



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:37 PM GMT

PDB ID : 4ITV
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, triple mutant, P212121 form
Authors : Lai, Y.-T.; Sawaya, M.R.; Yeates, T.O.
Deposited on : 2013-01-18
Resolution : 3.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

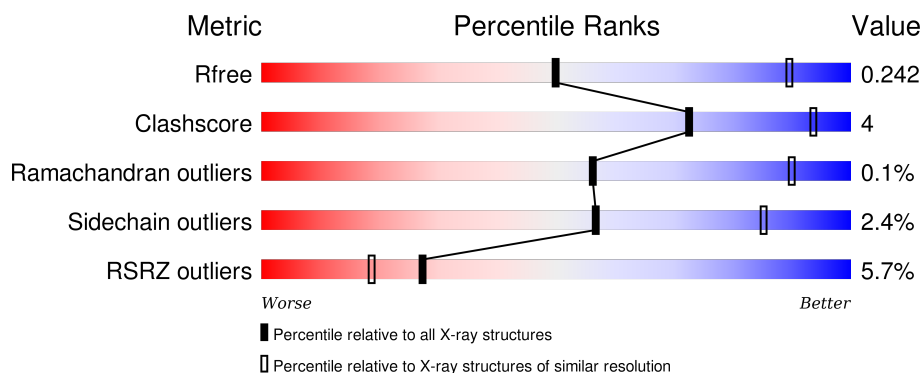
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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. 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 $\leq 5\%$. 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	456	<div> <div></div> <div>82%</div> <div>14%</div> <div>.</div> </div>
1	B	456	<div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div>
1	C	456	<div> <div>2%</div> <div></div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	D	456	<div> <div>8%</div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div>
1	E	456	<div> <div></div> <div>85%</div> <div>11%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	456	<div><div></div><div>12%</div><div>85%</div><div>11%</div><div></div></div>
1	G	456	<div><div></div><div>7%</div><div>86%</div><div>11%</div><div></div></div>
1	H	456	<div><div></div><div>18%</div><div>85%</div><div>11%</div><div></div></div>
1	I	456	<div><div></div><div>2%</div><div>86%</div><div>11%</div><div></div></div>
1	J	456	<div><div></div><div></div><div>86%</div><div>11%</div><div></div></div>
1	K	456	<div><div></div><div>2%</div><div>85%</div><div>11%</div><div></div></div>
1	L	456	<div><div></div><div>17%</div><div>84%</div><div>12%</div><div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40776 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 Non-haem bromoperoxidase BPO-A2, Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	B	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	C	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	D	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	E	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	F	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	G	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	H	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	I	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	J	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	K	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			
1	L	440	Total	C	N	O	S	0	0	0
			3398	2166	572	652	8			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
A	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
A	278	ALA	-	LINKER	UNP P03485
A	279	GLN	-	LINKER	UNP P03485
A	280	GLU	-	LINKER	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
A	281	ALA	-	LINKER	UNP P03485
A	282	GLN	-	LINKER	UNP P03485
A	283	LYS	-	LINKER	UNP P03485
A	284	GLN	-	LINKER	UNP P03485
A	285	LYS	-	LINKER	UNP P03485
A	448	LEU	-	EXPRESSION TAG	UNP P03485
A	449	GLU	-	EXPRESSION TAG	UNP P03485
A	450	HIS	-	EXPRESSION TAG	UNP P03485
A	451	HIS	-	EXPRESSION TAG	UNP P03485
A	452	HIS	-	EXPRESSION TAG	UNP P03485
A	453	HIS	-	EXPRESSION TAG	UNP P03485
A	454	HIS	-	EXPRESSION TAG	UNP P03485
A	455	HIS	-	EXPRESSION TAG	UNP P03485
B	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
B	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
B	278	ALA	-	LINKER	UNP P03485
B	279	GLN	-	LINKER	UNP P03485
B	280	GLU	-	LINKER	UNP P03485
B	281	ALA	-	LINKER	UNP P03485
B	282	GLN	-	LINKER	UNP P03485
B	283	LYS	-	LINKER	UNP P03485
B	284	GLN	-	LINKER	UNP P03485
B	285	LYS	-	LINKER	UNP P03485
B	448	LEU	-	EXPRESSION TAG	UNP P03485
