Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 10:42 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

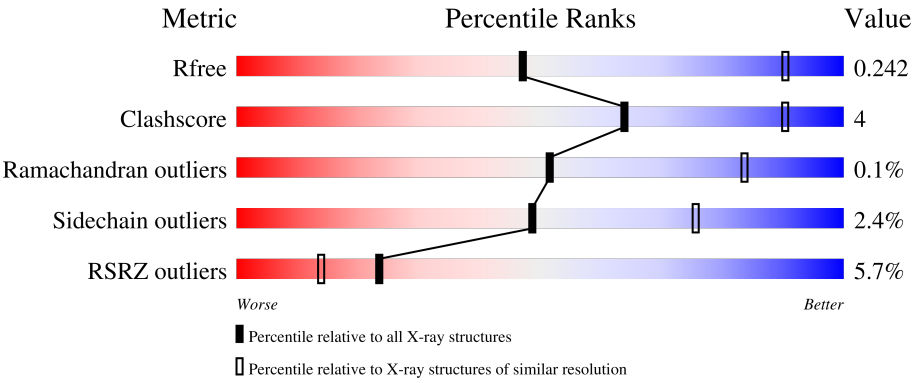
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	456	82% 14% ·
1	B	456	85% 11% ·
1	C	456	2% 86% 10% · ·
1	D	456	7% 85% 10% · ·
1	E	456	85% 11% ·

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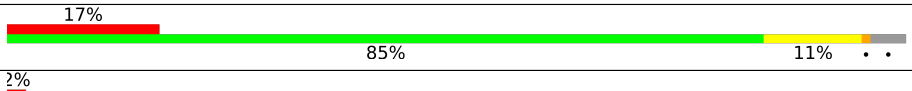
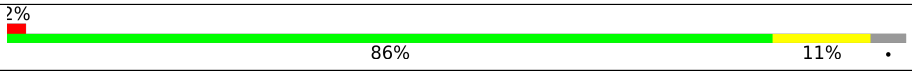
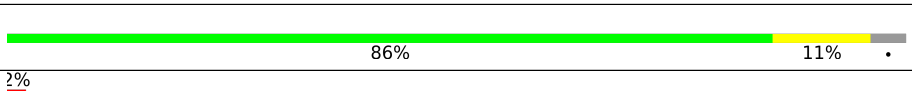
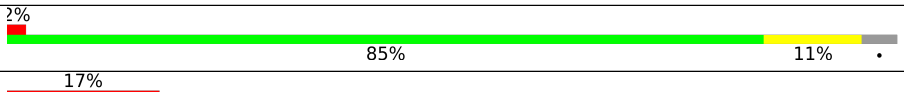
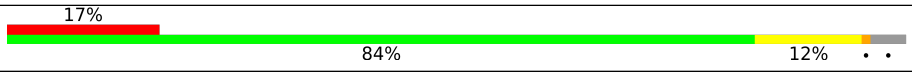
Mol	Chain	Length	Quality of chain
1	F	456	
1	G	456	
1	H	456	
1	I	456	
1	J	456	
1	K	456	
1	L	456	

2 Entry composition (i)

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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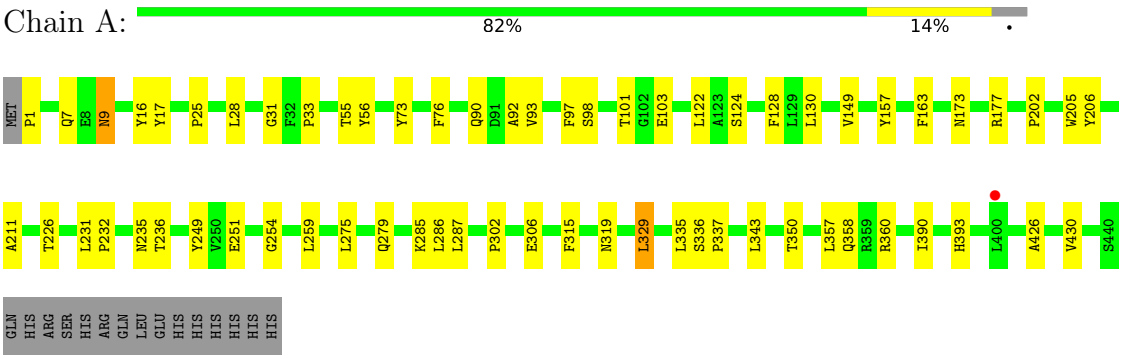
Chain	Residue	Modelled	Actual	Comment	Reference
L	455	HIS	-	expression tag	UNP P03485

3 Residue-property plots (i)

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

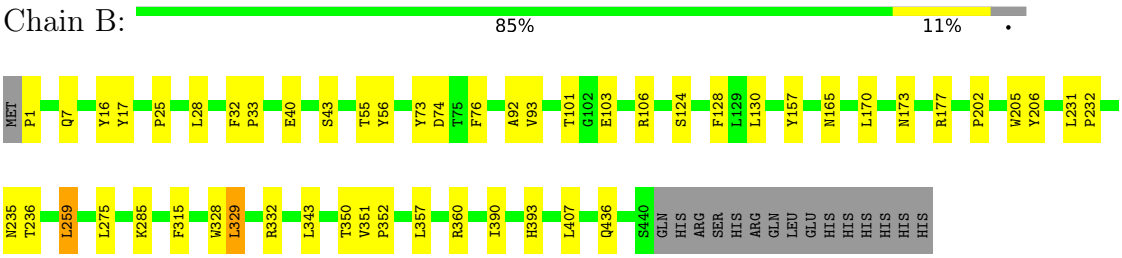
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain A:



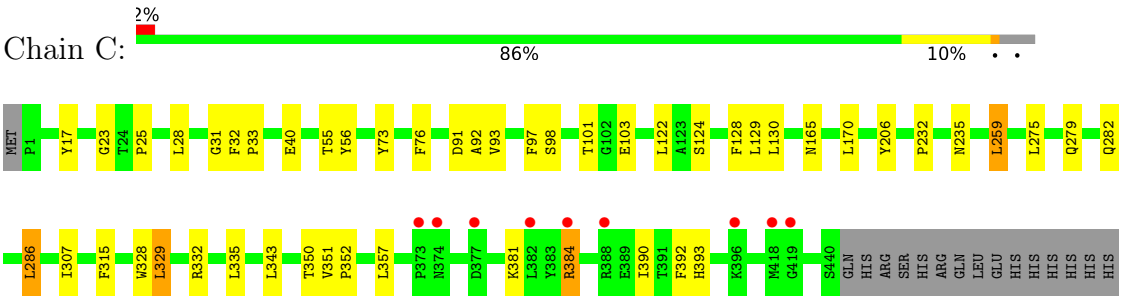
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain B:



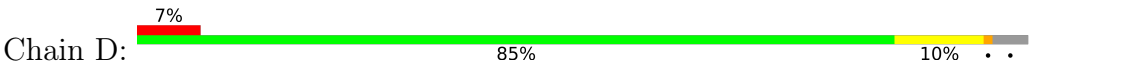
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

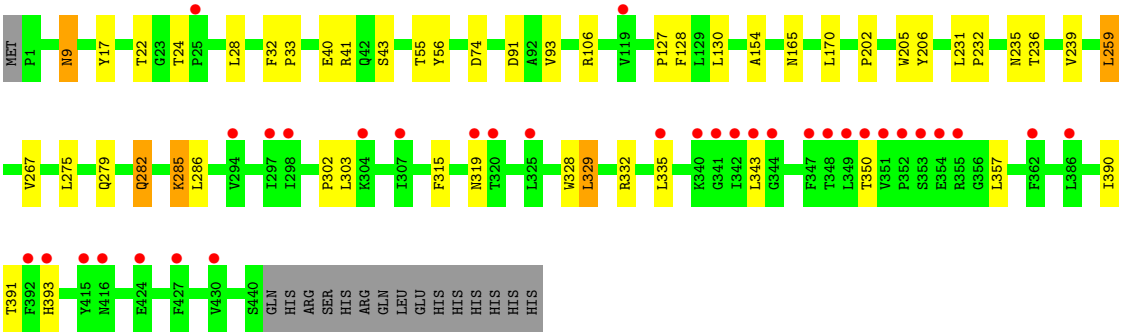
Chain C:



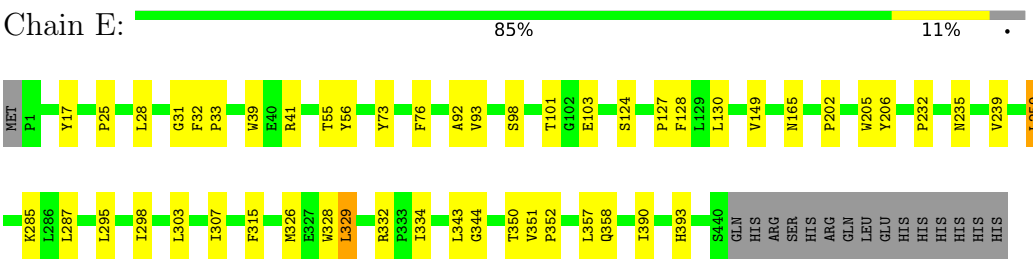
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1

Chain D:

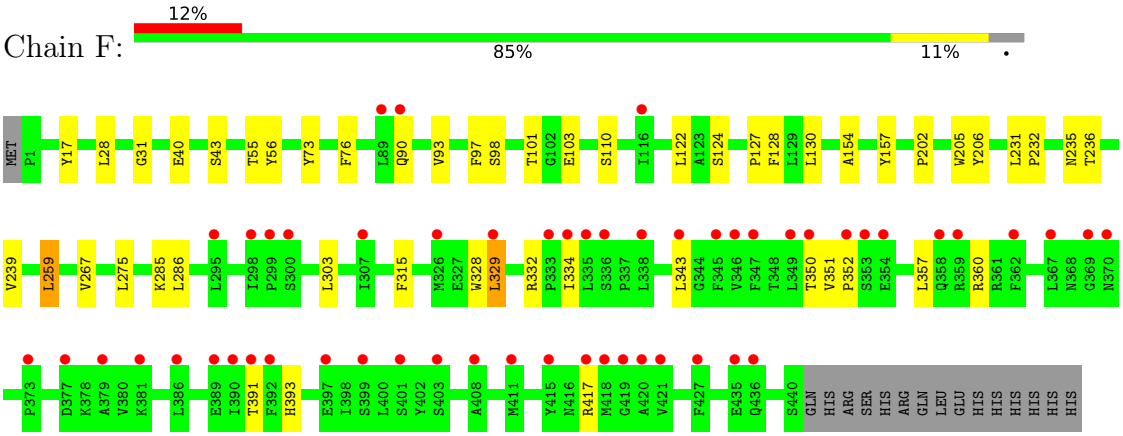




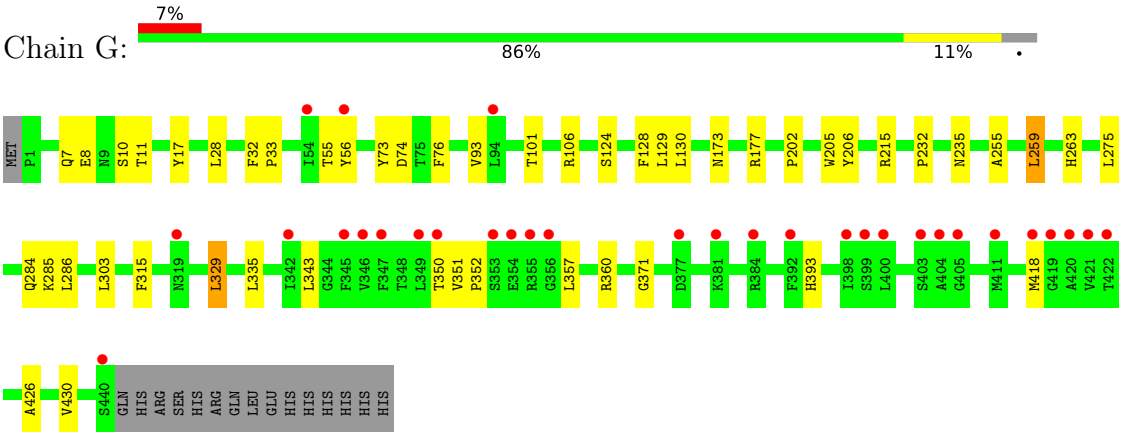
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



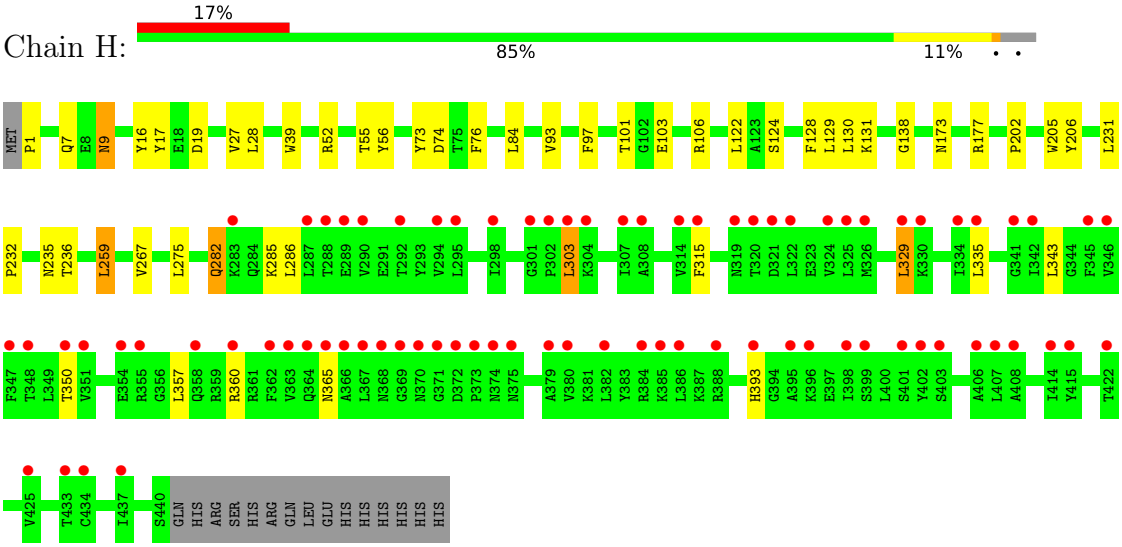
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



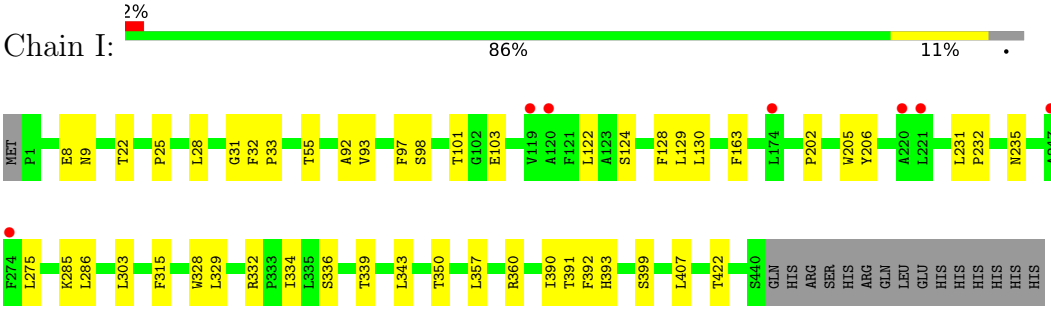
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



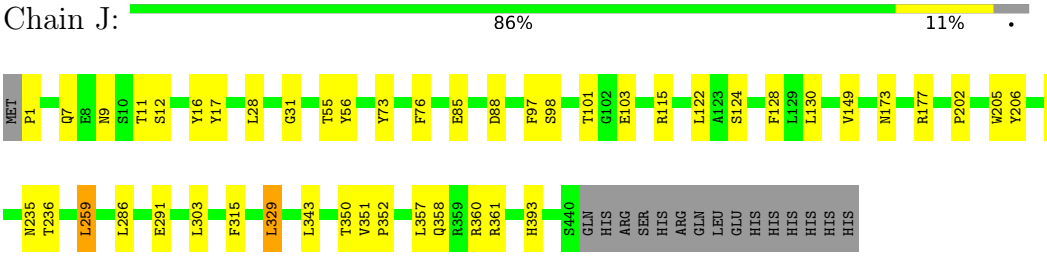
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



