Full wwPDB X-ray Structure Validation Report (i)

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 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 (i) symbol.

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

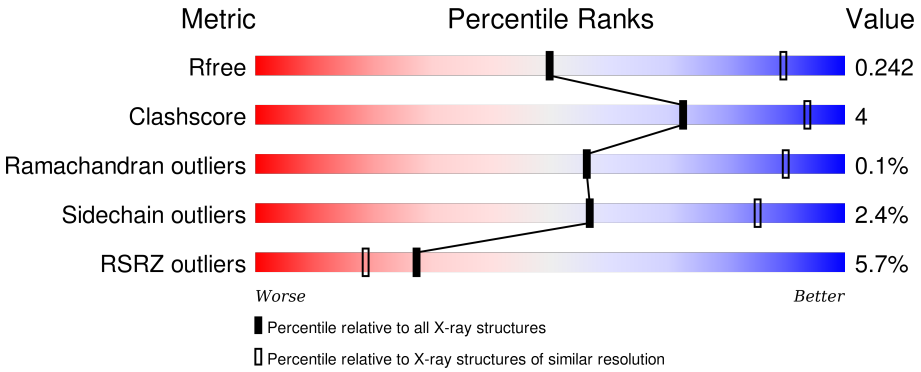
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	82% 14% •
1	B	456	85% 11% •
1	C	456	2% 86% 10% • •
1	D	456	8% 85% 10% • •
1	E	456	85% 11% •

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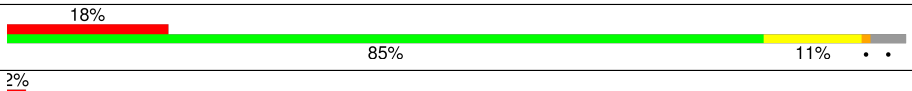
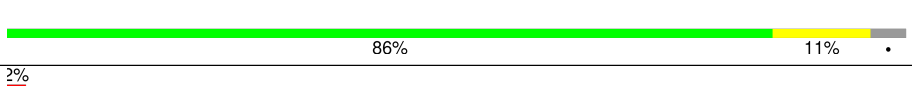
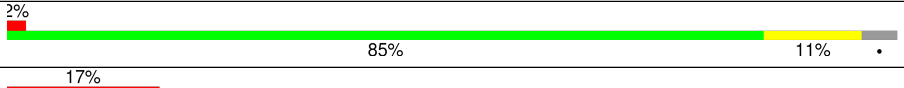
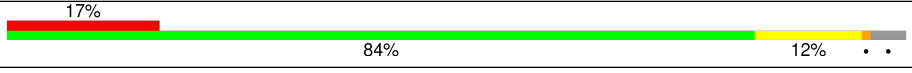
Mol	Chain	Length	Quality of chain
1	F	456	
1	G	456	
1	H	456	
1	I	456	
1	J	456	
1	K	456	
1	L	456	

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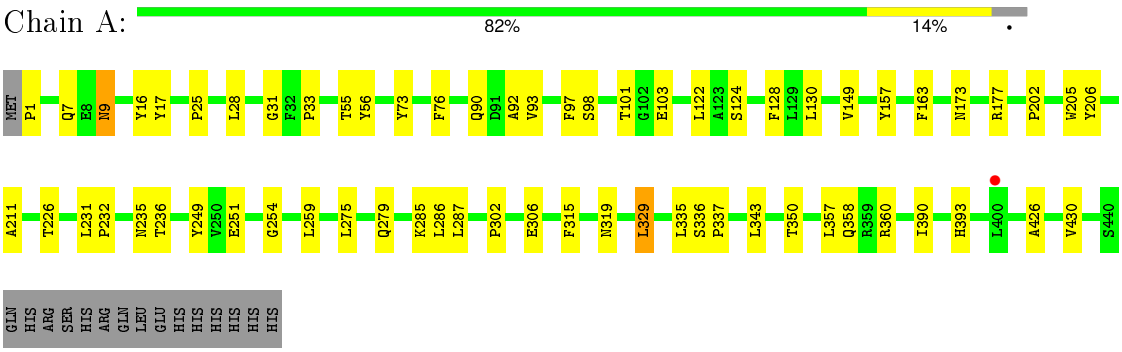
Chain	Residue	Modelled	Actual	Comment	Reference
L	455	HIS	-	EXPRESSION TAG	UNP P03485

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.

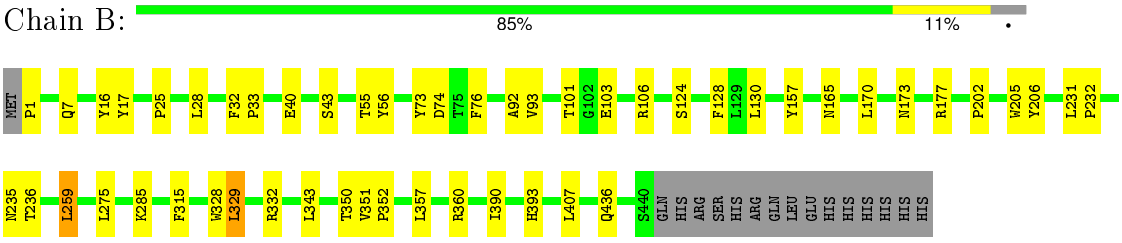
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain A:



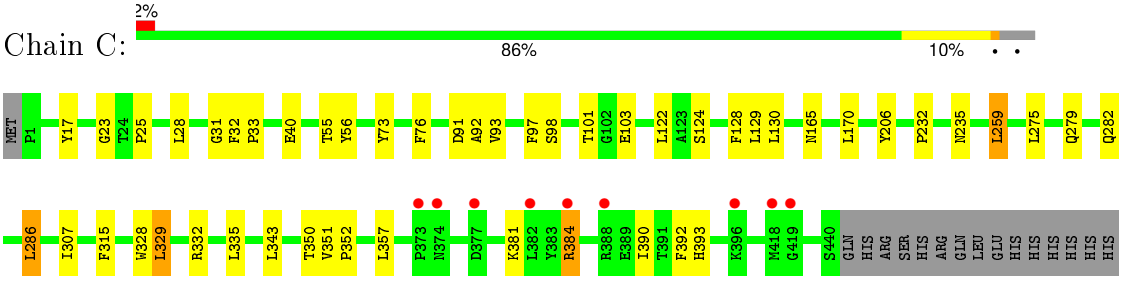
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain B:



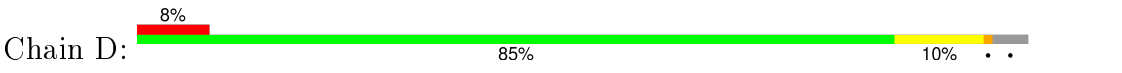
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

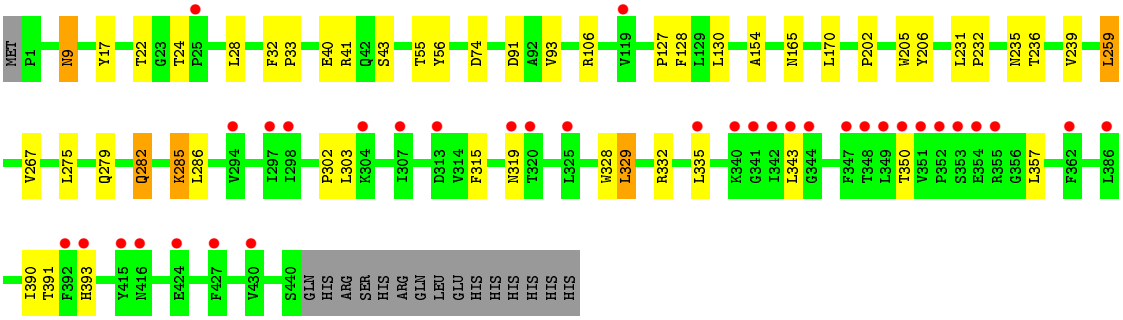
Chain C:



