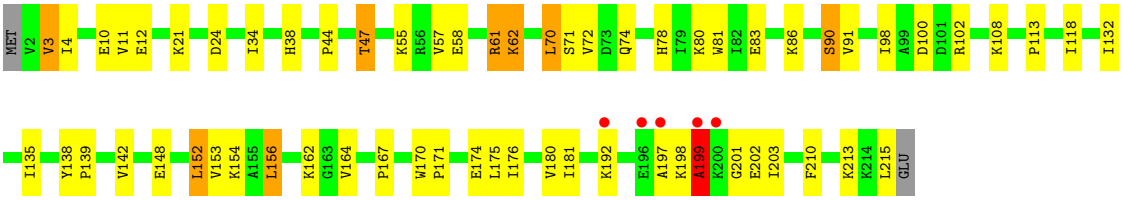
• Molecule 1: Peroxiredoxin

Chain N:



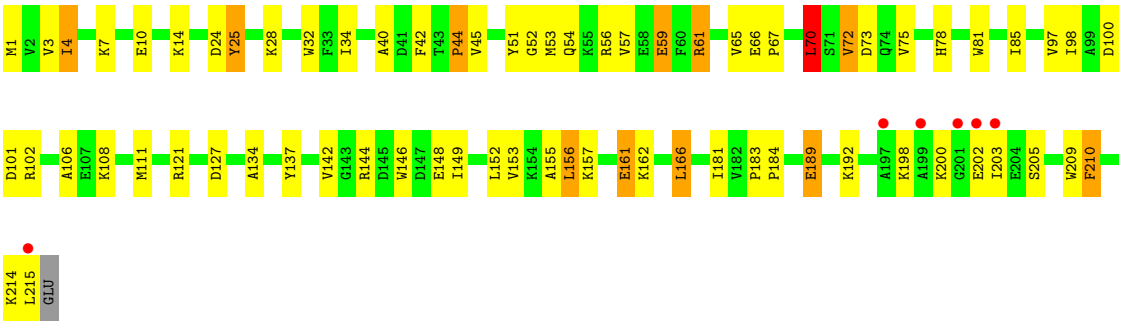
• Molecule 1: Peroxiredoxin

Chain O:



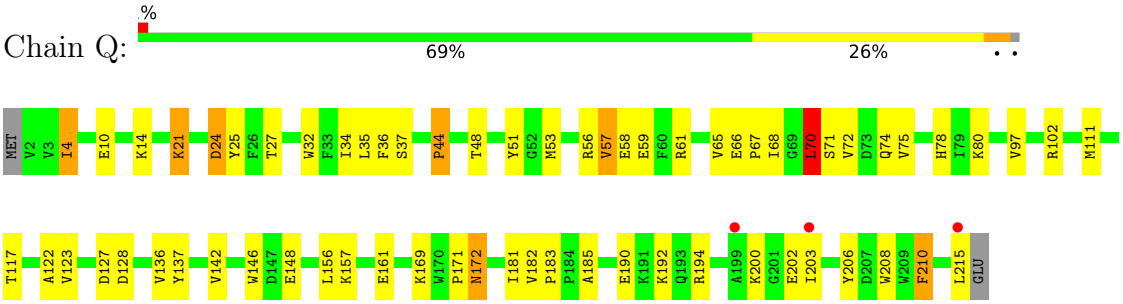
• Molecule 1: Peroxiredoxin

Chain P:



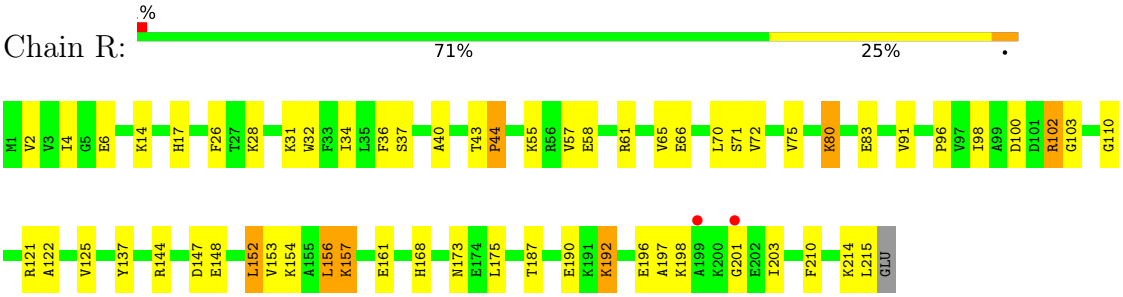
• Molecule 1: Peroxiredoxin

Chain Q:



