wwPDB X-ray Structure Validation Summary Report (i)

Feb 21, 2024 – 01:41 PM EST

PDB ID	:	4QFF
Title	:	Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains, quadruple mutant, P212121 form
Authors	:	Lai, Y.-T.; Yeates, T.O.
Deposited on	:	2014-05-20
Resolution	:	7.81 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 (1)) were used in the production of this report:

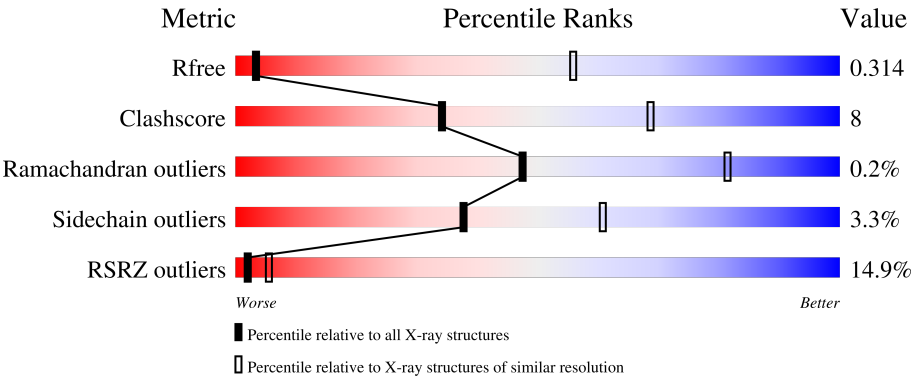
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 7.81 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	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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	456	10% 78% 17%
1	B	456	9% 80% 16%
1	C	456	11% 80% 15%
1	D	456	10% 79% 16%
1	E	456	11% 80% 16%

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Mol	Chain	Length	Quality of chain
1	F	456	9% 80% 16%
1	G	456	25% 80% 15%
1	H	456	9% 78% 17%
1	I	456	15% 79% 17%
1	J	456	13% 80% 15%
1	K	456	25% 75% 20%
1	L	456	26% 80% 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 40512 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 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	B	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	C	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	D	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	E	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	F	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	G	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	H	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	I	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	J	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	K	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			
1	L	441	Total	C	N	O	S	0	0	0
			3376	2151	569	648	8			

There are 228 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	THR	GLN	engineered mutation	UNP P29715
A	51	ALA	TYR	engineered mutation	UNP P29715
A	118	ALA	LYS	engineered mutation	UNP P29715
A	278	ALA	-	linker	UNP P03485
A	279	GLN	-	linker	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLU	-	linker	UNP P03485
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	51	ALA	TYR	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	51	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	284	GLN	-	linker	UNP P03485
C	285	LYS	-	linker	UNP P03485
C	448	LEU	-	expression tag	UNP P03485
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	51	ALA	TYR	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	51	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
E	455	HIS	-	expression tag	UNP P03485
F	24	THR	GLN	engineered mutation	UNP P29715
F	51	ALA	TYR	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	51	ALA	TYR	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

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Chain	Residue	Modelled	Actual	Comment	Reference
G	454	HIS	-	expression tag	UNP P03485
G	455	HIS	-	expression tag	UNP P03485
H	24	THR	GLN	engineered mutation	UNP P29715
H	51	ALA	TYR	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
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	51	ALA	TYR	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	51	ALA	TYR	engineered mutation	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	51	ALA	TYR	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	51	ALA	TYR	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