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

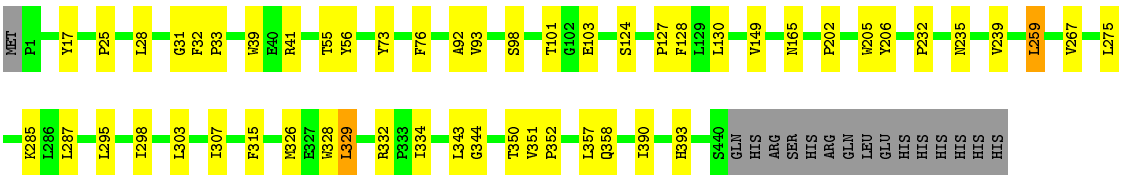
Chain D:





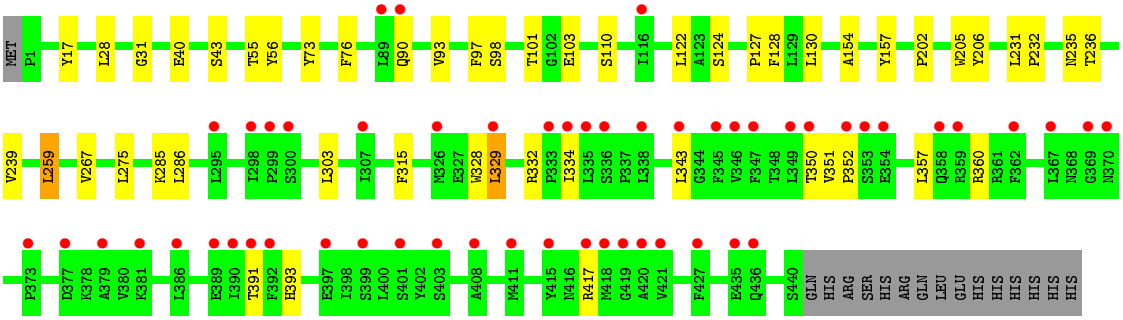
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain E:



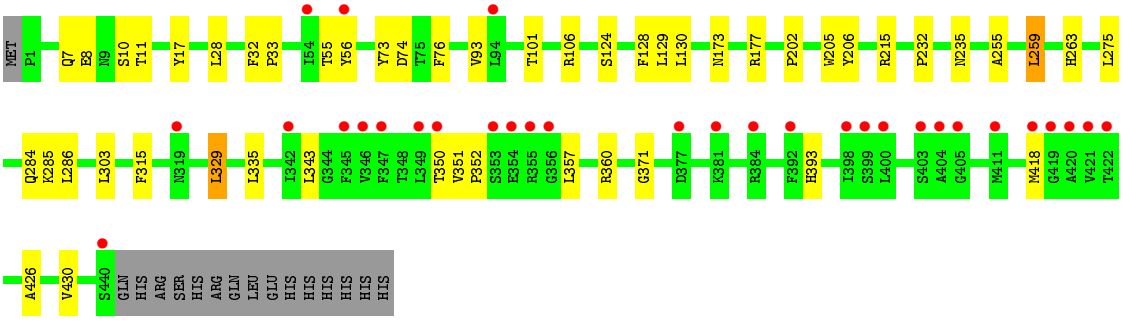
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain F:



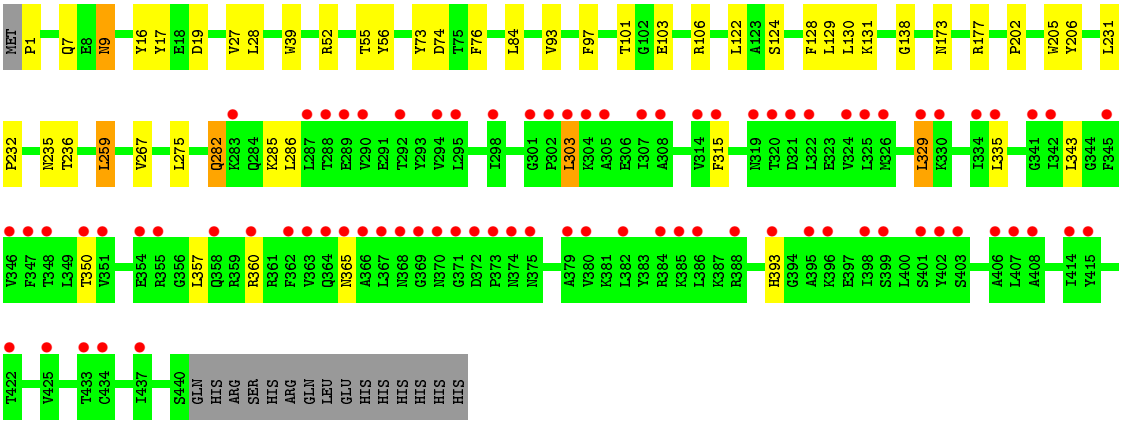
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain G:



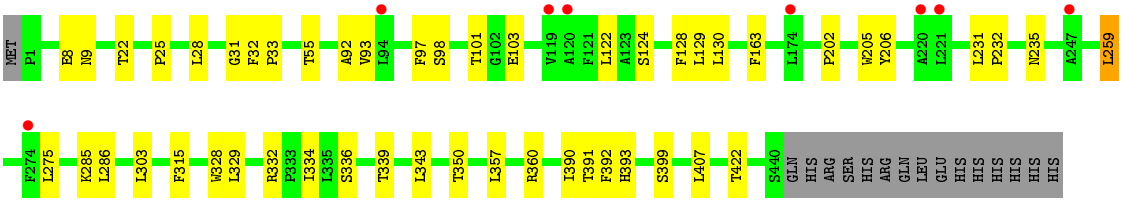
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain H:



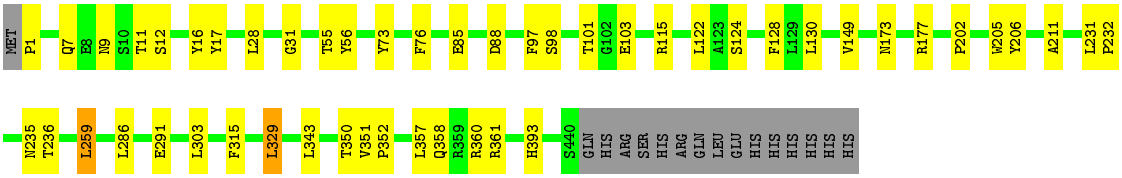
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain I:



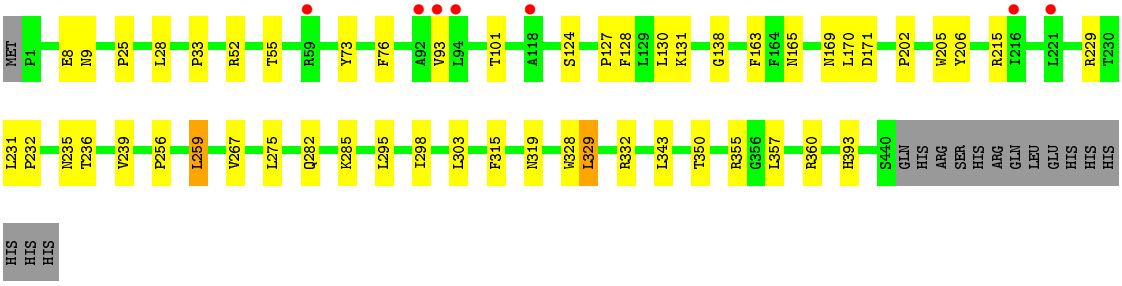
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain J:



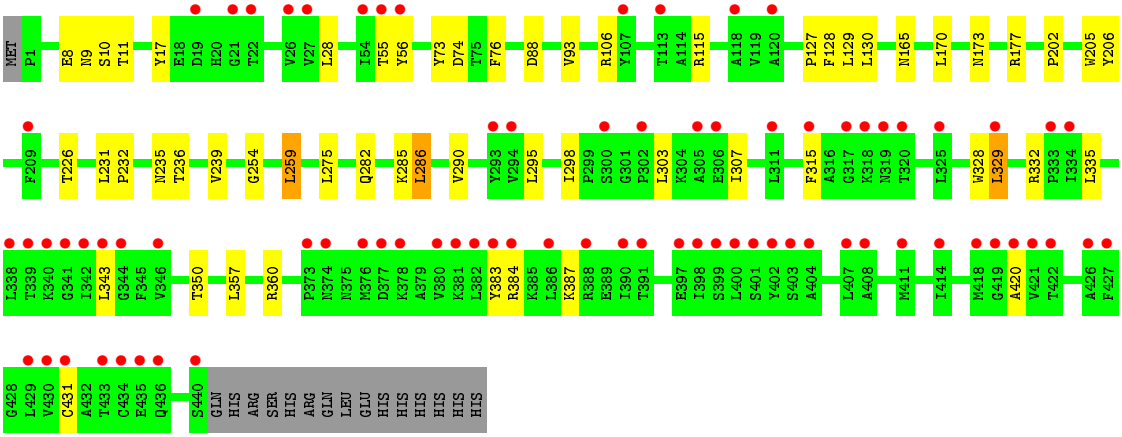
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain K:



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

Chain L:


MET P1 E8 N9 S10 T11 Y17 E18 D19 H20 G21 T22 V26 V27 L28 I54 T55 Y56 Y73 D74 T75 F76 D88 V93 R106 Y107 T113 A114 R115 A118 V119 A120 P127 F128 L129 L130 N165 L170 N173 R177 P202 W205 Y206
F209 T226 L231 P232 N235 T236 V239 G254 L259 L275 Q282 K285 L286 V290 Y293 V294 L295 I298 P299 S300 G301 P302 L303 K304 A305 E306 I307 L311 F315 A316 G317 K318 N319 T320 L325 W328 L329 R332 P333 I334 L335
L338 T339 K340 G341 I342 L343 G344 F345 V346 T350 L357 R360 P373 N374 N375 M376 D377 K378 A379 V380 K381 L382 Y383 R384 K385 L386 K387 R388 E389 I390 T391 E397 I398 S399 L400 S401 Y402 S403 A404 L407 A408 M411 I414 M418 G419 A420 V421 T422 A426 F427
G428 L429 V430 C431 A432 T433 C434 E435 Q436 S440 GLN HIS ARG SER HIS ARG GLN LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.24	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

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.