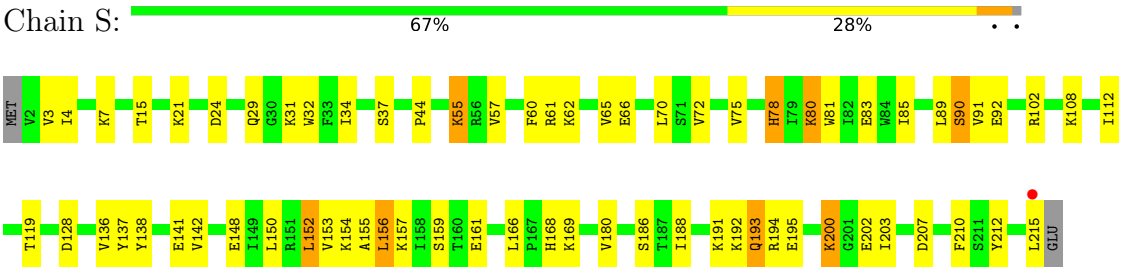
• Molecule 1: Peroxiredoxin

Chain R:



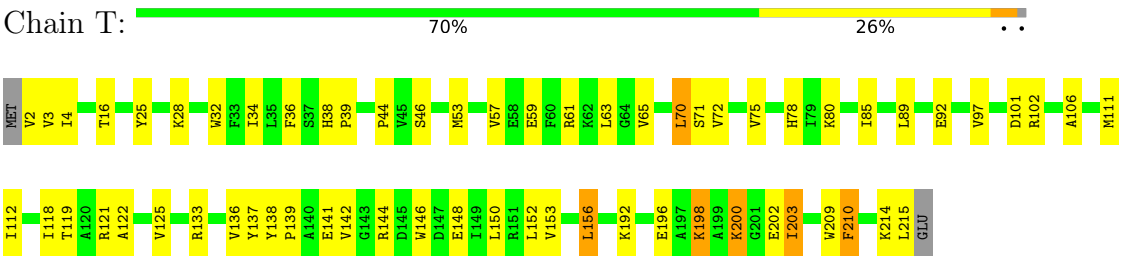
• Molecule 1: Peroxiredoxin

Chain S:



• Molecule 1: Peroxiredoxin

Chain T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	125.88Å 95.28Å 231.80Å 90.00° 104.43° 90.00°	Depositor
Resolution (Å)	39.09 – 2.89 39.09 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.2 (39.09-2.89) 98.3 (39.09-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.231 , 0.296 0.215 , 0.286	Depositor DCC
R_{free} test set	6141 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	44.3	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.002 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	34738	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 39.02 % 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 3.3804e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.62	0/1778	0.70	1/2410 (0.0%)
1	B	0.63	0/1778	0.70	0/2410
1	C	0.64	0/1778	0.75	1/2410 (0.0%)
1	D	0.63	0/1778	0.72	1/2410 (0.0%)
1	E	0.62	0/1778	0.74	1/2410 (0.0%)
1	F	0.68	0/1778	0.73	1/2410 (0.0%)
1	G	0.67	0/1778	0.73	1/2410 (0.0%)
1	H	0.70	0/1778	0.74	0/2410
1	I	0.62	0/1778	0.69	0/2410
1	J	0.64	0/1778	0.76	1/2410 (0.0%)
1	K	0.63	0/1778	0.71	1/2410 (0.0%)
1	L	0.65	0/1778	0.72	0/2410
1	M	0.63	0/1778	0.72	0/2410
1	N	0.67	0/1778	0.76	1/2410 (0.0%)
1	O	0.67	0/1778	0.74	0/2410
1	P	0.68	0/1786	0.78	1/2420 (0.0%)
1	Q	0.69	1/1778 (0.1%)	0.78	1/2410 (0.0%)
1	R	0.68	0/1786	0.78	0/2420
1	S	0.71	0/1778	0.77	0/2410
1	T	0.69	0/1778	0.74	1/2410 (0.0%)
All	All	0.66	1/35576 (0.0%)	0.74	12/48220 (0.0%)

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	L	0	1
1	M	0	1
1	O	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	58	GLU	CG-CD	5.22	1.59	1.51