B	449	GLU	-	EXPRESSION TAG	UNP P03485
B	450	HIS	-	EXPRESSION TAG	UNP P03485
B	451	HIS	-	EXPRESSION TAG	UNP P03485
B	452	HIS	-	EXPRESSION TAG	UNP P03485
B	453	HIS	-	EXPRESSION TAG	UNP P03485
B	454	HIS	-	EXPRESSION TAG	UNP P03485
B	455	HIS	-	EXPRESSION TAG	UNP P03485
C	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
C	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
C	278	ALA	-	LINKER	UNP P03485
C	279	GLN	-	LINKER	UNP P03485
C	280	GLU	-	LINKER	UNP P03485
C	281	ALA	-	LINKER	UNP P03485
C	282	GLN	-	LINKER	UNP P03485
C	283	LYS	-	LINKER	UNP P03485
C	284	GLN	-	LINKER	UNP P03485
C	285	LYS	-	LINKER	UNP P03485
C	448	LEU	-	EXPRESSION TAG	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
C	449	GLU	-	EXPRESSION TAG	UNP P03485
C	450	HIS	-	EXPRESSION TAG	UNP P03485
C	451	HIS	-	EXPRESSION TAG	UNP P03485
C	452	HIS	-	EXPRESSION TAG	UNP P03485
C	453	HIS	-	EXPRESSION TAG	UNP P03485
C	454	HIS	-	EXPRESSION TAG	UNP P03485
C	455	HIS	-	EXPRESSION TAG	UNP P03485
D	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
D	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
D	278	ALA	-	LINKER	UNP P03485
D	279	GLN	-	LINKER	UNP P03485
D	280	GLU	-	LINKER	UNP P03485
D	281	ALA	-	LINKER	UNP P03485
D	282	GLN	-	LINKER	UNP P03485
D	283	LYS	-	LINKER	UNP P03485
D	284	GLN	-	LINKER	UNP P03485
D	285	LYS	-	LINKER	UNP P03485
D	448	LEU	-	EXPRESSION TAG	UNP P03485
D	449	GLU	-	EXPRESSION TAG	UNP P03485
D	450	HIS	-	EXPRESSION TAG	UNP P03485
D	451	HIS	-	EXPRESSION TAG	UNP P03485
D	452	HIS	-	EXPRESSION TAG	UNP P03485
D	453	HIS	-	EXPRESSION TAG	UNP P03485
D	454	HIS	-	EXPRESSION TAG	UNP P03485
D	455	HIS	-	EXPRESSION TAG	UNP P03485
E	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
E	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
E	278	ALA	-	LINKER	UNP P03485
E	279	GLN	-	LINKER	UNP P03485
E	280	GLU	-	LINKER	UNP P03485
E	281	ALA	-	LINKER	UNP P03485
E	282	GLN	-	LINKER	UNP P03485
E	283	LYS	-	LINKER	UNP P03485
E	284	GLN	-	LINKER	UNP P03485
E	285	LYS	-	LINKER	UNP P03485
E	448	LEU	-	EXPRESSION TAG	UNP P03485
E	449	GLU	-	EXPRESSION TAG	UNP P03485
E	450	HIS	-	EXPRESSION TAG	UNP P03485
E	451	HIS	-	EXPRESSION TAG	UNP P03485
E	452	HIS	-	EXPRESSION TAG	UNP P03485
E	453	HIS	-	EXPRESSION TAG	UNP P03485
E	454	HIS	-	EXPRESSION TAG	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
E	455	HIS	-	EXPRESSION TAG	UNP P03485
F	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
F	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
F	278	ALA	-	LINKER	UNP P03485
F	279	GLN	-	LINKER	UNP P03485
F	280	GLU	-	LINKER	UNP P03485
F	281	ALA	-	LINKER	UNP P03485
F	282	GLN	-	LINKER	UNP P03485
F	283	LYS	-	LINKER	UNP P03485
F	284	GLN	-	LINKER	UNP P03485
F	285	LYS	-	LINKER	UNP P03485
F	448	LEU	-	EXPRESSION TAG	UNP P03485
F	449	GLU	-	EXPRESSION TAG	UNP P03485
F	450	HIS	-	EXPRESSION TAG	UNP P03485
F	451	HIS	-	EXPRESSION TAG	UNP P03485
F	452	HIS	-	EXPRESSION TAG	UNP P03485
F	453	HIS	-	EXPRESSION TAG	UNP P03485
F	454	HIS	-	EXPRESSION TAG	UNP P03485
F	455	HIS	-	EXPRESSION TAG	UNP P03485
G	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
G	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
G	278	ALA	-	LINKER	UNP P03485
G	279	GLN	-	LINKER	UNP P03485
G	280	GLU	-	LINKER	UNP P03485
G	281	ALA	-	LINKER	UNP P03485
G	282	GLN	-	LINKER	UNP P03485
G	283	LYS	-	LINKER	UNP P03485
G	284	GLN	-	LINKER	UNP P03485
G	285	LYS	-	LINKER	UNP P03485
G	448	LEU	-	EXPRESSION TAG	UNP P03485
G	449	GLU	-	EXPRESSION TAG	UNP P03485
G	450	HIS	-	EXPRESSION TAG	UNP P03485
G	451	HIS	-	EXPRESSION TAG	UNP P03485