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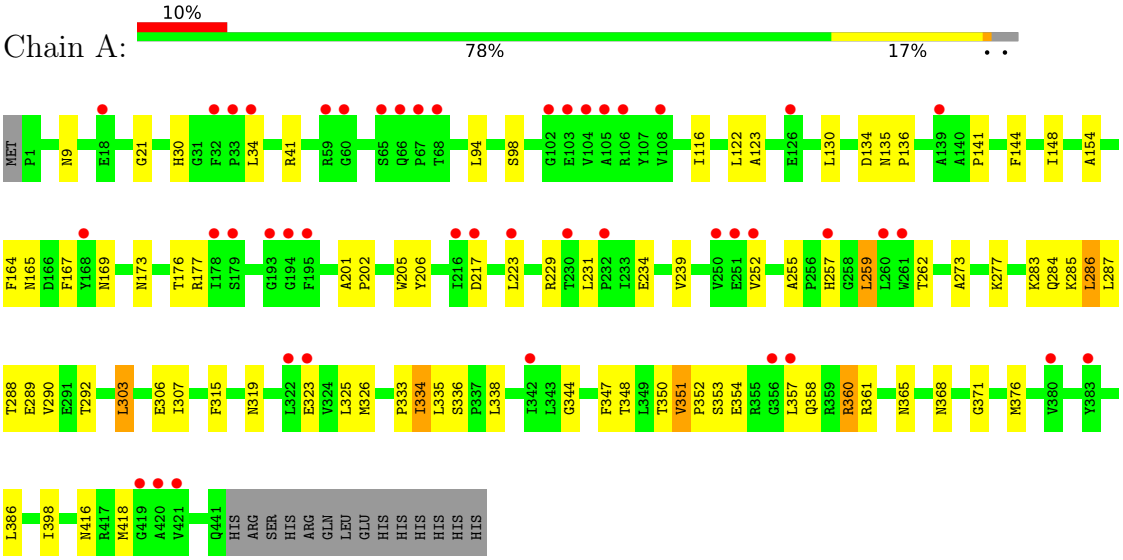
Chain	Residue	Modelled	Actual	Comment	Reference
L	281	ALA	-	linker	UNP P03485
L	282	GLN	-	linker	UNP P03485
L	283	LYS	-	linker	UNP P03485
L	284	GLN	-	linker	UNP P03485
L	285	LYS	-	linker	UNP P03485
L	448	LEU	-	expression tag	UNP P03485
L	449	GLU	-	expression tag	UNP P03485
L	450	HIS	-	expression tag	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
L	455	HIS	-	expression tag	UNP P03485

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.

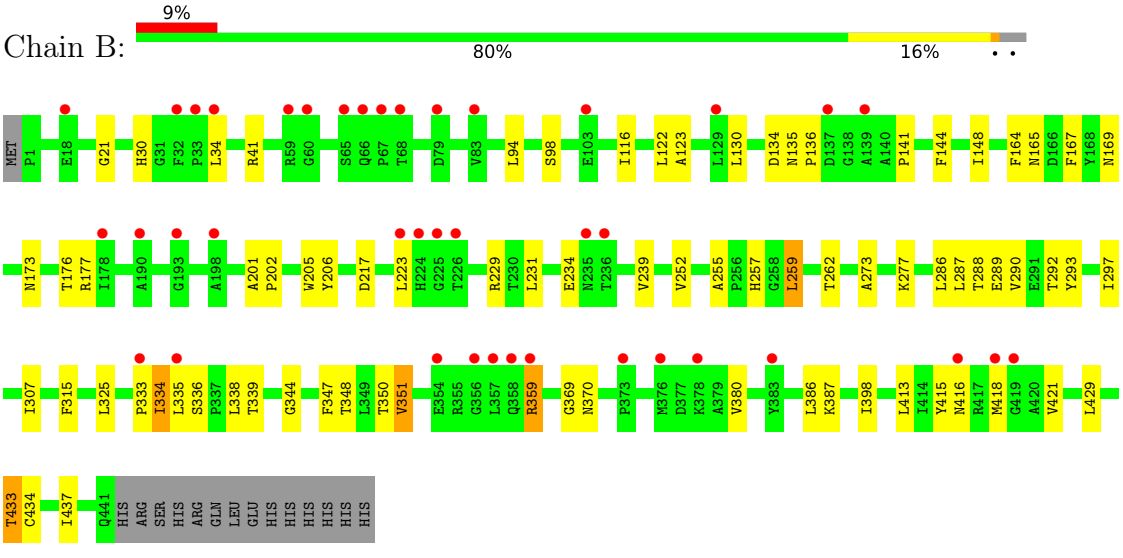
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain A:



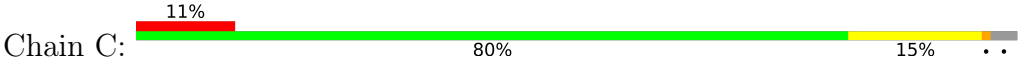
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