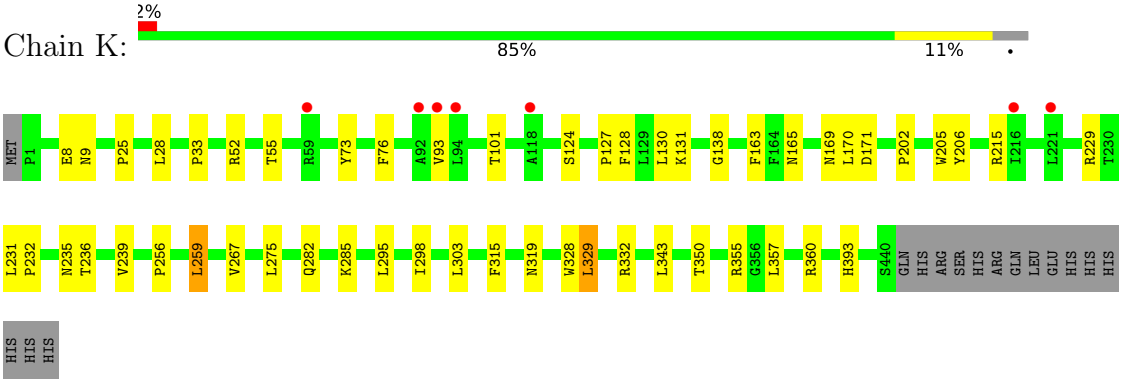
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



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

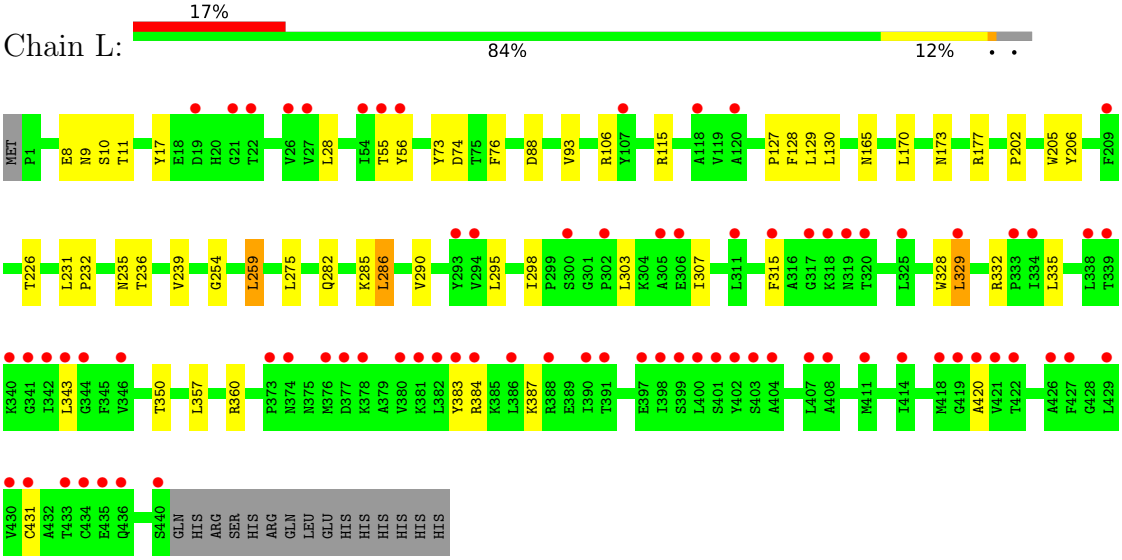


• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1



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

Chain L:



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 1.8.1_1168	Depositor
R, R_{free}	0.206 , 0.240 0.208 , 0.242	Depositor DCC
R_{free} test set	3824 reflections (5.00%)	wwPDB-VP
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 , 82.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.24	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:D:22:THR:HA	1:D:390:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:LEU:HB2	1:I:206:TYR:HB2	1.81	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:K:232:PRO:HG2	1:K:235:ASN:HB2	1.84	0.60
1:L:74:ASP:OD1	1:L:106:ARG:NH1	2.34	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:B:93:VAL:HG11	1:B:275:LEU:HD21	1.85	0.58
1:I:232:PRO:HG2	1:I:235:ASN:HB2	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:B:74:ASP:OD1	1:B:106:ARG:NH1	2.39	0.56
1:F:334:ILE:HD13	1:K:215:ARG:HH21	1.71	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:K:165:ASN:HA	1:K:170:LEU:HD12	1.87	0.56
1:L:329:LEU:HD11	1:L:343:LEU:HB3	1.88	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:A:93:VAL:HG11	1:A:275:LEU:HD21	1.88	0.55
1:E:232:PRO:HG2	1:E:235:ASN:HB2	1.87	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:A:9:ASN:HA	1:B:390:ILE:HD11	1.90	0.53
1:C:384:ARG:HG3	1:G:418:MET:HG2	1.91	0.53
1:G:173:ASN:HB3	1:G:177:ARG:HB2	1.91	0.53
1:G:259:LEU:HD13	1:G:259:LEU:H	1.74	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:H	1:L:259:LEU:HD13	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:F:259:LEU:HD13	1:F:259:LEU:H	1.75	0.51
1:K:259:LEU:HD13	1:K:259:LEU:H	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:C:286:LEU:HD11	1:C:392:PHE:CD1	2.47	0.50
1:I:93:VAL:HG11	1:I:275:LEU:HD21	1.93	0.50
1:D:9:ASN:HA	1:E:390:ILE:CD1	2.41	0.50
1:A:31:GLY:HA3	1:A:98:SER:HB3	1.94	0.50
1:H:259:LEU:HD13	1:H:259:LEU:H	1.76	0.50
1:A:173:ASN:HB3	1:A:177:ARG:HB2	1.92	0.50
1:C:384:ARG:NE	1:G:418:MET:HA	2.26	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:G:329:LEU:HD11	1:G:343:LEU:HB3	1.95	0.48
1:L:93:VAL:HG11	1:L:275:LEU:HD21	1.95	0.48
1:C:101:THR:HG21	1:C:124:SER:HA	1.96	0.48
1:E:17:TYR:HA	1:E:56:TYR:HA	1.95	0.48
1:I:286:LEU:HD21	1:I:392:PHE:CG	2.48	0.48
1:J:28:LEU:HB2	1:J:55:THR:HG22	1.94	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:B:315:PHE:HE1	1:B:350:THR:HG21	1.78	0.48
1:F:417:ARG:CD	1:L:387:LYS:HE2	2.44	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:C:259:LEU:HD13	1:C:259:LEU:H	1.78	0.48
1:D:259:LEU:HD13	1:D:259:LEU:H	1.78	0.48
1:I:202:PRO:HA	1:I:205:TRP:CE2	2.48	0.48
1:K:231:LEU:HB3	1:K:236:THR:HG21	1.96	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:C:31:GLY:HA3	1:C:98:SER:HB3	1.95	0.47
1:I:25:PRO:HG2	1:I:92:ALA:HA	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:F:329:LEU:HD11	1:F:343:LEU:HB3	1.96	0.47
1:L:202:PRO:HA	1:L:205:TRP:CD2	2.50	0.47
1:G:32:PHE:HA	1:G:33:PRO:HA	1.75	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:290:VAL:HG22	1:L:431:CYS:SG	2.55	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:G:73:TYR:HA	1:G:76:PHE: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: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:B:360:ARG:HE	1:B:360:ARG:HA	1.81	0.46
1:E:25:PRO:HG2	1:E:92:ALA:HA	1.96	0.46
1:K:328:TRP:O	1:K:332:ARG:HG2	2.16	0.46
1:L:88:ASP:HA	1:L:115:ARG:HH12	1.81	0.46
1:D:17:TYR:HA	1:D:56:TYR:HA	1.98	0.45
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: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:F:73:TYR:HA	1:F:76:PHE:HB2	1.98	0.45
1:K:101:THR:HG21	1:K:124:SER:HA	1.97	0.45
1:D:165:ASN:HA	1:D:170:LEU:HD12	1.98	0.45
1:H:329:LEU:HD11	1:H:343:LEU:HB3	1.97	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:D:41:ARG:NH2	1:F:154:ALA:O	2.48	0.45
1:H:73:TYR:HA	1:H:76:PHE:HB2	1.97	0.45
1:C:17:TYR:HA	1:C:56:TYR:HA	1.98	0.45
1:I:22:THR:HG21	1:I:422:THR:HG21	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:HE	1:G:360:ARG:HA	1.83	0.44
1:E:28:LEU:HB3	1:E:39:TRP:CE2	2.53	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:286:LEU:HD22	1:L:286:LEU:HA	1.86	0.44
1:D:202:PRO:HA	1:D:205:TRP:CD2	2.53	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:L:9:ASN:O	1:L:10:SER:OG	2.30	0.44
1:L:295:LEU:HA	1:L:298:ILE:HD12	2.00	0.44
1:H:315:PHE:HE1	1:H:350:THR:HG21	1.83	0.44
1:I:129:LEU:HB2	1:I:206:TYR:HA	1.99	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:H:173:ASN:HB3	1:H:177:ARG:HB2	1.99	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:D:24:THR:OG1	1:D:282:GLN:OE1	2.33	0.43
1:L:202:PRO:HA	1:L:205:TRP:CE2	2.52	0.43
