



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:45 PM GMT

PDB ID : 4D9J
Title : Structure of a 16 nm protein cage designed by fusing symmetric oligomeric domains
Authors : Lai, Y.-T.; Cascio, D.; Yeates, T.O.
Deposited on : 2012-01-11
Resolution : 3.92 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/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

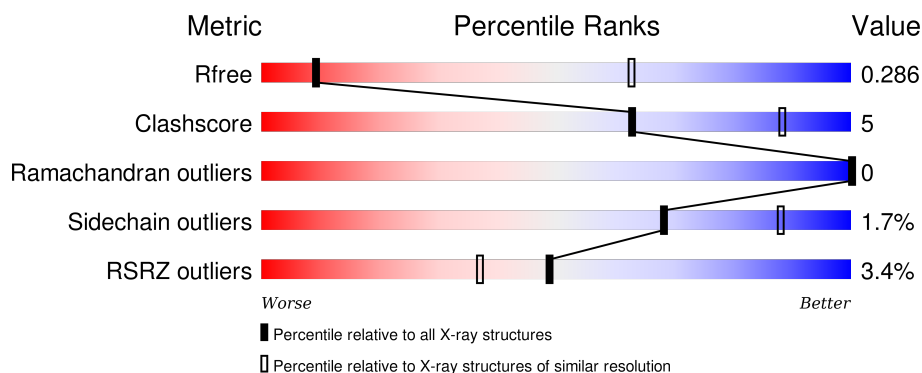
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.92 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	1047 (4.32-3.52)
Clashscore	102246	1008 (4.26-3.58)
Ramachandran outliers	100387	1044 (4.30-3.54)
Sidechain outliers	100360	1035 (4.30-3.54)
RSRZ outliers	91569	1002 (4.30-3.54)

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>7%</div> <div>80% 15% . .</div> </div>
1	B	456	<div> <div>4%</div> <div>81% 15% .</div> </div>
1	C	456	<div> <div>%</div> <div>82% 13% .</div> </div>
1	D	456	<div> <div>7%</div> <div>83% 13% . .</div> </div>
1	E	456	<div> <div>3%</div> <div>81% 15% .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	456	<div><div>%</div><div><div></div><div>82%</div><div>13%</div><div></div></div><div></div></div>
1	G	456	<div><div>4%</div><div><div></div><div>80%</div><div>16%</div><div></div></div><div></div></div>
1	H	456	<div><div>3%</div><div><div></div><div>81%</div><div>14%</div><div></div></div><div></div></div>
1	I	456	<div><div></div><div><div></div><div>85%</div><div>10%</div><div></div></div><div></div></div>
1	J	456	<div><div>3%</div><div><div></div><div>79%</div><div>16%</div><div></div></div><div></div></div>
1	K	456	<div><div></div><div><div></div><div>84%</div><div>12%</div><div></div></div><div></div></div>
1	L	456	<div><div>6%</div><div><div></div><div>83%</div><div>12%</div><div></div></div><div></div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 40596 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 Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	B	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	C	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	D	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	E	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	F	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	G	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	H	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	I	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	J	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	K	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			
1	L	438	Total	C	N	O	S	0	0	0
			3383	2161	569	645	8			

There are 216 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	VAL	GLN	CONFLICT	UNP P29715
A	118	ALA	LYS	CONFLICT	UNP P29715
A	278	ALA	-	LINKER	UNP P29715
A	279	LEU	-	LINKER	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLU	-	LINKER	UNP P29715
A	281	ALA	-	LINKER	UNP P29715
A	282	GLN	-	LINKER	UNP P29715
A	283	LYS	-	LINKER	UNP P29715
A	284	GLN	-	LINKER	UNP P29715
A	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
B	118	ALA	LYS	CONFLICT	UNP P29715
B	278	ALA	-	LINKER	UNP P29715
B	279	LEU	-	LINKER	UNP P29715
B	280	GLU	-	LINKER	UNP P29715
B	281	ALA	-	LINKER	UNP P29715
B	282	GLN	-	LINKER	UNP P29715
B	283	LYS	-	LINKER	UNP P29715
B	284	GLN	-	LINKER	UNP P29715
B	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
C	118	ALA	LYS	CONFLICT	UNP P29715
C	278	ALA	-	LINKER	UNP P29715
C	279	LEU	-	LINKER	UNP P29715
C	280	GLU	-	LINKER	UNP P29715
C	281	ALA	-	LINKER	UNP P29715
C	282	GLN	-	LINKER	UNP P29715
C	283	LYS	-	LINKER	UNP P29715
C	284	GLN	-	LINKER	UNP P29715
C	285	LYS	-	LINKER	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
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	VAL	GLN	CONFLICT	UNP P29715
D	118	ALA	LYS	CONFLICT	UNP P29715
D	278	ALA	-	LINKER	UNP P29715
D	279	LEU	-	LINKER	UNP P29715
D	280	GLU	-	LINKER	UNP P29715
D	281	ALA	-	LINKER	UNP P29715
D	282	GLN	-	LINKER	UNP P29715
D	283	LYS	-	LINKER	UNP P29715
D	284	GLN	-	LINKER	UNP P29715
D	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
E	118	ALA	LYS	CONFLICT	UNP P29715
E	278	ALA	-	LINKER	UNP P29715
E	279	LEU	-	LINKER	UNP P29715
E	280	GLU	-	LINKER	UNP P29715
E	281	ALA	-	LINKER	UNP P29715
E	282	GLN	-	LINKER	UNP P29715
E	283	LYS	-	LINKER	UNP P29715
E	284	GLN	-	LINKER	UNP P29715
E	285	LYS	-	LINKER	UNP P29715
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

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Chain	Residue	Modelled	Actual	Comment	Reference
E	454	HIS	-	EXPRESSION TAG	UNP P03485
E	455	HIS	-	EXPRESSION TAG	UNP P03485
F	24	VAL	GLN	CONFLICT	UNP P29715
F	118	ALA	LYS	CONFLICT	UNP P29715
F	278	ALA	-	LINKER	UNP P29715
F	279	LEU	-	LINKER	UNP P29715
F	280	GLU	-	LINKER	UNP P29715
F	281	ALA	-	LINKER	UNP P29715
F	282	GLN	-	LINKER	UNP P29715
F	283	LYS	-	LINKER	UNP P29715
F	284	GLN	-	LINKER	UNP P29715
F	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
G	118	ALA	LYS	CONFLICT	UNP P29715
G	278	ALA	-	LINKER	UNP P29715
G	279	LEU	-	LINKER	UNP P29715
G	280	GLU	-	LINKER	UNP P29715
G	281	ALA	-	LINKER	UNP P29715
G	282	GLN	-	LINKER	UNP P29715
G	283	LYS	-	LINKER	UNP P29715
G	284	GLN	-	LINKER	UNP P29715
G	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
H	118	ALA	LYS	CONFLICT	UNP P29715
H	278	ALA	-	LINKER	UNP P29715
H	279	LEU	-	LINKER	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
H	280	GLU	-	LINKER	UNP P29715
H	281	ALA	-	LINKER	UNP P29715
H	282	GLN	-	LINKER	UNP P29715
H	283	LYS	-	LINKER	UNP P29715
H	284	GLN	-	LINKER	UNP P29715
H	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
I	118	ALA	LYS	CONFLICT	UNP P29715
I	278	ALA	-	LINKER	UNP P29715
I	279	LEU	-	LINKER	UNP P29715
I	280	GLU	-	LINKER	UNP P29715
I	281	ALA	-	LINKER	UNP P29715
I	282	GLN	-	LINKER	UNP P29715
I	283	LYS	-	LINKER	UNP P29715
I	284	GLN	-	LINKER	UNP P29715
I	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
J	118	ALA	LYS	CONFLICT	UNP P29715
J	278	ALA	-	LINKER	UNP P29715
J	279	LEU	-	LINKER	UNP P29715
J	280	GLU	-	LINKER	UNP P29715
J	281	ALA	-	LINKER	UNP P29715
J	282	GLN	-	LINKER	UNP P29715
J	283	LYS	-	LINKER	UNP P29715
J	284	GLN	-	LINKER	UNP P29715
J	285	LYS	-	LINKER	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
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	VAL	GLN	CONFLICT	UNP P29715
K	118	ALA	LYS	CONFLICT	UNP P29715
K	278	ALA	-	LINKER	UNP P29715
K	279	LEU	-	LINKER	UNP P29715
K	280	GLU	-	LINKER	UNP P29715
K	281	ALA	-	LINKER	UNP P29715
K	282	GLN	-	LINKER	UNP P29715
K	283	LYS	-	LINKER	UNP P29715
K	284	GLN	-	LINKER	UNP P29715
K	285	LYS	-	LINKER	UNP P29715
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	VAL	GLN	CONFLICT	UNP P29715
L	118	ALA	LYS	CONFLICT	UNP P29715
L	278	ALA	-	LINKER	UNP P29715
L	279	LEU	-	LINKER	UNP P29715
L	280	GLU	-	LINKER	UNP P29715
L	281	ALA	-	LINKER	UNP P29715
L	282	GLN	-	LINKER	UNP P29715
L	283	LYS	-	LINKER	UNP P29715
L	284	GLN	-	LINKER	UNP P29715
L	285	LYS	-	LINKER	UNP P29715
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

