



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 PM GMT

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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

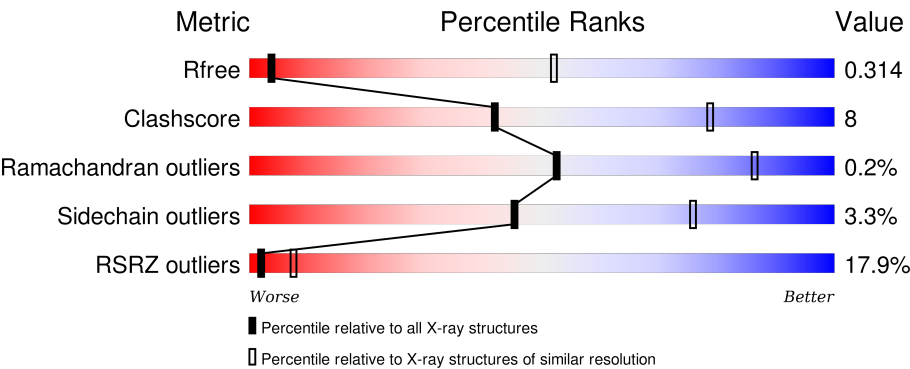
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance 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 <sub>free</sub>	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	456	<div><div>13%</div><div>78%</div><div>17%</div><div>• •</div></div>
1	B	456	<div><div>12%</div><div>80%</div><div>16%</div><div>• •</div></div>
1	C	456	<div><div>14%</div><div>80%</div><div>15%</div><div>• •</div></div>
1	D	456	<div><div>12%</div><div>79%</div><div>16%</div><div>• •</div></div>
1	E	456	<div><div>13%</div><div>80%</div><div>16%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
1	F	456	<div><div></div><div>11%</div><div>80%</div><div>16%</div><div></div><div></div></div>
1	G	456	<div><div></div><div>28%</div><div>80%</div><div>15%</div><div></div><div></div></div>
1	H	456	<div><div></div><div>12%</div><div>78%</div><div>17%</div><div></div><div></div></div>
1	I	456	<div><div></div><div>16%</div><div>79%</div><div>17%</div><div></div><div></div></div>
1	J	456	<div><div></div><div>16%</div><div>80%</div><div>15%</div><div></div><div></div></div>
1	K	456	<div><div></div><div>31%</div><div>75%</div><div>20%</div><div></div><div></div></div>
1	L	456	<div><div></div><div>29%</div><div>80%</div><div>15%</div><div></div><div></div></div>

## 2 Entry composition

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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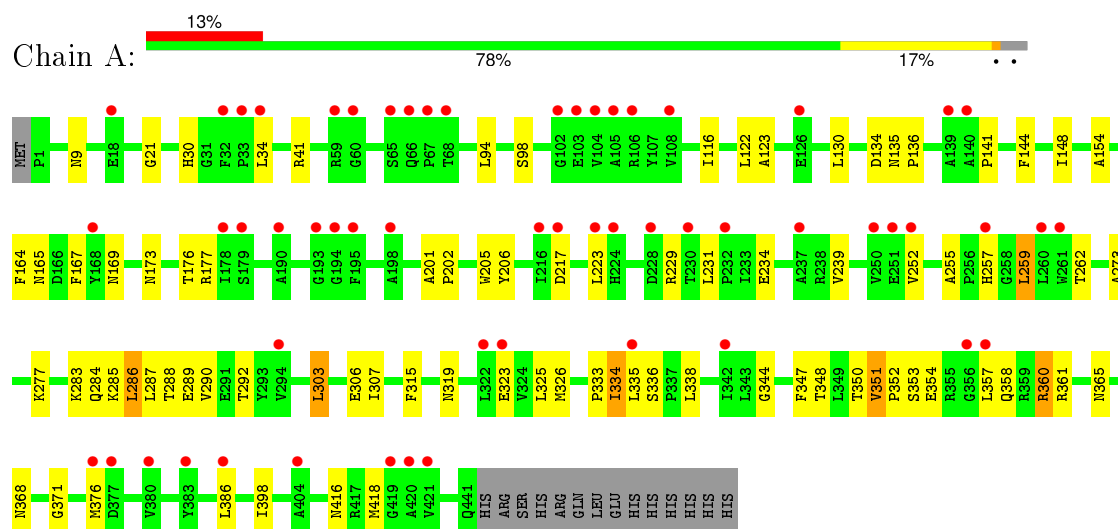
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Chain	Residue	Modelled	Actual	Comment	Reference
L	281	ALA	-	LINKER	UNP P03485
L	282	GLN	-	LINKER	UNP P03485
L	283	LYS	-	LINKER	UNP P03485
L	284	GLN	-	LINKER	UNP P03485
L	285	LYS	-	LINKER	UNP P03485
L	448	LEU	-	EXPRESSION TAG	UNP P03485
L	449	GLU	-	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