1:A:101:THR:HG21	1:A:124:SER:HA	1.99	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: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:I:31:GLY:HA3	1:I:98:SER:HB3	2.00	0.43
1:F:97:PHE:HA	1:F:122:LEU:O	2.18	0.43
1:F:101:THR:HG21	1:F:124:SER:HA	2.00	0.43
1:G:17:TYR:HA	1:G:56:TYR:HA	2.00	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:L:383:TYR:CZ	1:L:387:LYS:HD2	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:H:28:LEU:HB3	1:H:39:TRP:CE2	2.53	0.43
1:I:101:THR:HG21	1:I:124:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:360:ARG:HE	1:L:360:ARG:HA	1.84	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:C:73:TYR:HA	1:C:76:PHE:HB2	2.00	0.42
1:G:10:SER:O	1:H:17:TYR:OH	2.37	0.42
1:K:170:LEU:HD23	1:K:170:LEU:HA	1.88	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:H:19:ASP:OD2	1:H:52:ARG:NH2	2.44	0.42
1:I:202:PRO:HA	1:I:205:TRP:CD2	2.54	0.42
1:A:90:GLN:CB	1:A:390:ILE:HD13	2.45	0.42
1:G:7:GLN:HG3	1:G:8:GLU:N	2.34	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:D:282:GLN:HE21	1:D:282:GLN:HB2	1.68	0.42
1:L:129:LEU:HB2	1:L:206:TYR:HA	2.00	0.42
1:L:173:ASN:HB3	1:L:177:ARG:HB2	2.01	0.42
1:L:286:LEU:O	1:L:290:VAL:HG23	2.19	0.42
1:L:307:ILE:HD11	1:L:335:LEU:HD11	2.02	0.42
1:A:329:LEU:HD11	1:A:343:LEU:HB3	2.01	0.42
1:A:1:PRO:HD2	1:A:16:TYR:HE1	1.85	0.42
1:A:33:PRO:HD3	1:A:163:PHE:CE2	2.55	0.42
1:A:249:TYR:CE2	1:A:251:GLU:HG3	2.54	0.42
1:D:127:PRO:HD3	1:D:239:VAL:HG13	2.01	0.42
1:I:399:SER:O	1:I:407:LEU:HD21	2.19	0.42
1:J:291:GLU:HB2	1:J:315:PHE:HE2	1.85	0.42
1:K:127:PRO:HD3	1:K:239:VAL:HG13	2.01	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:J:97:PHE:HA	1:J:122:LEU:O	2.19	0.42
1:A:287:LEU:HD13	1:A:315:PHE:CD1	2.55	0.42
1:H:360:ARG:HE	1:H:360:ARG:HA	1.84	0.42
1:I:33:PRO:HD3	1:I:163:PHE:CE2	2.54	0.42
1:A:1:PRO:HD2	1:A:16:TYR:CE1	2.55	0.42
1:D:40:GLU:OE2	1:F:157:TYR:OH	2.28	0.42
1:D:315:PHE:HE1	1:D:350:THR:HG21	1.84	0.42
1:L:282:GLN:O	1:L:286:LEU:N	2.52	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:25:PRO:HG2	1:A:92:ALA:HA	2.02	0.41
1:A:149:VAL:HG22	1:A:202:PRO:HB2	2.02	0.41
1:A:358:GLN:OE1	1:J:361:ARG:N	2.54	0.41
1:B:25:PRO:HG2	1:B:92:ALA:HA	2.01	0.41
1:G:10:SER:OG	1:H:19:ASP:HB3	2.21	0.41
1:H:282:GLN:HA	1:H:285:LYS:HG2	2.02	0.41
1:A:231:LEU:HA	1:A:232:PRO:HD2	1.88	0.41
1:A:335:LEU:HD23	1:A:335:LEU:HA	1.90	0.41
1:D:93:VAL:HG11	1:D:275:LEU:HD21	2.03	0.41
1:F:259:LEU:HD23	1:F:267:VAL:HG21	2.02	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:B:202:PRO:HA	1:B:205:TRP:CE2	2.55	0.41
1:E:307:ILE:HD13	1:E:343:LEU:HD11	2.02	0.41
1:F:351:VAL:HA	1:F:352:PRO:HD3	1.90	0.41
1:H:1:PRO:HD2	1:H:16:TYR:HE1	1.85	0.41
1:K:360:ARG:HE	1:K:360:ARG:HA	1.85	0.41
1:B:32:PHE:HA	1:B:33:PRO:HA	1.76	0.41
1:B:40:GLU:HA	1:B:43:SER:HB2	2.03	0.41
1:C:129:LEU:HD23	1:C:129:LEU:HA	1.88	0.41
1:F:17:TYR:HA	1:F:56:TYR:HA	2.02	0.41
1:G:202:PRO:HA	1:G:205:TRP:CE2	2.56	0.41
1:G:255:ALA:HA	1:G:263:HIS:CE1	2.56	0.41
1:H:74:ASP:OD1	1:H:106:ARG:NH1	2.48	0.41
1:H:97:PHE:HA	1:H:122:LEU:O	2.21	0.41
1:H:129:LEU:HD23	1:H:129:LEU:HA	1.95	0.41
1:L:231:LEU:HA	1:L:232:PRO:HD2	1.89	0.41
1:A:426:ALA:O	1:A:430:VAL:HG23	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:D:335:LEU:HD23	1:D:335:LEU:HA	1.97	0.41
1:E:351:VAL:HA	1:E:352:PRO:HD3	1.87	0.41
1:F:31:GLY:HA3	1:F:98:SER:HB3	2.02	0.41
1:I:231:LEU:HA	1:I:232:PRO:HD2	1.86	0.41
1:I:336:SER:HB3	1:I:339:THR:OG1	2.21	0.41
1:I:390:ILE:HG23	1:I:391:THR:HG23	2.02	0.41
1:J:351:VAL:HA	1:J:352:PRO:HD3	1.92	0.41
1:C:307:ILE:HD11	1:C:335:LEU:HD11	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.57	0.40
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:A:336:SER:HA	1:A:337:PRO:HD3	1.98	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:259:LEU:HD23	1:E:267:VAL:HG21	2.03	0.40
1:E:326:MET:HE1	1:E:344:GLY:O	2.20	0.40
1:G:426:ALA:O	1:G:430:VAL:HG23	2.21	0.40
1:J:88:ASP:HA	1:J:115:ARG:HH12	1.87	0.40
1:B:407:LEU:HD12	1:B:436:GLN:HG3	2.03	0.40
1:C:315:PHE:CE1	1:C:350:THR:HG21	2.49	0.40
1:E:127:PRO:HD3	1:E:239:VAL:HG13	2.03	0.40
1:G:335:LEU:HD23	1:G:335:LEU:HA	1.97	0.40
1:I:328:TRP:O	1:I:332:ARG:HG2	2.21	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:F:40:GLU:HA	1:F:43:SER:HB2	2.03	0.40
1:J:73:TYR:HA	1:J:76:PHE:HB2	2.02	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%)	47 79
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%)	29	68
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%)	47	79
1	I	438/456 (96%)	412 (94%)	26 (6%)	0	100	100
1	J	438/456 (96%)	414 (94%)	23 (5%)	1 (0%)	47	79
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%)	51	83