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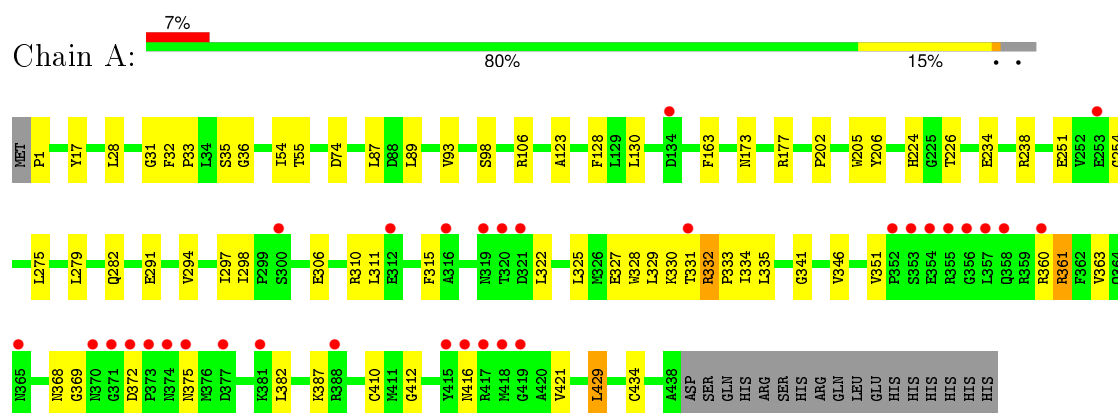
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Chain	Residue	Modelled	Actual	Comment	Reference
L	454	HIS	-	EXPRESSION TAG	UNP P03485
L	455	HIS	-	EXPRESSION TAG	UNP P03485

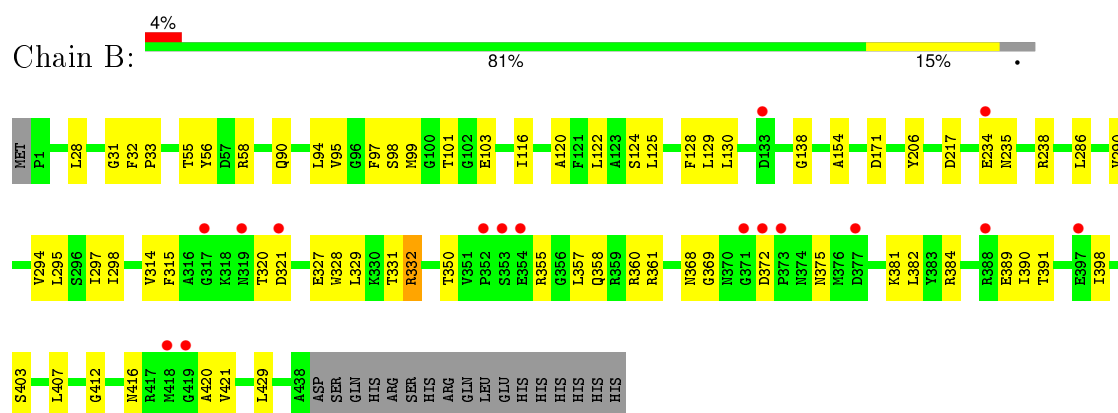
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

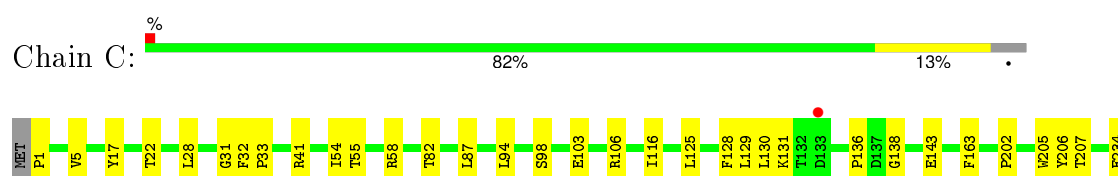
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

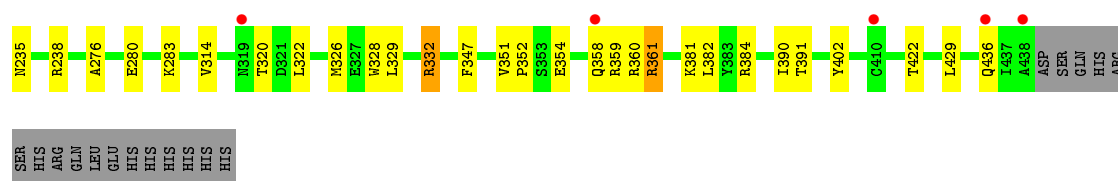


- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

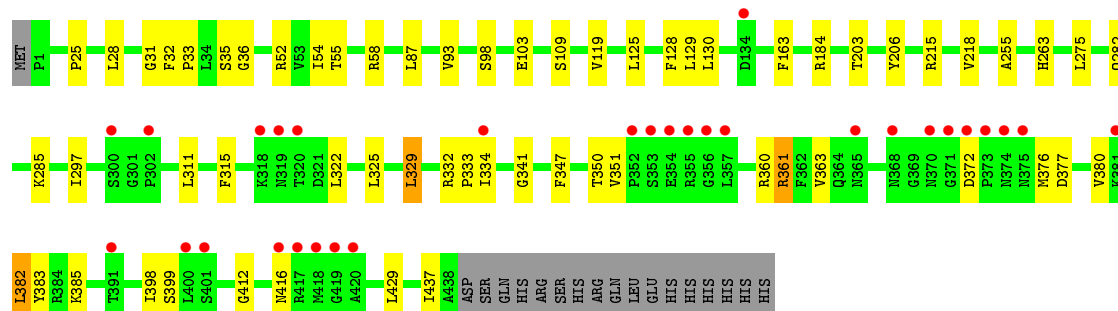
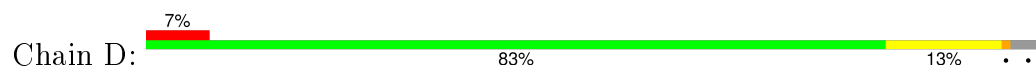


- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1

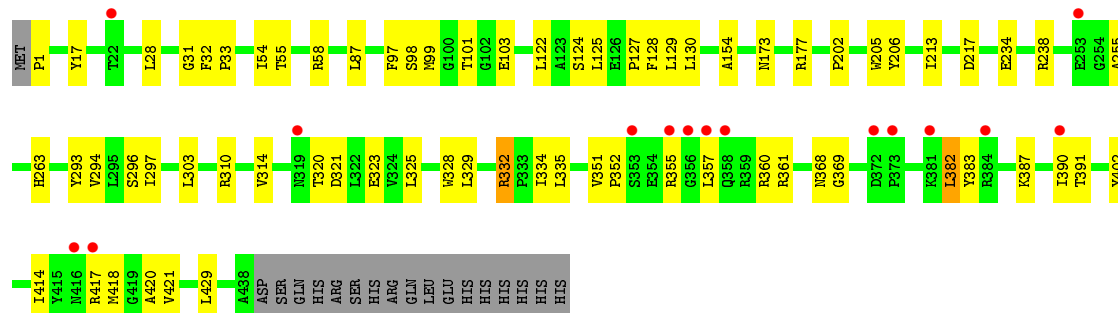
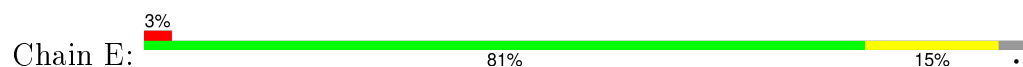




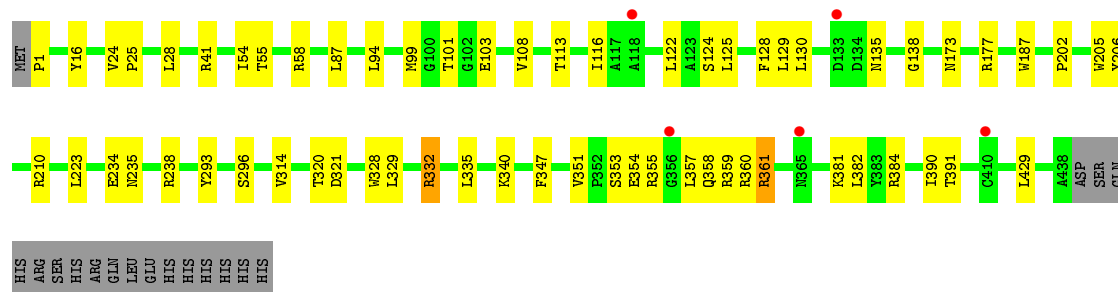
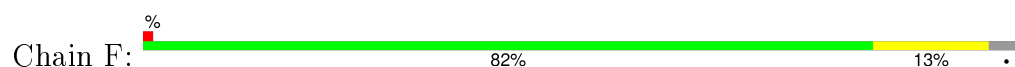
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