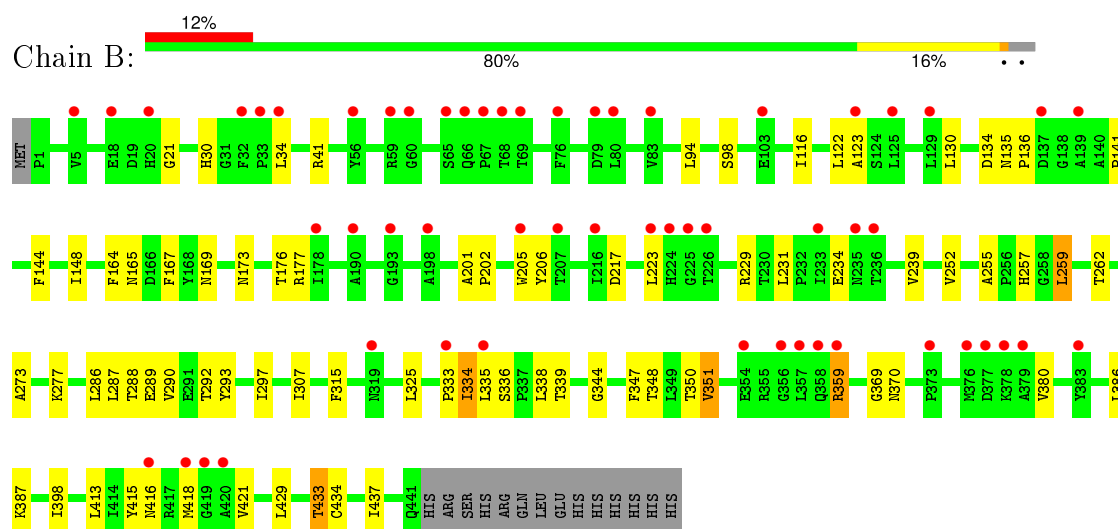
### 3 Residue-property plots [i](#)

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

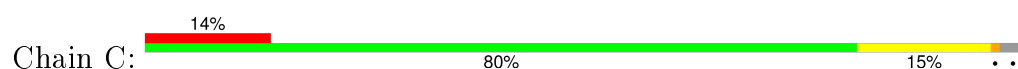
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