All (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
1:D:9:ASN:HA	1:E:390:ILE:HD11	1.73	0.69
1:C:23:GLY:HA2	1:C:390:ILE:HD13	1.74	0.69
1:F:417:ARG:HD2	1:L:387:LYS:HE2	1.74	0.68
1:K:130:LEU:HB2	1:K:206:TYR:HB2	1.75	0.68
1:H:130:LEU:HB2	1:H:206:TYR:HB2	1.74	0.68
1:F:28:LEU:HB2	1:F:55:THR:HG22	1.76	0.68
1:G:130:LEU:HB2	1:G:206:TYR:HB2	1.75	0.67
1:C:130:LEU:HB2	1:C:206:TYR:HB2	1.77	0.66
1:A:360:ARG:HH21	1:J:358:GLN:HG3	1.60	0.66
1:B:1:PRO:HD2	1:B:16:TYR:CE1	2.29	0.66
1:K:28:LEU:HB2	1:K:55:THR:HG22	1.77	0.66
1:C:315:PHE:HE1	1:C:350:THR:HG21	1.60	0.66
1:B:329:LEU:HD11	1:B:343:LEU:HB3	1.79	0.65
1:J:130:LEU:HB2	1:J:206:TYR:HB2	1.78	0.65
1:A:28:LEU:HB2	1:A:55:THR:HG22	1.78	0.65
1:L:130:LEU:HB2	1:L:206:TYR:HB2	1.79	0.64
1:L:8:GLU:HG2	1:L:9:ASN:H	1.62	0.64
1:D:302:PRO:HD2	1:G:215:ARG:HH22	1.63	0.64
1:K:315:PHE:HE1	1:K:350:THR:HG21	1.63	0.63
1:I:130:LEU:HB2	1:I:206:TYR:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:THR:HA	1:D:390:ILE:HD11	1.79	0.63
1:D:130:LEU:HB2	1:D:206:TYR:HB2	1.80	0.63
1:K:8:GLU:HG2	1:K:9:ASN:H	1.64	0.63
1:D:91:ASP:OD2	1:D:285:LYS:NZ	2.33	0.62
1:C:232:PRO:HG2	1:C:235:ASN:HB2	1.82	0.61
1:I:8:GLU:HG2	1:I:9:ASN:H	1.65	0.61
1:K:319:ASN:OD1	1:K:355:ARG:NH2	2.33	0.61
1:I:28:LEU:HB2	1:I:55:THR:HG22	1.82	0.61
1:D:231:LEU:HB3	1:D:236:THR:HG21	1.81	0.61
1:K:171:ASP:OD1	1:K:229:ARG:NH1	2.34	0.61
1:J:232:PRO:HG2	1:J:235:ASN:HB2	1.82	0.61
1:G:315:PHE:HE1	1:G:350:THR:HG21	1.66	0.61
1:L:28:LEU:HB2	1:L:55:THR:HG22	1.83	0.60
1:D:232:PRO:HG2	1:D:235:ASN:HB2	1.83	0.60
1:L:74:ASP:OD1	1:L:106:ARG:NH1	2.34	0.60
1:K:232:PRO:HG2	1:K:235:ASN:HB2	1.84	0.60
1:E:28:LEU:HB2	1:E:55:THR:HG22	1.84	0.60
1:L:232:PRO:HG2	1:L:235:ASN:HB2	1.83	0.60
1:L:315:PHE:HE1	1:L:350:THR:HG21	1.67	0.59
1:A:358:GLN:HG3	1:J:360:ARG:HH21	1.67	0.58
1:I:232:PRO:HG2	1:I:235:ASN:HB2	1.85	0.58
1:B:93:VAL:HG11	1:B:275:LEU:HD21	1.85	0.58
1:K:93:VAL:HG11	1:K:275:LEU:HD21	1.85	0.58
1:B:232:PRO:HG2	1:B:235:ASN:HB2	1.85	0.57
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.87	0.57
1:B:101:THR:HG21	1:B:124:SER:HA	1.87	0.57
1:E:93:VAL:HG11	1:E:275:LEU:HD21	1.86	0.57
1:D:28:LEU:HB2	1:D:55:THR:HG22	1.85	0.57
1:E:315:PHE:HE1	1:E:350:THR:HG21	1.69	0.56
1:G:232:PRO:HG2	1:G:235:ASN:HB2	1.87	0.56
1:F:232:PRO:HG2	1:F:235:ASN:HB2	1.87	0.56
1:J:7:GLN:HA	1:J:12:SER:HA	1.86	0.56
1:F:334:ILE:HD13	1:K:215:ARG:HH21	1.71	0.56
1:B:74:ASP:OD1	1:B:106:ARG:NH1	2.39	0.56
1:H:93:VAL:HG11	1:H:275:LEU:HD21	1.88	0.56
1:J:231:LEU:HB3	1:J:236:THR:HG21	1.86	0.56
1:L:329:LEU:HD11	1:L:343:LEU:HB3	1.88	0.56
1:K:165:ASN:HA	1:K:170:LEU:HD12	1.87	0.56
1:E:329:LEU:HD11	1:E:343:LEU:HB3	1.87	0.55
1:F:130:LEU:HB2	1:F:206:TYR:HB2	1.88	0.55
1:H:28:LEU:HB2	1:H:55:THR:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LEU:HB2	1:G:55:THR:HG22	1.89	0.55
1:K:329:LEU:HD11	1:K:343:LEU:HB3	1.86	0.55
1:E:232:PRO:HG2	1:E:235:ASN:HB2	1.87	0.55
1:A:93:VAL:HG11	1:A:275:LEU:HD21	1.88	0.55
1:A:211:ALA:HA	1:E:334:ILE:HA	1.90	0.55
1:B:7:GLN:HB2	1:G:371:GLY:HA3	1.89	0.54
1:E:101:THR:HG21	1:E:124:SER:HA	1.90	0.54
1:E:73:TYR:HA	1:E:76:PHE:HB2	1.89	0.53
1:G:173:ASN:HB3	1:G:177:ARG:HB2	1.91	0.53
1:A:9:ASN:HA	1:B:390:ILE:HD11	1.90	0.53
1:G:259:LEU:H	1:G:259:LEU:HD13	1.74	0.53
1:C:384:ARG:HG3	1:G:418:MET:HG2	1.91	0.53
1:F:315:PHE:HE1	1:F:350:THR:HG21	1.73	0.53
1:H:101:THR:HG21	1:H:124:SER:HA	1.90	0.53
1:B:28:LEU:HB2	1:B:55:THR:HG22	1.89	0.53
1:D:202:PRO:HA	1:D:205:TRP:CE2	2.45	0.52
1:L:259:LEU:HD13	1:L:259:LEU:H	1.73	0.52
1:D:329:LEU:HD11	1:D:343:LEU:HB3	1.91	0.52
1:H:232:PRO:HG2	1:H:235:ASN:HB2	1.90	0.52
1:F:231:LEU:HB3	1:F:236:THR:HG21	1.92	0.52
1:C:28:LEU:HB2	1:C:55:THR:HG22	1.92	0.51
1:B:173:ASN:HB3	1:B:177:ARG:HB2	1.93	0.51
1:J:329:LEU:HD11	1:J:343:LEU:HB3	1.92	0.51
1:K:259:LEU:HD13	1:K:259:LEU:H	1.75	0.51
1:F:259:LEU:H	1:F:259:LEU:HD13	1.75	0.51
1:F:93:VAL:HG11	1:F:275:LEU:HD21	1.92	0.51
1:L:226:THR:HG1	1:L:254:GLY:H	1.59	0.50
1:A:232:PRO:HG2	1:A:235:ASN:HB2	1.92	0.50
1:I:93:VAL:HG11	1:I:275:LEU:HD21	1.93	0.50
1:C:286:LEU:HD11	1:C:392:PHE:CD1	2.47	0.50
1:D:9:ASN:HA	1:E:390:ILE:CD1	2.41	0.50
1:H:259:LEU:H	1:H:259:LEU:HD13	1.76	0.50
1:A:31:GLY:HA3	1:A:98:SER:HB3	1.94	0.50
1:C:384:ARG:NE	1:G:418:MET:HA	2.26	0.50
1:A:173:ASN:HB3	1:A:177:ARG:HB2	1.92	0.50
1:F:110:SER:O	1:H:365:ASN:HB3	2.12	0.50
1:L:73:TYR:HA	1:L:76:PHE:HB2	1.94	0.49
1:G:74:ASP:OD1	1:G:106:ARG:NH1	2.45	0.49
1:B:157:TYR:OH	1:C:40:GLU:OE2	2.21	0.49
1:B:165:ASN:HA	1:B:170:LEU:HD12	1.94	0.49
1:J:17:TYR:HA	1:J:56:TYR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:TYR:HA	1:B:76:PHE:HB2	1.94	0.49
1:D:154:ALA:O	1:E:41:ARG:NH2	2.41	0.49
1:I:259:LEU:HD13	1:I:259:LEU:H	1.78	0.49
1:A:231:LEU:HB3	1:A:236:THR:HG21	1.93	0.48
1:L:93:VAL:HG11	1:L:275:LEU:HD21	1.95	0.48
1:G:329:LEU:HD11	1:G:343:LEU:HB3	1.95	0.48
1:E:17:TYR:HA	1:E:56:TYR:HA	1.95	0.48
1:J:28:LEU:HB2	1:J:55:THR:HG22	1.94	0.48