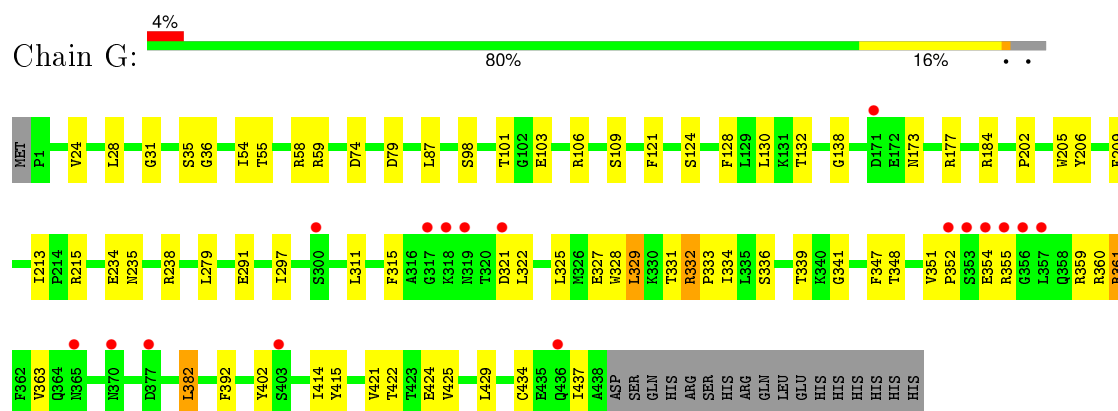
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



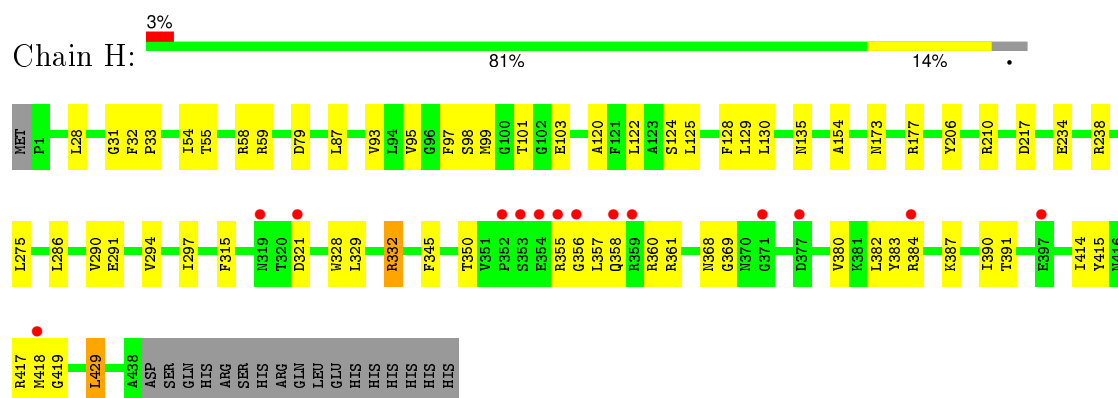
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



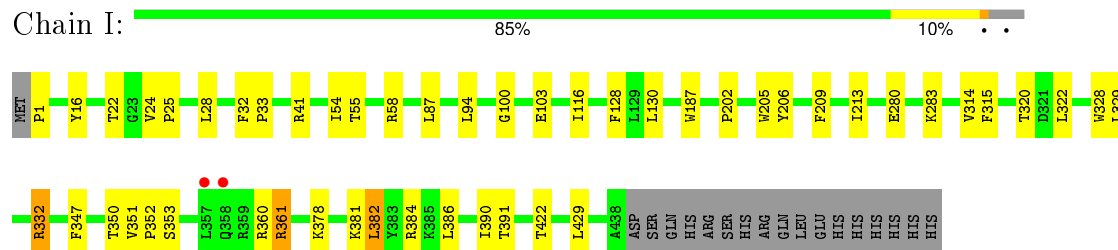
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



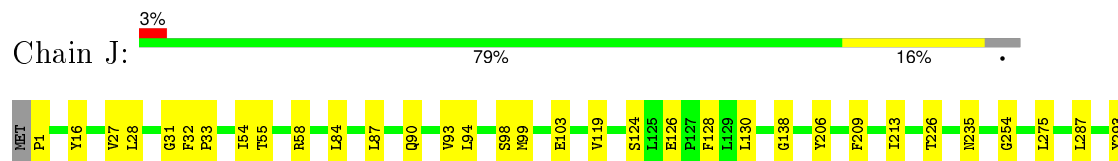
- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



- Molecule 1: Designed 16nm tetrahedral protein cage containing Non-haem bromoperoxidase BPO-A2 and Matrix protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	122.70Å 187.41Å 283.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 3.92 19.89 – 3.92	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.89-3.92) 99.1 (19.89-3.92)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.99 (at 3.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.282 , 0.294 0.272 , 0.286	Depositor DCC
R_{free} test set	2923 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	121.6	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 1.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 58471 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	40596	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% 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	0.22	0/3460	0.43	0/4709
1	B	0.23	0/3460	0.43	0/4709
1	C	0.22	0/3460	0.41	0/4709
1	D	0.22	0/3460	0.45	0/4709
1	E	0.22	0/3460	0.42	0/4709
1	F	0.22	0/3460	0.41	0/4709
1	G	0.22	0/3460	0.42	0/4709
1	H	0.22	0/3460	0.42	0/4709
1	I	0.22	0/3460	0.40	0/4709
1	J	0.22	0/3460	0.42	0/4709
1	K	0.22	0/3460	0.40	0/4709
1	L	0.26	0/3460	0.49	2/4709 (0.0%)
All	All	0.22	0/41520	0.42	2/56508 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	303	LEU	CB-CG-CD2	5.24	119.92	111.00
1	L	279	LEU	CA-CB-CG	5.19	127.25	115.30

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	3383	0	3322	43	0
1	B	3383	0	3322	36	0
1	C	3383	0	3322	34	0
1	D	3383	0	3322	34	0
1	E	3383	0	3322	39	0
1	F	3383	0	3322	35	0
1	G	3383	0	3322	40	0
1	H	3383	0	3322	41	0
1	I	3383	0	3322	30	0
1	J	3383	0	3322	43	0
1	K	3383	0	3322	27	0
1	L	3383	0	3322	38	0
All	All	40596	0	39864	427	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 5.