G	452	HIS	-	EXPRESSION TAG	UNP P03485
G	453	HIS	-	EXPRESSION TAG	UNP P03485
G	454	HIS	-	EXPRESSION TAG	UNP P03485
G	455	HIS	-	EXPRESSION TAG	UNP P03485
H	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
H	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
H	278	ALA	-	LINKER	UNP P03485
H	279	GLN	-	LINKER	UNP P03485
H	280	GLU	-	LINKER	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
H	281	ALA	-	LINKER	UNP P03485
H	282	GLN	-	LINKER	UNP P03485
H	283	LYS	-	LINKER	UNP P03485
H	284	GLN	-	LINKER	UNP P03485
H	285	LYS	-	LINKER	UNP P03485
H	448	LEU	-	EXPRESSION TAG	UNP P03485
H	449	GLU	-	EXPRESSION TAG	UNP P03485
H	450	HIS	-	EXPRESSION TAG	UNP P03485
H	451	HIS	-	EXPRESSION TAG	UNP P03485
H	452	HIS	-	EXPRESSION TAG	UNP P03485
H	453	HIS	-	EXPRESSION TAG	UNP P03485
H	454	HIS	-	EXPRESSION TAG	UNP P03485
H	455	HIS	-	EXPRESSION TAG	UNP P03485
I	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
I	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
I	278	ALA	-	LINKER	UNP P03485
I	279	GLN	-	LINKER	UNP P03485
I	280	GLU	-	LINKER	UNP P03485
I	281	ALA	-	LINKER	UNP P03485
I	282	GLN	-	LINKER	UNP P03485
I	283	LYS	-	LINKER	UNP P03485
I	284	GLN	-	LINKER	UNP P03485
I	285	LYS	-	LINKER	UNP P03485
I	448	LEU	-	EXPRESSION TAG	UNP P03485
I	449	GLU	-	EXPRESSION TAG	UNP P03485
I	450	HIS	-	EXPRESSION TAG	UNP P03485
I	451	HIS	-	EXPRESSION TAG	UNP P03485
I	452	HIS	-	EXPRESSION TAG	UNP P03485
I	453	HIS	-	EXPRESSION TAG	UNP P03485
I	454	HIS	-	EXPRESSION TAG	UNP P03485
I	455	HIS	-	EXPRESSION TAG	UNP P03485
J	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
J	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
J	278	ALA	-	LINKER	UNP P03485
J	279	GLN	-	LINKER	UNP P03485
J	280	GLU	-	LINKER	UNP P03485
J	281	ALA	-	LINKER	UNP P03485
J	282	GLN	-	LINKER	UNP P03485
J	283	LYS	-	LINKER	UNP P03485
J	284	GLN	-	LINKER	UNP P03485
J	285	LYS	-	LINKER	UNP P03485
J	448	LEU	-	EXPRESSION TAG	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
J	449	GLU	-	EXPRESSION TAG	UNP P03485
J	450	HIS	-	EXPRESSION TAG	UNP P03485
J	451	HIS	-	EXPRESSION TAG	UNP P03485
J	452	HIS	-	EXPRESSION TAG	UNP P03485
J	453	HIS	-	EXPRESSION TAG	UNP P03485
J	454	HIS	-	EXPRESSION TAG	UNP P03485
J	455	HIS	-	EXPRESSION TAG	UNP P03485
K	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
K	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
K	278	ALA	-	LINKER	UNP P03485
K	279	GLN	-	LINKER	UNP P03485
K	280	GLU	-	LINKER	UNP P03485
K	281	ALA	-	LINKER	UNP P03485
K	282	GLN	-	LINKER	UNP P03485
K	283	LYS	-	LINKER	UNP P03485
K	284	GLN	-	LINKER	UNP P03485
K	285	LYS	-	LINKER	UNP P03485
K	448	LEU	-	EXPRESSION TAG	UNP P03485
K	449	GLU	-	EXPRESSION TAG	UNP P03485
K	450	HIS	-	EXPRESSION TAG	UNP P03485
K	451	HIS	-	EXPRESSION TAG	UNP P03485
K	452	HIS	-	EXPRESSION TAG	UNP P03485
K	453	HIS	-	EXPRESSION TAG	UNP P03485
K	454	HIS	-	EXPRESSION TAG	UNP P03485
K	455	HIS	-	EXPRESSION TAG	UNP P03485
L	24	THR	GLN	ENGINEERED MUTATION	UNP P29715
L	118	ALA	LYS	ENGINEERED MUTATION	UNP P29715
L	278	ALA	-	LINKER	UNP P03485
L	279	GLN	-	LINKER	UNP P03485
L	280	GLU	-	LINKER	UNP P03485
L	281	ALA	-	LINKER	UNP P03485
L	282	GLN	-	LINKER	UNP P03485
L	283	LYS	-	LINKER	UNP P03485
L	284	GLN	-	LINKER	UNP P03485
L	285	LYS	-	LINKER	UNP P03485
L	448	LEU	-	EXPRESSION TAG	UNP P03485
L	449	GLU	-	EXPRESSION TAG	UNP P03485
L	450	HIS	-	EXPRESSION TAG	UNP P03485
L	451	HIS	-	EXPRESSION TAG	UNP P03485
L	452	HIS	-	EXPRESSION TAG	UNP P03485
L	453	HIS	-	EXPRESSION TAG	UNP P03485
L	454	HIS	-	EXPRESSION TAG	UNP P03485