1:I:286:LEU:HD21	1:I:392:PHE:CG	2.48	0.48
1:C:101:THR:HG21	1:C:124:SER:HA	1.96	0.48
1:I:315:PHE:HE1	1:I:350:THR:HG21	1.79	0.48
1:J:259:LEU:HD13	1:J:259:LEU:H	1.79	0.48
1:F:417:ARG:CD	1:L:387:LYS:HE2	2.44	0.48
1:B:315:PHE:HE1	1:B:350:THR:HG21	1.78	0.48
1:A:315:PHE:HE1	1:A:350:THR:HG21	1.78	0.48
1:J:85:GLU:OE1	1:J:115:ARG:NH2	2.44	0.48
1:J:315:PHE:HE1	1:J:350:THR:HG21	1.79	0.48
1:F:328:TRP:O	1:F:332:ARG:HG2	2.13	0.48
1:K:231:LEU:HB3	1:K:236:THR:HG21	1.96	0.48
1:C:259:LEU:H	1:C:259:LEU:HD13	1.78	0.48
1:D:259:LEU:H	1:D:259:LEU:HD13	1.78	0.48
1:I:202:PRO:HA	1:I:205:TRP:CE2	2.48	0.48
1:D:390:ILE:HG23	1:D:391:THR:HG23	1.96	0.48
1:E:31:GLY:HA3	1:E:98:SER:HB3	1.95	0.48
1:K:259:LEU:HD23	1:K:267:VAL:HG21	1.96	0.47
1:I:25:PRO:HG2	1:I:92:ALA:HA	1.95	0.47
1:C:31:GLY:HA3	1:C:98:SER:HB3	1.95	0.47
1:G:10:SER:HG	1:H:17:TYR:HE2	1.61	0.47
1:L:295:LEU:HD23	1:L:298:ILE:HD12	1.96	0.47
1:D:302:PRO:HD2	1:G:215:ARG:NH2	2.28	0.47
1:L:231:LEU:HB3	1:L:236:THR:HG21	1.97	0.47
1:J:173:ASN:HB3	1:J:177:ARG:HB2	1.96	0.47
1:G:202:PRO:HA	1:G:205:TRP:CD2	2.50	0.47
1:H:202:PRO:HA	1:H:205:TRP:CD2	2.50	0.47
1:B:1:PRO:HB2	1:B:17:TYR:O	2.15	0.47
1:B:17:TYR:HA	1:B:56:TYR:HA	1.96	0.47
1:H:202:PRO:HA	1:H:205:TRP:CE2	2.50	0.47
1:C:381:LYS:HG2	1:C:384:ARG:NH2	2.30	0.47
1:L:202:PRO:HA	1:L:205:TRP:CD2	2.50	0.47
1:F:329:LEU:HD11	1:F:343:LEU:HB3	1.96	0.47
1:L:290:VAL:HG22	1:L:431:CYS:SG	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:PHE:HA	1:G:33:PRO:HA	1.75	0.46
1:A:17:TYR:HA	1:A:56:TYR:HA	1.96	0.46
1:A:9:ASN:HA	1:B:390:ILE:CD1	2.45	0.46
1:A:202:PRO:HA	1:A:205:TRP:CE2	2.51	0.46
1:K:73:TYR:HA	1:K:76:PHE:HB2	1.96	0.46
1:A:73:TYR:HA	1:A:76:PHE:HB2	1.97	0.46
1:A:226:THR:HG1	1:A:254:GLY:H	1.60	0.46
1:J:149:VAL:HG22	1:J:202:PRO:HB2	1.97	0.46
1:J:11:THR:HG22	1:J:12:SER:N	2.31	0.46
1:J:31:GLY:HA3	1:J:98:SER:HB3	1.97	0.46
1:G:73:TYR:HA	1:G:76:PHE:HB2	1.97	0.46
1:C:93:VAL:HG11	1:C:275:LEU:HD21	1.98	0.46
1:K:202:PRO:HA	1:K:205:TRP:CE2	2.51	0.46
1:L:88:ASP:HA	1:L:115:ARG:HH12	1.81	0.46
1:K:328:TRP:O	1:K:332:ARG:HG2	2.16	0.46
1:B:360:ARG:HA	1:B:360:ARG:HE	1.81	0.46
1:E:25:PRO:HG2	1:E:92:ALA:HA	1.96	0.46
1:J:202:PRO:HA	1:J:205:TRP:CE2	2.50	0.45
1:L:165:ASN:HA	1:L:170:LEU:HD12	1.98	0.45
1:D:17:TYR:HA	1:D:56:TYR:HA	1.98	0.45
1:D:74:ASP:OD1	1:D:106:ARG:NH1	2.47	0.45
1:D:328:TRP:O	1:D:332:ARG:HG2	2.17	0.45
1:B:259:LEU:HD13	1:B:259:LEU:H	1.81	0.45
1:B:328:TRP:O	1:B:332:ARG:HG2	2.16	0.45
1:K:101:THR:HG21	1:K:124:SER:HA	1.97	0.45
1:F:73:TYR:HA	1:F:76:PHE:HB2	1.98	0.45
1:H:329:LEU:HD11	1:H:343:LEU:HB3	1.97	0.45
1:D:165:ASN:HA	1:D:170:LEU:HD12	1.98	0.45
1:A:202:PRO:HA	1:A:205:TRP:CD2	2.51	0.45
1:H:303:LEU:HD13	1:H:335:LEU:HG	1.99	0.45
1:G:129:LEU:HB2	1:G:206:TYR:HA	1.99	0.45
1:H:17:TYR:HA	1:H:56:TYR:HA	1.97	0.45
1:I:329:LEU:HD11	1:I:343:LEU:HB3	1.98	0.45
1:D:259:LEU:HD23	1:D:267:VAL:HG21	1.99	0.45
1:K:33:PRO:HD3	1:K:163:PHE:CE2	2.52	0.45
1:B:231:LEU:HB3	1:B:236:THR:HG21	1.98	0.45
1:D:32:PHE:HA	1:D:33:PRO:HA	1.81	0.45
1:H:73:TYR:HA	1:H:76:PHE:HB2	1.97	0.45
1:D:41:ARG:NH2	1:F:154:ALA:O	2.48	0.45
1:I:22:THR:HG21	1:I:422:THR:HG21	1.98	0.45
1:C:17:TYR:HA	1:C:56:TYR:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:287:LEU:HD13	1:E:315:PHE:CD1	2.52	0.44
1:C:32:PHE:HA	1:C:33:PRO:HA	1.77	0.44
1:G:360:ARG:HA	1:G:360:ARG:HE	1.83	0.44
1:E:28:LEU:HB3	1:E:39:TRP:CE2	2.53	0.44
1:L:286:LEU:HA	1:L:286:LEU:HD22	1.86	0.44
1:C:329:LEU:HD11	1:C:343:LEU:HB3	1.98	0.44
1:H:9:ASN:OD1	1:I:390:ILE:HD12	2.18	0.44
1:L:9:ASN:O	1:L:10:SER:OG	2.30	0.44
1:D:202:PRO:HA	1:D:205:TRP:CD2	2.53	0.44
1:L:295:LEU:HA	1:L:298:ILE:HD12	2.00	0.44
1:E:202:PRO:HA	1:E:205:TRP:CE2	2.51	0.44
1:G:11:THR:HB	1:H:1:PRO:HG3	1.98	0.44
1:I:129:LEU:HB2	1:I:206:TYR:HA	1.99	0.44
1:H:315:PHE:HE1	1:H:350:THR:HG21	1.83	0.44
1:L:17:TYR:HA	1:L:56:TYR:HA	1.99	0.44
1:C:165:ASN:HA	1:C:170:LEU:HD12	1.99	0.44
1:H:131:LYS:HA	1:H:138:GLY:HA3	2.00	0.44
1:L:9:ASN:C	1:L:11:THR:H	2.21	0.44
1:L:328:TRP:O	1:L:332:ARG:HG2	2.18	0.44
1:H:173:ASN:HB3	1:H:177:ARG:HB2	1.99	0.44
1:L:202:PRO:HA	1:L:205:TRP:CE2	2.52	0.43
1:D:24:THR:OG1	1:D:282:GLN:OE1	2.33	0.43
1:C:25:PRO:HG2	1:C:92:ALA:HA	2.00	0.43
1:F:90:GLN:HB3	1:F:391:THR:CG2	2.48	0.43
1:I:32:PHE:HA	1:I:33:PRO:HA	1.79	0.43
1:A:101:THR:HG21	1:A:124:SER:HA	1.99	0.43
1:I:31:GLY:HA3	1:I:98:SER:HB3	2.00	0.43
1:C:91:ASP:OD1	1:C:393:HIS:HB2	2.17	0.43
1:F:127:PRO:HD3	1:F:239:VAL:HG13	2.01	0.43
1:G:93:VAL:HG11	1:G:275:LEU:HD21	1.99	0.43
1:G:17:TYR:HA	1:G:56:TYR:HA	2.00	0.43
1:F:101:THR:HG21	1:F:124:SER:HA	2.00	0.43
1:F:97:PHE:HA	1:F:122:LEU:O	2.18	0.43
1:L:383:TYR:CZ	1:L:387:LYS:HD2	2.53	0.43
1:G:101:THR:HG21	1:G:124:SER:HA	2.01	0.43
1:K:169:ASN:HB2	1:K:256:PRO:HB3	1.99	0.43
1:H:28:LEU:HB3	1:H:39:TRP:CE2	2.53	0.43
1:C:328:TRP:O	1:C:332:ARG:HG2	2.19	0.43
1:C:351:VAL:HA	1:C:352:PRO:HD3	1.91	0.43
1:E:328:TRP:O	1:E:332:ARG:HG2	2.19	0.43