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	70	LEU	CA-CB-CG	7.38	132.28	115.30
1	J	70	LEU	CA-CB-CG	7.36	132.23	115.30
1	P	70	LEU	CA-CB-CG	7.11	131.65	115.30
1	D	70	LEU	CA-CB-CG	6.82	130.98	115.30
1	E	145	ASP	CB-CG-OD2	6.74	124.36	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	199	ALA	Peptide
1	M	199	ALA	Peptide
1	O	199	ALA	Peptide

5.2 Too-close contacts (i)

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	1732	0	1749	70	0
1	B	1732	0	1749	63	0
1	C	1732	0	1749	77	0
1	D	1732	0	1749	41	0
1	E	1732	0	1749	44	0
1	F	1732	0	1749	45	0
1	G	1732	0	1749	36	0
1	H	1732	0	1749	50	0
1	I	1732	0	1749	37	0
1	J	1732	0	1749	40	0
1	K	1732	0	1749	44	0
1	L	1732	0	1749	45	0
1	M	1732	0	1749	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	1732	0	1749	52	1
1	O	1732	0	1749	51	0
1	P	1740	0	1761	57	0
1	Q	1732	0	1749	44	0
1	R	1740	0	1761	36	0
1	S	1732	0	1749	42	1
1	T	1732	0	1749	48	0
2	A	2	0	0	1	0
2	B	5	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	6	0	0	0	0
2	H	4	0	0	0	0
2	I	3	0	0	1	0
2	J	5	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
2	M	3	0	0	0	0
2	N	3	0	0	0	0
2	O	4	0	0	0	0
2	P	5	0	0	0	0
2	Q	6	0	0	1	0
2	R	5	0	0	0	0
2	S	10	0	0	0	0
2	T	3	0	0	1	0
All	All	34738	0	35004	831	1

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 12.

The worst 5 of 831 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:192:LYS:N	1:C:193:GLN:HB2	1.53	1.23
1:C:201:GLY:HA3	1:C:202:GLU:CB	1.86	1.04
1:C:201:GLY:HA3	1:C:202:GLU:HB2	1.39	1.01
1:B:54:GLN:HA	1:B:57:VAL:HG23	1.42	1.01
1:K:196:GLU:O	1:K:200:LYS:HB2	1.63	0.99

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:88:ASN:O	1:S:90:SER:OG[1_655]	2.03	0.17

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	212/216 (98%)	185 (87%)	22 (10%)	5 (2%)	6	22
1	B	212/216 (98%)	186 (88%)	20 (9%)	6 (3%)	5	19
1	C	212/216 (98%)	187 (88%)	16 (8%)	9 (4%)	3	10
1	D	212/216 (98%)	185 (87%)	21 (10%)	6 (3%)	5	19
1	E	212/216 (98%)	194 (92%)	14 (7%)	4 (2%)	8	28
1	F	212/216 (98%)	194 (92%)	16 (8%)	2 (1%)	17	48
1	G	212/216 (98%)	193 (91%)	16 (8%)	3 (1%)	11	36
1	H	212/216 (98%)	199 (94%)	12 (6%)	1 (0%)	29	61
1	I	212/216 (98%)	181 (85%)	29 (14%)	2 (1%)	17	48
1	J	212/216 (98%)	190 (90%)	19 (9%)	3 (1%)	11	36
1	K	212/216 (98%)	194 (92%)	13 (6%)	5 (2%)	6	22
1	L	212/216 (98%)	185 (87%)	22 (10%)	5 (2%)	6	22
1	M	212/216 (98%)	196 (92%)	13 (6%)	3 (1%)	11	36
1	N	212/216 (98%)	192 (91%)	16 (8%)	4 (2%)	8	28
1	O	212/216 (98%)	188 (89%)	20 (9%)	4 (2%)	8	28
1	P	213/216 (99%)	197 (92%)	14 (7%)	2 (1%)	17	48
1	Q	212/216 (98%)	192 (91%)	16 (8%)	4 (2%)	8	28
1	R	213/216 (99%)	188 (88%)	22 (10%)	3 (1%)	11	36
1	S	212/216 (98%)	194 (92%)	15 (7%)	3 (1%)	11	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	T	212/216 (98%)	200 (94%)	11 (5%)	1 (0%)	29 61
All	All	4242/4320 (98%)	3820 (90%)	347 (8%)	75 (2%)	8 29

