Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2024 – 01:41 PM EST

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

This is a 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:

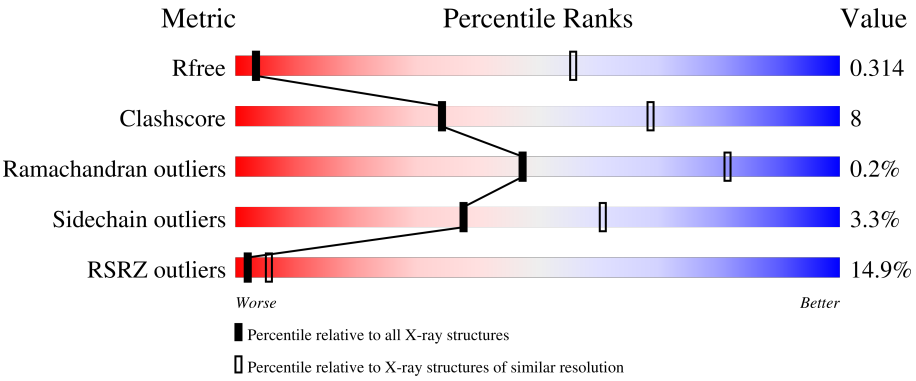
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 7.81 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	456	10% 78% 17%
1	B	456	9% 80% 16%
1	C	456	11% 80% 15%
1	D	456	10% 79% 16%
1	E	456	11% 80% 16%

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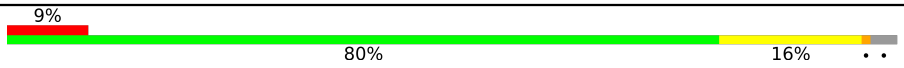
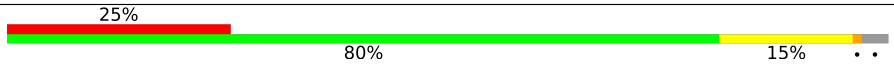
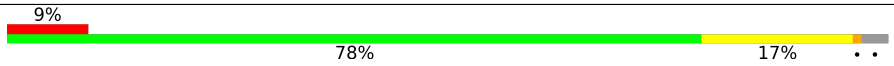
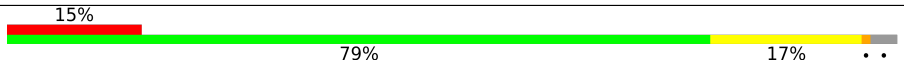
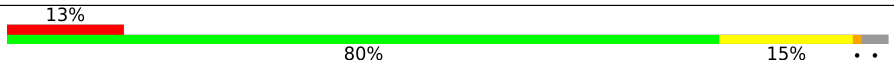
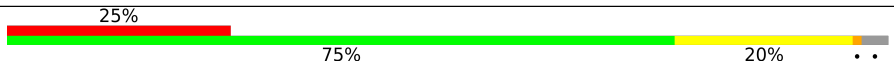
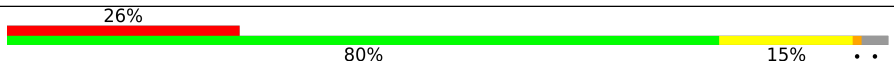
Mol	Chain	Length	Quality of chain
1	F	456	
1	G	456	
1	H	456	
1	I	456	
1	J	456	
1	K	456	
1	L	456	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 40512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera.

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

There are 228 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	280	GLU	-	linker	UNP P03485
A	281	ALA	-	linker	UNP P03485
A	282	GLN	-	linker	UNP P03485
A	283	LYS	-	linker	UNP P03485
A	284	GLN	-	linker	UNP P03485
A	285	LYS	-	linker	UNP P03485
A	448	LEU	-	expression tag	UNP P03485
A	449	GLU	-	expression tag	UNP P03485
A	450	HIS	-	expression tag	UNP P03485
A	451	HIS	-	expression tag	UNP P03485
A	452	HIS	-	expression tag	UNP P03485
A	453	HIS	-	expression tag	UNP P03485
A	454	HIS	-	expression tag	UNP P03485
A	455	HIS	-	expression tag	UNP P03485
B	24	THR	GLN	engineered mutation	UNP P29715
B	51	ALA	TYR	engineered mutation	UNP P29715
B	118	ALA	LYS	engineered mutation	UNP P29715
B	278	ALA	-	linker	UNP P03485
B	279	GLN	-	linker	UNP P03485
B	280	GLU	-	linker	UNP P03485
B	281	ALA	-	linker	UNP P03485
B	282	GLN	-	linker	UNP P03485
B	283	LYS	-	linker	UNP P03485
B	284	GLN	-	linker	UNP P03485
B	285	LYS	-	linker	UNP P03485
B	448	LEU	-	expression tag	UNP P03485
B	449	GLU	-	expression tag	UNP P03485
B	450	HIS	-	expression tag	UNP P03485
B	451	HIS	-	expression tag	UNP P03485
B	452	HIS	-	expression tag	UNP P03485
B	453	HIS	-	expression tag	UNP P03485
B	454	HIS	-	expression tag	UNP P03485
B	455	HIS	-	expression tag	UNP P03485
C	24	THR	GLN	engineered mutation	UNP P29715
C	51	ALA	TYR	engineered mutation	UNP P29715
C	118	ALA	LYS	engineered mutation	UNP P29715
C	278	ALA	-	linker	UNP P03485
C	279	GLN	-	linker	UNP P03485
C	280	GLU	-	linker	UNP P03485
C	281	ALA	-	linker	UNP P03485
C	282	GLN	-	linker	UNP P03485
C	283	LYS	-	linker	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
C	284	GLN	-	linker	UNP P03485
C	285	LYS	-	linker	UNP P03485
C	448	LEU	-	expression tag	UNP P03485
C	449	GLU	-	expression tag	UNP P03485
C	450	HIS	-	expression tag	UNP P03485
C	451	HIS	-	expression tag	UNP P03485
C	452	HIS	-	expression tag	UNP P03485
C	453	HIS	-	expression tag	UNP P03485
C	454	HIS	-	expression tag	UNP P03485
C	455	HIS	-	expression tag	UNP P03485
D	24	THR	GLN	engineered mutation	UNP P29715
D	51	ALA	TYR	engineered mutation	UNP P29715
D	118	ALA	LYS	engineered mutation	UNP P29715
D	278	ALA	-	linker	UNP P03485
D	279	GLN	-	linker	UNP P03485
D	280	GLU	-	linker	UNP P03485
D	281	ALA	-	linker	UNP P03485
D	282	GLN	-	linker	UNP P03485
D	283	LYS	-	linker	UNP P03485
D	284	GLN	-	linker	UNP P03485
D	285	LYS	-	linker	UNP P03485
D	448	LEU	-	expression tag	UNP P03485
D	449	GLU	-	expression tag	UNP P03485
D	450	HIS	-	expression tag	UNP P03485
D	451	HIS	-	expression tag	UNP P03485
D	452	HIS	-	expression tag	UNP P03485
D	453	HIS	-	expression tag	UNP P03485
D	454	HIS	-	expression tag	UNP P03485
D	455	HIS	-	expression tag	UNP P03485
E	24	THR	GLN	engineered mutation	UNP P29715
E	51	ALA	TYR	engineered mutation	UNP P29715
E	118	ALA	LYS	engineered mutation	UNP P29715
E	278	ALA	-	linker	UNP P03485
E	279	GLN	-	linker	UNP P03485
E	280	GLU	-	linker	UNP P03485
E	281	ALA	-	linker	UNP P03485
E	282	GLN	-	linker	UNP P03485
E	283	LYS	-	linker	UNP P03485
E	284	GLN	-	linker	UNP P03485
E	285	LYS	-	linker	UNP P03485
E	448	LEU	-	expression tag	UNP P03485
E	449	GLU	-	expression tag	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
E	450	HIS	-	expression tag	UNP P03485
E	451	HIS	-	expression tag	UNP P03485
E	452	HIS	-	expression tag	UNP P03485
E	453	HIS	-	expression tag	UNP P03485
E	454	HIS	-	expression tag	UNP P03485
E	455	HIS	-	expression tag	UNP P03485
F	24	THR	GLN	engineered mutation	UNP P29715
F	51	ALA	TYR	engineered mutation	UNP P29715
F	118	ALA	LYS	engineered mutation	UNP P29715
F	278	ALA	-	linker	UNP P03485
F	279	GLN	-	linker	UNP P03485
F	280	GLU	-	linker	UNP P03485
F	281	ALA	-	linker	UNP P03485
F	282	GLN	-	linker	UNP P03485
F	283	LYS	-	linker	UNP P03485
F	284	GLN	-	linker	UNP P03485
F	285	LYS	-	linker	UNP P03485
F	448	LEU	-	expression tag	UNP P03485
F	449	GLU	-	expression tag	UNP P03485
F	450	HIS	-	expression tag	UNP P03485
F	451	HIS	-	expression tag	UNP P03485
F	452	HIS	-	expression tag	UNP P03485
F	453	HIS	-	expression tag	UNP P03485
F	454	HIS	-	expression tag	UNP P03485
F	455	HIS	-	expression tag	UNP P03485
G	24	THR	GLN	engineered mutation	UNP P29715
G	51	ALA	TYR	engineered mutation	UNP P29715
G	118	ALA	LYS	engineered mutation	UNP P29715
G	278	ALA	-	linker	UNP P03485
G	279	GLN	-	linker	UNP P03485
G	280	GLU	-	linker	UNP P03485
G	281	ALA	-	linker	UNP P03485
G	282	GLN	-	linker	UNP P03485
G	283	LYS	-	linker	UNP P03485
G	284	GLN	-	linker	UNP P03485
G	285	LYS	-	linker	UNP P03485
G	448	LEU	-	expression tag	UNP P03485
G	449	GLU	-	expression tag	UNP P03485
G	450	HIS	-	expression tag	UNP P03485
G	451	HIS	-	expression tag	UNP P03485
G	452	HIS	-	expression tag	UNP P03485
G	453	HIS	-	expression tag	UNP P03485

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Chain	Residue	Modelled	Actual	Comment	Reference
G	454	HIS	-	expression tag	UNP P03485
G	455	HIS	-	expression tag	UNP P03485
H	24	THR	GLN	engineered mutation	UNP P29715
H	51	ALA	TYR	engineered mutation	UNP P29715
H	118	ALA	LYS	engineered mutation	UNP P29715
H	278	ALA	-	linker	UNP P03485
H	279	GLN	-	linker	UNP P03485
H	280	GLU	-	linker	UNP P03485
H	281	ALA	-	linker	UNP P03485
H	282	GLN	-	linker	UNP P03485
H	283	LYS	-	linker	UNP P03485
H	284	GLN	-	linker	UNP P03485
H	285	LYS	-	linker	UNP P03485
H	448	LEU	-	expression tag	UNP P03485
H	449	GLU	-	expression tag	UNP P03485
H	450	HIS	-	expression tag	UNP P03485
H	451	HIS	-	expression tag	UNP P03485
H	452	HIS	-	expression tag	UNP P03485
H	453	HIS	-	expression tag	UNP P03485
H	454	HIS	-	expression tag	UNP P03485
H	455	HIS	-	expression tag	UNP P03485
I	24	THR	GLN	engineered mutation	UNP P29715
I	51	ALA	TYR	engineered mutation	UNP P29715
I	118	ALA	LYS	engineered mutation	UNP P29715
I	278	ALA	-	linker	UNP P03485
I	279	GLN	-	linker	UNP P03485
I	280	GLU	-	linker	UNP P03485
I	281	ALA	-	linker	UNP P03485
I	282	GLN	-	linker	UNP P03485
I	283	LYS	-	linker	UNP P03485
I	284	GLN	-	linker	UNP P03485
I	285	LYS	-	linker	UNP P03485
I	448	LEU	-	expression tag	UNP P03485
I	449	GLU	-	expression tag	UNP P03485
I	450	HIS	-	expression tag	UNP P03485
I	451	HIS	-	expression tag	UNP P03485
I	452	HIS	-	expression tag	UNP P03485
I	453	HIS	-	expression tag	UNP P03485
I	454	HIS	-	expression tag	UNP P03485
I	455	HIS	-	expression tag	UNP P03485
J	24	THR	GLN	engineered mutation	UNP P29715
J	51	ALA	TYR	engineered mutation	UNP P29715

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Chain	Residue	Modelled	Actual	Comment	Reference
J	118	ALA	LYS	engineered mutation	UNP P29715
J	278	ALA	-	linker	UNP P03485
J	279	GLN	-	linker	UNP P03485
J	280	GLU	-	linker	UNP P03485
J	281	ALA	-	linker	UNP P03485
J	282	GLN	-	linker	UNP P03485
J	283	LYS	-	linker	UNP P03485
J	284	GLN	-	linker	UNP P03485
J	285	LYS	-	linker	UNP P03485
J	448	LEU	-	expression tag	UNP P03485
J	449	GLU	-	expression tag	UNP P03485
J	450	HIS	-	expression tag	UNP P03485
J	451	HIS	-	expression tag	UNP P03485
J	452	HIS	-	expression tag	UNP P03485
J	453	HIS	-	expression tag	UNP P03485
J	454	HIS	-	expression tag	UNP P03485
J	455	HIS	-	expression tag	UNP P03485
K	24	THR	GLN	engineered mutation	UNP P29715
K	51	ALA	TYR	engineered mutation	UNP P29715
K	118	ALA	LYS	engineered mutation	UNP P29715
K	278	ALA	-	linker	UNP P03485
K	279	GLN	-	linker	UNP P03485
K	280	GLU	-	linker	UNP P03485
K	281	ALA	-	linker	UNP P03485
K	282	GLN	-	linker	UNP P03485
K	283	LYS	-	linker	UNP P03485
K	284	GLN	-	linker	UNP P03485
K	285	LYS	-	linker	UNP P03485
K	448	LEU	-	expression tag	UNP P03485
K	449	GLU	-	expression tag	UNP P03485
K	450	HIS	-	expression tag	UNP P03485
K	451	HIS	-	expression tag	UNP P03485
K	452	HIS	-	expression tag	UNP P03485
K	453	HIS	-	expression tag	UNP P03485
K	454	HIS	-	expression tag	UNP P03485
K	455	HIS	-	expression tag	UNP P03485
L	24	THR	GLN	engineered mutation	UNP P29715
L	51	ALA	TYR	engineered mutation	UNP P29715
L	118	ALA	LYS	engineered mutation	UNP P29715
L	278	ALA	-	linker	UNP P03485
L	279	GLN	-	linker	UNP P03485
L	280	GLU	-	linker	UNP P03485

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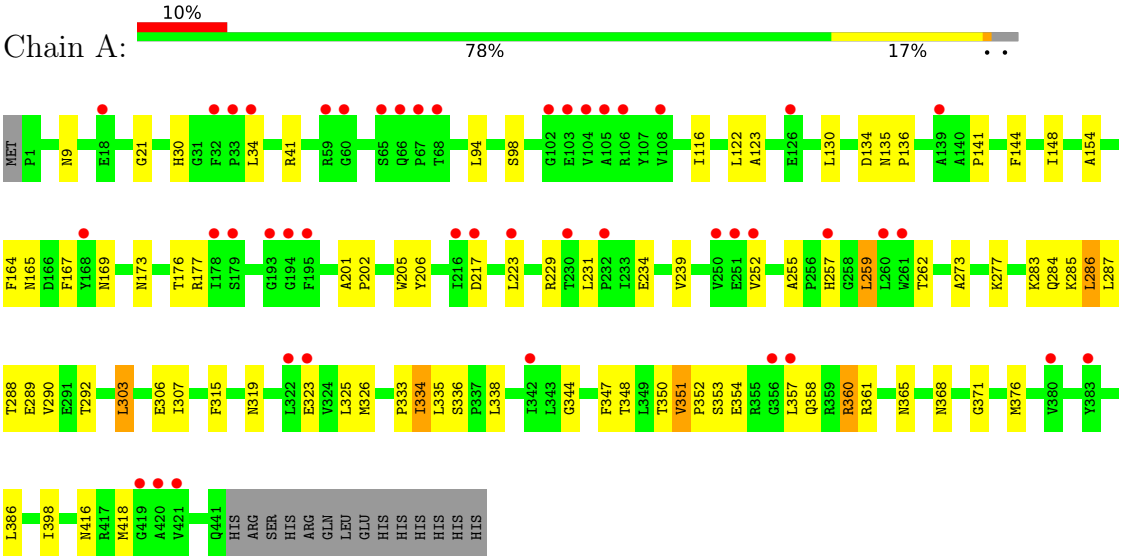
Chain	Residue	Modelled	Actual	Comment	Reference
L	281	ALA	-	linker	UNP P03485
L	282	GLN	-	linker	UNP P03485
L	283	LYS	-	linker	UNP P03485
L	284	GLN	-	linker	UNP P03485
L	285	LYS	-	linker	UNP P03485
L	448	LEU	-	expression tag	UNP P03485
L	449	GLU	-	expression tag	UNP P03485
L	450	HIS	-	expression tag	UNP P03485
L	451	HIS	-	expression tag	UNP P03485
L	452	HIS	-	expression tag	UNP P03485
L	453	HIS	-	expression tag	UNP P03485
L	454	HIS	-	expression tag	UNP P03485
L	455	HIS	-	expression tag	UNP P03485