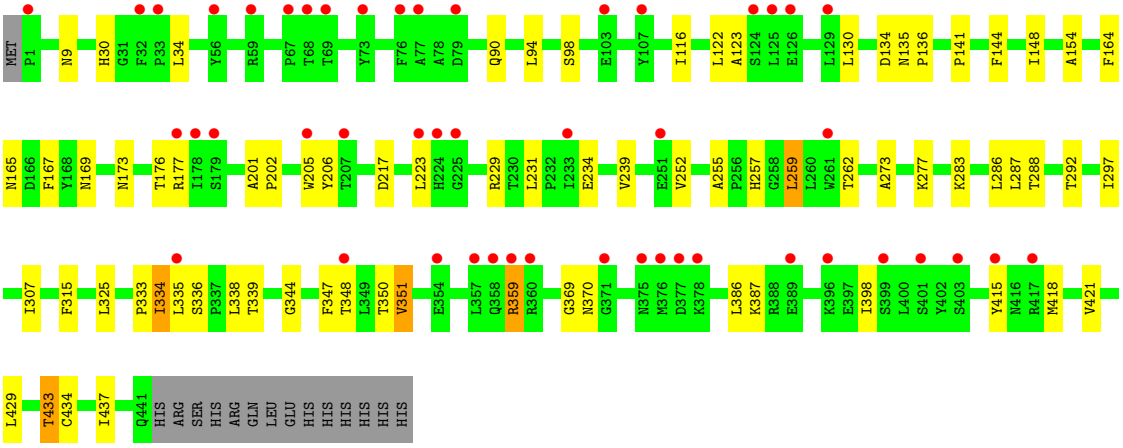
Chain B:



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

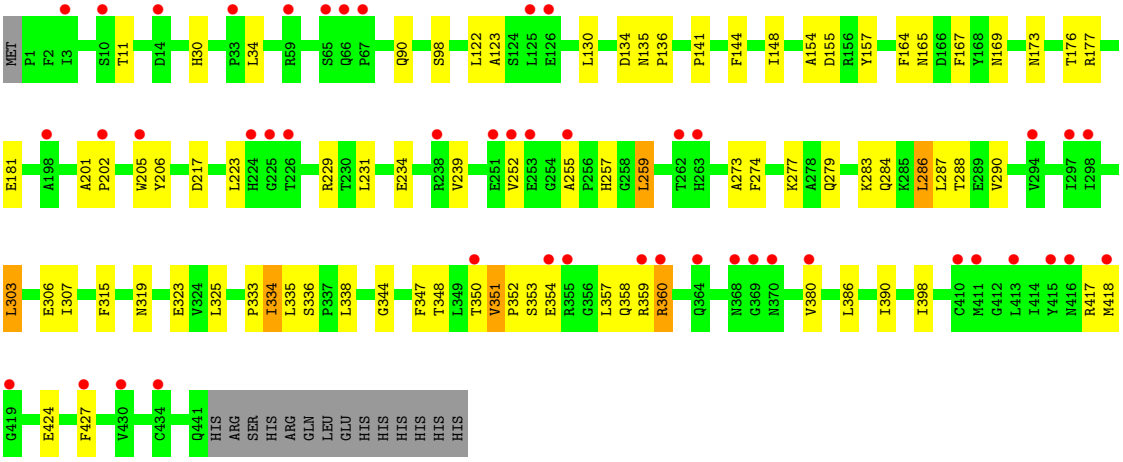
Chain C:





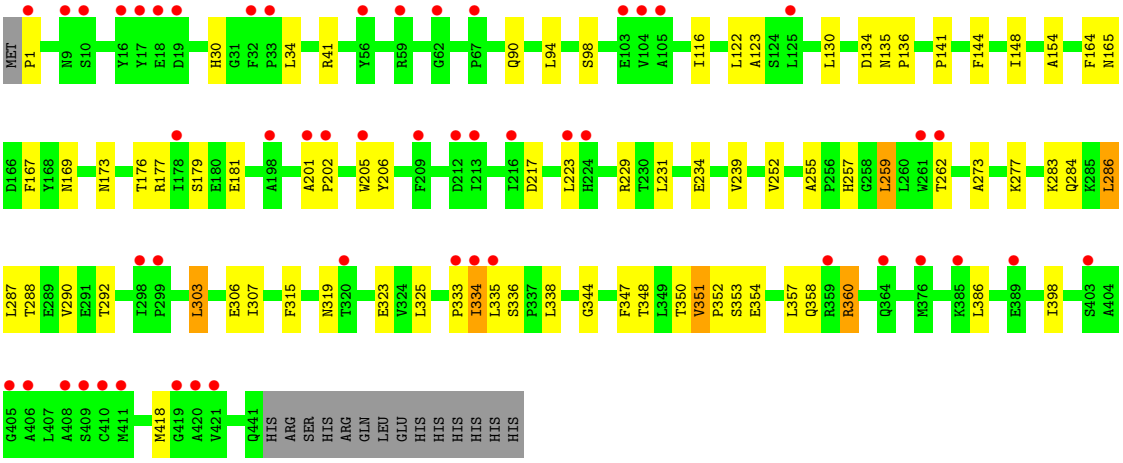
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain D:



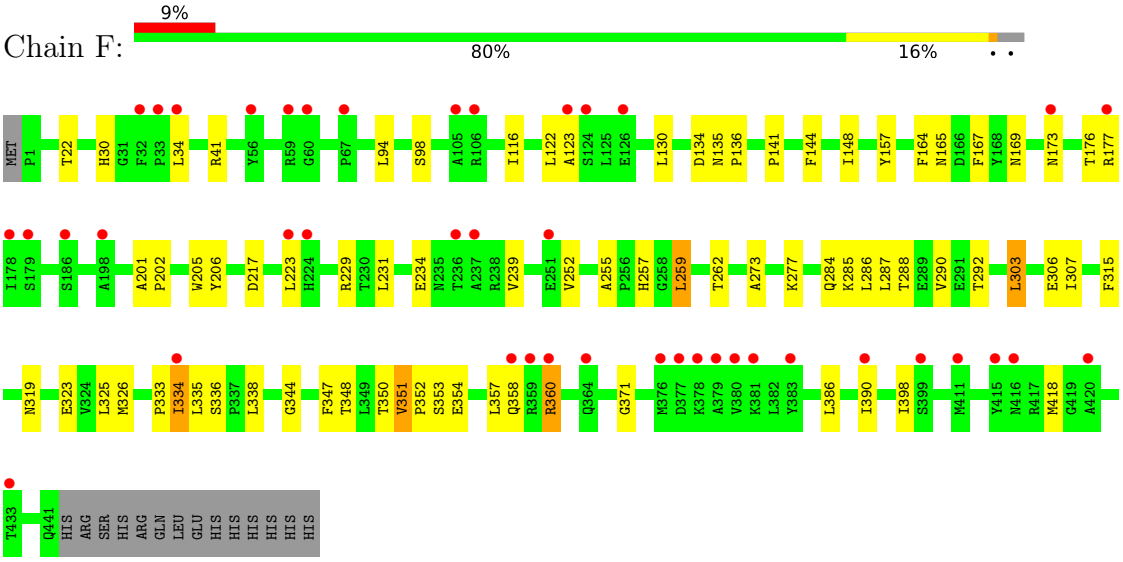
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain E:



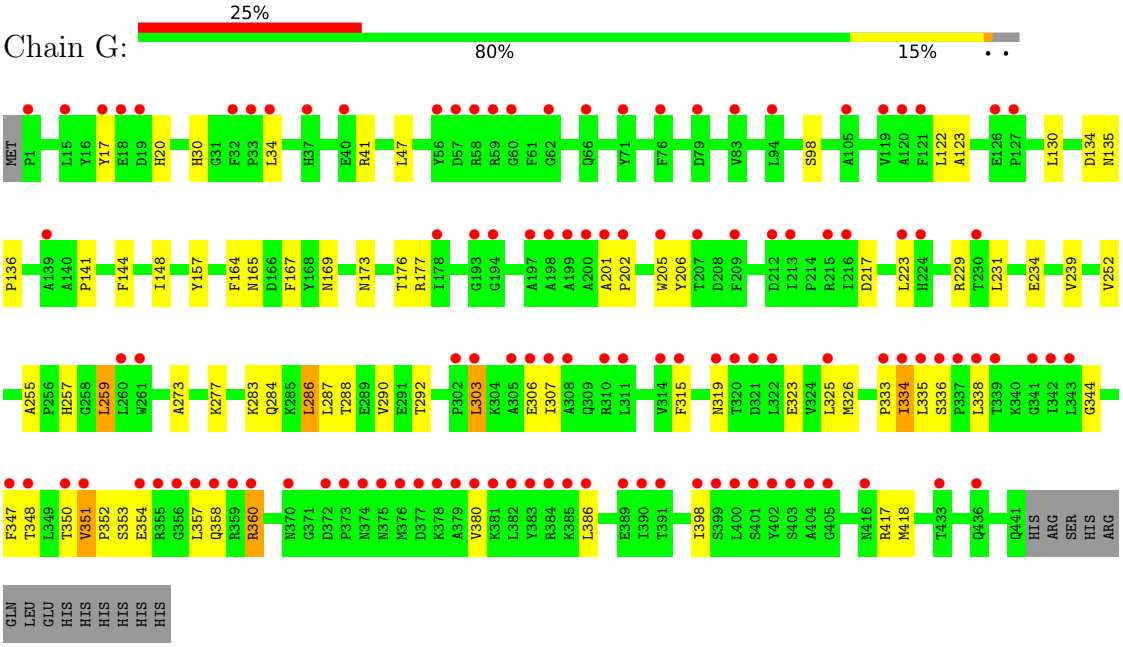
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain F:



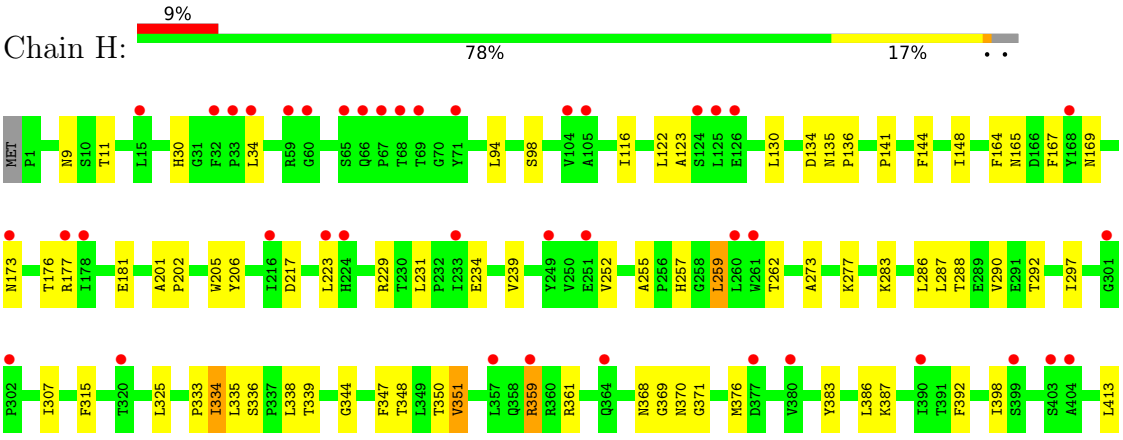
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

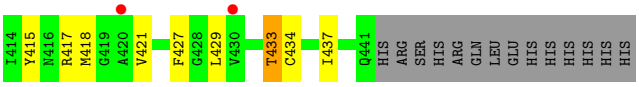
Chain G:



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

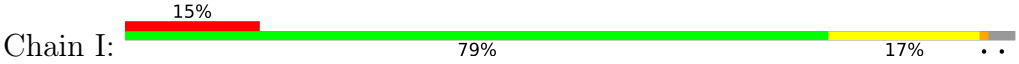
Chain H:

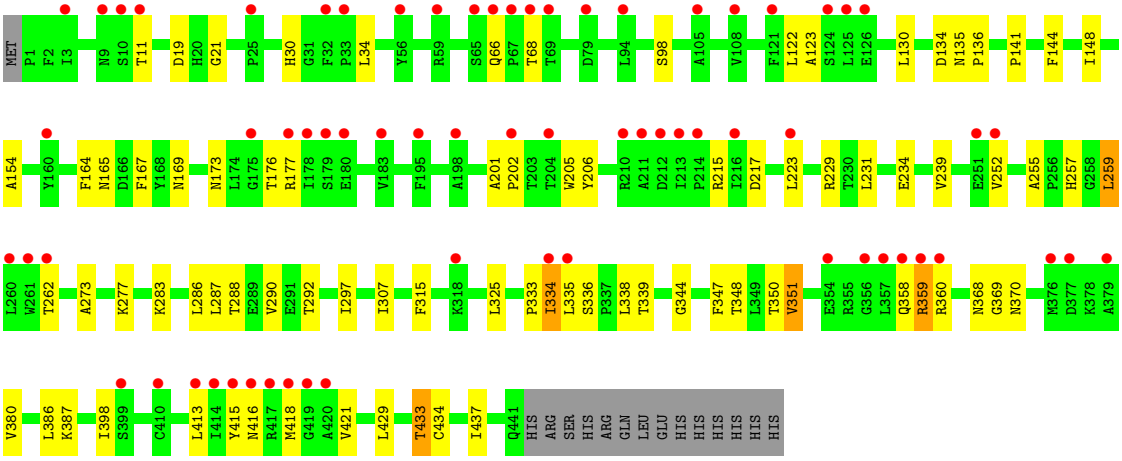




• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

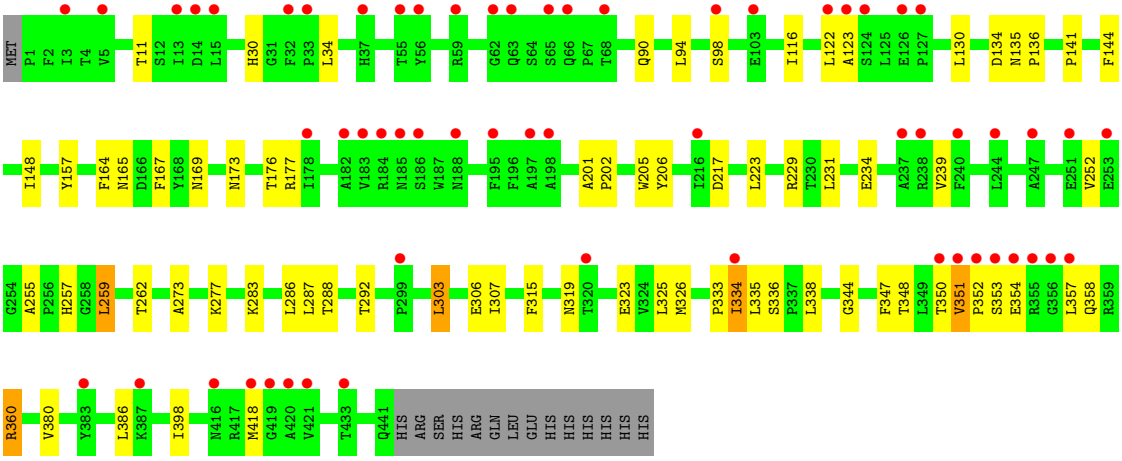
Chain I:





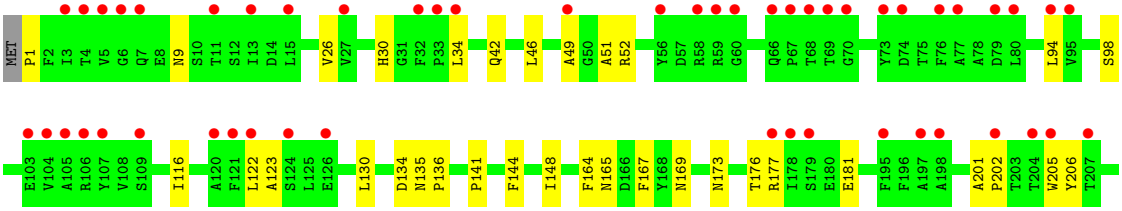
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