All (427) 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:L:303:LEU:HD22	1:L:328:TRP:CH2	2.16	0.80
1:A:291:GLU:HB2	1:A:315:PHE:HE2	1.49	0.77
1:F:130:LEU:HB2	1:F:206:TYR:HB2	1.70	0.73
1:A:322:LEU:HD11	1:A:351:VAL:HG21	1.71	0.70
1:G:74:ASP:OD1	1:G:106:ARG:NH1	2.23	0.70
1:I:28:LEU:HB2	1:I:55:THR:HG22	1.74	0.70
1:A:333:PRO:HG2	1:A:334:ILE:HD12	1.74	0.70
1:A:54:ILE:HD13	1:A:87:LEU:HD23	1.73	0.70
1:E:328:TRP:O	1:E:332:ARG:NH1	2.25	0.69
1:L:138:GLY:O	1:L:235:ASN:ND2	2.27	0.68
1:C:358:GLN:OE1	1:F:360:ARG:NH1	2.26	0.68
1:G:322:LEU:HD11	1:G:351:VAL:HG21	1.76	0.68
1:L:329:LEU:O	1:L:340:LYS:NZ	2.27	0.68
1:E:130:LEU:HB2	1:E:206:TYR:HB2	1.75	0.68
1:J:31:GLY:HA3	1:J:98:SER:HB3	1.76	0.67
1:F:355:ARG:HD2	1:F:357:LEU:HD12	1.74	0.67
1:G:130:LEU:HB2	1:G:206:TYR:HB2	1.77	0.67
1:H:321:ASP:HB3	1:H:355:ARG:HH21	1.60	0.67
1:H:417:ARG:NH1	1:J:416:ASN:O	2.28	0.67
1:D:380:VAL:HA	1:D:383:TYR:HB3	1.74	0.67
1:I:328:TRP:O	1:I:332:ARG:NH1	2.28	0.66
1:I:22:THR:HG21	1:I:422:THR:HG21	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ALA:O	1:F:41:ARG:NH2	2.29	0.66
1:K:360:ARG:HH11	1:K:361:ARG:HH12	1.42	0.66
1:B:412:GLY:O	1:B:416:ASN:ND2	2.28	0.65
1:C:328:TRP:O	1:C:332:ARG:NH1	2.30	0.64
1:J:328:TRP:O	1:J:332:ARG:NH1	2.30	0.64
1:H:31:GLY:HA3	1:H:98:SER:HB3	1.80	0.64
1:H:328:TRP:O	1:H:332:ARG:NH1	2.30	0.64
1:F:314:VAL:HG22	1:F:320:THR:HG21	1.80	0.64
1:F:28:LEU:HB2	1:F:55:THR:HG22	1.80	0.64
1:G:138:GLY:O	1:G:235:ASN:ND2	2.31	0.63
1:L:303:LEU:HD22	1:L:328:TRP:HH2	1.61	0.63
1:L:131:LYS:NZ	1:L:136:PRO:O	2.31	0.63
1:E:323:GLU:HB2	1:E:355:ARG:NH1	2.12	0.63
1:G:31:GLY:HA3	1:G:98:SER:HB3	1.81	0.63
1:E:58:ARG:NE	1:E:103:GLU:OE2	2.29	0.63
1:D:28:LEU:HB2	1:D:55:THR:HG22	1.79	0.63
1:K:130:LEU:HB2	1:K:206:TYR:HB2	1.81	0.62
1:B:58:ARG:NE	1:B:103:GLU:OE2	2.29	0.62
1:E:54:ILE:HD13	1:E:87:LEU:HD23	1.81	0.62
1:H:28:LEU:HB2	1:H:55:THR:HG22	1.82	0.61
1:F:381:LYS:HD3	1:F:384:ARG:HH12	1.65	0.61
1:H:130:LEU:HB2	1:H:206:TYR:HB2	1.81	0.61
1:B:314:VAL:HG22	1:B:320:THR:HG21	1.82	0.61
1:B:90:GLN:N	1:B:90:GLN:OE1	2.33	0.61
1:J:130:LEU:HB2	1:J:206:TYR:HB2	1.82	0.60
1:B:328:TRP:O	1:B:332:ARG:NH1	2.35	0.60
1:F:328:TRP:O	1:F:332:ARG:NH1	2.34	0.60
1:B:28:LEU:HB2	1:B:55:THR:HG22	1.82	0.60
1:A:412:GLY:O	1:A:416:ASN:ND2	2.34	0.60
1:A:368:ASN:OD1	1:A:369:GLY:N	2.34	0.59
1:J:28:LEU:HB2	1:J:55:THR:HG22	1.83	0.59
1:A:35:SER:OG	1:A:36:GLY:N	2.34	0.59
1:E:368:ASN:OD1	1:E:369:GLY:N	2.36	0.59
1:L:54:ILE:HD13	1:L:87:LEU:HD23	1.84	0.59
1:H:357:LEU:HA	1:J:357:LEU:HA	1.83	0.59
1:D:297:ILE:HD12	1:D:437:ILE:HB	1.84	0.59
1:C:381:LYS:HD3	1:C:384:ARG:HH12	1.67	0.59
1:K:28:LEU:HB2	1:K:55:THR:HG22	1.84	0.59
1:D:377:ASP:HA	1:D:380:VAL:HG22	1.83	0.59
1:D:35:SER:OG	1:D:36:GLY:N	2.35	0.59
1:K:54:ILE:HD13	1:K:87:LEU:HD23	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:345:PHE:HD2	1:L:415:TYR:HB2	1.68	0.58
1:D:322:LEU:HD11	1:D:351:VAL:HG11	1.85	0.58
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.84	0.58
1:C:58:ARG:NE	1:C:103:GLU:OE2	2.29	0.58
1:B:154:ALA:O	1:C:41:ARG:NH2	2.37	0.58
1:A:387:LYS:HG3	1:A:421:VAL:HG12	1.84	0.58
1:K:297:ILE:HD12	1:K:437:ILE:HB	1.86	0.58
1:E:31:GLY:HA3	1:E:98:SER:HB3	1.86	0.58
1:I:315:PHE:HE1	1:I:350:THR:HG21	1.68	0.58
1:L:58:ARG:NE	1:L:103:GLU:OE2	2.34	0.57
1:C:131:LYS:NZ	1:C:136:PRO:O	2.38	0.57
1:A:372:ASP:HB3	1:A:375:ASN:HB3	1.86	0.57
1:G:333:PRO:HG2	1:G:334:ILE:HD12	1.86	0.57
1:H:368:ASN:OD1	1:H:369:GLY:N	2.37	0.57
1:B:368:ASN:OD1	1:B:369:GLY:N	2.37	0.57
1:A:31:GLY:HA3	1:A:98:SER:HB3	1.85	0.57
1:I:314:VAL:HG22	1:I:320:THR:HG21	1.87	0.57
1:L:314:VAL:HG11	1:L:350:THR:HB	1.86	0.56
1:K:35:SER:OG	1:K:36:GLY:N	2.38	0.56
1:A:28:LEU:HB2	1:A:55:THR:HG22	1.87	0.56
1:G:291:GLU:HB2	1:G:315:PHE:HE2	1.70	0.56
1:L:297:ILE:HD12	1:L:437:ILE:HB	1.87	0.56
1:K:328:TRP:O	1:K:332:ARG:NH1	2.36	0.56
1:D:31:GLY:HA3	1:D:98:SER:HB3	1.87	0.56
1:J:390:ILE:HG13	1:J:391:THR:HG23	1.88	0.56
1:G:35:SER:OG	1:G:36:GLY:N	2.39	0.56
1:D:333:PRO:HG2	1:D:334:ILE:HD12	1.88	0.56
1:H:154:ALA:O	1:I:41:ARG:NH2	2.39	0.55
1:E:390:ILE:HG13	1:E:391:THR:HG23	1.88	0.55
1:K:74:ASP:OD1	1:K:106:ARG:NH1	2.38	0.55
1:E:321:ASP:HB2	1:E:355:ARG:NH1	2.20	0.55
1:L:402:TYR:O	1:L:436:GLN:NE2	2.39	0.55
1:J:93:VAL:HG11	1:J:275:LEU:HD21	1.88	0.55
1:A:226:THR:OG1	1:A:254:GLY:N	2.34	0.55
1:A:360:ARG:NH2	1:A:361:ARG:HH12	2.04	0.55
1:I:360:ARG:HH22	1:I:361:ARG:HE	1.55	0.55
1:L:280:GLU:OE2	1:L:284:GLN:NE2	2.40	0.55
1:H:93:VAL:HG11	1:H:275:LEU:HD21	1.89	0.55
1:L:52:ARG:HD2	1:L:390:ILE:HG21	1.89	0.55
1:B:138:GLY:O	1:B:235:ASN:ND2	2.40	0.54
1:I:130:LEU:HB2	1:I:206:TYR:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:LEU:HB2	1:C:55:THR:HG22	1.88	0.54
1:J:368:ASN:OD1	1:J:369:GLY:N	2.40	0.54
1:L:28:LEU:HB2	1:L:55:THR:HG22	1.90	0.54
1:C:347:PHE:O	1:C:351:VAL:HG22	2.08	0.54
1:I:58:ARG:NE	1:I:103:GLU:OE2	2.39	0.54
1:A:279:LEU:O	1:A:282:GLN:HG2	2.08	0.54
1:H:54:ILE:HD13	1:H:87:LEU:HD23	1.89	0.54
1:H:358:GLN:N	1:J:356:GLY:O	2.41	0.54
1:E:360:ARG:HA	1:E:360:ARG:HH11	1.73	0.54
1:C:31:GLY:HA3	1:C:98:SER:HB3	1.90	0.53
1:A:33:PRO:HD3	1:A:163:PHE:CE2	2.42	0.53
1:E:323:GLU:HG2	1:E:357:LEU:HD21	1.91	0.53
1:L:411:MET:HG3	1:L:429:LEU:HD22	1.91	0.53
1:C:322:LEU:HG	1:C:326:MET:HG2	1.89	0.53
1:C:143:GLU:OE1	1:C:143:GLU:N	2.42	0.53
1:C:130:LEU:HB2	1:C:206:TYR:HB2	1.90	0.53
1:C:125:LEU:HD22	1:C:129:LEU:HD11	1.91	0.53
1:G:234:GLU:HA	1:G:238:ARG:HG3	1.90	0.53
1:D:130:LEU:HB2	1:D:206:TYR:HB2	1.90	0.53
1:F:234:GLU:HA	1:F:238:ARG:HG3	1.90	0.53
1:F:390:ILE:HG13	1:F:391:THR:HG23	1.90	0.53
1:F:335:LEU:HB2	1:F:340:LYS:HZ3	1.74	0.52
1:G:328:TRP:O	1:G:332:ARG:NH1	2.42	0.52
1:C:54:ILE:HD13	1:C:87:LEU:HD23	1.90	0.52
1:G:392:PHE:HB2	1:G:424:GLU:HG2	1.92	0.52
1:L:51:TYR:HE1	1:L:279:LEU:HD21	1.74	0.52
1:A:327:GLU:OE1	1:A:360:ARG:NH2	2.43	0.52
1:B:360:ARG:HH11	1:B:360:ARG:HA	1.74	0.52
1:J:293:TYR:O	1:J:296:SER:OG	2.23	0.52
1:F:202:PRO:HA	1:F:205:TRP:CD2	2.45	0.52
1:F:173:ASN:HB3	1:F:177:ARG:HB2	1.90	0.51
1:D:25:PRO:HA	1:D:52:ARG:HB3	1.92	0.51
1:G:28:LEU:HB2	1:G:55:THR:HG22	1.92	0.51
1:D:315:PHE:HE1	1:D:350:THR:HG21	1.74	0.51
1:J:1:PRO:HD2	1:J:16:TYR:HE1	1.75	0.51
1:C:234:GLU:HA	1:C:238:ARG:HG3	1.91	0.51
1:E:303:LEU:HD12	1:E:334:ILE:HB	1.91	0.51
1:J:58:ARG:NE	1:J:103:GLU:OE2	2.43	0.51
1:A:234:GLU:HA	1:A:238:ARG:HG3	1.93	0.51
1:G:422:THR:HG22	1:G:425:VAL:HG22	1.92	0.51
1:H:390:ILE:HG13	1:H:391:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:ARG:HH11	1:L:360:ARG:HA	1.76	0.51
1:D:109:SER:HA	1:D:215:ARG:HH11	1.76	0.51
1:C:22:THR:HG21	1:C:422:THR:HG21	1.93	0.50
1:B:31:GLY:HA3	1:B:98:SER:HB3	1.94	0.50
1:E:234:GLU:HA	1:E:238:ARG:HG3	1.92	0.50
1:D:347:PHE:O	1:D:351:VAL:HG12	2.11	0.50