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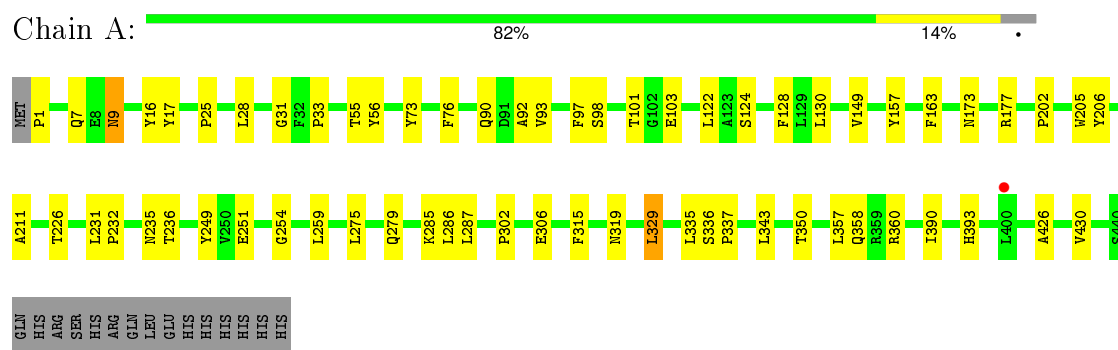
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Chain	Residue	Modelled	Actual	Comment	Reference
L	455	HIS	-	EXPRESSION TAG	UNP P03485