3 Residue-property plots (i)

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

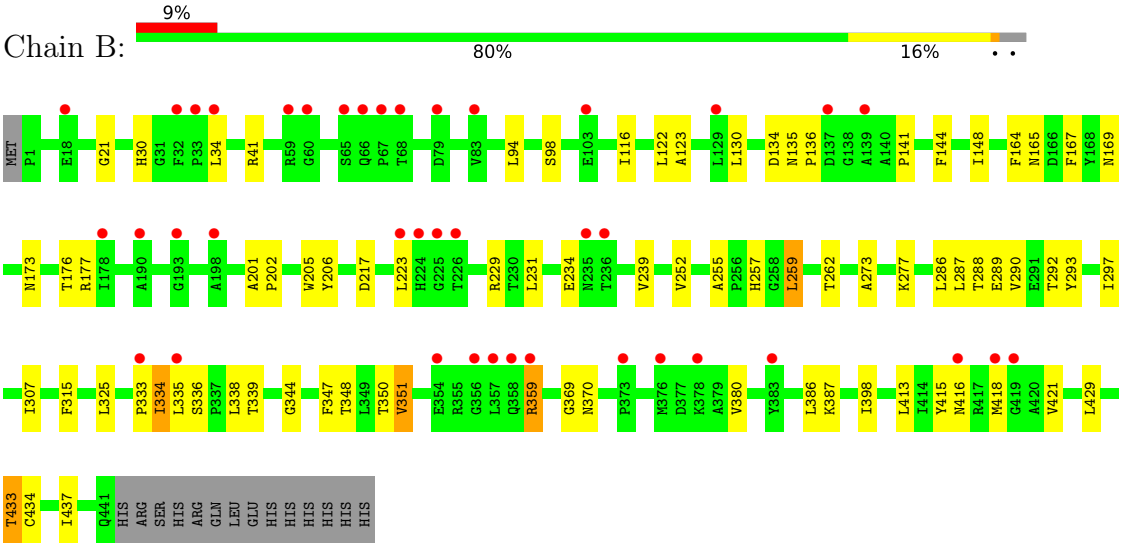
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain A:



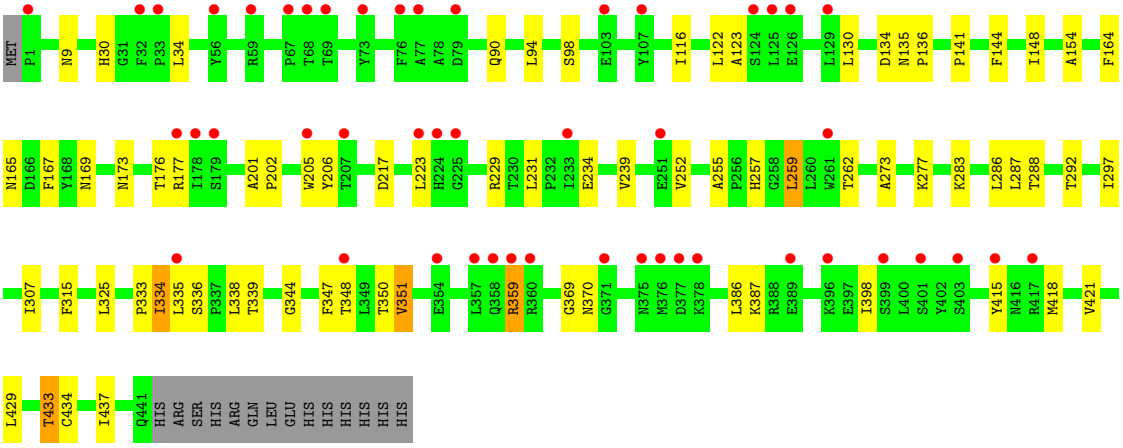
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain B:



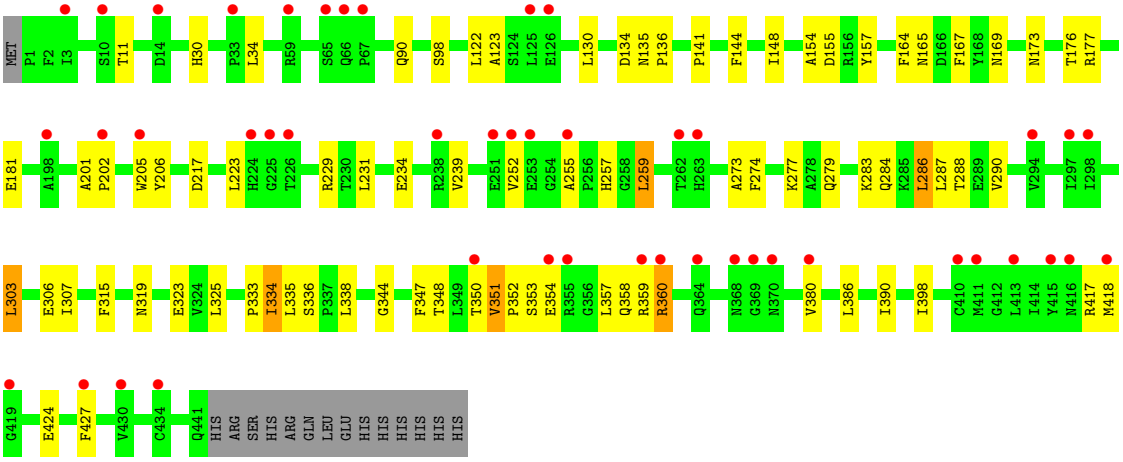
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain C:



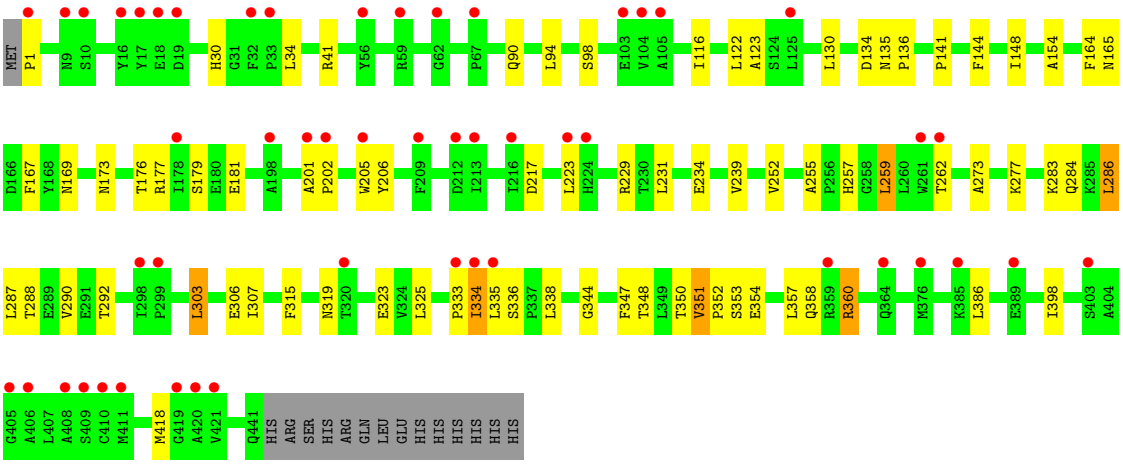
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain D:



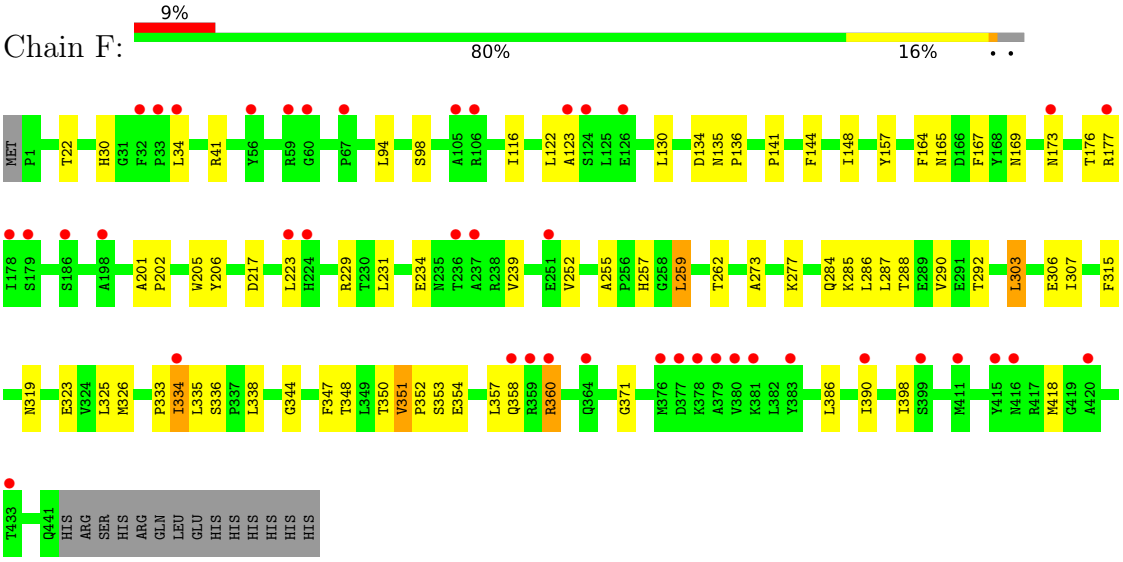
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain E:



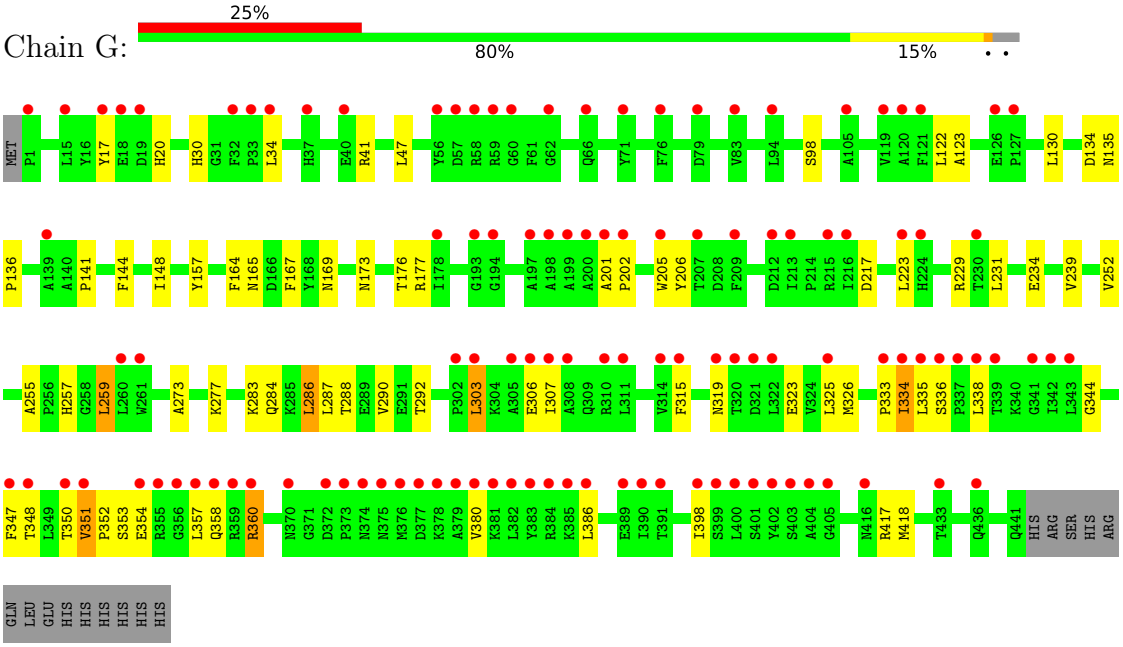
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain F:



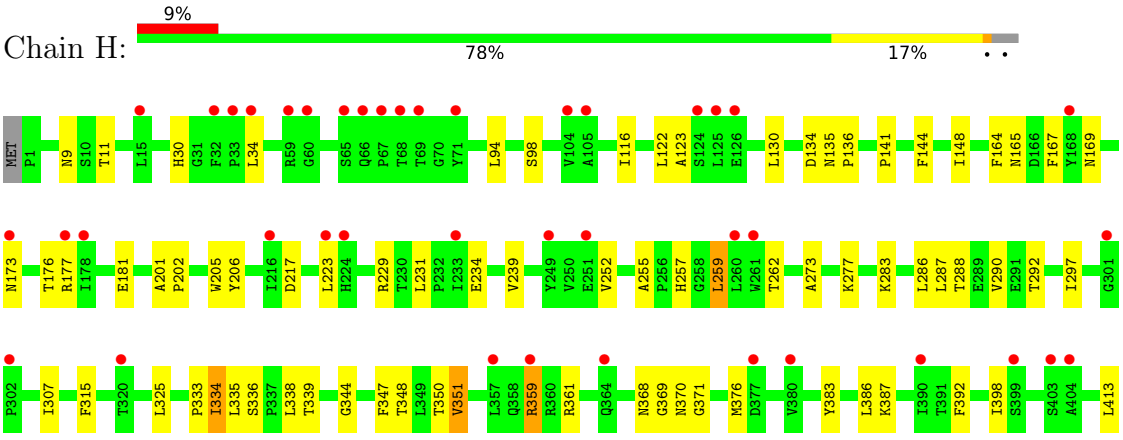
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

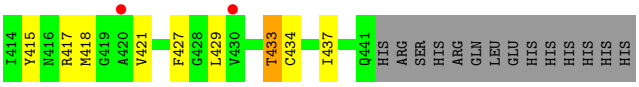
Chain G:



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

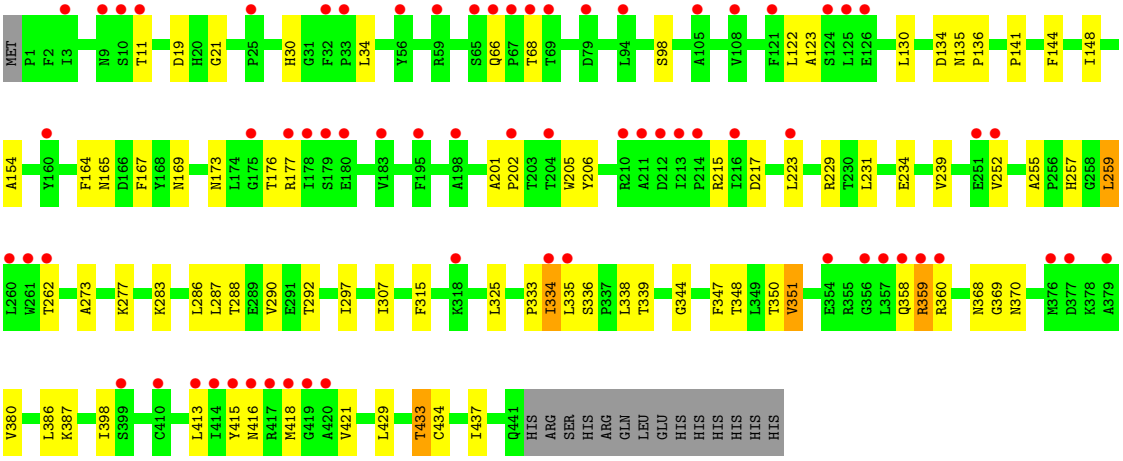
Chain H:





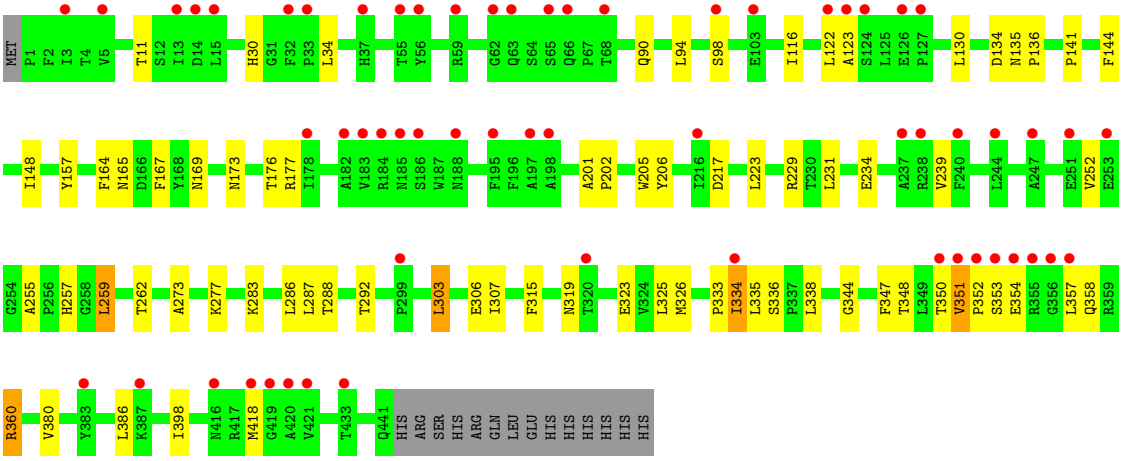
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

Chain I:



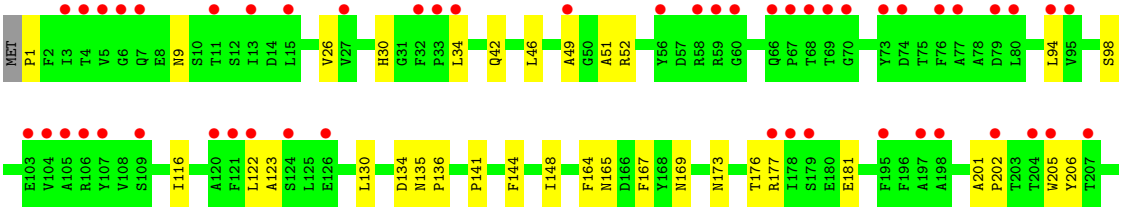
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

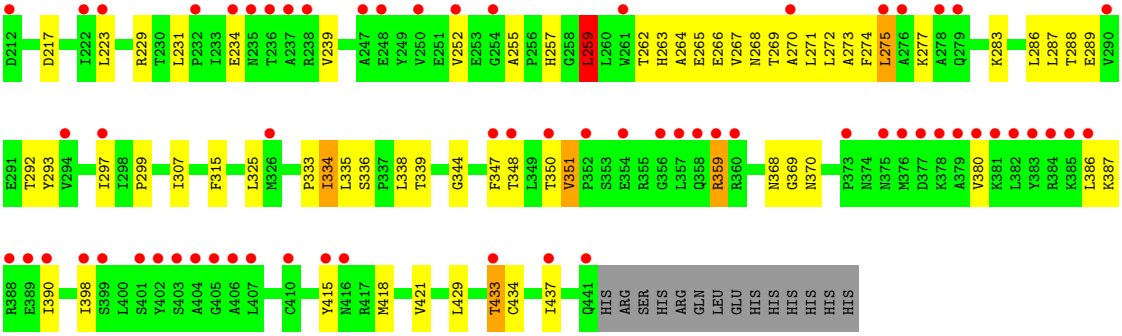
Chain J:



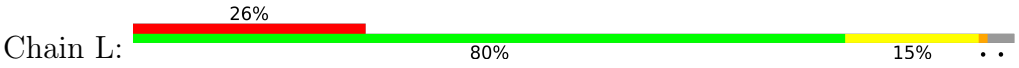
• Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

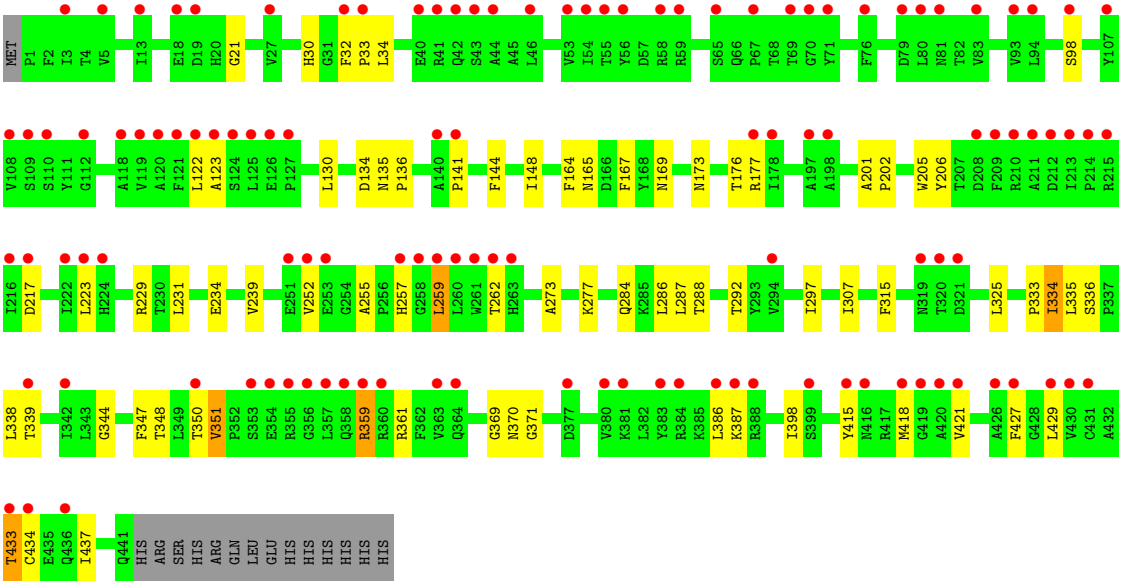
Chain K:





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





4 Data and refinement statistics (i)

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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/3452	0.75	2/4702 (0.0%)
1	B	0.53	0/3452	0.78	2/4702 (0.0%)
1	C	0.51	0/3452	0.77	2/4702 (0.0%)
1	D	0.51	0/3452	0.76	2/4702 (0.0%)
1	E	0.50	0/3452	0.75	2/4702 (0.0%)
1	F	0.51	0/3452	0.76	2/4702 (0.0%)
1	G	0.51	0/3452	0.76	2/4702 (0.0%)
1	H	0.51	0/3452	0.77	2/4702 (0.0%)
1	I	0.52	0/3452	0.78	2/4702 (0.0%)
1	J	0.51	0/3452	0.75	2/4702 (0.0%)
1	K	0.53	0/3452	0.77	2/4702 (0.0%)
1	L	0.52	0/3452	0.78	2/4702 (0.0%)
All	All	0.51	0/41424	0.76	24/56424 (0.0%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	J	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	259	LEU	CA-CB-CG	5.32	127.53	115.30
1	G	259	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	259	LEU	CA-CB-CG	5.31	127.52	115.30
1	C	259	LEU	CA-CB-CG	5.31	127.51	115.30
1	K	259	LEU	CA-CB-CG	5.31	127.51	115.30
1	H	259	LEU	CA-CB-CG	5.30	127.48	115.30
1	I	259	LEU	CA-CB-CG	5.30	127.49	115.30
1	F	259	LEU	CA-CB-CG	5.29	127.48	115.30
1	L	259	LEU	CA-CB-CG	5.29	127.47	115.30
1	E	259	LEU	CA-CB-CG	5.29	127.46	115.30
1	H	359	ARG	CG-CD-NE	5.19	122.69	111.80
1	A	360	ARG	CG-CD-NE	5.13	122.58	111.80
1	B	359	ARG	CG-CD-NE	5.13	122.57	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	360	ARG	CG-CD-NE	5.12	122.55	111.80
1	G	360	ARG	CG-CD-NE	5.12	122.55	111.80
1	L	359	ARG	CG-CD-NE	5.11	122.53	111.80
1	I	359	ARG	CG-CD-NE	5.08	122.47	111.80
1	J	360	ARG	CG-CD-NE	5.08	122.47	111.80
1	K	359	ARG	CG-CD-NE	5.08	122.47	111.80
1	E	360	ARG	CG-CD-NE	5.07	122.44	111.80
1	C	359	ARG	CG-CD-NE	5.06	122.43	111.80
1	D	360	ARG	CG-CD-NE	5.03	122.36	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3376	0	3286	69	0
1	B	3376	0	3286	46	0
1	C	3376	0	3286	44	0
1	D	3376	0	3286	86	0
1	E	3376	0	3286	54	0
1	F	3376	0	3286	53	0
1	G	3376	0	3286	54	0
1	H	3376	0	3286	73	0
1	I	3376	0	3286	67	0
1	J	3376	0	3286	48	0
1	K	3376	0	3286	83	0
1	L	3376	0	3286	61	0
All	All	40512	0	39432	671	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (671) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:MET:SD	1:I:418:MET:SD	2.38	1.21
1:K:264:ALA:O	1:K:268:ASN:HB2	1.39	1.19
1:L:284:GLN:HA	1:L:287:LEU:CD2	1.73	1.18
1:D:287:LEU:HD13	1:D:315:PHE:CD1	1.77	1.18
1:L:284:GLN:O	1:L:287:LEU:HG	1.41	1.16
1:C:287:LEU:HD13	1:C:315:PHE:HB3	1.16	1.13
1:B:418:MET:SD	1:J:418:MET:SD	2.47	1.12
1:I:287:LEU:HD13	1:I:315:PHE:HB3	1.32	1.12
1:K:46:LEU:HD22	1:K:275:LEU:HD22	1.21	1.10
1:D:286:LEU:CD2	1:D:424:GLU:HG3	1.85	1.07
1:I:287:LEU:HD13	1:I:315:PHE:CB	1.85	1.05
1:D:287:LEU:HB3	1:D:315:PHE:CD2	1.93	1.02
1:L:284:GLN:HA	1:L:287:LEU:HD23	1.40	1.02
1:K:266:GLU:O	1:K:269:THR:HG22	1.62	1.00
1:K:46:LEU:CD2	1:K:275:LEU:HD22	1.91	0.99
1:D:287:LEU:HD13	1:D:315:PHE:CG	1.96	0.99
1:G:418:MET:SD	1:K:418:MET:SD	2.60	0.99
1:L:286:LEU:HD13	1:L:427:PHE:HE2	1.26	0.98
1:K:42:GLN:HG3	1:K:268:ASN:OD1	1.66	0.95
1:L:287:LEU:HB2	1:L:315:PHE:CD2	2.02	0.94
1:D:90:GLN:HB3	1:D:390:ILE:HD13	1.47	0.94
1:D:287:LEU:CD1	1:D:315:PHE:HA	1.99	0.93
1:D:287:LEU:HB3	1:D:315:PHE:CG	2.05	0.92
1:E:287:LEU:HD13	1:E:315:PHE:HB3	1.51	0.92
1:A:368:ASN:HB2	1:H:418:MET:HA	1.51	0.91
1:K:287:LEU:HD13	1:K:315:PHE:HB3	1.53	0.90
1:D:90:GLN:HB3	1:D:390:ILE:CD1	2.01	0.90
1:A:371:GLY:HA2	1:H:418:MET:O	1.73	0.89
1:D:287:LEU:HD13	1:D:315:PHE:HA	1.54	0.89
1:I:287:LEU:CD1	1:I:315:PHE:HB3	2.02	0.89
1:F:22:THR:HG22	1:F:390:ILE:HD11	1.56	0.88
1:H:287:LEU:HD13	1:H:315:PHE:HB3	1.56	0.88
1:F:287:LEU:HD13	1:F:315:PHE:HB3	1.54	0.87
1:E:287:LEU:HD13	1:E:315:PHE:CB	2.05	0.86
1:B:287:LEU:HD13	1:B:315:PHE:HB3	1.57	0.86
1:K:264:ALA:O	1:K:268:ASN:CB	2.23	0.86
1:I:287:LEU:HD13	1:I:315:PHE:CG	2.10	0.85
1:K:26:VAL:HG21	1:K:275:LEU:HD13	1.59	0.84
1:L:284:GLN:HA	1:L:287:LEU:HD21	1.60	0.83
1:D:287:LEU:HD22	1:D:315:PHE:CE1	2.13	0.83
1:H:287:LEU:HD13	1:H:315:PHE:CB	2.08	0.82
1:D:286:LEU:HD23	1:D:424:GLU:HG3	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:386:LEU:HD23	1:J:398:ILE:HD11	1.63	0.81
1:G:386:LEU:HD23	1:G:398:ILE:HD11	1.63	0.81
1:L:287:LEU:CB	1:L:315:PHE:CD2	2.63	0.81
1:L:386:LEU:HD23	1:L:398:ILE:HD11	1.63	0.81
1:A:386:LEU:HD23	1:A:398:ILE:HD11	1.63	0.81
1:I:288:THR:O	1:I:292:THR:HG23	1.81	0.80
1:E:386:LEU:HD23	1:E:398:ILE:HD11	1.63	0.80
1:D:386:LEU:HD23	1:D:398:ILE:HD11	1.63	0.80
1:F:386:LEU:HD23	1:F:398:ILE:HD11	1.63	0.80
1:H:386:LEU:HD23	1:H:398:ILE:HD11	1.63	0.80
1:B:288:THR:O	1:B:292:THR:HG23	1.82	0.79
1:F:287:LEU:HD13	1:F:315:PHE:CB	2.11	0.79
1:I:215:ARG:NH2	1:K:299:PRO:HG3	1.98	0.79
1:I:386:LEU:HD23	1:I:398:ILE:HD11	1.63	0.79
1:C:386:LEU:HD23	1:C:398:ILE:HD11	1.63	0.79
1:L:284:GLN:O	1:L:287:LEU:CG	2.29	0.79
1:B:386:LEU:HD23	1:B:398:ILE:HD11	1.63	0.78
1:K:263:HIS:HB3	1:K:266:GLU:HB2	1.66	0.78
1:K:386:LEU:HD23	1:K:398:ILE:HD11	1.63	0.78
1:D:287:LEU:HD13	1:D:315:PHE:CA	2.13	0.78
1:I:287:LEU:HB3	1:I:315:PHE:CD2	2.19	0.78
1:L:286:LEU:HD13	1:L:427:PHE:CE2	2.15	0.78
1:A:361:ARG:HH11	1:H:417:ARG:NH1	1.81	0.77
1:D:286:LEU:HG	1:D:427:PHE:CD2	2.19	0.77
1:K:288:THR:O	1:K:292:THR:HG23	1.85	0.77
1:D:287:LEU:HD13	1:D:315:PHE:CB	2.14	0.76
1:K:49:ALA:HB2	1:K:272:LEU:HD21	1.66	0.76
1:K:51:ALA:HB2	1:K:275:LEU:HD11	1.67	0.76
1:C:418:MET:SD	1:E:418:MET:SD	2.84	0.76
1:A:418:MET:O	1:H:371:GLY:HA2	1.86	0.75
1:K:223:LEU:HD21	1:K:267:VAL:HG22	1.68	0.75
1:G:287:LEU:HD13	1:G:315:PHE:HB3	1.69	0.74
1:H:9:ASN:ND2	1:I:21:GLY:O	2.20	0.74
1:H:344:GLY:O	1:H:348:THR:HG23	1.88	0.73
1:F:344:GLY:O	1:F:348:THR:HG23	1.88	0.73
1:L:287:LEU:HD12	1:L:288:THR:N	2.03	0.73
1:I:344:GLY:O	1:I:348:THR:HG23	1.88	0.73
1:A:287:LEU:HD13	1:A:315:PHE:HB3	1.71	0.73
1:A:361:ARG:HD2	1:H:417:ARG:CZ	2.19	0.73
1:B:289:GLU:HG2	1:B:293:TYR:CE2	2.23	0.73
1:D:287:LEU:CD1	1:D:315:PHE:CD1	2.67	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:344:GLY:O	1:J:348:THR:HG23	1.89	0.73
1:C:30:HIS:CE1	1:C:34:LEU:O	2.42	0.73
1:B:30:HIS:CE1	1:B:34:LEU:O	2.42	0.72
1:B:344:GLY:O	1:B:348:THR:HG23	1.88	0.72
1:E:30:HIS:CE1	1:E:34:LEU:O	2.42	0.72
1:E:344:GLY:O	1:E:348:THR:HG23	1.89	0.72
1:F:30:HIS:CE1	1:F:34:LEU:O	2.43	0.72
1:H:30:HIS:CE1	1:H:34:LEU:O	2.43	0.72
1:L:344:GLY:O	1:L:348:THR:HG23	1.88	0.72
1:I:30:HIS:CE1	1:I:34:LEU:O	2.43	0.72
1:A:30:HIS:CE1	1:A:34:LEU:O	2.43	0.72
1:D:344:GLY:O	1:D:348:THR:HG23	1.89	0.72
1:G:30:HIS:CE1	1:G:34:LEU:O	2.42	0.72
1:K:30:HIS:CE1	1:K:34:LEU:O	2.42	0.72
1:C:344:GLY:O	1:C:348:THR:HG23	1.88	0.72
1:J:30:HIS:CE1	1:J:34:LEU:O	2.42	0.72
1:L:30:HIS:CE1	1:L:34:LEU:O	2.43	0.72
1:K:259:LEU:HG	1:K:267:VAL:HG21	1.71	0.72
1:K:344:GLY:O	1:K:348:THR:HG23	1.88	0.72
1:G:344:GLY:O	1:G:348:THR:HG23	1.89	0.71
1:A:344:GLY:O	1:A:348:THR:HG23	1.89	0.71
1:D:30:HIS:CE1	1:D:34:LEU:O	2.42	0.71
1:C:287:LEU:HD13	1:C:315:PHE:CB	2.10	0.71
1:H:286:LEU:HD13	1:H:290:VAL:CG2	2.20	0.71
1:D:273:ALA:O	1:D:277:LYS:HG2	1.91	0.71
1:L:287:LEU:HB2	1:L:315:PHE:HD2	1.55	0.70
1:D:319:ASN:HA	1:D:352:PRO:HG2	1.74	0.70
1:A:371:GLY:O	1:H:383:TYR:HE2	1.73	0.70
1:H:286:LEU:CD1	1:H:427:PHE:CD2	2.75	0.70
1:B:273:ALA:O	1:B:277:LYS:HG3	1.92	0.70
1:B:289:GLU:HG2	1:B:293:TYR:HE2	1.57	0.70
1:G:319:ASN:HA	1:G:352:PRO:HG2	1.74	0.70
1:J:319:ASN:HA	1:J:352:PRO:HG2	1.74	0.69
1:D:417:ARG:O	1:I:368:ASN:ND2	2.26	0.69
1:E:319:ASN:HA	1:E:352:PRO:HG2	1.74	0.69
1:A:319:ASN:HA	1:A:352:PRO:HG2	1.74	0.68
1:D:287:LEU:CD1	1:D:315:PHE:CA	2.67	0.68
1:A:376:MET:CE	1:H:413:LEU:HD22	2.23	0.68
1:C:288:THR:O	1:C:292:THR:HG23	1.93	0.68
1:L:284:GLN:C	1:L:287:LEU:HG	2.14	0.68
1:F:319:ASN:HA	1:F:352:PRO:HG2	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:MET:HE2	1:H:376:MET:SD	2.34	0.67
1:G:157:TYR:HB3	1:H:181:GLU:HB3	1.77	0.67
1:H:286:LEU:HD13	1:H:290:VAL:HG23	1.77	0.66
1:F:273:ALA:O	1:F:277:LYS:HG3	1.94	0.66
1:E:287:LEU:CD1	1:E:315:PHE:HB3	2.25	0.66
1:K:286:LEU:HD13	1:K:286:LEU:C	2.17	0.66
1:E:154:ALA:O	1:F:41:ARG:NH2	2.27	0.65
1:I:215:ARG:HH22	1:K:299:PRO:HG3	1.60	0.65
1:K:26:VAL:HG21	1:K:275:LEU:CD1	2.24	0.65
1:D:286:LEU:O	1:D:290:VAL:HG23	1.97	0.65
1:H:286:LEU:HD12	1:H:427:PHE:CD2	2.32	0.65
1:A:9:ASN:ND2	1:B:21:GLY:O	2.26	0.64
1:D:380:VAL:HG21	1:I:380:VAL:HG21	1.79	0.64
1:A:273:ALA:O	1:A:277:LYS:HG3	1.97	0.64
1:G:287:LEU:HD13	1:G:315:PHE:CB	2.28	0.64
1:J:273:ALA:O	1:J:277:LYS:HG3	1.98	0.64
1:D:287:LEU:CD1	1:D:315:PHE:CB	2.76	0.64
1:D:418:MET:HE1	1:I:413:LEU:HD23	1.79	0.64
1:D:287:LEU:HD13	1:D:315:PHE:HD1	1.58	0.64
1:H:273:ALA:O	1:H:277:LYS:HG3	1.98	0.63
1:D:287:LEU:CD1	1:D:315:PHE:CG	2.78	0.63
1:D:286:LEU:HD21	1:D:424:GLU:HG3	1.77	0.63
1:E:273:ALA:O	1:E:277:LYS:HG3	1.98	0.63
1:K:269:THR:HG23	1:K:270:ALA:N	2.13	0.63
1:I:273:ALA:O	1:I:277:LYS:HG3	1.97	0.63
1:F:371:GLY:HA2	1:L:418:MET:O	1.99	0.63
1:J:283:LYS:O	1:J:287:LEU:HG	1.99	0.63
1:L:273:ALA:O	1:L:277:LYS:HG3	1.98	0.63
1:C:273:ALA:O	1:C:277:LYS:HG3	1.99	0.62
1:A:376:MET:HE3	1:H:413:LEU:HD22	1.80	0.62
1:G:283:LYS:O	1:G:287:LEU:HG	1.99	0.62
1:H:286:LEU:O	1:H:290:VAL:HG23	2.00	0.62
1:A:371:GLY:O	1:H:383:TYR:CE2	2.53	0.61
1:H:286:LEU:HD11	1:H:427:PHE:CD2	2.35	0.61
1:H:287:LEU:HB3	1:H:315:PHE:CD2	2.35	0.61
1:F:22:THR:CG2	1:F:390:ILE:HD11	2.31	0.60
1:G:273:ALA:O	1:G:277:LYS:HG3	2.01	0.60
1:K:286:LEU:HD13	1:K:286:LEU:O	2.00	0.60
1:G:17:TYR:CZ	1:I:11:THR:HG22	2.37	0.60
1:G:417:ARG:O	1:K:368:ASN:ND2	2.35	0.59
1:K:273:ALA:O	1:K:277:LYS:HE3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG12	1:A:255:ALA:HB2	1.84	0.59
1:A:286:LEU:O	1:A:290:VAL:HG23	2.02	0.59
1:B:252:VAL:HG12	1:B:255:ALA:HB2	1.85	0.59
1:I:252:VAL:HG12	1:I:255:ALA:HB2	1.85	0.59
1:F:284:GLN:O	1:F:288:THR:HG23	2.02	0.59
1:G:252:VAL:HG12	1:G:255:ALA:HB2	1.84	0.59
1:D:252:VAL:HG12	1:D:255:ALA:HB2	1.85	0.59
1:D:286:LEU:CD2	1:D:424:GLU:CG	2.74	0.59
1:F:287:LEU:CD1	1:F:315:PHE:HB3	2.28	0.59
1:H:252:VAL:HG12	1:H:255:ALA:HB2	1.84	0.59
1:B:416:ASN:ND2	1:J:418:MET:SD	2.69	0.59
1:K:51:ALA:CB	1:K:275:LEU:HD11	2.32	0.59
1:E:333:PRO:O	1:E:334:ILE:HG12	2.03	0.59
1:E:252:VAL:HG12	1:E:255:ALA:HB2	1.85	0.58
1:H:287:LEU:CD1	1:H:315:PHE:HB3	2.32	0.58
1:J:333:PRO:O	1:J:334:ILE:HG12	2.03	0.58
1:J:252:VAL:HG12	1:J:255:ALA:HB2	1.84	0.58
1:E:287:LEU:HB3	1:E:315:PHE:CD2	2.37	0.58
1:F:252:VAL:HG12	1:F:255:ALA:HB2	1.84	0.58
1:F:333:PRO:O	1:F:334:ILE:HG12	2.03	0.58
1:K:252:VAL:HG12	1:K:255:ALA:HB2	1.85	0.58
1:L:252:VAL:HG12	1:L:255:ALA:HB2	1.84	0.58
1:A:154:ALA:O	1:B:41:ARG:NH2	2.35	0.58
1:D:283:LYS:O	1:D:287:LEU:HG	2.04	0.58
1:D:358:GLN:HG3	1:I:360:ARG:NH2	2.18	0.58
1:A:333:PRO:O	1:A:334:ILE:HG12	2.03	0.58
1:A:287:LEU:HD13	1:A:315:PHE:CB	2.33	0.57
1:H:333:PRO:O	1:H:334:ILE:HG12	2.04	0.57
1:C:252:VAL:HG12	1:C:255:ALA:HB2	1.84	0.57
1:I:333:PRO:O	1:I:334:ILE:HG12	2.05	0.57
1:D:333:PRO:O	1:D:334:ILE:HG12	2.03	0.57