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.47	0.50
1:J:314:VAL:HG22	1:J:320:THR:HG21	1.92	0.50
1:H:58:ARG:NE	1:H:103:GLU:OE2	2.40	0.50
1:K:234:GLU:HA	1:K:238:ARG:HG3	1.93	0.50
1:G:202:PRO:HA	1:G:205:TRP:CD2	2.47	0.49
1:A:279:LEU:HD22	1:A:282:GLN:NE2	2.27	0.49
1:K:412:GLY:O	1:K:416:ASN:ND2	2.25	0.49
1:J:138:GLY:O	1:J:235:ASN:ND2	2.45	0.49
1:H:360:ARG:HA	1:H:360:ARG:HH11	1.77	0.49
1:C:360:ARG:HA	1:C:360:ARG:HH11	1.77	0.49
1:F:122:LEU:HD22	1:F:223:LEU:HD22	1.95	0.49
1:J:383:TYR:CZ	1:J:387:LYS:HE3	2.47	0.49
1:E:310:ARG:HD3	1:E:325:LEU:HD11	1.94	0.49
1:J:226:THR:HB	1:J:254:GLY:H	1.78	0.49
1:H:291:GLU:HB2	1:H:315:PHE:HE2	1.78	0.48
1:K:94:LEU:HB2	1:K:119:VAL:HG12	1.95	0.48
1:G:348:THR:HG21	1:G:415:TYR:HE1	1.78	0.48
1:G:24:VAL:HG11	1:G:279:LEU:HD13	1.95	0.48
1:F:360:ARG:HH11	1:F:360:ARG:HA	1.79	0.48
1:L:378:LYS:HE3	1:L:402:TYR:HD1	1.79	0.48
1:I:360:ARG:HH11	1:I:360:ARG:HA	1.78	0.48
1:G:209:PHE:O	1:G:213:ILE:HG13	2.14	0.48
1:I:381:LYS:HD3	1:I:384:ARG:HH12	1.78	0.48
1:G:130:LEU:HG	1:G:132:THR:HG23	1.96	0.48
1:B:321:ASP:HB3	1:B:355:ARG:HH21	1.77	0.48
1:D:385:LYS:HB3	1:D:398:ILE:HD13	1.96	0.48
1:C:402:TYR:O	1:C:436:GLN:NE2	2.41	0.48
1:E:383:TYR:CZ	1:E:387:LYS:HE3	2.49	0.48
1:K:73:TYR:HA	1:K:76:PHE:HB2	1.94	0.48
1:G:321:ASP:HB2	1:G:355:ARG:HH22	1.78	0.48
1:J:54:ILE:HD13	1:J:87:LEU:HD23	1.96	0.48
1:L:348:THR:HG1	1:L:415:TYR:HE1	1.61	0.47
1:G:173:ASN:HB3	1:G:177:ARG:HB2	1.96	0.47
1:J:327:GLU:O	1:J:331:THR:HG22	2.14	0.47
1:I:202:PRO:HA	1:I:205:TRP:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:315:PHE:HE1	1:H:350:THR:HG21	1.79	0.47
1:C:202:PRO:HA	1:C:205:TRP:CD2	2.49	0.47
1:L:345:PHE:CD2	1:L:415:TYR:HB2	2.49	0.47
1:G:58:ARG:NE	1:G:103:GLU:OE2	2.41	0.47
1:D:341:GLY:HA2	1:D:363:VAL:HG23	1.96	0.47
1:D:360:ARG:HH11	1:D:361:ARG:HH12	1.61	0.47
1:I:1:PRO:HD2	1:I:16:TYR:HE1	1.78	0.47
1:K:31:GLY:HA3	1:K:98:SER:HB3	1.96	0.47
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.95	0.47
1:A:341:GLY:HA2	1:A:363:VAL:HG23	1.97	0.47
1:J:27:VAL:HG21	1:J:84:LEU:HD21	1.97	0.47
1:C:360:ARG:HH22	1:C:361:ARG:HE	1.63	0.47
1:L:125:LEU:HD22	1:L:129:LEU:HD11	1.96	0.47
1:G:325:LEU:O	1:G:329:LEU:HB2	2.14	0.47
1:D:315:PHE:CE1	1:D:350:THR:HG21	2.50	0.47
1:K:327:GLU:O	1:K:331:THR:HG22	2.15	0.47
1:J:360:ARG:HH11	1:J:360:ARG:HA	1.80	0.47
1:A:327:GLU:O	1:A:331:THR:HG22	2.15	0.46
1:B:286:LEU:O	1:B:290:VAL:HG23	2.16	0.46
1:L:325:LEU:O	1:L:329:LEU:HB2	2.14	0.46
1:D:58:ARG:NE	1:D:103:GLU:OE2	2.43	0.46
1:E:125:LEU:HD22	1:E:129:LEU:HD11	1.97	0.46
1:L:108:VAL:HG23	1:L:113:THR:HG22	1.97	0.46
1:I:351:VAL:HG22	1:I:353:SER:H	1.79	0.46
1:H:417:ARG:NE	1:H:417:ARG:HA	2.31	0.46
1:C:360:ARG:NH1	1:F:358:GLN:OE1	2.48	0.46
1:K:293:TYR:O	1:K:296:SER:OG	2.25	0.46
1:A:1:PRO:HB2	1:A:17:TYR:O	2.16	0.46
1:E:417:ARG:HA	1:E:417:ARG:NE	2.31	0.46
1:L:234:GLU:HA	1:L:238:ARG:HG3	1.98	0.46
1:H:32:PHE:HB2	1:H:99:MET:SD	2.55	0.46
1:H:383:TYR:CZ	1:H:387:LYS:HE3	2.51	0.46
1:G:327:GLU:O	1:G:331:THR:HG22	2.16	0.46
1:A:74:ASP:OD1	1:A:106:ARG:NH1	2.47	0.46
1:B:97:PHE:HA	1:B:122:LEU:O	2.16	0.46
1:C:314:VAL:HG22	1:C:320:THR:HG21	1.98	0.46
1:E:314:VAL:HG22	1:E:320:THR:HG21	1.98	0.46
1:A:330:LYS:HZ1	1:A:360:ARG:HH22	1.63	0.46
1:C:276:ALA:O	1:C:280:GLU:HB2	2.15	0.46
1:J:287:LEU:HD13	1:J:315:PHE:CD1	2.51	0.46
1:F:58:ARG:NE	1:F:103:GLU:OE2	2.37	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:O	1:B:297:ILE:HG22	2.16	0.46
1:J:321:ASP:HB3	1:J:355:ARG:NH2	2.31	0.46
1:E:28:LEU:HB2	1:E:55:THR:HG22	1.98	0.46
1:L:51:TYR:CE1	1:L:279:LEU:HD21	2.51	0.46
1:G:54:ILE:HD13	1:G:87:LEU:HD23	1.97	0.46
1:I:390:ILE:HG13	1:I:391:THR:HG23	1.97	0.46
1:I:315:PHE:CE1	1:I:350:THR:HG21	2.50	0.45
1:J:321:ASP:HA	1:J:355:ARG:HE	1.80	0.45
1:H:356:GLY:O	1:J:358:GLN:N	2.49	0.45
1:I:58:ARG:NH2	1:I:100:GLY:HA2	2.31	0.45
1:L:51:TYR:CZ	1:L:279:LEU:HD11	2.50	0.45
1:B:390:ILE:HG13	1:B:391:THR:HG23	1.97	0.45
1:E:97:PHE:HA	1:E:122:LEU:O	2.15	0.45
1:B:295:LEU:HD23	1:B:298:ILE:HD12	1.97	0.45
1:D:33:PRO:HD3	1:D:163:PHE:CE2	2.51	0.45
1:K:322:LEU:HD11	1:K:351:VAL:HG21	1.99	0.45
1:H:418:MET:HA	1:H:419:GLY:HA2	1.75	0.45
1:K:422:THR:HG22	1:K:425:VAL:HG22	1.98	0.45
1:F:1:PRO:HD2	1:F:16:TYR:HE1	1.82	0.45
1:H:173:ASN:HB3	1:H:177:ARG:HB2	1.98	0.45
1:F:94:LEU:HG	1:F:116:ILE:HD12	1.97	0.45
1:D:203:THR:HA	1:D:206:TYR:CE1	2.52	0.45
1:B:315:PHE:HE1	1:B:350:THR:HG21	1.81	0.45
1:J:294:VAL:O	1:J:297:ILE:HG22	2.16	0.45
1:E:32:PHE:HB2	1:E:99:MET:SD	2.57	0.45
1:H:417:ARG:HA	1:H:417:ARG:HE	1.81	0.45
1:L:51:TYR:OH	1:L:275:LEU:HB3	2.17	0.45
1:A:310:ARG:HD2	1:A:325:LEU:HD11	1.97	0.45
1:G:341:GLY:HA2	1:G:363:VAL:HG23	1.99	0.45
1:K:125:LEU:HD22	1:K:129:LEU:HD11	1.99	0.45
1:E:127:PRO:HB3	1:E:213:ILE:HD11	1.99	0.45
1:C:5:VAL:HA	1:C:82:THR:HG21	1.99	0.45
1:C:390:ILE:HG13	1:C:391:THR:HG23	1.98	0.45
1:I:280:GLU:HA	1:I:283:LYS:HD2	1.99	0.45
1:A:173:ASN:HB3	1:A:177:ARG:HB2	1.99	0.44
1:K:95:VAL:HG22	1:K:120:ALA:HB3	1.98	0.44
1:J:94:LEU:HB2	1:J:119:VAL:HG12	1.99	0.44
1:B:389:GLU:OE1	1:B:398:ILE:HD11	2.17	0.44
1:G:297:ILE:HD12	1:G:437:ILE:HB	1.98	0.44
1:B:381:LYS:HD3	1:B:384:ARG:HH21	1.82	0.44
1:D:54:ILE:HD13	1:D:87:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:VAL:HG22	1:B:120:ALA:HB3	1.97	0.44
1:G:184:ARG:HD2	1:I:187:TRP:CZ3	2.52	0.44
1:K:202:PRO:HA	1:K:205:TRP:CD2	2.51	0.44
1:E:101:THR:HG21	1:E:124:SER:HA	1.99	0.44
1:J:395:ALA:HB2	1:J:425:VAL:HG13	1.99	0.44
1:B:32:PHE:HB2	1:B:99:MET:SD	2.58	0.44
1:J:209:PHE:O	1:J:213:ILE:HG13	2.18	0.44
1:F:360:ARG:HH22	1:F:361:ARG:HE	1.66	0.44
1:E:1:PRO:HB2	1:E:17:TYR:O	2.17	0.44
1:E:332:ARG:HG2	1:E:335:LEU:HD12	1.99	0.44
1:C:351:VAL:HA	1:C:352:PRO:HD3	1.83	0.44
1:F:354:GLU:OE1	1:F:359:ARG:NH2	2.49	0.44
1:L:332:ARG:HG2	1:L:335:LEU:HG	1.99	0.44
1:H:417:ARG:CD	1:J:417:ARG:HG2	2.48	0.44
1:A:330:LYS:HZ1	1:A:361:ARG:HH22	1.66	0.44
1:L:271:LEU:O	1:L:275:LEU:HG	2.18	0.44
1:K:94:LEU:HG	1:K:116:ILE:HD12	1.99	0.44
1:H:95:VAL:HG22	1:H:120:ALA:HB3	1.99	0.44
1:H:97:PHE:HA	1:H:122:LEU:O	2.18	0.44
1:G:382:LEU:HG	1:G:402:TYR:CD2	2.53	0.44
1:B:372:ASP:HB2	1:B:375:ASN:HB2	1.99	0.44
1:A:202:PRO:HA	1:A:205:TRP:CD2	2.53	0.44
1:A:328:TRP:O	1:A:332:ARG:NH1	2.51	0.44
1:A:238:ARG:NE	1:A:251:GLU:OE2	2.49	0.43
1:L:33:PRO:HD3	1:L:163:PHE:CE2	2.52	0.43
1:G:59:ARG:NE	1:G:79:ASP:OD2	2.51	0.43
1:H:294:VAL:O	1:H:297:ILE:HG22	2.18	0.43
1:J:295:LEU:HD23	1:J:298:ILE:HD12	2.00	0.43
1:A:372:ASP:HB3	1:A:375:ASN:CB	2.46	0.43
1:L:328:TRP:O	1:L:332:ARG:NH1	2.50	0.43
1:E:417:ARG:HA	1:E:417:ARG:HE	1.82	0.43
1:G:414:ILE:HD13	1:G:421:VAL:HG22	2.00	0.43
1:B:420:ALA:HA	1:B:421:VAL:HA	1.74	0.43
1:E:294:VAL:O	1:E:297:ILE:HG22	2.19	0.43
1:I:382:LEU:HD22	1:I:386:LEU:HG	2.00	0.43
1:F:135:ASN:HB3	1:F:210:ARG:NH1	2.34	0.43