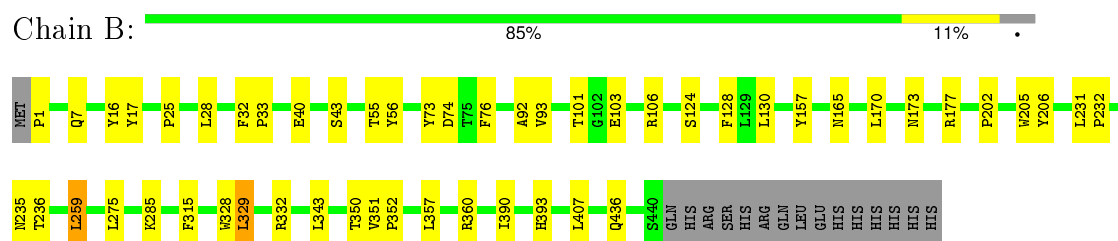
3 Residue-property plots [i](#)

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

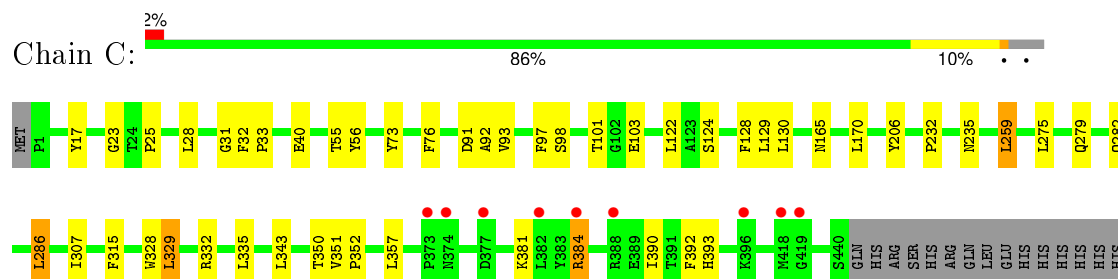
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



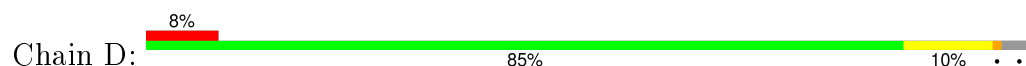
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

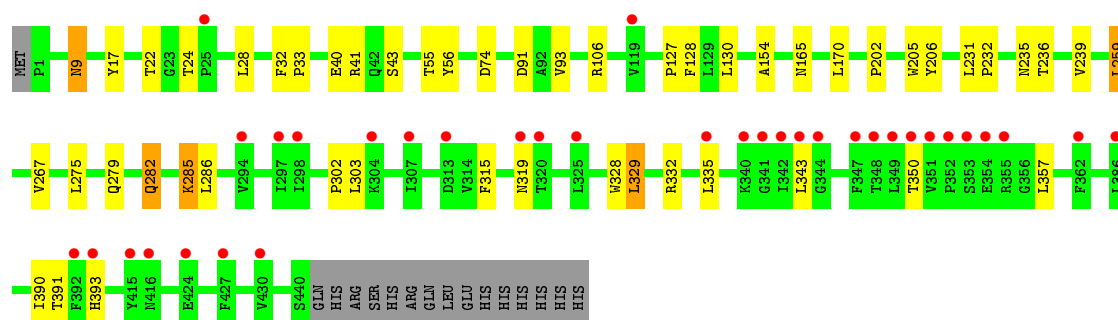


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



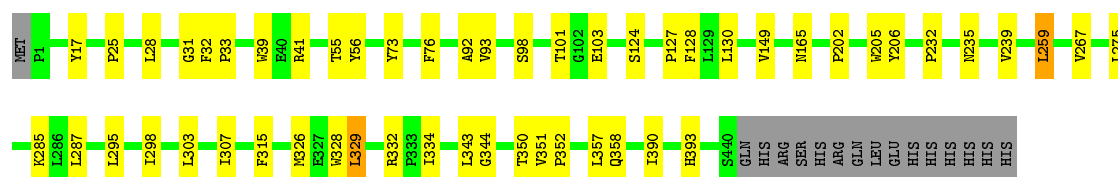
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1





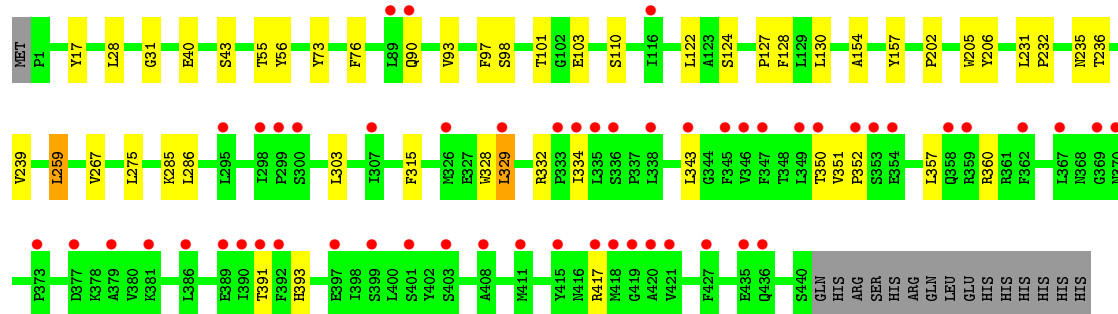
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain E: 85% 11%