1:L:360:ARG:HA	1:L:360:ARG:HE	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:THR:HG21	1:I:124:SER:HA	2.00	0.43
1:E:149:VAL:HG22	1:E:202:PRO:HB2	2.00	0.43
1:K:25:PRO:HA	1:K:52:ARG:HB3	2.01	0.43
1:K:170:LEU:HA	1:K:170:LEU:HD23	1.88	0.42
1:G:10:SER:O	1:H:17:TYR:OH	2.37	0.42
1:C:73:TYR:HA	1:C:76:PHE:HB2	2.00	0.42
1:I:202:PRO:HA	1:I:205:TRP:CD2	2.54	0.42
1:H:19:ASP:OD2	1:H:52:ARG:NH2	2.44	0.42
1:B:360:ARG:HH21	1:E:358:GLN:HG3	1.84	0.42
1:F:202:PRO:HA	1:F:205:TRP:CD2	2.53	0.42
1:A:90:GLN:CB	1:A:390:ILE:HD13	2.45	0.42
1:H:259:LEU:HD23	1:H:267:VAL:HG21	2.01	0.42
1:L:282:GLN:HA	1:L:285:LYS:HB3	2.00	0.42
1:G:7:GLN:HG3	1:G:8:GLU:N	2.34	0.42
1:L:129:LEU:HB2	1:L:206:TYR:HA	2.00	0.42
1:L:286:LEU:O	1:L:290:VAL:HG23	2.19	0.42
1:D:282:GLN:HB2	1:D:282:GLN:HE21	1.68	0.42
1:L:307:ILE:HD11	1:L:335:LEU:HD11	2.02	0.42
1:L:173:ASN:HB3	1:L:177:ARG:HB2	2.01	0.42
1:A:329:LEU:HD11	1:A:343:LEU:HB3	2.01	0.42
1:J:291:GLU:HB2	1:J:315:PHE:HE2	1.85	0.42
1:A:249:TYR:CE2	1:A:251:GLU:HG3	2.54	0.42
1:A:33:PRO:HD3	1:A:163:PHE:CE2	2.55	0.42
1:A:1:PRO:HD2	1:A:16:TYR:HE1	1.85	0.42
1:D:127:PRO:HD3	1:D:239:VAL:HG13	2.01	0.42
1:K:127:PRO:HD3	1:K:239:VAL:HG13	2.01	0.42
1:I:399:SER:O	1:I:407:LEU:HD21	2.19	0.42
1:J:97:PHE:HA	1:J:122:LEU:O	2.19	0.42
1:A:97:PHE:HA	1:A:122:LEU:O	2.20	0.42
1:A:157:TYR:OH	1:B:40:GLU:OE2	2.27	0.42
1:E:32:PHE:HA	1:E:33:PRO:HA	1.80	0.42
1:A:287:LEU:HD13	1:A:315:PHE:CD1	2.55	0.42
1:I:33:PRO:HD3	1:I:163:PHE:CE2	2.54	0.42
1:H:360:ARG:HA	1:H:360:ARG:HE	1.84	0.42
1:L:282:GLN:O	1:L:286:LEU:N	2.52	0.42
1:A:1:PRO:HD2	1:A:16:TYR:CE1	2.55	0.42
1:D:315:PHE:HE1	1:D:350:THR:HG21	1.84	0.42
1:D:40:GLU:OE2	1:F:157:TYR:OH	2.28	0.42
1:A:302:PRO:O	1:A:306:GLU:HG3	2.20	0.41
1:I:97:PHE:HA	1:I:122:LEU:O	2.20	0.41
1:D:40:GLU:HA	1:D:43:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:231:LEU:HB3	1:H:236:THR:HG21	2.01	0.41
1:G:351:VAL:HA	1:G:352:PRO:HD3	1.91	0.41
1:I:334:ILE:HA	1:J:211:ALA:HA	2.02	0.41
1:A:149:VAL:HG22	1:A:202:PRO:HB2	2.02	0.41
1:A:25:PRO:HG2	1:A:92:ALA:HA	2.02	0.41
1:A:358:GLN:OE1	1:J:361:ARG:N	2.54	0.41
1:G:10:SER:OG	1:H:19:ASP:HB3	2.21	0.41
1:B:25:PRO:HG2	1:B:92:ALA:HA	2.01	0.41
1:H:282:GLN:HA	1:H:285:LYS:HG2	2.02	0.41
1:F:259:LEU:HD23	1:F:267:VAL:HG21	2.02	0.41
1:A:231:LEU:HA	1:A:232:PRO:HD2	1.88	0.41
1:K:295:LEU:HD23	1:K:298:ILE:HD12	2.02	0.41
1:L:127:PRO:HD3	1:L:239:VAL:HG13	2.02	0.41
1:A:335:LEU:HA	1:A:335:LEU:HD23	1.90	0.41
1:D:93:VAL:HG11	1:D:275:LEU:HD21	2.03	0.41
1:E:307:ILE:HD13	1:E:343:LEU:HD11	2.02	0.41
1:H:1:PRO:HD2	1:H:16:TYR:HE1	1.85	0.41
1:K:360:ARG:HA	1:K:360:ARG:HE	1.85	0.41
1:B:202:PRO:HA	1:B:205:TRP:CE2	2.55	0.41
1:F:351:VAL:HA	1:F:352:PRO:HD3	1.90	0.41
1:L:231:LEU:HA	1:L:232:PRO:HD2	1.89	0.41
1:G:202:PRO:HA	1:G:205:TRP:CE2	2.56	0.41
1:B:40:GLU:HA	1:B:43:SER:HB2	2.03	0.41
1:G:255:ALA:HA	1:G:263:HIS:CE1	2.56	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.88	0.41
1:H:97:PHE:HA	1:H:122:LEU:O	2.21	0.41
1:B:32:PHE:HA	1:B:33:PRO:HA	1.76	0.41
1:H:129:LEU:HA	1:H:129:LEU:HD23	1.95	0.41
1:H:74:ASP:OD1	1:H:106:ARG:NH1	2.48	0.41
1:F:17:TYR:HA	1:F:56:TYR:HA	2.02	0.41
1:I:231:LEU:HA	1:I:232:PRO:HD2	1.86	0.41
1:I:390:ILE:HG23	1:I:391:THR:HG23	2.02	0.41
1:A:426:ALA:O	1:A:430:VAL:HG23	2.21	0.41
1:F:31:GLY:HA3	1:F:98:SER:HB3	2.02	0.41
1:I:336:SER:HB3	1:I:339:THR:OG1	2.21	0.41
1:B:351:VAL:HA	1:B:352:PRO:HD3	1.86	0.41
1:C:279:GLN:O	1:C:282:GLN:HG3	2.21	0.41
1:J:351:VAL:HA	1:J:352:PRO:HD3	1.92	0.41
1:D:335:LEU:HA	1:D:335:LEU:HD23	1.97	0.41
1:E:351:VAL:HA	1:E:352:PRO:HD3	1.87	0.41
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:LEU:HD23	1:E:298:ILE:HD12	2.03	0.40
1:J:101:THR:HG21	1:J:124:SER:HA	2.03	0.40
1:K:131:LYS:HA	1:K:138:GLY:HA3	2.03	0.40
1:C:307:ILE:HD11	1:C:335:LEU:HD11	2.04	0.40
1:J:88:ASP:HA	1:J:115:ARG:HH12	1.87	0.40
1:B:202:PRO:HA	1:B:205:TRP:CD2	2.57	0.40
1:C:97:PHE:HA	1:C:122:LEU:O	2.20	0.40
1:E:326:MET:HE1	1:E:344:GLY:O	2.20	0.40
1:E:259:LEU:HD23	1:E:267:VAL:HG21	2.03	0.40
1:A:336:SER:HA	1:A:337:PRO:HD3	1.98	0.40
1:G:426:ALA:O	1:G:430:VAL:HG23	2.21	0.40
1:C:315:PHE:CE1	1:C:350:THR:HG21	2.49	0.40
1:I:328:TRP:O	1:I:332:ARG:HG2	2.21	0.40
1:B:407:LEU:HD12	1:B:436:GLN:HG3	2.03	0.40
1:E:127:PRO:HD3	1:E:239:VAL:HG13	2.03	0.40
1:G:335:LEU:HA	1:G:335:LEU:HD23	1.97	0.40
1:I:360:ARG:HE	1:I:360:ARG:HA	1.86	0.40
1:J:1:PRO:HD2	1:J:16:TYR:HE1	1.86	0.40
1:D:275:LEU:O	1:D:279:GLN:N	2.47	0.40
1:J:73:TYR:HA	1:J:76:PHE:HB2	2.02	0.40
1:F:40:GLU:HA	1:F:43:SER:HB2	2.03	0.40
1:F:360:ARG:HE	1:F:360:ARG:HA	1.86	0.40
1:H:27:VAL:HG21	1:H:84:LEU:HD21	2.04	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	438/456 (96%)	415 (95%)	23 (5%)	0	100 100
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 (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	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	354/370 (96%)	345 (98%)	9 (2%)	55 84
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