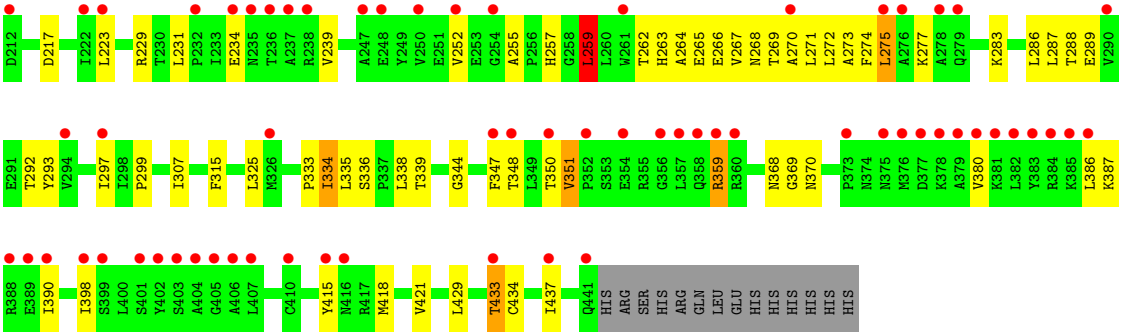
Chain J:



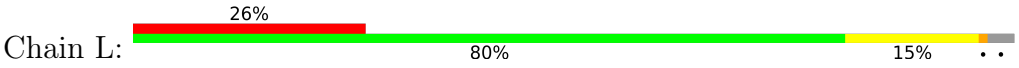
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

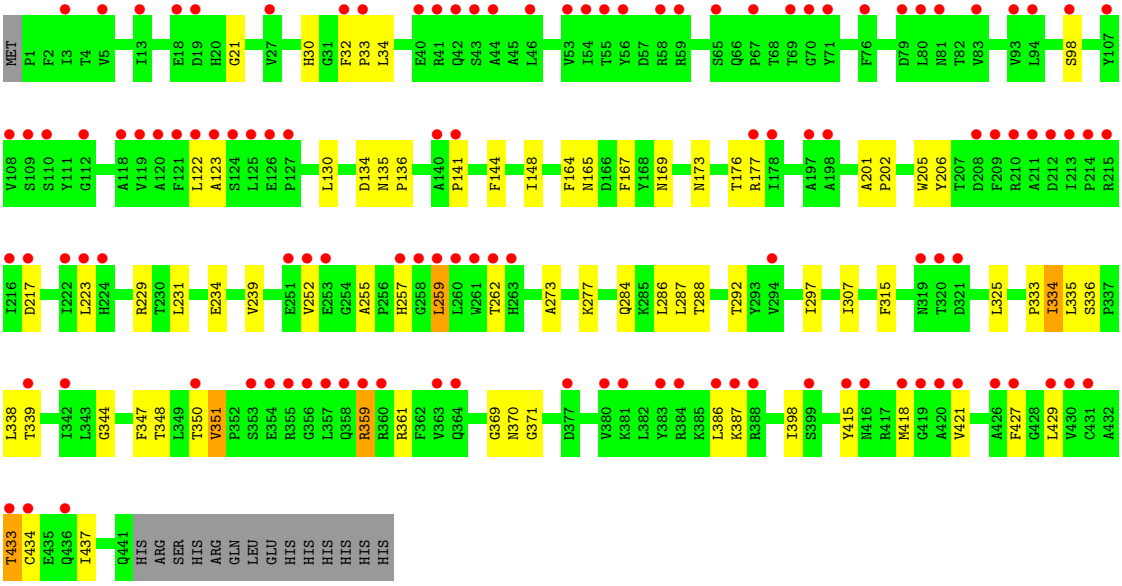
Chain K:





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





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	155.50Å 156.52Å 325.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.27 – 7.81 91.27 – 7.81	Depositor EDS
% Data completeness (in resolution range)	92.1 (91.27-7.81) 92.2 (91.27-7.81)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 7.43Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.288 , 0.339 0.278 , 0.314	Depositor DCC
R_{free} test set	437 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	250.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 295.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.057 for k,h,-l	Xtriage
F_o,F_c correlation	0.72	EDS
Total number of atoms	40512	wwPDB-VP
Average B, all atoms (Å^2)	244.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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

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	0.50	0/3452	0.75	2/4702 (0.0%)
1	B	0.53	0/3452	0.78	2/4702 (0.0%)
1	C	0.51	0/3452	0.77	2/4702 (0.0%)
1	D	0.51	0/3452	0.76	2/4702 (0.0%)
1	E	0.50	0/3452	0.75	2/4702 (0.0%)
1	F	0.51	0/3452	0.76	2/4702 (0.0%)
1	G	0.51	0/3452	0.76	2/4702 (0.0%)
1	H	0.51	0/3452	0.77	2/4702 (0.0%)
1	I	0.52	0/3452	0.78	2/4702 (0.0%)
1	J	0.51	0/3452	0.75	2/4702 (0.0%)
1	K	0.53	0/3452	0.77	2/4702 (0.0%)
1	L	0.52	0/3452	0.78	2/4702 (0.0%)
All	All	0.51	0/41424	0.76	24/56424 (0.0%)