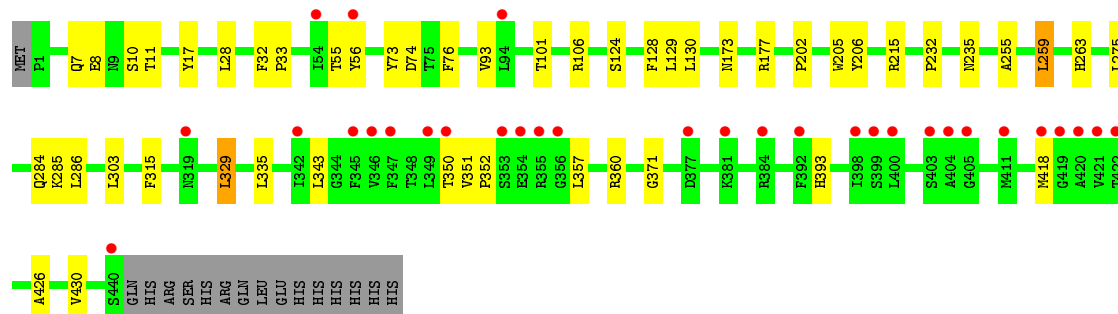
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain F: 85% 11%



- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

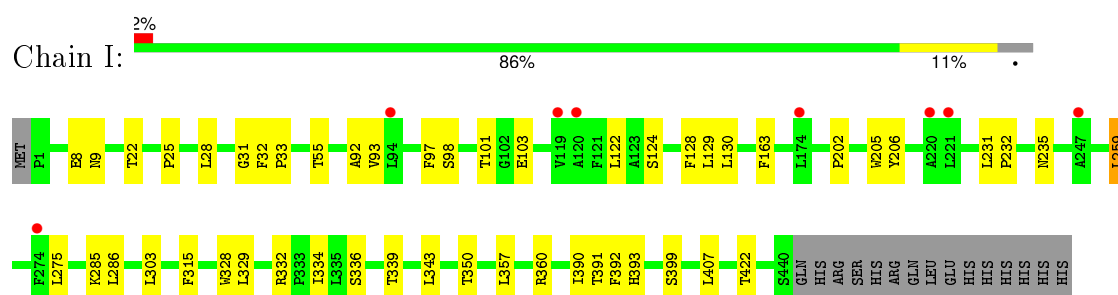
Chain G: 86% 11%



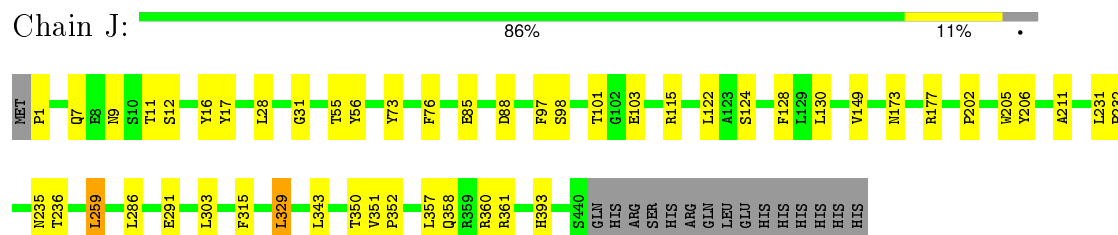
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain H: 85% 11%