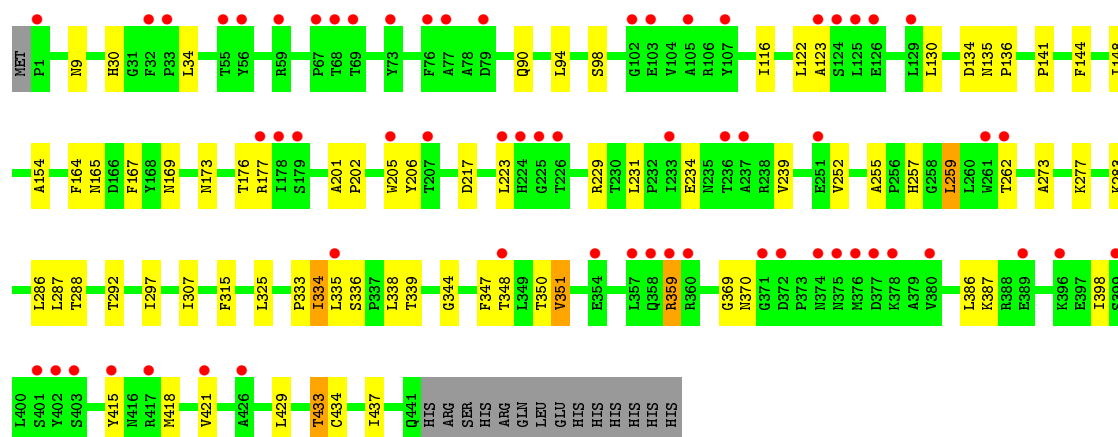


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

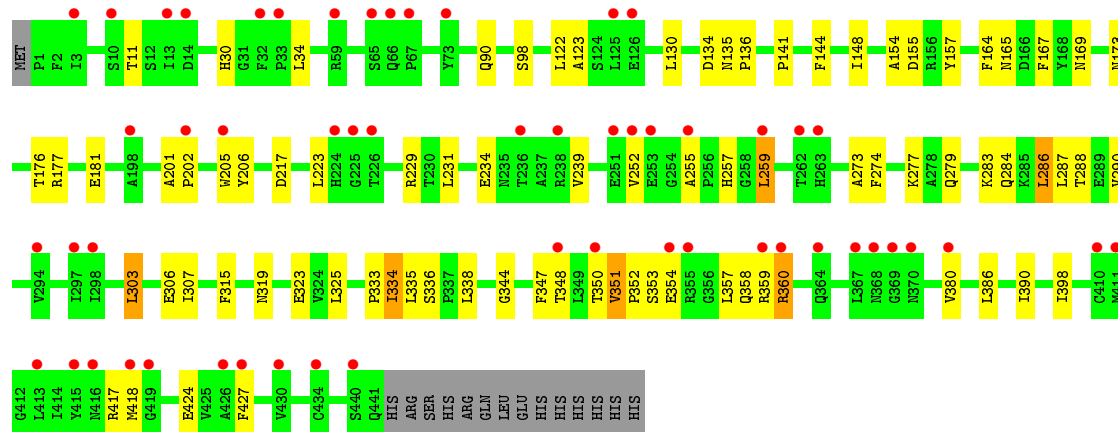
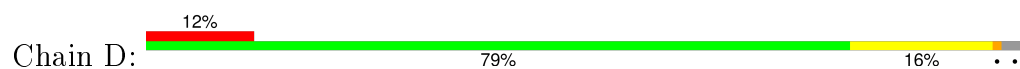


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

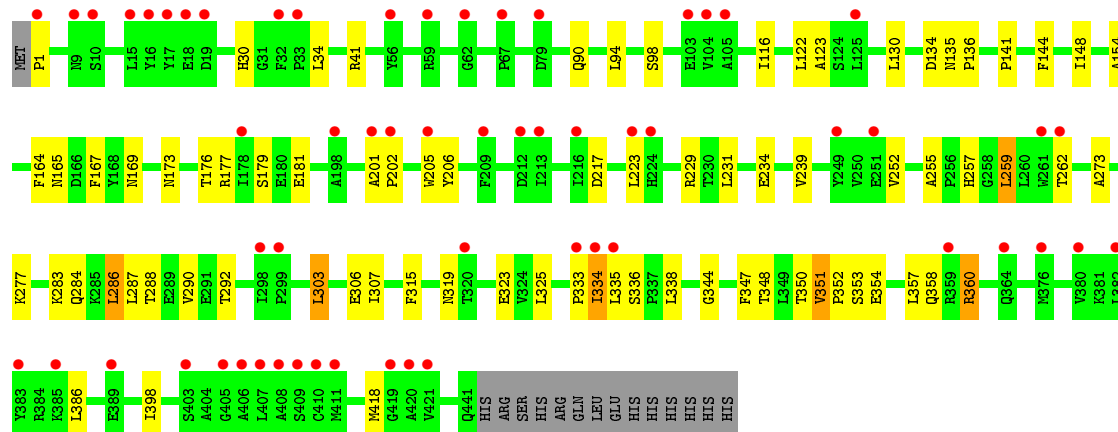
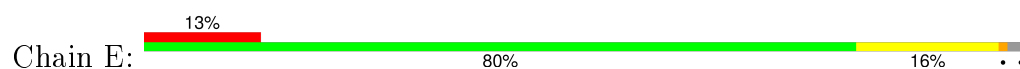