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%)	40	71
1	B	354/370 (96%)	347 (98%)	7 (2%)	55	79
1	C	354/370 (96%)	347 (98%)	7 (2%)	55	79
1	D	354/370 (96%)	345 (98%)	9 (2%)	47	75
1	E	354/370 (96%)	345 (98%)	9 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	354/370 (96%)	345 (98%)	9 (2%)	47 75
1	G	354/370 (96%)	345 (98%)	9 (2%)	47 75
1	H	354/370 (96%)	344 (97%)	10 (3%)	43 72
1	I	354/370 (96%)	347 (98%)	7 (2%)	55 79
1	J	354/370 (96%)	346 (98%)	8 (2%)	50 76
1	K	354/370 (96%)	346 (98%)	8 (2%)	50 76
1	L	354/370 (96%)	347 (98%)	7 (2%)	55 79
All	All	4248/4440 (96%)	4147 (98%)	101 (2%)	49 75

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

Sometimes 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 (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	440/456 (96%)	-0.09	1 (0%) 95 91	63, 94, 154, 182	0
1	B	440/456 (96%)	-0.17	0 100 100	72, 106, 155, 220	0
1	C	440/456 (96%)	-0.05	9 (2%) 65 49	68, 122, 214, 270	0
1	D	440/456 (96%)	0.33	34 (7%) 13 8	84, 135, 228, 266	0
1	E	440/456 (96%)	-0.19	0 100 100	74, 114, 155, 200	0
1	F	440/456 (96%)	0.54	54 (12%) 4 3	113, 184, 300, 340	0
1	G	440/456 (96%)	0.24	31 (7%) 16 9	118, 167, 247, 287	0
1	H	440/456 (96%)	0.75	79 (17%) 1 0	87, 129, 332, 377	0
1	I	440/456 (96%)	-0.01	7 (1%) 72 57	90, 132, 168, 218	0
1	J	440/456 (96%)	-0.15	0 100 100	81, 118, 153, 187	0
1	K	440/456 (96%)	0.00	7 (1%) 72 57	93, 156, 213, 271	0
1	L	440/456 (96%)	0.76	77 (17%) 1 1	130, 211, 375, 404	0
All	All	5280/5472 (96%)	0.16	299 (5%) 23 14	63, 134, 291, 404	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	399	SER	12.7
1	H	321	ASP	10.7
1	F	334	ILE	9.8
1	F	359	ARG	9.0
1	D	353	SER	8.8
1	H	354	GLU	8.8
1	H	367	LEU	8.4
1	H	302	PRO	8.1
1	H	301	GLY	7.7
1	L	398	ILE	7.5
1	L	401	SER	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	7.0
1	L	419	GLY	6.9
1	H	320	THR	6.7
1	H	366	ALA	6.7
1	F	420	ALA	6.7
1	L	374	ASN	6.6
1	L	377	ASP	6.2
1	L	320	THR	6.1
1	D	352	PRO	6.0
1	H	363	VAL	6.0
1	F	329	LEU	5.9
1	L	420	ALA	5.9
1	F	421	VAL	5.7
1	G	419	GLY	5.5
1	L	430	VAL	5.4
1	L	344	GLY	5.3
1	H	385	LYS	5.2
1	H	370	ASN	5.2
1	L	378	LYS	5.1
1	L	390	ILE	5.1
1	L	373	PRO	5.1
1	F	350	THR	5.0
1	L	343	LEU	5.0
1	H	319	ASN	5.0
1	H	362	PHE	5.0
1	H	322	LEU	4.9
1	H	373	PRO	4.9
1	F	353	SER	4.9
1	L	319	ASN	4.8
1	L	382	LEU	4.8
1	F	335	LEU	4.7
1	G	421	VAL	4.7
1	L	340	LYS	4.7
1	H	307	ILE	4.7
1	G	399	SER	4.6
1	F	298	ILE	4.6
1	F	419	GLY	4.5
1	H	406	ALA	4.5
1	H	364	GLN	4.5
1	L	408	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	L	436	GLN	4.5
1	D	347	PHE	4.5
1	L	380	VAL	4.4
1	L	317	GLY	4.4
1	L	429	LEU	4.4
1	F	300	SER	4.3
1	H	369	GLY	4.3
1	L	418	MET	4.3
1	H	402	TYR	4.3
1	H	347	PHE	4.2
1	G	418	MET	4.2
1	H	386	LEU	4.2
1	H	368	ASN	4.2
1	F	386	LEU	4.2
1	L	427	PHE	4.1
1	G	356	GLY	4.1
1	D	341	GLY	4.1
1	F	418	MET	4.1
1	F	299	PRO	4.0
1	H	324	VAL	4.0
1	D	335	LEU	4.0
1	G	403	SER	4.0
1	H	330	LYS	4.0
1	G	398	ILE	4.0
1	L	388	ARG	4.0
1	H	348	THR	4.0
1	D	355	ARG	3.9
1	L	56	TYR	3.9
1	H	384	ARG	3.9
1	L	421	VAL	3.9
1	L	431	CYS	3.9
1	H	287	LEU	3.8
1	I	120	ALA	3.8
1	L	400	LEU	3.8
1	C	418	MET	3.8
1	L	383	TYR	3.7
1	H	308	ALA	3.7
1	H	358	GLN	3.7
1	F	411	MET	3.6
1	L	55	THR	3.6
1	D	362	PHE	3.6
1	H	434	CYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	G	420	ALA	3.6
1	H	304	LYS	3.6
1	F	399	SER	3.5
1	L	302	PRO	3.5
1	H	298	ILE	3.5
1	G	345	PHE	3.5
1	F	408	ALA	3.5
1	K	216	ILE	3.5
1	F	349	LEU	3.5