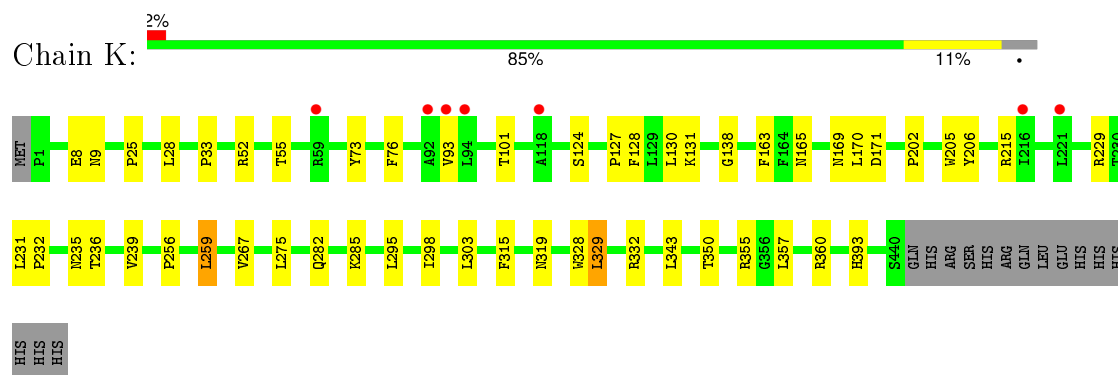
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



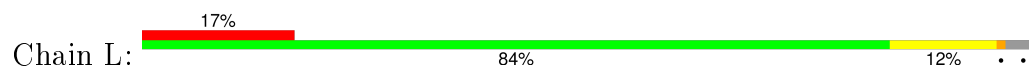
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

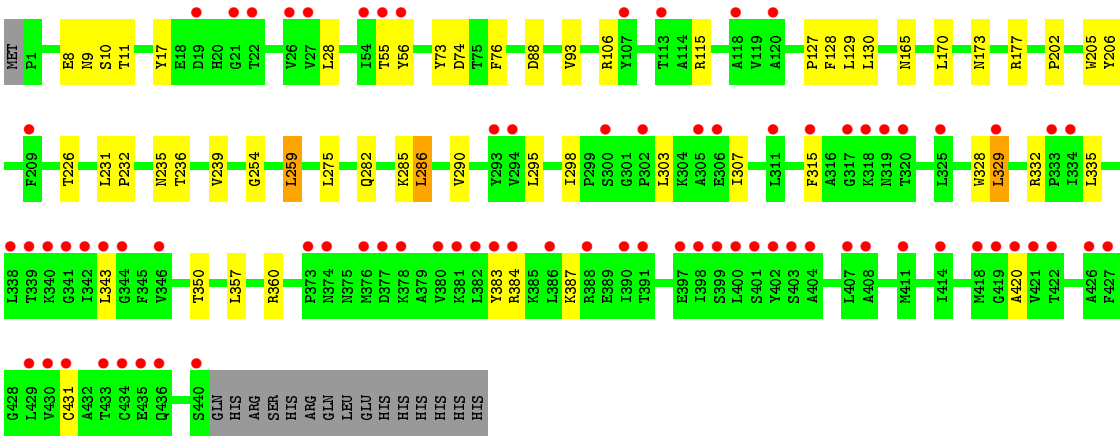


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.62Å 156.61Å 321.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.14 – 3.60 96.14 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (96.14-3.60) 98.3 (96.14-3.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.206 , 0.240 0.207 , 0.242	Depositor DCC
R_{free} test set	3822 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	114.8	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 76475 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	40776	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/3475	0.41	0/4729
1	B	0.23	0/3475	0.40	0/4729
1	C	0.22	0/3475	0.40	0/4729
1	D	0.22	0/3475	0.39	0/4729
1	E	0.23	0/3475	0.40	0/4729
1	F	0.22	0/3475	0.39	0/4729
1	G	0.23	0/3475	0.40	0/4729
1	H	0.22	0/3475	0.40	0/4729
1	I	0.22	0/3475	0.39	0/4729
1	J	0.23	0/3475	0.40	0/4729
1	K	0.22	0/3475	0.40	0/4729
1	L	0.22	0/3475	0.39	0/4729
All	All	0.22	0/41700	0.40	0/56748

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3398	0	3326	37	0
1	B	3398	0	3326	32	0
1	C	3398	0	3326	28	0
1	D	3398	0	3326	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3398	0	3326	29	0
1	F	3398	0	3326	27	0
1	G	3398	0	3326	31	0
1	H	3398	0	3326	32	0
1	I	3398	0	3326	27	0
1	J	3398	0	3326	26	0
1	K	3398	0	3326	26	0
1	L	3398	0	3326	37	0
All	All	40776	0	39912	335	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 4.