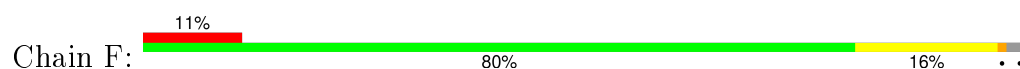
- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

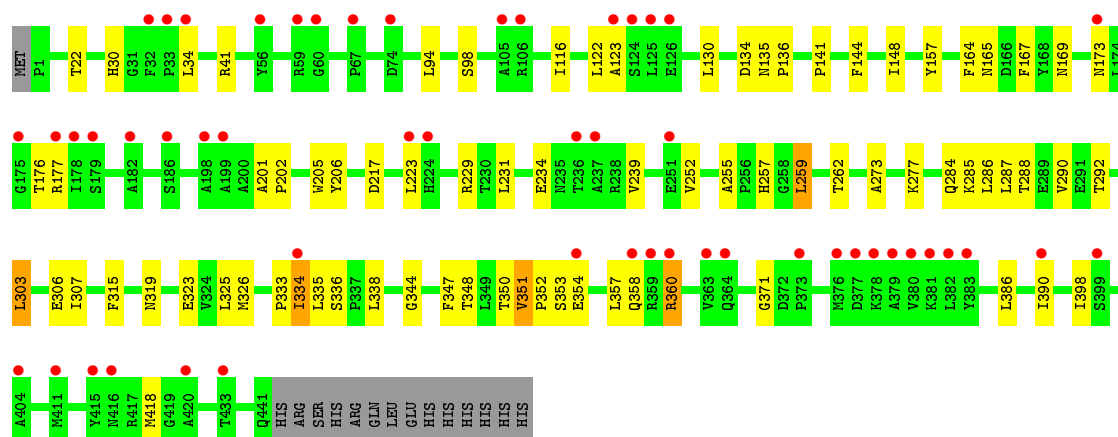


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

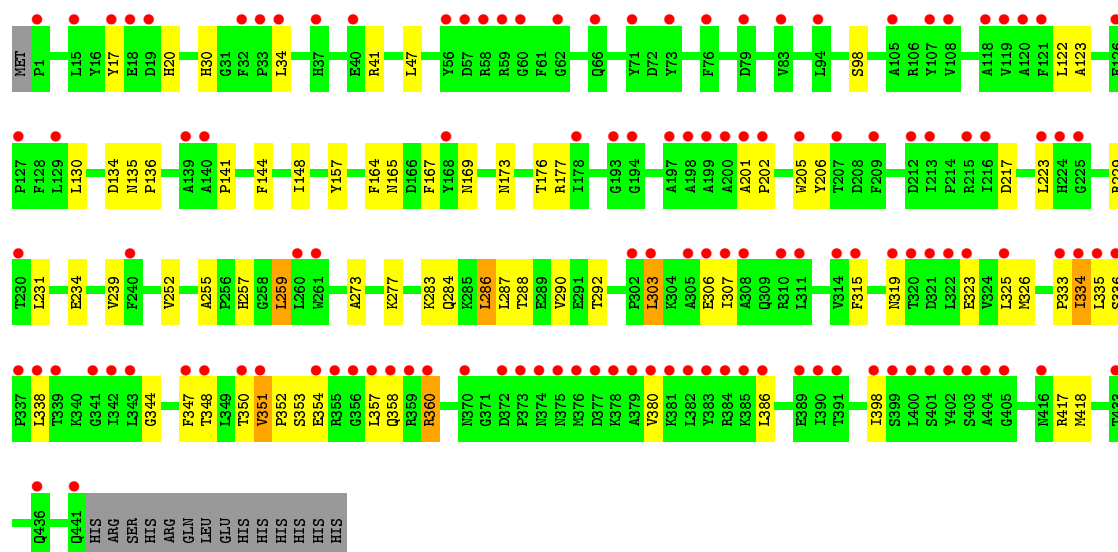
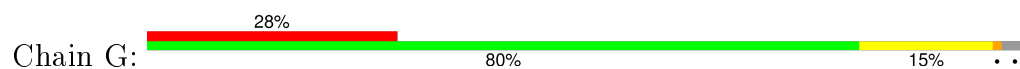


- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera

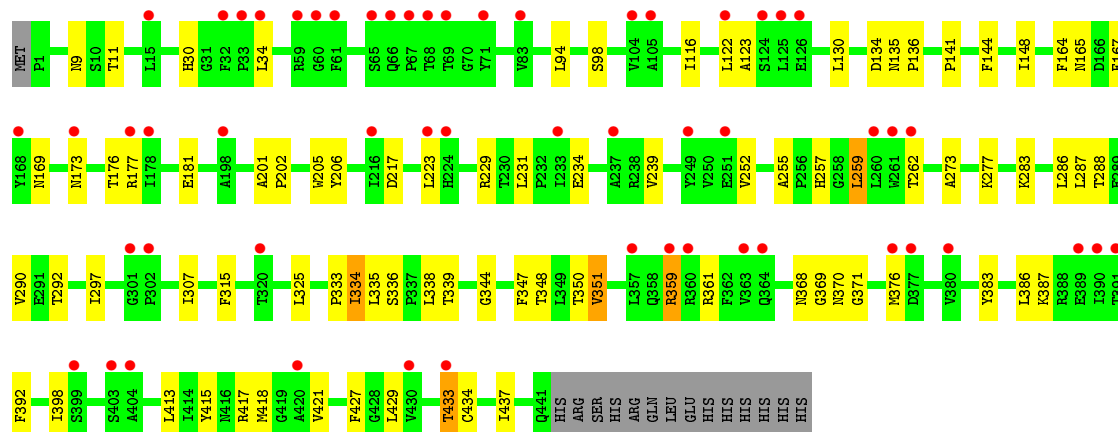
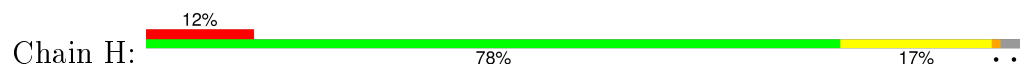




- Molecule 1: Non-haem bromoperoxidase BPO-A2, Matrix protein 1 chimera



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



- Chain I:
- 
- 16% 79% 17%
- Chain I:
- Sequence of amino acids (from left to right): MET, P1, F2, I3, N9, S10, T11, D19, H20, G21, T24, P25, H30, G31, F32, P33, L34, Y56, H59, S65, D66, P67, T68, T69, D79, L94, S98, V104, A105, V108, G112, F121, L122, A123, S124, L125, E126, L130, D134, M135, P136, P144, F144, I148, A154, Y150, F164, D166, F167, Y168, M169, M173, L174, G175, T176, R177, L178, S179, E180, Y183, F195, P196, A197, A198, A201, T202, T203, T204, T205, Y206, R210, A211, D212, T213, T214, R215, D216, L217, L223, T226, R229, T230, L231, E234, V239, T241, V252, A255, P256, H257, G258, L259, L260, H261, T262, A273, K277, K283, L286, T287, L288, E289, I414, Y415, N416, F291, T292, T297, I307, F315, K318, N319, C320, L325, P333, A334, S335, S336, P337, L338, T339, G344, F347, T348, L349, T350, V351, E354, R355, G356, L357, Q358, R359, P360.