1:G:291:GLU:HG3	1:G:311:LEU:HD13	2.00	0.43
1:G:336:SER:OG	1:G:339:THR:HG23	2.18	0.43
1:L:357:LEU:HD23	1:L:357:LEU:HA	1.86	0.43
1:B:125:LEU:HD22	1:B:129:LEU:HD11	2.00	0.43
1:D:119:VAL:HG22	1:D:218:VAL:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLY:O	1:C:235:ASN:ND2	2.52	0.43
1:D:93:VAL:HG11	1:D:275:LEU:HD21	2.00	0.43
1:H:101:THR:HG21	1:H:124:SER:HA	2.01	0.43
1:D:372:ASP:O	1:D:376:MET:N	2.39	0.43
1:B:101:THR:HG21	1:B:124:SER:HA	2.00	0.43
1:G:351:VAL:HA	1:G:352:PRO:HD3	1.91	0.43
1:A:32:PHE:HA	1:A:33:PRO:HA	1.77	0.43
1:L:281:ALA:O	1:L:285:LYS:HG3	2.19	0.43
1:G:109:SER:HA	1:G:215:ARG:HH11	1.84	0.43
1:G:297:ILE:HD11	1:G:434:CYS:O	2.19	0.43
1:B:403:SER:O	1:B:407:LEU:HG	2.19	0.43
1:G:101:THR:HB	1:G:121:PHE:HD1	1.84	0.43
1:F:125:LEU:HD22	1:F:129:LEU:HD11	1.99	0.43
1:D:255:ALA:HA	1:D:263:HIS:CE1	2.54	0.43
1:J:90:GLN:NE2	1:J:390:ILE:HG22	2.34	0.42
1:I:322:LEU:HD13	1:I:351:VAL:HG11	2.01	0.42
1:E:293:TYR:O	1:E:296:SER:OG	2.28	0.42
1:D:325:LEU:O	1:D:329:LEU:HB2	2.19	0.42
1:E:351:VAL:HA	1:E:352:PRO:HD3	1.87	0.42
1:A:291:GLU:HG3	1:A:311:LEU:HD13	2.01	0.42
1:F:347:PHE:O	1:F:351:VAL:HG23	2.19	0.42
1:G:360:ARG:HH11	1:G:361:ARG:HH12	1.67	0.42
1:D:412:GLY:O	1:D:416:ASN:ND2	2.27	0.42
1:C:354:GLU:OE1	1:C:359:ARG:NH2	2.52	0.42
1:G:347:PHE:O	1:G:351:VAL:HG22	2.19	0.42
1:C:1:PRO:HB2	1:C:17:TYR:O	2.18	0.42
1:B:171:ASP:N	1:B:171:ASP:OD1	2.52	0.42
1:H:135:ASN:HB2	1:H:210:ARG:NH1	2.35	0.42
1:H:417:ARG:HD2	1:J:417:ARG:HG2	2.02	0.42
1:B:234:GLU:HA	1:B:238:ARG:HG3	2.01	0.42
1:I:54:ILE:HD13	1:I:87:LEU:HD23	2.01	0.42
1:F:54:ILE:HD13	1:F:87:LEU:HD23	2.01	0.42
1:A:291:GLU:HB2	1:A:315:PHE:CE2	2.41	0.42
1:F:99:MET:HA	1:F:125:LEU:HD11	2.01	0.42
1:C:94:LEU:HG	1:C:116:ILE:HD12	2.01	0.42
1:J:32:PHE:HB2	1:J:99:MET:SD	2.60	0.42
1:J:32:PHE:HA	1:J:33:PRO:HA	1.81	0.42
1:E:255:ALA:HA	1:E:263:HIS:CE1	2.54	0.42
1:A:310:ARG:NH1	1:A:325:LEU:HD21	2.35	0.42
1:A:297:ILE:HD11	1:A:434:CYS:O	2.19	0.42
1:F:332:ARG:HB3	1:F:340:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:297:ILE:HD11	1:L:434:CYS:O	2.19	0.42
1:E:202:PRO:HA	1:E:205:TRP:CE2	2.55	0.42
1:A:306:GLU:O	1:A:310:ARG:HG2	2.20	0.42
1:D:184:ARG:HD2	1:F:187:TRP:CZ3	2.55	0.42
1:A:298:ILE:HG23	1:A:335:LEU:HD21	2.02	0.42
1:A:93:VAL:HG11	1:A:275:LEU:HD21	2.00	0.42
1:F:321:ASP:HB2	1:F:355:ARG:HH22	1.85	0.42
1:G:354:GLU:OE2	1:G:359:ARG:NH2	2.41	0.42
1:L:209:PHE:O	1:L:213:ILE:HG13	2.18	0.42
1:K:297:ILE:HD11	1:K:434:CYS:O	2.19	0.41
1:D:32:PHE:HA	1:D:33:PRO:HA	1.78	0.41
1:J:310:ARG:HD3	1:J:325:LEU:HD11	2.02	0.41
1:D:311:LEU:HB3	1:D:315:PHE:CE2	2.55	0.41
1:E:32:PHE:HA	1:E:33:PRO:HA	1.82	0.41
1:J:420:ALA:HA	1:J:421:VAL:HA	1.80	0.41
1:L:27:VAL:HG21	1:L:84:LEU:HD21	2.02	0.41
1:E:217:ASP:N	1:E:217:ASP:OD2	2.53	0.41
1:J:365:ASN:O	1:J:368:ASN:ND2	2.53	0.41
1:K:303:LEU:HD12	1:K:334:ILE:HB	2.01	0.41
1:C:32:PHE:HA	1:C:33:PRO:HA	1.78	0.41
1:K:341:GLY:HA2	1:K:363:VAL:HG23	2.02	0.41
1:G:101:THR:HG21	1:G:124:SER:HA	2.01	0.41
1:E:173:ASN:HB3	1:E:177:ARG:HB2	2.02	0.41
1:H:414:ILE:HD12	1:H:429:LEU:HD12	2.03	0.41
1:B:94:LEU:HG	1:B:116:ILE:HD12	2.01	0.41
1:A:123:ALA:HA	1:A:224:HIS:CD2	2.55	0.41
1:H:59:ARG:NE	1:H:79:ASP:OD2	2.54	0.41
1:J:372:ASP:HA	1:J:373:PRO:HD2	1.93	0.41
1:I:347:PHE:O	1:I:351:VAL:HG12	2.20	0.41
1:C:280:GLU:HA	1:C:283:LYS:HD2	2.03	0.41
1:L:304:LYS:HA	1:L:307:ILE:HG22	2.01	0.41
1:I:32:PHE:HA	1:I:33:PRO:HA	1.81	0.41
1:J:297:ILE:HA	1:J:297:ILE:HD12	1.85	0.41
1:F:351:VAL:HG12	1:F:353:SER:H	1.85	0.41
1:F:293:TYR:O	1:F:296:SER:OG	2.31	0.41
1:F:138:GLY:O	1:F:235:ASN:ND2	2.54	0.41
1:A:294:VAL:HG21	1:A:346:VAL:HG21	2.02	0.41
1:D:282:GLN:HA	1:D:285:LYS:HB3	2.02	0.41
1:K:32:PHE:HA	1:K:33:PRO:HA	1.78	0.41
1:B:56:TYR:OH	1:B:103:GLU:OE1	2.38	0.41
1:D:322:LEU:HD11	1:D:351:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:202:PRO:HA	1:I:205:TRP:CE2	2.55	0.41
1:I:351:VAL:HA	1:I:352:PRO:HD3	1.83	0.41
1:H:32:PHE:HA	1:H:33:PRO:HA	1.81	0.41
1:D:125:LEU:HD22	1:D:129:LEU:HD11	2.03	0.41
1:F:101:THR:HG21	1:F:124:SER:HA	2.02	0.41
1:I:209:PHE:O	1:I:213:ILE:HG13	2.20	0.41
1:F:24:VAL:HA	1:F:25:PRO:HD3	1.93	0.41
1:H:345:PHE:HD2	1:H:415:TYR:HD1	1.69	0.41
1:I:94:LEU:HG	1:I:116:ILE:HD12	2.03	0.41
1:E:414:ILE:O	1:E:418:MET:HB3	2.21	0.41
1:L:130:LEU:HG	1:L:132:THR:HG23	2.03	0.41
1:H:380:VAL:O	1:H:384:ARG:HG3	2.20	0.41
1:J:414:ILE:O	1:J:418:MET:HB3	2.21	0.41
1:A:410:CYS:HB3	1:A:429:LEU:HD11	2.02	0.40
1:K:101:THR:HG21	1:K:124:SER:HA	2.02	0.40
1:B:357:LEU:HB3	1:B:358:GLN:H	1.76	0.40
1:E:382:LEU:HG	1:E:402:TYR:CE2	2.56	0.40
1:H:125:LEU:HD22	1:H:129:LEU:HD11	2.03	0.40
1:A:54:ILE:HD12	1:A:89:LEU:HD11	2.03	0.40
1:B:32:PHE:HA	1:B:33:PRO:HA	1.80	0.40
1:H:297:ILE:HA	1:H:297:ILE:HD12	1.86	0.40
1:H:286:LEU:O	1:H:290:VAL:HG23	2.21	0.40
1:B:217:ASP:OD2	1:B:217:ASP:N	2.52	0.40
1:I:378:LYS:HE3	1:I:378:LYS:HB3	1.91	0.40
1:H:217:ASP:OD2	1:H:217:ASP:N	2.52	0.40
1:J:380:VAL:O	1:J:384:ARG:HG3	2.21	0.40
1:J:124:SER:HB2	1:J:126:GLU:OE1	2.22	0.40
1:C:106:ARG:HH22	1:C:207:THR:CG2	2.35	0.40
1:C:33:PRO:HD3	1:C:163:PHE:CE2	2.56	0.40
1:H:234:GLU:HA	1:H:238:ARG:HG3	2.03	0.40
1:D:382:LEU:HD21	1:D:399:SER:HB3	2.03	0.40
1:B:327:GLU:O	1:B:331:THR:HG22	2.21	0.40
1:K:58:ARG:NE	1:K:103:GLU:OE2	2.52	0.40
1:F:108:VAL:HG23	1:F:113:THR:HG22	2.04	0.40
1:I:24:VAL:HA	1:I:25:PRO:HD3	1.95	0.40
1:E:420:ALA:HA	1:E:421:VAL:HA	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/456 (96%)	411 (94%)	25 (6%)	0	100	100
1	B	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	C	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	D	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	E	436/456 (96%)	412 (94%)	24 (6%)	0	100	100
1	F	436/456 (96%)	411 (94%)	25 (6%)	0	100	100
1	G	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	H	436/456 (96%)	411 (94%)	25 (6%)	0	100	100
1	I	436/456 (96%)	411 (94%)	25 (6%)	0	100	100
1	J	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	K	436/456 (96%)	410 (94%)	26 (6%)	0	100	100
1	L	436/456 (96%)	412 (94%)	24 (6%)	0	100	100
All	All	5232/5472 (96%)	4928 (94%)	304 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	B	352/370 (95%)	346 (98%)	6 (2%)	68	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	D	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	E	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	F	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	G	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	H	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	I	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	J	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	K	352/370 (95%)	346 (98%)	6 (2%)	68	88
1	L	352/370 (95%)	346 (98%)	6 (2%)	68	88
All	All	4224/4440 (95%)	4152 (98%)	72 (2%)	68	88