1:E:164:PHE:HA	1:E:167:PHE:HB3	1.87	0.57
1:E:360:ARG:HG2	1:E:360:ARG:HH11	1.70	0.57
1:G:333:PRO:O	1:G:334:ILE:HG12	2.03	0.57
1:B:333:PRO:O	1:B:334:ILE:HG12	2.05	0.57
1:G:284:GLN:O	1:G:288:THR:HG23	2.05	0.57
1:L:164:PHE:HA	1:L:167:PHE:HB3	1.87	0.57
1:F:287:LEU:HB3	1:F:315:PHE:CD2	2.39	0.57
1:F:360:ARG:HG2	1:F:360:ARG:HH11	1.70	0.57
1:J:164:PHE:HA	1:J:167:PHE:HB3	1.87	0.57
1:K:283:LYS:O	1:K:287:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:333:PRO:O	1:K:334:ILE:HG12	2.05	0.57
1:C:333:PRO:O	1:C:334:ILE:HG12	2.05	0.57
1:A:284:GLN:O	1:A:288:THR:HG23	2.05	0.57
1:F:164:PHE:HA	1:F:167:PHE:HB3	1.87	0.57
1:I:336:SER:HB3	1:I:339:THR:HG23	1.87	0.57
1:K:164:PHE:HA	1:K:167:PHE:HB3	1.86	0.57
1:D:279:GLN:O	1:D:283:LYS:CB	2.53	0.57
1:D:164:PHE:HA	1:D:167:PHE:HB3	1.86	0.57
1:D:360:ARG:HH11	1:D:360:ARG:HG2	1.70	0.57
1:A:358:GLN:OE1	1:H:361:ARG:HB2	2.05	0.56
1:B:380:VAL:HG21	1:J:380:VAL:HG21	1.87	0.56
1:A:164:PHE:HA	1:A:167:PHE:HB3	1.87	0.56
1:C:164:PHE:HA	1:C:167:PHE:HB3	1.87	0.56
1:C:336:SER:HB3	1:C:339:THR:HG23	1.87	0.56
1:G:360:ARG:HH11	1:G:360:ARG:HG2	1.70	0.56
1:L:333:PRO:O	1:L:334:ILE:HG12	2.04	0.56
1:B:336:SER:HB3	1:B:339:THR:HG23	1.87	0.56
1:K:336:SER:HB3	1:K:339:THR:HG23	1.87	0.56
1:J:360:ARG:HG2	1:J:360:ARG:HH11	1.70	0.56
1:F:285:LYS:HA	1:F:288:THR:OG1	2.05	0.56
1:H:164:PHE:HA	1:H:167:PHE:HB3	1.87	0.56
1:H:287:LEU:HD13	1:H:315:PHE:CG	2.40	0.56
1:I:164:PHE:HA	1:I:167:PHE:HB3	1.87	0.56
1:L:336:SER:HB3	1:L:339:THR:HG23	1.87	0.56
1:B:164:PHE:HA	1:B:167:PHE:HB3	1.87	0.56
1:F:288:THR:O	1:F:292:THR:HG23	2.06	0.56
1:I:283:LYS:O	1:I:287:LEU:HG	2.06	0.56
1:E:284:GLN:O	1:E:288:THR:HG23	2.06	0.55
1:G:164:PHE:HA	1:G:167:PHE:HB3	1.87	0.55
1:A:360:ARG:HG2	1:A:360:ARG:HH11	1.70	0.55
1:D:274:PHE:HA	1:D:277:LYS:CG	2.36	0.55
1:D:157:TYR:HB3	1:E:181:GLU:HB3	1.87	0.55
1:K:49:ALA:CB	1:K:272:LEU:HD21	2.36	0.55
1:K:130:LEU:HB2	1:K:206:TYR:HB2	1.89	0.55
1:K:266:GLU:O	1:K:269:THR:CG2	2.45	0.55
1:K:265:GLU:O	1:K:269:THR:HB	2.07	0.55
1:D:130:LEU:HB2	1:D:206:TYR:HB2	1.89	0.55
1:H:283:LYS:O	1:H:287:LEU:HG	2.06	0.55
1:C:429:LEU:O	1:C:433:THR:HG23	2.07	0.55
1:I:130:LEU:HB2	1:I:206:TYR:HB2	1.89	0.54
1:K:429:LEU:O	1:K:433:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:130:LEU:HB2	1:F:206:TYR:HB2	1.89	0.54
1:F:286:LEU:O	1:F:290:VAL:HG23	2.08	0.54
1:D:284:GLN:O	1:D:288:THR:HG23	2.08	0.54
1:H:336:SER:HB3	1:H:339:THR:HG23	1.87	0.54
1:B:130:LEU:HB2	1:B:206:TYR:HB2	1.89	0.54
1:B:201:ALA:HB3	1:B:202:PRO:HD3	1.90	0.54
1:H:130:LEU:HB2	1:H:206:TYR:HB2	1.89	0.54
1:B:429:LEU:O	1:B:433:THR:HG23	2.08	0.54
1:H:429:LEU:O	1:H:433:THR:HG23	2.08	0.54
1:A:283:LYS:O	1:A:287:LEU:HG	2.08	0.54
1:D:358:GLN:CB	1:I:358:GLN:HB2	2.37	0.54
1:H:286:LEU:HD13	1:H:290:VAL:HG21	1.90	0.54
1:K:223:LEU:CD2	1:K:267:VAL:HG22	2.35	0.54
1:L:130:LEU:HB2	1:L:206:TYR:HB2	1.89	0.54
1:D:274:PHE:HA	1:D:277:LYS:HG2	1.89	0.54
1:K:201:ALA:HB3	1:K:202:PRO:HD3	1.90	0.54
1:C:201:ALA:HB3	1:C:202:PRO:HD3	1.90	0.54
1:E:130:LEU:HB2	1:E:206:TYR:HB2	1.89	0.54
1:D:154:ALA:O	1:E:41:ARG:NH2	2.39	0.53
1:I:201:ALA:HB3	1:I:202:PRO:HD3	1.90	0.53
1:I:429:LEU:O	1:I:433:THR:HG23	2.08	0.53
1:G:130:LEU:HB2	1:G:206:TYR:HB2	1.89	0.53
1:B:359:ARG:NH1	1:B:415:TYR:O	2.39	0.53
1:D:201:ALA:HB3	1:D:202:PRO:HD3	1.90	0.53
1:D:418:MET:CG	1:I:416:ASN:HD22	2.21	0.53
1:G:201:ALA:HB3	1:G:202:PRO:HD3	1.90	0.53
1:H:288:THR:O	1:H:292:THR:HG23	2.07	0.53
1:K:359:ARG:NH1	1:K:415:TYR:O	2.39	0.53
1:L:429:LEU:O	1:L:433:THR:HG23	2.08	0.53
1:A:130:LEU:HB2	1:A:206:TYR:HB2	1.89	0.53
1:A:288:THR:O	1:A:292:THR:HG23	2.08	0.53
1:C:176:THR:HG22	1:C:177:ARG:N	2.24	0.53
1:E:176:THR:HG22	1:E:177:ARG:N	2.24	0.53
1:E:287:LEU:HD13	1:E:315:PHE:CG	2.43	0.53
1:G:288:THR:O	1:G:292:THR:HG23	2.08	0.53
1:C:130:LEU:HB2	1:C:206:TYR:HB2	1.90	0.53
1:F:201:ALA:HB3	1:F:202:PRO:HD3	1.90	0.53
1:I:176:THR:HG22	1:I:177:ARG:N	2.24	0.53
1:A:176:THR:HG22	1:A:177:ARG:N	2.24	0.53
1:A:201:ALA:HB3	1:A:202:PRO:HD3	1.90	0.53
1:B:176:THR:HG22	1:B:177:ARG:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:THR:HG22	1:F:177:ARG:N	2.24	0.53
1:D:176:THR:HG22	1:D:177:ARG:N	2.24	0.53
1:D:274:PHE:O	1:D:277:LYS:HG3	2.09	0.53
1:G:176:THR:HG22	1:G:177:ARG:N	2.24	0.53
1:I:215:ARG:HH22	1:K:299:PRO:CG	2.21	0.53
1:H:201:ALA:HB3	1:H:202:PRO:HD3	1.90	0.53
1:A:418:MET:CE	1:H:376:MET:SD	2.96	0.53
1:G:286:LEU:O	1:G:290:VAL:HG23	2.09	0.53
1:E:286:LEU:O	1:E:290:VAL:HG23	2.09	0.53
1:E:288:THR:O	1:E:292:THR:HG23	2.08	0.52
1:J:130:LEU:HB2	1:J:206:TYR:HB2	1.89	0.52
1:J:201:ALA:HB3	1:J:202:PRO:HD3	1.90	0.52
1:J:288:THR:O	1:J:292:THR:HG23	2.09	0.52
1:L:176:THR:HG22	1:L:177:ARG:N	2.24	0.52
1:E:201:ALA:HB3	1:E:202:PRO:HD3	1.90	0.52
1:F:358:GLN:OE1	1:L:361:ARG:HB2	2.09	0.52
1:J:176:THR:HG22	1:J:177:ARG:N	2.24	0.52
1:K:176:THR:HG22	1:K:177:ARG:N	2.24	0.52
1:L:201:ALA:HB3	1:L:202:PRO:HD3	1.90	0.52
1:D:286:LEU:HG	1:D:427:PHE:HD2	1.71	0.52
1:H:176:THR:HG22	1:H:177:ARG:N	2.24	0.52
1:I:359:ARG:NH1	1:I:415:TYR:O	2.39	0.52
1:K:266:GLU:N	1:K:266:GLU:OE1	2.42	0.52
1:K:289:GLU:O	1:K:293:TYR:HD2	1.92	0.52
1:D:287:LEU:HD22	1:D:315:PHE:CD1	2.44	0.51
1:K:271:LEU:O	1:K:274:PHE:N	2.40	0.51
1:A:41:ARG:NH2	1:C:154:ALA:O	2.43	0.51
1:G:98:SER:HA	1:G:123:ALA:O	2.11	0.51
1:J:98:SER:HA	1:J:123:ALA:O	2.11	0.51
1:K:98:SER:HA	1:K:123:ALA:O	2.11	0.51
1:D:359:ARG:O	1:I:358:GLN:OE1	2.28	0.51
1:L:173:ASN:HD22	1:L:177:ARG:HG3	1.76	0.51
1:A:21:GLY:O	1:C:9:ASN:ND2	2.39	0.51
1:C:98:SER:HA	1:C:123:ALA:O	2.11	0.51
1:B:98:SER:HA	1:B:123:ALA:O	2.11	0.51
1:C:130:LEU:O	1:C:135:ASN:ND2	2.38	0.51
1:F:418:MET:O	1:L:371:GLY:HA2	2.10	0.51
1:G:17:TYR:OH	1:I:11:THR:HG22	2.10	0.51
1:G:173:ASN:HD22	1:G:177:ARG:HG3	1.76	0.51
1:J:157:TYR:HB3	1:K:181:GLU:HB3	1.92	0.51
1:E:98:SER:HA	1:E:123:ALA:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:297:ILE:HD11	1:I:434:CYS:O	2.11	0.51
1:L:297:ILE:HD11	1:L:434:CYS:O	2.11	0.51
1:H:98:SER:HA	1:H:123:ALA:O	2.11	0.50
1:L:130:LEU:O	1:L:135:ASN:ND2	2.38	0.50
1:A:130:LEU:O	1:A:135:ASN:ND2	2.38	0.50
1:C:297:ILE:HD11	1:C:434:CYS:O	2.11	0.50
1:H:173:ASN:HD22	1:H:177:ARG:HG3	1.76	0.50
1:A:173:ASN:HD22	1:A:177:ARG:HG3	1.76	0.50
1:F:98:SER:HA	1:F:123:ALA:O	2.11	0.50
1:I:286:LEU:O	1:I:290:VAL:HG23	2.12	0.50
1:K:173:ASN:HD22	1:K:177:ARG:HG3	1.76	0.50
1:F:173:ASN:HD22	1:F:177:ARG:HG3	1.76	0.50
1:L:287:LEU:CD2	1:L:315:PHE:HB3	2.41	0.50
1:B:297:ILE:HD11	1:B:434:CYS:O	2.11	0.50
1:H:297:ILE:HD11	1:H:434:CYS:O	2.12	0.50
1:I:173:ASN:HD22	1:I:177:ARG:HG3	1.76	0.50
1:J:173:ASN:HD22	1:J:177:ARG:HG3	1.76	0.50
1:K:259:LEU:HG	1:K:267:VAL:CG2	2.38	0.50
1:E:354:GLU:O	1:E:357:LEU:HG	2.12	0.50
1:L:98:SER:HA	1:L:123:ALA:O	2.11	0.50
1:D:354:GLU:O	1:D:357:LEU:HG	2.12	0.50
1:G:130:LEU:O	1:G:135:ASN:ND2	2.38	0.50
1:K:269:THR:CG2	1:K:270:ALA:N	2.74	0.50
1:I:98:SER:HA	1:I:123:ALA:O	2.11	0.50
1:J:354:GLU:O	1:J:357:LEU:HG	2.12	0.50
1:A:98:SER:HA	1:A:123:ALA:O	2.11	0.50
1:A:354:GLU:O	1:A:357:LEU:HG	2.12	0.50
1:B:173:ASN:HD22	1:B:177:ARG:HG3	1.76	0.50
1:D:98:SER:HA	1:D:123:ALA:O	2.11	0.50
1:F:354:GLU:O	1:F:357:LEU:HG	2.12	0.50
1:I:231:LEU:HD12	1:I:257:HIS:HE1	1.77	0.50
1:K:9:ASN:ND2	1:L:21:GLY:O	2.43	0.50
1:F:231:LEU:HD12	1:F:257:HIS:HE1	1.77	0.49
1:J:130:LEU:O	1:J:135:ASN:ND2	2.38	0.49
1:G:41:ARG:NH2	1:I:154:ALA:O	2.44	0.49
1:L:231:LEU:HD12	1:L:257:HIS:HE1	1.78	0.49
1:E:231:LEU:HD12	1:E:257:HIS:HE1	1.77	0.49
1:K:297:ILE:HD11	1:K:434:CYS:O	2.12	0.49
1:B:297:ILE:HD11	1:B:437:ILE:HB	1.95	0.49
1:C:359:ARG:NH1	1:C:415:TYR:O	2.39	0.49
1:D:173:ASN:HD22	1:D:177:ARG:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:LEU:CD2	1:F:223:LEU:HB3	2.43	0.49
1:G:122:LEU:CD2	1:G:223:LEU:HB3	2.42	0.49
1:G:231:LEU:HD12	1:G:257:HIS:HE1	1.77	0.49
1:G:283:LYS:O	1:G:287:LEU:N	2.32	0.49
1:J:122:LEU:CD2	1:J:223:LEU:HB3	2.43	0.49
1:K:122:LEU:CD2	1:K:223:LEU:HB3	2.43	0.49
1:A:361:ARG:NH1	1:H:417:ARG:NH1	2.57	0.49
1:C:173:ASN:HD22	1:C:177:ARG:HG3	1.76	0.49
1:D:122:LEU:CD2	1:D:223:LEU:HB3	2.43	0.49
1:I:297:ILE:HD11	1:I:437:ILE:HB	1.95	0.49
1:J:231:LEU:HD12	1:J:257:HIS:HE1	1.77	0.49
1:C:297:ILE:HD11	1:C:437:ILE:HB	1.94	0.49
1:D:231:LEU:HD12	1:D:257:HIS:HE1	1.77	0.49
1:K:287:LEU:CD1	1:K:315:PHE:HB3	2.36	0.49
1:L:287:LEU:HB3	1:L:315:PHE:CD2	2.43	0.49
1:L:297:ILE:HD11	1:L:437:ILE:HB	1.95	0.49
1:H:130:LEU:O	1:H:135:ASN:ND2	2.38	0.49
1:K:231:LEU:HD12	1:K:257:HIS:HE1	1.77	0.49
1:K:297:ILE:HD11	1:K:437:ILE:HB	1.95	0.49
1:C:122:LEU:CD2	1:C:223:LEU:HB3	2.43	0.49
1:G:354:GLU:O	1:G:357:LEU:HG	2.12	0.49
1:L:122:LEU:CD2	1:L:223:LEU:HB3	2.43	0.49
1:E:173:ASN:HD22	1:E:177:ARG:HG3	1.76	0.48
1:H:122:LEU:CD2	1:H:223:LEU:HB3	2.43	0.48
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.78	0.48
1:A:365:ASN:OD1	1:H:417:ARG:HD2	2.13	0.48
1:C:231:LEU:HD12	1:C:257:HIS:HE1	1.77	0.48
1:H:231:LEU:HD12	1:H:257:HIS:HE1	1.78	0.48
1:H:359:ARG:NH1	1:H:415:TYR:O	2.39	0.48
1:K:52:ARG:CZ	1:K:390:ILE:HD11	2.43	0.48
1:B:122:LEU:CD2	1:B:223:LEU:HB3	2.43	0.48
1:B:413:LEU:HD23	1:J:418:MET:HE1	1.95	0.48
1:K:283:LYS:O	1:K:287:LEU:CB	2.62	0.48
1:E:122:LEU:CD2	1:E:223:LEU:HB3	2.43	0.48
1:H:297:ILE:HD11	1:H:437:ILE:HB	1.95	0.48
1:I:122:LEU:CD2	1:I:223:LEU:HB3	2.43	0.48
1:D:181:GLU:HB3	1:F:157:TYR:HB3	1.95	0.48
1:B:231:LEU:HD12	1:B:257:HIS:HE1	1.78	0.48
1:J:347:PHE:O	1:J:351:VAL:HB	2.14	0.48
1:L:288:THR:O	1:L:292:THR:HG23	2.13	0.48
1:E:283:LYS:O	1:E:287:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:LEU:CD2	1:A:223:LEU:HB3	2.43	0.47
1:E:347:PHE:O	1:E:351:VAL:HB	2.14	0.47
1:H:307:ILE:HD11	1:H:335:LEU:HD11	1.97	0.47
1:K:307:ILE:HD11	1:K:335:LEU:HD11	1.97	0.47
1:A:347:PHE:O	1:A:351:VAL:HB	2.14	0.47
1:D:418:MET:HE1	1:I:413:LEU:CD2	2.43	0.47
1:I:286:LEU:HD13	1:I:290:VAL:HG23	1.96	0.47
1:K:369:GLY:O	1:K:370:ASN:OD1	2.33	0.47
1:L:347:PHE:O	1:L:351:VAL:HB	2.15	0.47
1:C:347:PHE:O	1:C:351:VAL:HB	2.15	0.47
1:D:418:MET:CG	1:I:416:ASN:ND2	2.78	0.47
1:E:173:ASN:ND2	1:E:177:ARG:HG3	2.30	0.47
1:I:173:ASN:ND2	1:I:177:ARG:HG3	2.30	0.47
1:L:359:ARG:NH1	1:L:415:TYR:O	2.39	0.47
1:D:287:LEU:CB	1:D:315:PHE:CG	2.90	0.47
1:F:173:ASN:ND2	1:F:177:ARG:HG3	2.30	0.47
1:F:347:PHE:O	1:F:351:VAL:HB	2.14	0.47
1:I:307:ILE:HD11	1:I:335:LEU:HD11	1.97	0.47
1:K:347:PHE:O	1:K:351:VAL:HB	2.15	0.47
1:B:369:GLY:O	1:B:370:ASN:OD1	2.33	0.47
1:C:173:ASN:ND2	1:C:177:ARG:HG3	2.30	0.47
1:L:307:ILE:HD11	1:L:335:LEU:HD11	1.97	0.47
1:A:173:ASN:ND2	1:A:177:ARG:HG3	2.30	0.47
1:A:307:ILE:HD11	1:A:335:LEU:HD11	1.97	0.47
1:D:303:LEU:HA	1:D:306:GLU:OE1	2.15	0.47
1:G:347:PHE:O	1:G:351:VAL:HB	2.14	0.47
1:C:369:GLY:O	1:C:370:ASN:OD1	2.33	0.47
1:E:303:LEU:HA	1:E:306:GLU:OE1	2.15	0.47
1:I:347:PHE:O	1:I:351:VAL:HB	2.15	0.47
1:J:30:HIS:ND1	1:J:34:LEU:O	2.48	0.47
1:J:307:ILE:HD11	1:J:335:LEU:HD11	1.97	0.47
1:A:303:LEU:HA	1:A:306:GLU:OE1	2.15	0.46
1:B:307:ILE:HD11	1:B:335:LEU:HD11	1.97	0.46