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	103	GLU
1	A	128	PHE
1	A	259	LEU
1	A	279	GLN
1	A	285	LYS
1	A	286	LEU
1	A	319	ASN
1	A	329	LEU
1	A	357	LEU
1	A	393	HIS
1	B	103	GLU
1	B	128	PHE
1	B	259	LEU
1	B	285	LYS
1	B	329	LEU
1	B	357	LEU
1	B	393	HIS
1	C	103	GLU
1	C	128	PHE
1	C	259	LEU
1	C	286	LEU
1	C	329	LEU
1	C	357	LEU
1	C	384	ARG
1	D	128	PHE
1	D	259	LEU
1	D	282	GLN

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Mol	Chain	Res	Type
1	D	285	LYS
1	D	286	LEU
1	D	303	LEU
1	D	329	LEU
1	D	357	LEU
1	D	393	HIS
1	E	103	GLU
1	E	128	PHE
1	E	165	ASN
1	E	259	LEU
1	E	285	LYS
1	E	303	LEU
1	E	329	LEU
1	E	357	LEU
1	E	393	HIS
1	F	103	GLU
1	F	128	PHE
1	F	259	LEU
1	F	285	LYS
1	F	286	LEU
1	F	303	LEU
1	F	329	LEU
1	F	357	LEU
1	F	393	HIS
1	G	128	PHE
1	G	259	LEU
1	G	284	GLN
1	G	285	LYS
1	G	286	LEU
1	G	303	LEU
1	G	329	LEU
1	G	357	LEU
1	G	393	HIS
1	H	7	GLN
1	H	103	GLU
1	H	128	PHE
1	H	259	LEU
1	H	282	GLN
1	H	286	LEU
1	H	303	LEU
1	H	329	LEU
1	H	357	LEU