1	L	433	THR	3.5
1	L	376	MET	3.5
1	H	351	VAL	3.5
1	L	397	GLU	3.4
1	L	403	SER	3.4
1	D	294	VAL	3.4
1	F	415	TYR	3.4
1	F	338	LEU	3.4
1	L	54	ILE	3.4
1	L	440	SER	3.4
1	L	120	ALA	3.4
1	H	372	ASP	3.4
1	L	21	GLY	3.4
1	H	334	ILE	3.4
1	H	388	ARG	3.3
1	D	350	THR	3.3
1	G	392	PHE	3.3
1	L	27	VAL	3.3
1	L	346	VAL	3.3
1	L	407	LEU	3.3
1	G	404	ALA	3.3
1	F	397	GLU	3.3
1	L	19	ASP	3.3
1	G	354	GLU	3.3
1	K	92	ALA	3.3
1	F	345	PHE	3.2
1	G	381	LYS	3.2
1	F	370	ASN	3.2
1	H	303	LEU	3.2
1	L	318	LYS	3.2
1	G	422	THR	3.2
1	L	305	ALA	3.2
1	L	426	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	290	VAL	3.2
1	I	119	VAL	3.2
1	G	355	ARG	3.2
1	F	347	PHE	3.1
1	G	346	VAL	3.1
1	F	354	GLU	3.1
1	D	340	LYS	3.1
1	D	427	PHE	3.1
1	L	338	LEU	3.1
1	G	319	ASN	3.1
1	H	408	ALA	3.1
1	C	419	GLY	3.1
1	H	371	GLY	3.1
1	H	399	SER	3.1
1	H	382	LEU	3.1
1	D	344	GLY	3.0
1	F	336	SER	3.0
1	F	326	MET	3.0
1	F	362	PHE	3.0
1	G	349	LEU	3.0
1	H	315	PHE	3.0
1	G	342	ILE	2.9
1	K	93	VAL	2.9
1	H	342	ILE	2.9
1	D	319	ASN	2.9
1	H	288	THR	2.9
1	H	375	ASN	2.9
1	H	401	SER	2.8
1	H	437	ILE	2.8
1	H	365	ASN	2.8
1	H	325	LEU	2.8
1	H	403	SER	2.8
1	L	402	TYR	2.8
1	H	314	VAL	2.8
1	D	342	ILE	2.8
1	L	293	TYR	2.8
1	F	377	ASP	2.8
1	L	422	THR	2.8
1	L	294	VAL	2.8
1	D	392	PHE	2.8
1	H	415	TYR	2.8
1	D	304	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	94	LEU	2.8
1	G	377	ASP	2.8
1	L	404	ALA	2.8
1	D	25	PRO	2.7
1	F	367	LEU	2.7
1	D	386	LEU	2.7
1	D	119	VAL	2.7
1	D	415	TYR	2.7
1	D	298	ILE	2.7
1	D	343	LEU	2.7
1	D	348	THR	2.7
1	D	416	ASN	2.7
1	F	427	PHE	2.7
1	H	355	ARG	2.7
1	F	401	SER	2.7
1	L	342	ILE	2.7
1	G	54	ILE	2.6
1	F	352	PRO	2.6
1	L	334	ILE	2.6
1	L	329	LEU	2.6
1	L	381	LYS	2.6
1	H	395	ALA	2.6
1	G	350	THR	2.6
1	F	346	VAL	2.6
1	H	379	ALA	2.6
1	L	209	PHE	2.5
1	L	311	LEU	2.5
1	L	22	THR	2.5
1	H	326	MET	2.5
1	F	116	ILE	2.5
1	L	341	GLY	2.5
1	H	341	GLY	2.5
1	D	351	VAL	2.5
1	F	379	ALA	2.5
1	H	422	THR	2.4
1	D	297	ILE	2.4
1	L	300	SER	2.4
1	G	384	ARG	2.4
1	H	360	ARG	2.4
1	F	391	THR	2.4
1	H	295	LEU	2.4
1	F	89	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	247	ALA	2.4
1	L	107	TYR	2.4
1	C	377	ASP	2.4
1	K	59	ARG	2.4
1	K	118	ALA	2.4
1	D	354	GLU	2.4
1	A	400	LEU	2.4
1	C	396	LYS	2.4
1	F	358	GLN	2.3
1	H	294	VAL	2.3
1	H	292	THR	2.3
1	F	435	GLU	2.3
1	L	306	GLU	2.3
1	G	353	SER	2.3
1	I	221	LEU	2.3
1	G	56	TYR	2.3
1	G	411	MET	2.3
1	H	433	THR	2.3
1	D	325	LEU	2.3
1	F	390	ILE	2.3
1	D	393	HIS	2.3
1	F	295	LEU	2.3
1	G	400	LEU	2.3
1	F	417	ARG	2.3
1	C	373	PRO	2.3
1	G	347	PHE	2.3
1	D	349	LEU	2.3
1	F	381	LYS	2.3
1	H	414	ILE	2.3
1	H	335	LEU	2.3
1	L	411	MET	2.2
1	C	382	LEU	2.2
1	H	346	VAL	2.2
1	L	26	VAL	2.2
1	L	118	ALA	2.2
1	L	386	LEU	2.2
1	L	414	ILE	2.2
1	H	345	PHE	2.2
1	C	384	ARG	2.2
1	H	425	VAL	2.2
1	G	440	SER	2.2
1	H	374	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	396	LYS	2.2
1	F	307	ILE	2.2
1	C	388	ARG	2.2
1	F	90	GLN	2.2
1	L	384	ARG	2.2
1	F	343	LEU	2.2
1	H	283	LYS	2.2
1	G	405	GLY	2.2
1	I	174	LEU	2.2
1	L	325	LEU	2.2
1	F	403	SER	2.2
1	F	333	PRO	2.2
1	L	391	THR	2.2
1	D	320	THR	2.1
1	F	389	GLU	2.1
1	F	392	PHE	2.1
1	D	307	ILE	2.1
1	H	289	GLU	2.1
1	H	329	LEU	2.1
1	L	435	GLU	2.1
1	F	373	PRO	2.1
1	D	430	VAL	2.1
1	G	94	LEU	2.1
1	F	369	GLY	2.1
1	K	221	LEU	2.1
1	H	393	HIS	2.1
1	C	374	ASN	2.1
1	H	398	ILE	2.1
1	H	380	VAL	2.0
1	D	424	GLU	2.0
1	L	434	CYS	2.0
1	F	436	GLN	2.0
1	I	220	ALA	2.0
1	L	315	PHE	2.0
1	H	407	LEU	2.0
1	I	274	PHE	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.