1:E:130:LEU:O	1:E:135:ASN:ND2	2.38	0.46
1:K:283:LYS:O	1:K:287:LEU:N	2.41	0.46
1:C:307:ILE:HD11	1:C:335:LEU:HD11	1.97	0.46
1:D:347:PHE:O	1:D:351:VAL:HB	2.15	0.46
1:F:30:HIS:ND1	1:F:34:LEU:O	2.48	0.46
1:G:173:ASN:ND2	1:G:177:ARG:HG3	2.30	0.46
1:J:303:LEU:HA	1:J:306:GLU:OE1	2.15	0.46
1:C:30:HIS:ND1	1:C:34:LEU:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:HIS:ND1	1:E:34:LEU:O	2.48	0.46
1:H:173:ASN:ND2	1:H:177:ARG:HG3	2.30	0.46
1:J:173:ASN:ND2	1:J:177:ARG:HG3	2.30	0.46
1:L:173:ASN:ND2	1:L:177:ARG:HG3	2.30	0.46
1:H:347:PHE:O	1:H:351:VAL:HB	2.15	0.46
1:D:358:GLN:CB	1:I:358:GLN:CB	2.93	0.46
1:D:30:HIS:ND1	1:D:34:LEU:O	2.48	0.46
1:D:307:ILE:HD11	1:D:335:LEU:HD11	1.97	0.46
1:G:30:HIS:ND1	1:G:34:LEU:O	2.48	0.46
1:G:303:LEU:HA	1:G:306:GLU:OE1	2.15	0.46
1:G:307:ILE:HD11	1:G:335:LEU:HD11	1.97	0.46
1:K:30:HIS:ND1	1:K:34:LEU:O	2.48	0.46
1:K:173:ASN:ND2	1:K:177:ARG:HG3	2.30	0.46
1:B:173:ASN:ND2	1:B:177:ARG:HG3	2.30	0.46
1:F:287:LEU:HD13	1:F:315:PHE:CG	2.50	0.46
1:F:303:LEU:HA	1:F:306:GLU:OE1	2.15	0.46
1:B:30:HIS:ND1	1:B:34:LEU:O	2.48	0.46
1:D:173:ASN:ND2	1:D:177:ARG:HG3	2.30	0.46
1:H:369:GLY:O	1:H:370:ASN:OD1	2.33	0.46
1:L:315:PHE:HE1	1:L:350:THR:HG21	1.81	0.46
1:B:347:PHE:O	1:B:351:VAL:HB	2.15	0.46
1:I:30:HIS:ND1	1:I:34:LEU:O	2.49	0.46
1:L:287:LEU:HB3	1:L:315:PHE:CG	2.51	0.46
1:F:307:ILE:HD11	1:F:335:LEU:HD11	1.97	0.45
1:G:319:ASN:CA	1:G:352:PRO:HG2	2.46	0.45
1:L:284:GLN:CA	1:L:287:LEU:CD2	2.67	0.45
1:C:141:PRO:O	1:C:144:PHE:HB3	2.17	0.45
1:D:141:PRO:O	1:D:144:PHE:HB3	2.17	0.45
1:A:141:PRO:O	1:A:144:PHE:HB3	2.17	0.45
1:B:141:PRO:O	1:B:144:PHE:HB3	2.17	0.45
1:E:307:ILE:HD11	1:E:335:LEU:HD11	1.98	0.45
1:I:369:GLY:O	1:I:370:ASN:OD1	2.33	0.45
1:L:30:HIS:ND1	1:L:34:LEU:O	2.49	0.45
1:A:365:ASN:OD1	1:H:417:ARG:CD	2.65	0.45
1:G:141:PRO:O	1:G:144:PHE:HB3	2.17	0.45
1:H:141:PRO:O	1:H:144:PHE:HB3	2.17	0.45
1:D:130:LEU:O	1:D:135:ASN:ND2	2.38	0.45
1:E:315:PHE:HE1	1:E:350:THR:HG21	1.82	0.45
1:G:283:LYS:O	1:G:287:LEU:CB	2.64	0.45
1:H:30:HIS:ND1	1:H:34:LEU:O	2.48	0.45
1:J:141:PRO:O	1:J:144:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:ND1	1:A:34:LEU:O	2.48	0.45
1:A:315:PHE:HE1	1:A:350:THR:HG21	1.81	0.45
1:B:130:LEU:O	1:B:135:ASN:ND2	2.38	0.45
1:F:141:PRO:O	1:F:144:PHE:HB3	2.17	0.45
1:I:315:PHE:HE1	1:I:350:THR:HG21	1.82	0.45
1:K:315:PHE:HE1	1:K:350:THR:HG21	1.82	0.45
1:L:369:GLY:O	1:L:370:ASN:OD1	2.33	0.45
1:F:319:ASN:CA	1:F:352:PRO:HG2	2.46	0.45
1:H:315:PHE:HE1	1:H:350:THR:HG21	1.82	0.45
1:E:141:PRO:O	1:E:144:PHE:HB3	2.17	0.45
1:A:358:GLN:O	1:A:360:ARG:NH1	2.50	0.45
1:B:122:LEU:HD23	1:B:223:LEU:HB3	1.99	0.45
1:G:122:LEU:HD23	1:G:223:LEU:HB3	1.99	0.45
1:G:315:PHE:HE1	1:G:350:THR:HG21	1.82	0.45
1:D:122:LEU:HD23	1:D:223:LEU:HB3	1.99	0.44
1:E:358:GLN:O	1:E:360:ARG:NH1	2.50	0.44
1:H:122:LEU:HD23	1:H:223:LEU:HB3	1.99	0.44
1:D:319:ASN:CA	1:D:352:PRO:HG2	2.46	0.44
1:I:141:PRO:O	1:I:144:PHE:HB3	2.17	0.44
1:L:287:LEU:HD12	1:L:288:THR:CA	2.47	0.44
1:E:319:ASN:CA	1:E:352:PRO:HG2	2.46	0.44
1:F:315:PHE:HE1	1:F:350:THR:HG21	1.82	0.44
1:K:141:PRO:O	1:K:144:PHE:HB3	2.17	0.44
1:A:361:ARG:HD2	1:H:417:ARG:NH2	2.32	0.44
1:B:286:LEU:O	1:B:290:VAL:HG23	2.18	0.44
1:B:289:GLU:O	1:B:293:TYR:HD2	2.00	0.44
1:G:358:GLN:O	1:G:360:ARG:NH1	2.50	0.44
1:F:358:GLN:O	1:F:360:ARG:NH1	2.50	0.44
1:J:315:PHE:HE1	1:J:350:THR:HG21	1.81	0.44
1:J:358:GLN:O	1:J:360:ARG:NH1	2.50	0.44
1:A:285:LYS:O	1:A:289:GLU:HG3	2.18	0.44
1:C:315:PHE:HE1	1:C:350:THR:HG21	1.82	0.44
1:K:122:LEU:HD23	1:K:223:LEU:HB3	1.99	0.44
1:D:155:ASP:OD2	1:E:179:SER:OG	2.25	0.44
1:D:358:GLN:O	1:D:360:ARG:NH1	2.51	0.44
1:F:122:LEU:HD23	1:F:223:LEU:HB3	1.99	0.43
1:L:141:PRO:O	1:L:144:PHE:HB3	2.17	0.43
1:L:284:GLN:CA	1:L:287:LEU:HD21	2.39	0.43
1:A:122:LEU:HD23	1:A:223:LEU:HB3	2.00	0.43
1:D:315:PHE:HE1	1:D:350:THR:HG21	1.83	0.43
1:E:122:LEU:HD23	1:E:223:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:122:LEU:HD23	1:I:223:LEU:HB3	1.99	0.43
1:J:122:LEU:HD23	1:J:223:LEU:HB3	1.99	0.43
1:K:42:GLN:O	1:K:46:LEU:HG	2.17	0.43
1:D:358:GLN:HB3	1:I:358:GLN:CB	2.48	0.43
1:B:315:PHE:HE1	1:B:350:THR:HG21	1.82	0.43
1:G:169:ASN:HA	1:G:229:ARG:NH1	2.33	0.43
1:I:130:LEU:O	1:I:135:ASN:ND2	2.38	0.43
1:D:90:GLN:HB3	1:D:390:ILE:HD11	1.92	0.43
1:F:130:LEU:O	1:F:135:ASN:ND2	2.38	0.43
1:J:11:THR:HG21	1:K:1:PRO:HG2	2.01	0.43
1:K:130:LEU:O	1:K:135:ASN:ND2	2.38	0.43
1:L:122:LEU:HD23	1:L:223:LEU:HB3	1.99	0.43
1:L:284:GLN:HA	1:L:287:LEU:CG	2.41	0.43
1:C:122:LEU:HD23	1:C:223:LEU:HB3	1.99	0.43
1:G:20:HIS:CE1	1:I:66:GLN:O	2.72	0.43
1:G:47:LEU:HD11	1:I:68:THR:HG21	2.01	0.43
1:J:319:ASN:CA	1:J:352:PRO:HG2	2.46	0.43
1:C:283:LYS:O	1:C:287:LEU:HG	2.19	0.42
1:A:169:ASN:HA	1:A:229:ARG:NH1	2.35	0.42
1:A:319:ASN:CA	1:A:352:PRO:HG2	2.46	0.42
1:D:252:VAL:CG1	1:D:255:ALA:HB2	2.50	0.42
1:K:252:VAL:CG1	1:K:255:ALA:HB2	2.50	0.42
1:A:416:ASN:O	1:H:368:ASN:ND2	2.53	0.42
1:D:144:PHE:CZ	1:D:148:ILE:HD11	2.55	0.42
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.55	0.42
1:E:252:VAL:CG1	1:E:255:ALA:HB2	2.50	0.42
1:J:360:ARG:HG2	1:J:360:ARG:NH1	2.34	0.42
1:B:169:ASN:HA	1:B:229:ARG:NH1	2.35	0.42
1:C:202:PRO:HA	1:C:205:TRP:CD2	2.55	0.42
1:E:134:ASP:C	1:E:136:PRO:HD3	2.40	0.42
1:H:286:LEU:HD21	1:H:392:PHE:CD1	2.55	0.42
1:L:202:PRO:HA	1:L:205:TRP:CD2	2.54	0.42
1:F:202:PRO:HA	1:F:205:TRP:CD2	2.55	0.42
1:I:252:VAL:CG1	1:I:255:ALA:HB2	2.50	0.42
1:L:252:VAL:CG1	1:L:255:ALA:HB2	2.49	0.42
1:D:202:PRO:HA	1:D:205:TRP:CD2	2.55	0.42
1:F:134:ASP:C	1:F:136:PRO:HD3	2.40	0.42
1:I:202:PRO:HA	1:I:205:TRP:CD2	2.54	0.42
1:G:360:ARG:HG2	1:G:360:ARG:NH1	2.34	0.42
1:A:360:ARG:HG2	1:A:360:ARG:NH1	2.34	0.42
1:B:202:PRO:HA	1:B:205:TRP:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:GLU:HB2	1:F:357:LEU:HD11	2.02	0.42
1:J:144:PHE:CZ	1:J:148:ILE:HD11	2.55	0.42
1:K:169:ASN:HA	1:K:229:ARG:NH1	2.35	0.42
1:K:202:PRO:HA	1:K:205:TRP:CD2	2.55	0.42
1:B:134:ASP:C	1:B:136:PRO:HD3	2.40	0.42
1:J:134:ASP:C	1:J:136:PRO:HD3	2.40	0.42
1:A:202:PRO:HA	1:A:205:TRP:CD2	2.54	0.41
1:A:323:GLU:HB2	1:A:357:LEU:HD11	2.02	0.41
1:G:144:PHE:CZ	1:G:148:ILE:HD11	2.55	0.41
1:H:134:ASP:C	1:H:136:PRO:HD3	2.41	0.41
1:H:144:PHE:CZ	1:H:148:ILE:HD11	2.55	0.41
1:I:134:ASP:C	1:I:136:PRO:HD3	2.41	0.41
1:J:169:ASN:HA	1:J:229:ARG:NH1	2.35	0.41
1:K:144:PHE:CZ	1:K:148:ILE:HD11	2.55	0.41
1:A:418:MET:HG2	1:H:368:ASN:CG	2.40	0.41
1:B:144:PHE:CZ	1:B:148:ILE:HD11	2.55	0.41
1:C:169:ASN:HA	1:C:229:ARG:NH1	2.35	0.41
1:D:169:ASN:HA	1:D:229:ARG:NH1	2.35	0.41
1:G:252:VAL:CG1	1:G:255:ALA:HB2	2.49	0.41
1:I:169:ASN:HA	1:I:229:ARG:NH1	2.35	0.41
1:J:202:PRO:HA	1:J:205:TRP:CD2	2.54	0.41
1:F:169:ASN:HA	1:F:229:ARG:NH1	2.35	0.41
1:G:134:ASP:C	1:G:136:PRO:HD3	2.40	0.41
1:H:11:THR:HG23	1:I:19:ASP:HB3	2.02	0.41
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.55	0.41
1:G:202:PRO:HA	1:G:205:TRP:CD2	2.55	0.41
1:G:323:GLU:HB2	1:G:357:LEU:HD11	2.02	0.41
1:I:144:PHE:CZ	1:I:148:ILE:HD11	2.56	0.41
1:J:323:GLU:HB2	1:J:357:LEU:HD11	2.02	0.41
1:K:52:ARG:NH1	1:K:390:ILE:HD11	2.36	0.41
1:L:134:ASP:C	1:L:136:PRO:HD3	2.41	0.41
1:L:297:ILE:CD1	1:L:437:ILE:HB	2.51	0.41
1:B:177:ARG:HD3	1:B:262:THR:O	2.21	0.41
1:C:297:ILE:CD1	1:C:437:ILE:HB	2.50	0.41
1:H:202:PRO:HA	1:H:205:TRP:CD2	2.54	0.41
1:K:263:HIS:O	1:K:266:GLU:HB2	2.21	0.41
1:A:134:ASP:C	1:A:136:PRO:HD3	2.40	0.41
1:C:94:LEU:HG	1:C:116:ILE:HD12	2.03	0.41
1:H:94:LEU:HG	1:H:116:ILE:HD12	2.03	0.41
1:J:252:VAL:CG1	1:J:255:ALA:HB2	2.49	0.41
1:K:94:LEU:HG	1:K:116:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:134:ASP:C	1:K:136:PRO:HD3	2.41	0.41
1:L:169:ASN:HA	1:L:229:ARG:NH1	2.35	0.41
1:D:134:ASP:C	1:D:136:PRO:HD3	2.41	0.41
1:G:326:MET:CE	1:G:347:PHE:HB2	2.51	0.41
1:H:169:ASN:HA	1:H:229:ARG:NH1	2.35	0.41
1:I:177:ARG:HD3	1:I:262:THR:O	2.21	0.41
1:I:297:ILE:CD1	1:I:437:ILE:HB	2.51	0.41
1:J:360:ARG:HH11	1:J:360:ARG:CG	2.34	0.41
1:A:94:LEU:HG	1:A:116:ILE:HD12	2.03	0.41
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.95	0.41
1:E:94:LEU:HG	1:E:116:ILE:HD12	2.03	0.41
1:E:144:PHE:CZ	1:E:148:ILE:HD11	2.55	0.41
1:E:169:ASN:HA	1:E:229:ARG:NH1	2.35	0.41
1:I:286:LEU:HD13	1:I:290:VAL:CG2	2.51	0.41
1:A:177:ARG:HD3	1:A:262:THR:O	2.21	0.41
1:A:361:ARG:HD2	1:H:417:ARG:NH1	2.36	0.41
1:C:144:PHE:CZ	1:C:148:ILE:HD11	2.55	0.41
1:D:286:LEU:HD21	1:D:424:GLU:CG	2.49	0.41
1:E:360:ARG:HG2	1:E:360:ARG:NH1	2.34	0.41
1:G:380:VAL:HG21	1:K:380:VAL:HG21	2.03	0.41
1:H:177:ARG:HD3	1:H:262:THR:O	2.21	0.41
1:J:326:MET:CE	1:J:347:PHE:HB2	2.51	0.41
1:L:144:PHE:CZ	1:L:148:ILE:HD11	2.55	0.41
1:A:360:ARG:HH11	1:A:360:ARG:CG	2.34	0.41
1:E:323:GLU:HB2	1:E:357:LEU:HD11	2.02	0.41
1:J:94:LEU:HG	1:J:116:ILE:HD12	2.03	0.41
1:D:323:GLU:HB2	1:D:357:LEU:HD11	2.02	0.40
1:F:144:PHE:CZ	1:F:148:ILE:HD11	2.55	0.40
1:F:326:MET:CE	1:F:347:PHE:HB2	2.51	0.40
1:H:297:ILE:CD1	1:H:437:ILE:HB	2.51	0.40
1:K:52:ARG:CZ	1:K:390:ILE:CD1	3.00	0.40
1:K:177:ARG:HD3	1:K:262:THR:O	2.21	0.40
1:K:263:HIS:O	1:K:266:GLU:N	2.54	0.40
1:A:358:GLN:OE1	1:H:361:ARG:CB	2.69	0.40
1:C:90:GLN:NE2	1:C:90:GLN:HA	2.37	0.40
1:J:177:ARG:HD3	1:J:262:THR:O	2.21	0.40
1:L:32:PHE:HA	1:L:33:PRO:HA	1.95	0.40
1:L:177:ARG:HD3	1:L:262:THR:O	2.21	0.40
1:B:94:LEU:HG	1:B:116:ILE:HD12	2.03	0.40
1:C:130:LEU:HD12	1:C:130:LEU:HA	1.95	0.40
1:C:134:ASP:C	1:C:136:PRO:HD3	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:THR:HB	1:E:1:PRO:HG3	2.03	0.40
1:E:177:ARG:HD3	1:E:262:THR:O	2.21	0.40
1:G:283:LYS:O	1:G:287:LEU:HB2	2.22	0.40
1:L:286:LEU:HD22	1:L:427:PHE:CD2	2.56	0.40
1:C:177:ARG:HD3	1:C:262:THR:O	2.21	0.40
1:D:360:ARG:HG2	1:D:360:ARG:NH1	2.34	0.40
1:F:94:LEU:HG	1:F:116:ILE:HD12	2.03	0.40
1:F:177:ARG:HD3	1:F:262:THR:O	2.21	0.40
1:F:360:ARG:HH11	1:F:360:ARG:CG	2.34	0.40
1:J:90:GLN:NE2	1:J:90:GLN:HA	2.37	0.40
1:K:297:ILE:CD1	1:K:437:ILE:HB	2.51	0.40
1:A:326:MET:CE	1:A:347:PHE:HB2	2.51	0.40
1:E:90:GLN:NE2	1:E:90:GLN:HA	2.37	0.40
1:E:287:LEU:HD13	1:E:315:PHE:CA	2.50	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	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47 81
1	B	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47 81
1	C	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47 81
1	D	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47 81
1	E	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47 81
1	F	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47 81
1	G	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	47 81
1	H	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47 81
1	I	439/456 (96%)	425 (97%)	13 (3%)	1 (0%)	47 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	47 81
1	K	439/456 (96%)	424 (97%)	14 (3%)	1 (0%)	47 81
1	L	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	47 81
All	All	5268/5472 (96%)	5118 (97%)	138 (3%)	12 (0%)	47 81