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	PHE
1	A	329	LEU
1	A	332	ARG
1	A	361	ARG
1	A	382	LEU
1	A	429	LEU
1	B	128	PHE
1	B	329	LEU
1	B	332	ARG
1	B	361	ARG
1	B	382	LEU
1	B	429	LEU
1	C	128	PHE
1	C	329	LEU
1	C	332	ARG
1	C	361	ARG
1	C	382	LEU
1	C	429	LEU
1	D	128	PHE
1	D	329	LEU
1	D	332	ARG
1	D	361	ARG
1	D	382	LEU

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Mol	Chain	Res	Type
1	D	429	LEU
1	E	128	PHE
1	E	329	LEU
1	E	332	ARG
1	E	361	ARG
1	E	382	LEU
1	E	429	LEU
1	F	128	PHE
1	F	329	LEU
1	F	332	ARG
1	F	361	ARG
1	F	382	LEU
1	F	429	LEU
1	G	128	PHE
1	G	329	LEU
1	G	332	ARG
1	G	361	ARG
1	G	382	LEU
1	G	429	LEU
1	H	128	PHE
1	H	329	LEU
1	H	332	ARG
1	H	361	ARG
1	H	382	LEU
1	H	429	LEU
1	I	128	PHE
1	I	329	LEU
1	I	332	ARG
1	I	361	ARG
1	I	382	LEU
1	I	429	LEU
1	J	128	PHE
1	J	329	LEU
1	J	332	ARG
1	J	361	ARG
1	J	382	LEU
1	J	429	LEU
1	K	128	PHE
1	K	329	LEU
1	K	332	ARG
1	K	361	ARG
1	K	382	LEU