The worst 5 of 335 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:E:130:LEU:HB2	1:E:206:TYR:HB2	1.70	0.73
1:A:90:GLN:HB2	1:A:390:ILE:HD13	1.71	0.73
1:L:387:LYS:NZ	1:L:420:ALA:O	2.22	0.72
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.71	0.72
1:B:1:PRO:HD2	1:B:16:TYR:HE1	1.57	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	438/456 (96%)	414 (94%)	23 (5%)	1 (0%)	52	87
1	B	438/456 (96%)	416 (95%)	22 (5%)	0	100	100
1	C	438/456 (96%)	415 (95%)	23 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	438/456 (96%)	414 (94%)	22 (5%)	2 (0%)	34	77
1	E	438/456 (96%)	413 (94%)	25 (6%)	0	100	100
1	F	438/456 (96%)	414 (94%)	24 (6%)	0	100	100
1	G	438/456 (96%)	418 (95%)	20 (5%)	0	100	100
1	H	438/456 (96%)	418 (95%)	19 (4%)	1 (0%)	52	87
1	I	438/456 (96%)	412 (94%)	26 (6%)	0	100	100
1	J	438/456 (96%)	414 (94%)	23 (5%)	1 (0%)	52	87
1	K	438/456 (96%)	414 (94%)	24 (6%)	0	100	100
1	L	438/456 (96%)	414 (94%)	24 (6%)	0	100	100
All	All	5256/5472 (96%)	4976 (95%)	275 (5%)	5 (0%)	56	90

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	D	9	ASN
1	H	9	ASN
1	J	9	ASN
1	D	319	ASN

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	354/370 (96%)	343 (97%)	11 (3%)	47	81
1	B	354/370 (96%)	347 (98%)	7 (2%)	63	87
1	C	354/370 (96%)	347 (98%)	7 (2%)	63	87
1	D	354/370 (96%)	345 (98%)	9 (2%)	55	84
1	E	354/370 (96%)	345 (98%)	9 (2%)	55	84
1	F	354/370 (96%)	345 (98%)	9 (2%)	55	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	354/370 (96%)	345 (98%)	9 (2%)	55	84
1	H	354/370 (96%)	344 (97%)	10 (3%)	51	82
1	I	354/370 (96%)	347 (98%)	7 (2%)	63	87
1	J	354/370 (96%)	346 (98%)	8 (2%)	58	85
1	K	354/370 (96%)	346 (98%)	8 (2%)	58	85
1	L	354/370 (96%)	347 (98%)	7 (2%)	63	87
All	All	4248/4440 (96%)	4147 (98%)	101 (2%)	57	85

5 of 101 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	259	LEU
1	G	286	LEU
1	K	393	HIS
1	F	286	LEU
1	F	393	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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, 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	440/456 (96%)	-0.07	1 (0%) 95 92	63, 94, 154, 182	0
1	B	440/456 (96%)	-0.14	0 100 100	72, 106, 155, 220	0
1	C	440/456 (96%)	-0.03	9 (2%) 68 54	68, 122, 214, 270	0
1	D	440/456 (96%)	0.35	35 (7%) 15 10	85, 135, 228, 266	0
1	E	440/456 (96%)	-0.17	0 100 100	74, 114, 155, 200	0
1	F	440/456 (96%)	0.57	54 (12%) 5 5	113, 184, 300, 340	0
1	G	440/456 (96%)	0.26	31 (7%) 19 13	118, 167, 247, 287	0
1	H	440/456 (96%)	0.78	80 (18%) 2 1	87, 129, 332, 377	0
1	I	440/456 (96%)	0.01	8 (1%) 71 58	90, 132, 168, 219	0
1	J	440/456 (96%)	-0.12	0 100 100	81, 118, 153, 187	0
1	K	440/456 (96%)	0.03	7 (1%) 74 61	93, 156, 213, 271	0
1	L	440/456 (96%)	0.78	78 (17%) 2 2	130, 211, 375, 404	0
All	All	5280/5472 (96%)	0.19	303 (5%) 27 19	63, 134, 291, 404	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	399	SER	12.9
1	H	321	ASP	10.9
1	F	334	ILE	9.6
1	H	354	GLU	9.0
1	D	353	SER	8.9

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 [i](#)

There are no carbohydrates 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.