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	334	ILE
1	B	334	ILE
1	D	334	ILE
1	F	334	ILE
1	G	334	ILE
1	H	334	ILE
1	I	334	ILE
1	J	334	ILE
1	K	334	ILE
1	L	334	ILE
1	C	334	ILE
1	E	334	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	348/369 (94%)	336 (97%)	12 (3%)	37 60
1	B	348/369 (94%)	337 (97%)	11 (3%)	39 61
1	C	348/369 (94%)	336 (97%)	12 (3%)	37 60
1	D	348/369 (94%)	336 (97%)	12 (3%)	37 60
1	E	348/369 (94%)	336 (97%)	12 (3%)	37 60
1	F	348/369 (94%)	337 (97%)	11 (3%)	39 61
1	G	348/369 (94%)	336 (97%)	12 (3%)	37 60

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

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ASN
1	A	217	ASP
1	A	234	GLU
1	A	239	VAL
1	A	259	LEU
1	A	286	LEU
1	A	303	LEU
1	A	325	LEU
1	A	336	SER
1	A	338	LEU
1	A	351	VAL
1	A	353	SER
1	B	165	ASN
1	B	217	ASP
1	B	234	GLU
1	B	239	VAL
1	B	259	LEU
1	B	325	LEU
1	B	338	LEU
1	B	351	VAL
1	B	387	LYS
1	B	421	VAL
1	B	433	THR
1	C	165	ASN
1	C	217	ASP
1	C	234	GLU
1	C	239	VAL
1	C	259	LEU
1	C	286	LEU
1	C	325	LEU

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Mol	Chain	Res	Type
1	C	338	LEU
1	C	351	VAL
1	C	387	LYS
1	C	421	VAL
1	C	433	THR
1	D	165	ASN
1	D	217	ASP
1	D	234	GLU
1	D	239	VAL
1	D	259	LEU
1	D	286	LEU
1	D	303	LEU
1	D	325	LEU
1	D	336	SER
1	D	338	LEU
1	D	351	VAL
1	D	353	SER
1	E	165	ASN
1	E	217	ASP
1	E	234	GLU
1	E	239	VAL
1	E	259	LEU
1	E	286	LEU
1	E	303	LEU
1	E	325	LEU
1	E	336	SER
1	E	338	LEU
1	E	351	VAL
1	E	353	SER
1	F	165	ASN
1	F	217	ASP
1	F	234	GLU
1	F	239	VAL
1	F	259	LEU
1	F	303	LEU
1	F	325	LEU
1	F	336	SER
1	F	338	LEU
1	F	351	VAL
1	F	353	SER
1	G	165	ASN
1	G	217	ASP

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Mol	Chain	Res	Type
1	G	234	GLU
1	G	239	VAL
1	G	259	LEU
1	G	286	LEU
1	G	303	LEU
1	G	325	LEU
1	G	336	SER
1	G	338	LEU
1	G	351	VAL
1	G	353	SER
1	H	165	ASN
1	H	217	ASP
1	H	234	GLU
1	H	239	VAL
1	H	259	LEU
1	H	325	LEU
1	H	338	LEU
1	H	351	VAL
1	H	387	LYS
1	H	421	VAL
1	H	433	THR
1	I	165	ASN
1	I	217	ASP
1	I	234	GLU
1	I	239	VAL
1	I	259	LEU
1	I	325	LEU
1	I	338	LEU
1	I	351	VAL
1	I	387	LYS
1	I	421	VAL
1	I	433	THR
1	J	165	ASN
1	J	217	ASP
1	J	234	GLU
1	J	239	VAL
1	J	259	LEU
1	J	286	LEU
1	J	303	LEU
1	J	325	LEU
1	J	336	SER
1	J	338	LEU

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Mol	Chain	Res	Type
1	J	351	VAL
1	J	353	SER
1	K	165	ASN
1	K	217	ASP
1	K	234	GLU
1	K	239	VAL
1	K	259	LEU
1	K	275	LEU
1	K	325	LEU
1	K	338	LEU
1	K	351	VAL
1	K	387	LYS
1	K	421	VAL
1	K	433	THR
1	L	165	ASN
1	L	217	ASP
1	L	234	GLU
1	L	239	VAL
1	L	259	LEU
1	L	325	LEU
1	L	338	LEU
1	L	351	VAL
1	L	387	LYS
1	L	421	VAL
1	L	433	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	173	ASN
1	A	188	ASN
1	B	90	GLN
1	B	173	ASN
1	B	188	ASN
1	B	375	ASN
1	C	90	GLN
1	C	173	ASN
1	C	188	ASN
1	C	375	ASN
1	D	173	ASN
1	D	188	ASN

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Mol	Chain	Res	Type
1	E	90	GLN
1	E	173	ASN
1	E	188	ASN
1	F	90	GLN
1	F	173	ASN
1	F	188	ASN
1	G	90	GLN
1	G	173	ASN
1	G	188	ASN
1	H	90	GLN
1	H	173	ASN
1	H	188	ASN
1	H	375	ASN
1	I	90	GLN
1	I	173	ASN
1	I	188	ASN
1	I	375	ASN
1	J	90	GLN
1	J	173	ASN
1	J	188	ASN
1	K	90	GLN
1	K	173	ASN
1	K	188	ASN
1	K	375	ASN
1	L	90	GLN
1	L	173	ASN
1	L	188	ASN
1	L	375	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 monosaccharides 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	441/456 (96%)	0.86	45 (10%) 6 10	120, 209, 300, 386	0
1	B	441/456 (96%)	0.83	40 (9%) 9 11	93, 191, 267, 346	0
1	C	441/456 (96%)	0.88	48 (10%) 5 9	114, 196, 263, 325	0
1	D	441/456 (96%)	0.84	46 (10%) 6 9	110, 223, 370, 443	0
1	E	441/456 (96%)	0.86	51 (11%) 4 8	122, 196, 275, 336	0
1	F	441/456 (96%)	0.77	42 (9%) 8 11	117, 208, 305, 393	0
1	G	441/456 (96%)	1.30	116 (26%) 0 2	142, 284, 420, 498	0
1	H	441/456 (96%)	0.86	43 (9%) 7 10	130, 228, 310, 365	0
1	I	441/456 (96%)	0.96	67 (15%) 2 5	179, 269, 364, 453	0
1	J	441/456 (96%)	0.99	60 (13%) 3 6	127, 225, 323, 448	0
1	K	441/456 (96%)	1.39	116 (26%) 0 2	194, 329, 412, 474	0
1	L	441/456 (96%)	1.36	117 (26%) 0 2	179, 305, 412, 500	0
All	All	5292/5472 (96%)	0.99	791 (14%) 2 5	93, 233, 368, 500	0