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Mol	Chain	Res	Type
1	K	429	LEU
1	L	128	PHE
1	L	329	LEU
1	L	332	ARG
1	L	361	ARG
1	L	382	LEU
1	L	429	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

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	438/456 (96%)	0.21	32 (7%) 18 12	24, 43, 76, 127	0
1	B	438/456 (96%)	-0.04	16 (3%) 45 34	25, 48, 96, 136	0
1	C	438/456 (96%)	-0.16	6 (1%) 78 68	29, 53, 98, 143	0
1	D	438/456 (96%)	0.21	30 (6%) 20 13	24, 43, 76, 127	0
1	E	438/456 (96%)	-0.04	15 (3%) 49 37	25, 48, 96, 136	0
1	F	438/456 (96%)	-0.07	5 (1%) 82 75	29, 53, 98, 143	0
1	G	438/456 (96%)	-0.07	17 (3%) 43 32	24, 43, 76, 127	0
1	H	438/456 (96%)	-0.06	14 (3%) 51 38	25, 48, 96, 136	0
1	I	438/456 (96%)	-0.14	2 (0%) 91 88	29, 53, 98, 143	0
1	J	438/456 (96%)	-0.07	13 (2%) 54 40	25, 48, 96, 136	0
1	K	438/456 (96%)	-0.28	1 (0%) 95 94	24, 43, 76, 127	0
1	L	438/456 (96%)	0.11	26 (5%) 26 17	29, 53, 98, 143	0
All	All	5256/5472 (96%)	-0.03	177 (3%) 49 37	24, 47, 95, 143	0

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	353	SER	8.2
1	L	319	ASN	6.5
1	G	356	GLY	6.3
1	A	373	PRO	6.0
1	H	353	SER	5.9
1	A	370	ASN	5.8
1	D	374	ASN	5.6
1	D	371	GLY	5.6
1	D	352	PRO	5.5
1	D	370	ASN	5.5
1	D	354	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	372	ASP	5.4
1	A	372	ASP	5.3
1	D	319	ASN	5.2
1	J	384	ARG	4.9
1	L	357	LEU	4.6
1	H	352	PRO	4.6
1	A	371	GLY	4.4
1	A	377	ASP	4.4
1	A	353	SER	4.4
1	A	319	ASN	4.3
1	B	354	GLU	4.3
1	L	356	GLY	4.2
1	J	353	SER	4.2
1	E	358	GLN	4.2
1	F	356	GLY	4.1
1	D	417	ARG	4.1
1	L	393	HIS	4.1
1	J	373	PRO	4.0
1	J	388	ARG	3.9
1	A	331	THR	3.9
1	G	353	SER	3.9
1	A	354	GLU	3.8
1	B	377	ASP	3.8
1	A	418	MET	3.8
1	H	358	GLN	3.7
1	L	353	SER	3.7
1	A	374	ASN	3.7
1	J	354	GLU	3.7
1	G	300	SER	3.6
1	L	352	PRO	3.6
1	A	416	ASN	3.6
1	I	358	GLN	3.5
1	J	355	ARG	3.5
1	D	419	GLY	3.5
1	D	420	ALA	3.5
1	J	358	GLN	3.4
1	A	355	ARG	3.3
1	G	171	ASP	3.3
1	A	358	GLN	3.3
1	A	312	GLU	3.3
1	E	357	LEU	3.2
1	G	318	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	321	ASP	3.2
1	G	319	ASN	3.2
1	L	365	ASN	3.2
1	D	375	ASN	3.2
1	B	353	SER	3.2
1	L	358	GLN	3.2
1	L	435	GLU	3.1
1	A	316	ALA	3.1
1	J	319	ASN	3.1
1	E	417	ARG	3.1
1	D	368	ASN	3.1
1	E	416	ASN	3.1
1	D	302	PRO	3.0
1	B	418	MET	3.0
1	E	355	ARG	3.0
1	H	355	ARG	2.9
1	K	134	ASP	2.9
1	G	317	GLY	2.9
1	G	354	GLU	2.9
1	A	320	THR	2.9
1	L	401	SER	2.9
1	A	417	ARG	2.9
1	G	355	ARG	2.9
1	B	388	ARG	2.8
1	A	253	GLU	2.8
1	D	391	THR	2.8
1	H	321	ASP	2.8
1	D	373	PRO	2.8
1	E	353	SER	2.8
1	E	381	LYS	2.8
1	D	418	MET	2.7
1	L	300	SER	2.7
1	B	371	GLY	2.7
1	L	320	THR	2.7
1	D	355	ARG	2.7
1	D	416	ASN	2.7
1	H	319	ASN	2.7
1	J	301	GLY	2.7
1	H	397	GLU	2.6
1	L	333	PRO	2.6
1	A	381	LYS	2.6
1	L	422	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	133	ASP	2.6
1	A	419	GLY	2.6
1	L	351	VAL	2.6
1	F	365	ASN	2.6
1	A	357	LEU	2.6
1	D	134	ASP	2.5
1	L	321	ASP	2.5
1	E	373	PRO	2.5
1	H	359	ARG	2.5
1	A	356	GLY	2.5
1	F	118	ALA	2.5
1	B	319	ASN	2.5
1	I	357	LEU	2.5
1	G	403	SER	2.5
1	L	318	LYS	2.5
1	B	352	PRO	2.5
1	A	365	ASN	2.5
1	G	436	GLN	2.5
1	C	319	ASN	2.5
1	H	356	GLY	2.5
1	L	317	GLY	2.5
1	G	321	ASP	2.4
1	L	282	GLN	2.4
1	A	375	ASN	2.4
1	B	397	GLU	2.4
1	E	356	GLY	2.4
1	G	357	LEU	2.4
1	J	356	GLY	2.4
1	B	373	PRO	2.4
1	B	317	GLY	2.4
1	A	352	PRO	2.4
1	D	357	LEU	2.4
1	J	357	LEU	2.3
1	J	381	LYS	2.3
1	D	356	GLY	2.3
1	C	438	ALA	2.3
1	E	384	ARG	2.3
1	H	371	GLY	2.3
1	B	133	ASP	2.3
1	A	388	ARG	2.3
1	D	381	LYS	2.2
1	A	321	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	384	ARG	2.2
1	L	283	LYS	2.2
1	B	234	GLU	2.2
1	L	388	ARG	2.2
1	E	319	ASN	2.2
1	E	22	THR	2.2
1	A	415	TYR	2.2
1	G	365	ASN	2.2
1	L	327	GLU	2.2
1	D	334	ILE	2.2
1	A	360	ARG	2.2
1	H	377	ASP	2.2
1	A	300	SER	2.1
1	L	334	ILE	2.1
1	G	352	PRO	2.1
1	L	301	GLY	2.1
1	A	134	ASP	2.1
1	H	418	MET	2.1
1	E	253	GLU	2.1
1	H	354	GLU	2.1
1	C	358	GLN	2.1
1	C	436	GLN	2.1
1	D	320	THR	2.1
1	E	372	ASP	2.1
1	G	370	ASN	2.1
1	D	365	ASN	2.1
1	D	400	LEU	2.1
1	L	397	GLU	2.1
1	E	390	ILE	2.1
1	D	401	SER	2.0
1	F	410	CYS	2.0
1	C	133	ASP	2.0
1	B	419	GLY	2.0
1	C	410	CYS	2.0
1	D	300	SER	2.0
1	B	372	ASP	2.0
1	J	321	ASP	2.0
1	D	318	LYS	2.0
1	G	377	ASP	2.0
1	L	316	ALA	2.0

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 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.