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Mol	Chain	Res	Type
1	H	393	HIS
1	I	103	GLU
1	I	128	PHE
1	I	259	LEU
1	I	285	LYS
1	I	303	LEU
1	I	357	LEU
1	I	393	HIS
1	J	103	GLU
1	J	128	PHE
1	J	259	LEU
1	J	286	LEU
1	J	303	LEU
1	J	329	LEU
1	J	357	LEU
1	J	393	HIS
1	K	128	PHE
1	K	259	LEU
1	K	282	GLN
1	K	285	LYS
1	K	303	LEU
1	K	329	LEU
1	K	357	LEU
1	K	393	HIS
1	L	128	PHE
1	L	259	LEU
1	L	286	LEU
1	L	303	LEU
1	L	329	LEU
1	L	357	LEU
1	L	384	ARG

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	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

All (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
1	F	359	ARG	8.7
1	H	367	LEU	8.3
1	H	302	PRO	8.0
1	H	301	GLY	7.7
1	L	401	SER	7.7
1	L	398	ILE	7.5

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Mol	Chain	Res	Type	RSRZ
1	H	350	THR	7.4
1	L	339	THR	7.3
1	L	333	PRO	6.9
1	L	419	GLY	6.8
1	F	420	ALA	6.8
1	H	320	THR	6.7
1	H	366	ALA	6.7
1	L	374	ASN	6.7
1	L	377	ASP	6.3
1	L	320	THR	6.1
1	D	352	PRO	5.9
1	H	363	VAL	5.9
1	L	420	ALA	5.9
1	F	329	LEU	5.9
1	F	421	VAL	5.7
1	G	419	GLY	5.4
1	L	430	VAL	5.4
1	L	344	GLY	5.2
1	H	370	ASN	5.2
1	H	385	LYS	5.1
1	L	373	PRO	5.1
1	H	319	ASN	5.1
1	F	350	THR	5.1
1	L	378	LYS	5.0
1	L	390	ILE	5.0
1	H	362	PHE	5.0
1	L	343	LEU	5.0
1	F	353	SER	4.9
1	H	322	LEU	4.9
1	L	319	ASN	4.9
1	H	373	PRO	4.8
1	L	382	LEU	4.8
1	G	399	SER	4.7
1	G	421	VAL	4.7
1	F	335	LEU	4.7
1	H	307	ILE	4.6
1	L	340	LYS	4.6
1	H	406	ALA	4.5
1	L	436	GLN	4.5
1	L	408	ALA	4.5
1	H	364	GLN	4.5
1	F	298	ILE	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	419	GLY	4.5
1	D	347	PHE	4.5
1	F	300	SER	4.4
1	L	380	VAL	4.4
1	L	317	GLY	4.4
1	L	429	LEU	4.3
1	H	402	TYR	4.3
1	L	418	MET	4.3
1	H	368	ASN	4.3
1	H	347	PHE	4.2
1	H	369	GLY	4.2
1	G	418	MET	4.2
1	H	386	LEU	4.2
1	L	427	PHE	4.1
1	F	386	LEU	4.1
1	L	431	CYS	4.1
1	G	403	SER	4.1
1	G	356	GLY	4.0
1	D	341	GLY	4.0
1	F	418	MET	4.0
1	H	324	VAL	4.0
1	F	299	PRO	4.0
1	D	335	LEU	4.0
1	H	348	THR	4.0
1	H	330	LYS	3.9
1	G	398	ILE	3.9
1	L	56	TYR	3.9
1	L	388	ARG	3.9
1	L	421	VAL	3.9
1	I	120	ALA	3.8
1	H	287	LEU	3.8
1	H	434	CYS	3.8
1	D	355	ARG	3.8
1	H	384	ARG	3.8
1	L	400	LEU	3.8
1	L	383	TYR	3.8
1	C	418	MET	3.7
1	H	308	ALA	3.7
1	H	358	GLN	3.7
1	L	55	THR	3.6
1	F	411	MET	3.6
1	F	399	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	362	PHE	3.6
1	G	420	ALA	3.6
1	L	397	GLU	3.5
1	F	408	ALA	3.5
1	L	302	PRO	3.5
1	G	345	PHE	3.5
1	L	433	THR	3.5
1	H	304	LYS	3.5
1	L	403	SER	3.5
1	L	440	SER	3.5
1	F	349	LEU	3.5
1	H	298	ILE	3.5
1	L	376	MET	3.5
1	H	351	VAL	3.4
1	F	415	TYR	3.4
1	K	216	ILE	3.4
1	H	372	ASP	3.4
1	F	338	LEU	3.4
1	D	294	VAL	3.4
1	L	120	ALA	3.4
1	G	354	GLU	3.4
1	L	54	ILE	3.3
1	F	397	GLU	3.3
1	L	19	ASP	3.3
1	L	21	GLY	3.3
1	D	350	THR	3.3
1	G	404	ALA	3.3
1	G	392	PHE	3.3
1	H	334	ILE	3.3
1	L	407	LEU	3.3
1	L	27	VAL	3.3
1	K	92	ALA	3.3
1	L	346	VAL	3.3
1	F	370	ASN	3.3
1	F	345	PHE	3.3
1	H	303	LEU	3.2
1	H	388	ARG	3.2
1	G	422	THR	3.2
1	L	426	ALA	3.2
1	F	354	GLU	3.2
1	L	305	ALA	3.2
1	G	381	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	290	VAL	3.2
1	F	347	PHE	3.1
1	H	399	SER	3.1
1	G	319	ASN	3.1
1	G	346	VAL	3.1
1	I	119	VAL	3.1
1	L	318	LYS	3.1
1	F	336	SER	3.1
1	H	408	ALA	3.1
1	D	427	PHE	3.1
1	G	355	ARG	3.1
1	L	338	LEU	3.1
1	H	371	GLY	3.1
1	D	340	LYS	3.1
1	H	382	LEU	3.0
1	F	362	PHE	3.0
1	C	419	GLY	3.0
1	D	344	GLY	3.0
1	F	326	MET	3.0
1	H	315	PHE	3.0
1	G	349	LEU	3.0
1	D	319	ASN	3.0
1	H	375	ASN	3.0
1	K	93	VAL	2.9
1	H	365	ASN	2.9
1	H	403	SER	2.9
1	H	401	SER	2.9
1	G	342	ILE	2.9
1	H	288	THR	2.9
1	H	342	ILE	2.9
1	F	377	ASP	2.9
1	L	402	TYR	2.9
1	G	377	ASP	2.9
1	H	314	VAL	2.8
1	L	293	TYR	2.8
1	L	422	THR	2.8
1	H	325	LEU	2.8
1	D	342	ILE	2.8
1	H	437	ILE	2.8
1	H	415	TYR	2.8
1	L	404	ALA	2.8
1	D	392	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	94	LEU	2.8
1	L	294	VAL	2.8
1	D	416	ASN	2.7
1	D	304	LYS	2.7
1	D	25	PRO	2.7
1	F	401	SER	2.7
1	D	119	VAL	2.7
1	D	386	LEU	2.7
1	F	367	LEU	2.7
1	D	348	THR	2.7
1	D	415	TYR	2.7
1	D	343	LEU	2.7
1	F	427	PHE	2.7
1	D	298	ILE	2.7
1	L	342	ILE	2.6
1	F	352	PRO	2.6
1	G	54	ILE	2.6
1	H	395	ALA	2.6
1	L	329	LEU	2.6
1	G	350	THR	2.6
1	H	379	ALA	2.6
1	F	346	VAL	2.6
1	L	334	ILE	2.6
1	H	355	ARG	2.6
1	L	381	LYS	2.6
1	L	209	PHE	2.6
1	L	22	THR	2.5
1	L	311	LEU	2.5
1	H	326	MET	2.5
1	L	300	SER	2.5
1	H	422	THR	2.5
1	H	341	GLY	2.5
1	F	379	ALA	2.5
1	D	351	VAL	2.5
1	F	116	ILE	2.5
1	L	341	GLY	2.5
1	C	377	ASP	2.5
1	F	391	THR	2.4
1	D	354	GLU	2.4
1	I	247	ALA	2.4
1	H	295	LEU	2.4
1	D	297	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	107	TYR	2.4
1	F	435	GLU	2.4
1	K	118	ALA	2.4
1	L	306	GLU	2.4
1	F	89	LEU	2.4
1	G	353	SER	2.4
1	F	358	GLN	2.4
1	G	384	ARG	2.4
1	H	360	ARG	2.4
1	H	292	THR	2.4
1	A	400	LEU	2.4
1	H	294	VAL	2.3
1	G	56	TYR	2.3
1	H	433	THR	2.3
1	C	396	LYS	2.3
1	K	59	ARG	2.3
1	G	411	MET	2.3
1	G	440	SER	2.3
1	C	373	PRO	2.3
1	D	325	LEU	2.3
1	I	221	LEU	2.3
1	G	347	PHE	2.3
1	G	400	LEU	2.3
1	D	349	LEU	2.3
1	F	295	LEU	2.3
1	H	345	PHE	2.3
1	H	335	LEU	2.3
1	H	374	ASN	2.3
1	H	346	VAL	2.3
1	L	118	ALA	2.3
1	F	390	ILE	2.2
1	F	417	ARG	2.2
1	F	403	SER	2.2
1	H	425	VAL	2.2
1	L	26	VAL	2.2
1	H	414	ILE	2.2
1	L	411	MET	2.2
1	D	393	HIS	2.2
1	C	382	LEU	2.2
1	L	386	LEU	2.2
1	F	381	LYS	2.2
1	F	90	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	414	ILE	2.2
1	L	434	CYS	2.2
1	F	343	LEU	2.2
1	H	289	GLU	2.2
1	L	325	LEU	2.2
1	F	389	GLU	2.2
1	I	174	LEU	2.2
1	G	405	GLY	2.2
1	L	435	GLU	2.2
1	H	396	LYS	2.2
1	F	307	ILE	2.2
1	C	384	ARG	2.2
1	L	391	THR	2.2
1	F	333	PRO	2.2
1	H	283	LYS	2.2
1	D	320	THR	2.2
1	L	384	ARG	2.2
1	F	392	PHE	2.2
1	C	388	ARG	2.1
1	C	374	ASN	2.1
1	D	424	GLU	2.1
1	D	307	ILE	2.1
1	D	430	VAL	2.1
1	H	329	LEU	2.1
1	F	373	PRO	2.1
1	G	94	LEU	2.1
1	K	221	LEU	2.1
1	D	313	ASP	2.1
1	H	380	VAL	2.1
1	F	369	GLY	2.1
1	F	436	GLN	2.1
1	H	398	ILE	2.0
1	I	220	ALA	2.0
1	L	315	PHE	2.0
1	L	113	THR	2.0
1	H	407	LEU	2.0
1	I	274	PHE	2.0
1	H	305	ALA	2.0
1	H	393	HIS	2.0
1	I	94	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.