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	J	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	G	259	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	259	LEU	CA-CB-CG	5.31	127.52	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	3376	0	3286	69	0
1	B	3376	0	3286	46	0
1	C	3376	0	3286	44	0
1	D	3376	0	3286	86	0
1	E	3376	0	3286	54	0
1	F	3376	0	3286	53	0
1	G	3376	0	3286	54	0
1	H	3376	0	3286	73	0
1	I	3376	0	3286	67	0
1	J	3376	0	3286	48	0
1	K	3376	0	3286	83	0
1	L	3376	0	3286	61	0
All	All	40512	0	39432	671	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 671 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:D:418:MET:SD	1:I:418:MET:SD	2.38	1.21
1:K:264:ALA:O	1:K:268:ASN:HB2	1.39	1.19
1:L:284:GLN:HA	1:L:287:LEU:CD2	1.73	1.18
1:D:287:LEU:HD13	1:D:315:PHE:CD1	1.77	1.18
1:L:284:GLN:O	1:L:287:LEU:HG	1.41	1.16

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	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47	81
1	B	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47	81
1	C	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47	81
1	D	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47	81
1	E	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47	81
1	F	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47	81
1	G	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47	81
1	H	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47	81
1	I	439/456 (96%)	425 (97%)	13 (3%)	1 (0%)	47	81
1	J	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47	81
1	K	439/456 (96%)	424 (97%)	14 (3%)	1 (0%)	47	81
1	L	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47	81
All	All	5268/5472 (96%)	5118 (97%)	138 (3%)	12 (0%)	47	81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	ILE
1	B	334	ILE
1	D	334	ILE
1	F	334	ILE
1	G	334	ILE

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	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	B	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	C	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	D	348/369 (94%)	336 (97%)	12 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	F	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	G	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	H	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	I	348/369 (94%)	337 (97%)	11 (3%)	39	61
1	J	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	K	348/369 (94%)	336 (97%)	12 (3%)	37	60
1	L	348/369 (94%)	337 (97%)	11 (3%)	39	61
All	All	4176/4428 (94%)	4037 (97%)	139 (3%)	38	61

5 of 139 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	353	SER
1	K	239	VAL
1	L	234	GLU
1	E	217	ASP
1	E	165	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	188	ASN
1	K	188	ASN
1	I	375	ASN
1	J	188	ASN
1	L	90	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	441/456 (96%)	0.86	45 (10%) 6 10	120, 209, 300, 386	0
1	B	441/456 (96%)	0.83	40 (9%) 9 11	93, 191, 267, 346	0
1	C	441/456 (96%)	0.88	48 (10%) 5 9	114, 196, 263, 325	0
1	D	441/456 (96%)	0.84	46 (10%) 6 9	110, 223, 370, 443	0
1	E	441/456 (96%)	0.86	51 (11%) 4 8	122, 196, 275, 336	0
1	F	441/456 (96%)	0.77	42 (9%) 8 11	117, 208, 305, 393	0
1	G	441/456 (96%)	1.30	116 (26%) 0 2	142, 284, 420, 498	0
1	H	441/456 (96%)	0.86	43 (9%) 7 10	130, 228, 310, 365	0
1	I	441/456 (96%)	0.96	67 (15%) 2 5	179, 269, 364, 453	0
1	J	441/456 (96%)	0.99	60 (13%) 3 6	127, 225, 323, 448	0
1	K	441/456 (96%)	1.39	116 (26%) 0 2	194, 329, 412, 474	0
1	L	441/456 (96%)	1.36	117 (26%) 0 2	179, 305, 412, 500	0
All	All	5292/5472 (96%)	0.99	791 (14%) 2 5	93, 233, 368, 500	0

The worst 5 of 791 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	GLN	7.3
1	L	120	ALA	7.0
1	K	359	ARG	6.9
1	L	119	VAL	6.7
1	A	33	PRO	6.5

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 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.