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	ALA
1	C	90	SER
1	C	193	GLN
1	C	196	GLU
1	C	197	ALA

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	187/189 (99%)	164 (88%)	23 (12%)	4 14
1	B	187/189 (99%)	165 (88%)	22 (12%)	5 16
1	C	187/189 (99%)	163 (87%)	24 (13%)	4 13
1	D	187/189 (99%)	170 (91%)	17 (9%)	9 28
1	E	187/189 (99%)	174 (93%)	13 (7%)	15 41
1	F	187/189 (99%)	165 (88%)	22 (12%)	5 16
1	G	187/189 (99%)	169 (90%)	18 (10%)	8 25
1	H	187/189 (99%)	171 (91%)	16 (9%)	10 30
1	I	187/189 (99%)	168 (90%)	19 (10%)	7 22
1	J	187/189 (99%)	171 (91%)	16 (9%)	10 30
1	K	187/189 (99%)	168 (90%)	19 (10%)	7 22
1	L	187/189 (99%)	168 (90%)	19 (10%)	7 22
1	M	187/189 (99%)	175 (94%)	12 (6%)	17 45
1	N	187/189 (99%)	173 (92%)	14 (8%)	13 37
1	O	187/189 (99%)	172 (92%)	15 (8%)	12 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	P	188/189 (100%)	163 (87%)	25 (13%)	4 11
1	Q	187/189 (99%)	175 (94%)	12 (6%)	17 45
1	R	188/189 (100%)	171 (91%)	17 (9%)	9 29
1	S	187/189 (99%)	167 (89%)	20 (11%)	6 20
1	T	187/189 (99%)	173 (92%)	14 (8%)	13 37
All	All	3742/3780 (99%)	3385 (90%)	357 (10%)	8 26

5 of 357 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	55	LYS
1	P	189	GLU
1	M	203	ILE
1	O	80	LYS
1	Q	156	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	M	172	ASN
1	Q	172	ASN
1	T	78	HIS
1	Q	29	GLN
1	R	74	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	214/216 (99%)	0.18	7 (3%)	46	41	33, 48, 62, 72	0
1	B	214/216 (99%)	0.14	9 (4%)	36	32	32, 46, 63, 69	0
1	C	214/216 (99%)	-0.10	7 (3%)	46	41	29, 42, 58, 64	0
1	D	214/216 (99%)	-0.23	5 (2%)	60	58	25, 40, 61, 67	0
1	E	214/216 (99%)	-0.35	1 (0%)	91	91	16, 35, 50, 55	0
1	F	214/216 (99%)	-0.31	3 (1%)	75	75	18, 31, 53, 58	0
1	G	214/216 (99%)	-0.40	2 (0%)	84	84	13, 28, 52, 57	0
1	H	214/216 (99%)	-0.45	2 (0%)	84	84	13, 28, 47, 54	0
1	I	214/216 (99%)	-0.27	1 (0%)	91	91	21, 39, 60, 65	0
1	J	214/216 (99%)	-0.24	3 (1%)	75	75	25, 36, 53, 61	0
1	K	214/216 (99%)	-0.19	6 (2%)	53	49	23, 36, 58, 67	0
1	L	214/216 (99%)	-0.16	1 (0%)	91	91	19, 36, 51, 59	0
1	M	214/216 (99%)	-0.19	3 (1%)	75	75	23, 38, 56, 66	0
1	N	214/216 (99%)	-0.27	4 (1%)	66	65	20, 36, 55, 65	0
1	O	214/216 (99%)	-0.40	5 (2%)	60	58	20, 32, 45, 56	0
1	P	215/216 (99%)	-0.25	6 (2%)	53	49	16, 31, 54, 61	0
1	Q	214/216 (99%)	-0.36	3 (1%)	75	75	11, 24, 43, 49	0
1	R	215/216 (99%)	-0.42	2 (0%)	84	84	6, 25, 44, 52	0
1	S	214/216 (99%)	-0.49	1 (0%)	91	91	14, 27, 42, 50	0
1	T	214/216 (99%)	-0.43	0	100	100	11, 28, 38, 44	0
All	All	4282/4320 (99%)	-0.26	71 (1%)	70	69	6, 34, 55, 72	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	LEU	4.6
1	B	199	ALA	4.5
1	L	199	ALA	4.4
1	N	200	LYS	4.2
1	P	215	LEU	4.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.