All (791) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	GLN	7.3
1	L	120	ALA	7.0
1	K	359	ARG	6.9
1	L	119	VAL	6.7
1	A	33	PRO	6.5
1	K	32	PHE	6.1
1	F	359	ARG	6.0
1	H	67	PRO	5.9
1	B	33	PRO	5.9
1	L	212	ASP	5.8
1	K	33	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	L	123	ALA	5.5
1	G	357	LEU	5.5
1	I	211	ALA	5.5
1	L	223	LEU	5.4
1	J	420	ALA	5.3
1	C	33	PRO	5.1
1	J	419	GLY	5.1
1	G	381	LYS	5.1
1	L	59	ARG	5.0
1	L	320	THR	5.0
1	L	213	ILE	5.0
1	K	357	LEU	5.0
1	G	59	ARG	5.0
1	J	33	PRO	5.0
1	L	94	LEU	5.0
1	F	377	ASP	5.0
1	L	214	PRO	4.9
1	L	211	ALA	4.9
1	L	359	ARG	4.9
1	C	178	ILE	4.8
1	B	67	PRO	4.8
1	K	358	GLN	4.8
1	L	124	SER	4.7
1	K	59	ARG	4.7
1	G	380	VAL	4.7
1	L	178	ILE	4.7
1	G	307	ILE	4.7
1	I	33	PRO	4.7
1	K	3	ILE	4.7
1	H	261	TRP	4.7
1	K	379	ALA	4.6
1	L	215	ARG	4.6
1	L	121	PHE	4.6
1	J	13	ILE	4.5
1	L	55	THR	4.5
1	I	416	ASN	4.5
1	H	178	ILE	4.5
1	A	67	PRO	4.5
1	I	418	MET	4.4
1	L	216	ILE	4.4
1	H	65	SER	4.4
1	K	382	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	L	122	LEU	4.4
1	C	125	LEU	4.3
1	L	5	VAL	4.3
1	I	419	GLY	4.3
1	L	222	ILE	4.3
1	F	33	PRO	4.3
1	K	5	VAL	4.2
1	K	79	ASP	4.2
1	I	67	PRO	4.2
1	L	257	HIS	4.2
1	L	357	LEU	4.1
1	G	359	ARG	4.1
1	H	33	PRO	4.1
1	J	421	VAL	4.1
1	G	377	ASP	4.1
1	C	124	SER	4.1
1	G	382	LEU	4.1
1	G	403	SER	4.1
1	C	359	ARG	4.1
1	J	126	GLU	4.1
1	L	258	GLY	4.1
1	J	65	SER	4.1
1	G	198	ALA	4.0
1	G	376	MET	4.0
1	D	359	ARG	4.0
1	L	118	ALA	4.0
1	I	213	ILE	4.0
1	G	354	GLU	4.0
1	G	333	PRO	4.0
1	A	251	GLU	4.0
1	E	18	GLU	4.0
1	J	124	SER	4.0
1	A	419	GLY	4.0
1	K	198	ALA	4.0
1	G	385	LYS	4.0
1	L	420	ALA	4.0
1	E	33	PRO	3.9
1	G	1	PRO	3.9
1	A	60	GLY	3.9
1	C	179	SER	3.9
1	B	65	SER	3.9
1	K	94	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	J	185	ASN	3.9
1	D	368	ASN	3.9
1	K	67	PRO	3.9
1	K	69	THR	3.9
1	G	338	LEU	3.9
1	A	194	GLY	3.9
1	G	197	ALA	3.8
1	C	67	PRO	3.8
1	F	380	VAL	3.8
1	K	204	THR	3.8
1	L	224	HIS	3.8
1	G	399	SER	3.8
1	H	251	GLU	3.8
1	G	223	LEU	3.8
1	K	399	SER	3.8
1	K	406	ALA	3.7
1	B	66	GLN	3.7
1	C	126	GLU	3.7
1	D	251	GLU	3.7
1	L	56	TYR	3.7
1	B	32	PHE	3.7
1	G	404	ALA	3.7
1	F	379	ALA	3.7
1	K	195	PHE	3.7
1	G	120	ALA	3.7
1	C	68	THR	3.7
1	L	416	ASN	3.7
1	J	14	ASP	3.7
1	L	43	SER	3.6
1	G	384	ARG	3.6
1	K	385	LYS	3.6
1	C	224	HIS	3.6
1	G	402	TYR	3.6
1	C	261	TRP	3.6
1	L	18	GLU	3.6
1	G	17	TYR	3.6
1	H	69	THR	3.6
1	H	59	ARG	3.6
1	L	126	GLU	3.6
1	F	224	HIS	3.6
1	G	33	PRO	3.6
1	I	318	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	212	ASP	3.6
1	L	108	VAL	3.6
1	B	59	ARG	3.6
1	L	79	ASP	3.6
1	K	80	LEU	3.6
1	I	413	LEU	3.6
1	K	376	MET	3.6
1	K	212	ASP	3.5
1	F	178	ILE	3.5
1	K	380	VAL	3.5
1	L	54	ILE	3.5
1	G	358	GLN	3.5
1	I	252	VAL	3.5
1	G	19	ASP	3.5
1	I	59	ARG	3.5
1	A	103	GLU	3.5
1	I	178	ILE	3.5
1	L	321	ASP	3.5
1	A	421	VAL	3.5
1	F	126	GLU	3.5
1	H	224	HIS	3.5
1	B	359	ARG	3.5
1	G	375	ASN	3.5
1	A	230	THR	3.5
1	E	410	CYS	3.4
1	H	104	VAL	3.4
1	F	381	LYS	3.4
1	I	414	ILE	3.4
1	H	377	ASP	3.4
1	G	339	THR	3.4
1	J	238	ARG	3.4
1	K	11	THR	3.4
1	L	434	CYS	3.4
1	J	186	SER	3.4
1	L	262	THR	3.4
1	E	32	PHE	3.4
1	C	225	GLY	3.4
1	C	376	MET	3.4
1	K	354	GLU	3.4
1	F	378	LYS	3.4
1	H	126	GLU	3.4
1	J	299	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	387	LYS	3.4
1	E	178	ILE	3.4
1	I	10	SER	3.4
1	G	212	ASP	3.4
1	J	251	GLU	3.3
1	L	209	PHE	3.3
1	F	358	GLN	3.3
1	K	410	CYS	3.3
1	K	13	ILE	3.3
1	C	77	ALA	3.3
1	K	398	ILE	3.3
1	I	359	ARG	3.3
1	A	193	GLY	3.3
1	B	225	GLY	3.3
1	E	419	GLY	3.3
1	K	120	ALA	3.3
1	A	178	ILE	3.3
1	K	60	GLY	3.3
1	L	355	ARG	3.3
1	G	390	ILE	3.3
1	D	65	SER	3.3
1	L	70	GLY	3.3
1	L	364	GLN	3.3
1	G	56	TYR	3.3
1	A	59	ARG	3.3
1	B	79	ASP	3.2
1	D	252	VAL	3.2
1	H	68	THR	3.2
1	K	386	LEU	3.2
1	D	225	GLY	3.2
1	A	32	PHE	3.2
1	G	119	VAL	3.2
1	K	222	ILE	3.2
1	G	18	GLU	3.2
1	L	253	GLU	3.2
1	J	183	VAL	3.2
1	E	212	ASP	3.2
1	K	223	LEU	3.2
1	C	354	GLU	3.2
1	L	354	GLU	3.2
1	B	224	HIS	3.2
1	J	178	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	379	ALA	3.2
1	G	320	THR	3.2
1	F	124	SER	3.2
1	K	279	GLN	3.2
1	A	18	GLU	3.2
1	G	356	GLY	3.2
1	L	42	GLN	3.2
1	L	261	TRP	3.1
1	J	5	VAL	3.1
1	I	198	ALA	3.1
1	L	386	LEU	3.1
1	L	40	GLU	3.1
1	L	107	TYR	3.1
1	J	354	GLU	3.1
1	L	210	ARG	3.1
1	F	420	ALA	3.1
1	I	179	SER	3.1
1	L	32	PHE	3.1
1	K	121	PHE	3.1
1	L	358	GLN	3.1
1	L	430	VAL	3.1
1	F	416	ASN	3.1
1	B	60	GLY	3.1
1	G	321	ASP	3.1
1	J	383	TYR	3.1
1	K	178	ILE	3.1
1	I	420	ALA	3.1
1	G	383	TYR	3.1
1	J	59	ARG	3.1
1	G	79	ASP	3.0
1	A	223	LEU	3.0
1	L	433	THR	3.0
1	H	320	THR	3.0
1	D	59	ARG	3.0
1	L	112	GLY	3.0
1	D	370	ASN	3.0
1	D	419	GLY	3.0
1	E	224	HIS	3.0
1	I	415	TYR	3.0
1	A	105	ALA	3.0
1	G	303	LEU	3.0
1	K	4	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	261	TRP	3.0
1	L	263	HIS	3.0
1	L	429	LEU	3.0
1	J	182	ALA	3.0
1	D	262	THR	3.0
1	E	209	PHE	3.0
1	D	298	ILE	3.0
1	G	71	TYR	3.0
1	A	217	ASP	3.0
1	L	58	ARG	3.0
1	J	32	PHE	3.0
1	J	353	SER	3.0
1	K	105	ALA	3.0
1	L	259	LEU	3.0
1	J	56	TYR	3.0
1	J	123	ALA	3.0
1	H	177	ARG	2.9
1	K	95	VAL	2.9
1	G	401	SER	2.9
1	G	94	LEU	2.9
1	K	350	THR	2.9
1	A	357	LEU	2.9
1	L	71	TYR	2.9
1	K	106	ARG	2.9
1	J	334	ILE	2.9
1	K	179	SER	2.9
1	G	337	PRO	2.9
1	K	76	PHE	2.9
1	D	369	GLY	2.9
1	D	430	VAL	2.9
1	A	68	THR	2.9
1	L	141	PRO	2.9
1	K	197	ALA	2.9
1	F	105	ALA	2.9
1	B	236	THR	2.9
1	B	235	ASN	2.9
1	G	350	THR	2.9
1	F	360	ARG	2.9
1	G	336	SER	2.9
1	K	27	VAL	2.9
1	L	421	VAL	2.9
1	E	408	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	105	ALA	2.8
1	D	3	ILE	2.8
1	G	302	PRO	2.8
1	C	399	SER	2.8
1	E	334	ILE	2.8
1	F	433	THR	2.8
1	B	419	GLY	2.8
1	D	10	SER	2.8
1	K	103	GLU	2.8
1	K	381	LYS	2.8
1	I	417	ARG	2.8
1	K	294	VAL	2.8
1	K	402	TYR	2.8
1	I	356	GLY	2.8
1	L	109	SER	2.8
1	G	325	LEU	2.8
1	D	360	ARG	2.8
1	D	126	GLU	2.8
1	G	398	ILE	2.8
1	J	350	THR	2.8
1	K	278	ALA	2.8
1	B	68	THR	2.8
1	G	373	PRO	2.8
1	J	253	GLU	2.8
1	I	11	THR	2.8
1	E	202	PRO	2.8
1	I	65	SER	2.8
1	E	213	ILE	2.8
1	K	248	GLU	2.8
1	L	127	PRO	2.8
1	K	416	ASN	2.8
1	C	417	ARG	2.8
1	K	388	ARG	2.8
1	F	198	ALA	2.8
1	I	334	ILE	2.8
1	I	223	LEU	2.7
1	B	416	ASN	2.7
1	C	103	GLU	2.7
1	G	105	ALA	2.7
1	G	319	ASN	2.7
1	I	358	GLN	2.7
1	K	375	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	411	MET	2.7
1	J	352	PRO	2.7
1	K	378	LYS	2.7
1	G	342	ILE	2.7
1	E	223	LEU	2.7
1	L	83	VAL	2.7
1	L	426	ALA	2.7
1	D	297	ILE	2.7
1	G	213	ILE	2.7
1	L	319	ASN	2.7
1	F	376	MET	2.7
1	K	290	VAL	2.7
1	A	65	SER	2.7
1	J	55	THR	2.7
1	C	73	TYR	2.7
1	J	3	ILE	2.7
1	I	210	ARG	2.7
1	G	207	THR	2.7
1	L	44	ALA	2.7
1	J	357	LEU	2.7
1	E	10	SER	2.7
1	E	420	ALA	2.7
1	I	56	TYR	2.7
1	K	202	PRO	2.7
1	I	410	CYS	2.7
1	G	40	GLU	2.7
1	I	68	THR	2.7
1	G	62	GLY	2.7
1	G	405	GLY	2.7
1	K	205	TRP	2.7
1	G	391	THR	2.7
1	K	384	ARG	2.7
1	L	384	ARG	2.7
1	L	399	SER	2.7
1	I	66	GLN	2.7
1	I	216	ILE	2.6
1	A	420	ALA	2.6
1	B	356	GLY	2.6
1	F	236	THR	2.6
1	B	103	GLU	2.6
1	C	32	PHE	2.6
1	I	124	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	125	LEU	2.6
1	G	372	ASP	2.6
1	L	217	ASP	2.6
1	H	399	SER	2.6
1	C	79	ASP	2.6
1	I	108	VAL	2.6
1	E	103	GLU	2.6
1	G	341	GLY	2.6
1	L	13	ILE	2.6
1	K	124	SER	2.6
1	D	255	ALA	2.6
1	F	334	ILE	2.6
1	J	197	ALA	2.6
1	G	335	LEU	2.6
1	L	350	THR	2.6
1	D	354	GLU	2.6
1	I	195	PHE	2.6
1	C	177	ARG	2.6
1	K	15	LEU	2.6
1	G	433	THR	2.6
1	G	202	PRO	2.6
1	L	46	LEU	2.6
1	A	179	SER	2.6
1	G	261	TRP	2.6
1	B	83	VAL	2.6
1	I	105	ALA	2.6
1	K	326	MET	2.6
1	E	19	ASP	2.6
1	D	198	ALA	2.6
1	K	377	ASP	2.6
1	H	124	SER	2.6
1	L	98	SER	2.6
1	L	19	ASP	2.6
1	F	34	LEU	2.6
1	K	235	ASN	2.6
1	E	389	GLU	2.6
1	D	14	ASP	2.6
1	E	364	GLN	2.5
1	L	431	CYS	2.5
1	G	310	ARG	2.5
1	D	416	ASN	2.5
1	F	186	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	68	THR	2.5
1	G	374	ASN	2.5
1	H	66	GLN	2.5
1	E	205	TRP	2.5
1	G	360	ARG	2.5
1	J	433	THR	2.5
1	D	410	CYS	2.5
1	E	1	PRO	2.5
1	E	406	ALA	2.5
1	G	216	ILE	2.5
1	H	223	LEU	2.5
1	L	41	ARG	2.5
1	L	356	GLY	2.5
1	C	389	GLU	2.5
1	H	260	LEU	2.5
1	B	358	GLN	2.5
1	C	223	LEU	2.5
1	C	377	ASP	2.5
1	K	270	ALA	2.5
1	B	34	LEU	2.5
1	D	66	GLN	2.5
1	I	32	PHE	2.5
1	G	379	ALA	2.5
1	A	257	HIS	2.5
1	A	216	ILE	2.5
1	G	83	VAL	2.5
1	J	351	VAL	2.5
1	K	405	GLY	2.5
1	E	201	ALA	2.5
1	K	74	ASP	2.5
1	A	356	GLY	2.5
1	H	168	TYR	2.5
1	H	71	TYR	2.5
1	H	233	ILE	2.5
1	J	63	GLN	2.5
1	J	247	ALA	2.5
1	G	121	PHE	2.5
1	K	68	THR	2.5
1	K	207	THR	2.5
1	H	15	LEU	2.5
1	K	441	GLN	2.5
1	C	69	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	32	PHE	2.5
1	A	126	GLU	2.5
1	E	17	TYR	2.5
1	H	380	VAL	2.5
1	K	407	LEU	2.5
1	C	76	PHE	2.5
1	B	223	LEU	2.5
1	K	70	GLY	2.4
1	L	360	ARG	2.4
1	L	208	ASP	2.4
1	E	216	ILE	2.4
1	A	108	VAL	2.4
1	E	376	MET	2.4
1	F	32	PHE	2.4
1	I	126	GLU	2.4
1	K	347	PHE	2.4
1	L	53	VAL	2.4
1	B	178	ILE	2.4
1	D	224	HIS	2.4
1	K	107	TYR	2.4
1	L	67	PRO	2.4
1	I	357	LEU	2.4
1	J	188	ASN	2.4
1	D	202	PRO	2.4
1	F	237	ALA	2.4
1	G	378	LYS	2.4
1	C	360	ARG	2.4
1	F	415	TYR	2.4
1	J	15	LEU	2.4
1	L	93	VAL	2.4
1	L	294	VAL	2.4
1	L	383	TYR	2.4
1	G	34	LEU	2.4
1	G	139	ALA	2.4
1	I	376	MET	2.4
1	K	275	LEU	2.4
1	K	360	ARG	2.4
1	D	205	TRP	2.4
1	K	77	ALA	2.4
1	L	436	GLN	2.4
1	K	415	TYR	2.4
1	K	404	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	404	ALA	2.4
1	A	383	TYR	2.4
1	K	122	LEU	2.4
1	F	251	GLU	2.4
1	B	193	GLY	2.4
1	H	125	LEU	2.4
1	G	260	LEU	2.4
1	G	209	PHE	2.4
1	G	178	ILE	2.4
1	K	126	GLU	2.4
1	B	129	LEU	2.4
1	G	200	ALA	2.4
1	I	180	GLU	2.4
1	L	418	MET	2.4
1	G	201	ALA	2.4
1	L	65	SER	2.3
1	E	333	PRO	2.3
1	I	261	TRP	2.3
1	G	306	GLU	2.3
1	E	62	GLY	2.3
1	G	348	THR	2.3
1	K	403	SER	2.3
1	D	427	PHE	2.3
1	G	76	PHE	2.3
1	J	244	LEU	2.3
1	L	377	ASP	2.3
1	J	198	ALA	2.3
1	G	311	LEU	2.3
1	G	400	LEU	2.3
1	K	177	ARG	2.3
1	J	195	PHE	2.3
1	F	390	ILE	2.3
1	K	433	THR	2.3
1	F	179	SER	2.3
1	J	66	GLN	2.3
1	J	356	GLY	2.3
1	J	103	GLU	2.3
1	J	418	MET	2.3
1	D	364	GLN	2.3
1	D	413	LEU	2.3
1	D	33	PRO	2.3
1	C	415	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	405	GLY	2.3
1	C	251	GLU	2.3
1	K	348	THR	2.3
1	C	1	PRO	2.3
1	D	67	PRO	2.3
1	F	364	GLN	2.3
1	G	199	ALA	2.3
1	D	411	MET	2.3
1	H	390	ILE	2.3
1	I	335	LEU	2.3
1	H	359	ARG	2.3
1	L	110	SER	2.3
1	G	66	GLN	2.3
1	G	193	GLY	2.3
1	G	416	ASN	2.3
1	K	66	GLN	2.3
1	J	237	ALA	2.3
1	E	125	LEU	2.3
1	I	160	TYR	2.3
1	L	251	GLU	2.3
1	C	403	SER	2.3
1	C	358	GLN	2.3
1	K	109	SER	2.3
1	C	375	ASN	2.3
1	H	173	ASN	2.3
1	I	25	PRO	2.3
1	K	390	ILE	2.3
1	A	104	VAL	2.3
1	E	403	SER	2.3
1	G	315	PHE	2.3
1	I	354	GLU	2.3
1	G	386	LEU	2.2
1	I	94	LEU	2.2
1	J	216	ILE	2.2
1	C	348	THR	2.2
1	I	183	VAL	2.2
1	E	409	SER	2.2
1	H	301	GLY	2.2
1	I	204	THR	2.2
1	I	214	PRO	2.2
1	I	260	LEU	2.2
1	G	37	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	6	GLY	2.2
1	L	27	VAL	2.2
1	L	198	ALA	2.2
1	K	401	SER	2.2
1	L	140	ALA	2.2
1	A	323	GLU	2.2
1	C	357	LEU	2.2
1	E	67	PRO	2.2
1	H	302	PRO	2.2
1	L	76	PHE	2.2
1	A	34	LEU	2.2
1	L	125	LEU	2.2
1	G	389	GLU	2.2
1	I	177	ARG	2.2
1	C	129	LEU	2.2
1	I	377	ASP	2.2
1	L	419	GLY	2.2
1	K	232	PRO	2.2
1	L	381	LYS	2.2
1	B	418	MET	2.2
1	L	380	VAL	2.2
1	K	56	TYR	2.2
1	C	205	TRP	2.2
1	B	18	GLU	2.2
1	K	250	VAL	2.2
1	L	260	LEU	2.2
1	C	371	GLY	2.2
1	E	385	LYS	2.2
1	G	322	LEU	2.2
1	B	226	THR	2.2
1	K	373	PRO	2.2
1	L	197	ALA	2.2
1	E	198	ALA	2.2
1	F	59	ARG	2.2
1	K	7	GLN	2.2
1	K	238	ARG	2.2
1	B	373	PRO	2.2
1	D	253	GLU	2.2
1	G	126	GLU	2.2
1	K	276	ALA	2.2
1	B	376	MET	2.2
1	K	104	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	177	ARG	2.2
1	J	320	THR	2.2
1	D	418	MET	2.2
1	D	350	THR	2.2
1	H	430	VAL	2.2
1	E	299	PRO	2.2
1	K	352	PRO	2.2
1	A	139	ALA	2.2
1	G	343	LEU	2.2
1	H	403	SER	2.2
1	K	383	TYR	2.2
1	K	356	GLY	2.2
1	L	363	VAL	2.2
1	D	434	CYS	2.2
1	E	16	TYR	2.2
1	I	175	GLY	2.2
1	J	184	ARG	2.2
1	C	401	SER	2.2
1	K	437	ILE	2.2
1	L	177	ARG	2.2
1	K	247	ALA	2.2
1	D	355	ARG	2.1
1	G	205	TRP	2.2
1	A	195	PHE	2.1
1	A	250	VAL	2.1
1	C	335	LEU	2.1
1	L	33	PRO	2.1
1	C	207	THR	2.1
1	D	263	HIS	2.1
1	F	173	ASN	2.1
1	H	60	GLY	2.1
1	A	168	TYR	2.1
1	F	399	SER	2.1
1	I	399	SER	2.1
1	B	333	PRO	2.1
1	K	389	GLU	2.1
1	K	297	ILE	2.1
1	B	139	ALA	2.1
1	B	190	ALA	2.1
1	D	238	ARG	2.1
1	G	58	ARG	2.1
1	G	370	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	80	LEU	2.1
1	C	233	ILE	2.1
1	C	378	LYS	2.1
1	G	60	GLY	2.1
1	I	262	THR	2.1
1	G	127	PRO	2.1
1	G	314	VAL	2.1
1	C	59	ARG	2.1
1	D	380	VAL	2.1
1	A	342	ILE	2.1
1	B	335	LEU	2.1
1	J	240	PHE	2.1
1	K	49	ALA	2.1
1	D	415	TYR	2.1
1	E	335	LEU	2.1
1	G	351	VAL	2.1
1	K	237	ALA	2.1
1	B	354	GLU	2.1
1	F	56	TYR	2.1
1	G	15	LEU	2.1
1	E	262	THR	2.1
1	H	420	ALA	2.1
1	J	416	ASN	2.1
1	I	202	PRO	2.1
1	L	353	SER	2.1
1	A	260	LEU	2.1
1	F	383	TYR	2.1
1	G	334	ILE	2.1
1	I	3	ILE	2.1
1	K	234	GLU	2.1
1	L	415	TYR	2.1
1	I	121	PHE	2.1
1	B	357	LEU	2.1
1	C	56	TYR	2.1
1	G	194	GLY	2.1
1	I	251	GLU	2.1
1	K	58	ARG	2.1
1	C	107	TYR	2.1
1	E	56	TYR	2.1
1	G	215	ARG	2.1
1	H	249	TYR	2.1
1	D	294	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	252	VAL	2.1
1	I	360	ARG	2.1
1	J	37	HIS	2.1
1	B	198	ALA	2.1
1	L	81	ASN	2.1
1	K	236	THR	2.1
1	E	298	ILE	2.1
1	F	123	ALA	2.1
1	G	305	ALA	2.1
1	E	59	ARG	2.1
1	E	320	THR	2.1
1	L	339	THR	2.1
1	L	388	ARG	2.1
1	I	125	LEU	2.1
1	J	98	SER	2.1
1	E	359	ARG	2.0
1	L	427	PHE	2.0
1	C	396	LYS	2.0
1	F	60	GLY	2.0
1	F	67	PRO	2.0
1	G	57	ASP	2.0
1	B	383	TYR	2.0
1	I	9	ASN	2.0
1	K	34	LEU	2.0
1	J	355	ARG	2.0
1	B	137	ASP	2.0
1	H	357	LEU	2.0
1	A	232	PRO	2.0
1	D	226	THR	2.0
1	H	216	ILE	2.0
1	I	69	THR	2.0
1	L	3	ILE	2.0
1	K	252	VAL	2.0
1	E	9	ASN	2.0
1	G	308	ALA	2.0
1	A	380	VAL	2.0
1	G	347	PHE	2.0
1	L	342	ILE	2.0
1	G	224	HIS	2.0
1	H	34	LEU	2.0
1	I	79	ASP	2.0
1	A	261	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	322	LEU	2.0
1	E	105	ALA	2.0
1	F	223	LEU	2.0
1	G	355	ARG	2.0
1	E	104	VAL	2.0
1	G	230	THR	2.0
1	A	106	ARG	2.0
1	F	106	ARG	2.0
1	J	62	GLY	2.0
1	L	387	LYS	2.0
1	F	411	MET	2.0
1	L	69	THR	2.0
1	E	261	TRP	2.0
1	G	436	GLN	2.0
1	A	102	GLY	2.0
1	K	73	TYR	2.0
1	A	252	VAL	2.0
1	J	127	PRO	2.0
1	H	32	PHE	2.0
1	H	364	GLN	2.0
1	J	122	LEU	2.0
1	B	378	LYS	2.0
1	E	421	VAL	2.0
1	K	254	GLY	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.