- [illegible]

- Chain K:



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	250.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 295.2	EDS
Estimated twinning fraction	0.057 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 8723 reflections	Xtriage
$F_o, F_c$ correlation	0.72	EDS
Total number of atoms	40512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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(°)	Ideal(°)
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

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:L:284:GLN:HA	1:L:287:LEU:HD23	1.40	1.02
1:D:287:LEU:HB3	1:D:315:PHE:CD2	1.93	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:K:264:ALA:O	1:K:268:ASN:CB	2.23	0.86
1:B:287:LEU:HD13	1:B:315:PHE:HB3	1.57	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: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:G:386:LEU:HD23	1:G: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:L:284:GLN:O	1:L:287:LEU:CG	2.29	0.79
1:C:386:LEU:HD23	1:C:398:ILE:HD11	1.63	0.79
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:B:386:LEU:HD23	1:B: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:51:ALA:HB2	1:K:275:LEU:HD11	1.67	0.76
1:K:49:ALA:HB2	1:K:272:LEU:HD21	1.66	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:H:9:ASN:ND2	1:I:21:GLY:O	2.20	0.74
1:G:287:LEU:HD13	1:G:315:PHE:HB3	1.69	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:361:ARG:HD2	1:H:417:ARG:CZ	2.19	0.73
1:A:287:LEU:HD13	1:A:315:PHE:HB3	1.71	0.73
1:D:287:LEU:CD1	1:D:315:PHE:CD1	2.67	0.73
1:B:289:GLU:HG2	1:B:293:TYR:CE2	2.23	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:344:GLY:O	1:B:348:THR:HG23	1.88	0.72
1:B:30:HIS:CE1	1:B:34:LEU:O	2.42	0.72
1:E:30:HIS:CE1	1:E:34:LEU:O	2.42	0.72
1:F:30:HIS:CE1	1:F:34:LEU:O	2.43	0.72
1:E:344:GLY:O	1:E:348:THR:HG23	1.89	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:G:30:HIS:CE1	1:G:34:LEU:O	2.42	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: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:L:30:HIS:CE1	1:L:34:LEU:O	2.43	0.72
1:J:30:HIS:CE1	1:J:34:LEU:O	2.42	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:D:287:LEU:CD1	1:D:315:PHE:CA	2.67	0.68
1:A:319:ASN:HA	1:A:352:PRO:HG2	1.74	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:C	1:K:286:LEU:HD13	2.17	0.66
1:E:154:ALA:O	1:F:41:ARG:NH2	2.27	0.65
1:K:26:VAL:HG21	1:K:275:LEU:CD1	2.24	0.65
1:I:215:ARG:HH22	1:K:299:PRO:HG3	1.60	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:G:287:LEU:HD13	1:G:315:PHE:CB	2.28	0.64
1:A:273:ALA:O	1:A:277:LYS:HG3	1.97	0.64
1:J:273:ALA:O	1:J:277:LYS:HG3	1.98	0.64
1:D:418:MET:HE1	1:I:413:LEU:HD23	1.79	0.64
1:D:287:LEU:CD1	1:D:315:PHE:CB	2.76	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:J:283:LYS:O	1:J:287:LEU:HG	1.99	0.63
1:F:371:GLY:HA2	1:L:418:MET:O	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:G:283:LYS:O	1:G:287:LEU:HG	1.99	0.62
1:A:376:MET:HE3	1:H:413:LEU:HD22	1.80	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:K:286:LEU:HD13	1:K:286:LEU:O	2.00	0.60
1:G:273:ALA:O	1:G:277:LYS:HG3	2.01	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: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:A:286:LEU:O	1:A:290:VAL:HG23	2.02	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:286:LEU:CD2	1:D:424:GLU:CG	2.74	0.59
1:D:252:VAL:HG12	1:D:255:ALA:HB2	1.85	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:K:51:ALA:CB	1:K:275:LEU:HD11	2.32	0.59
1:B:416:ASN:ND2	1:J:418:MET:SD	2.69	0.59
1:E:333:PRO:O	1:E:334:ILE:HG12	2.03	0.59
1:H:287:LEU:CD1	1:H:315:PHE:HB3	2.32	0.58
1:E:252:VAL:HG12	1:E:255:ALA:HB2	1.85	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:333:PRO:O	1:F:334:ILE:HG12	2.03	0.58
1:F:252:VAL:HG12	1:F:255:ALA:HB2	1.84	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:D:283:LYS:O	1:D:287:LEU:HG	2.04	0.58
1:A:154:ALA:O	1:B:41:ARG:NH2	2.35	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:I:333:PRO:O	1:I:334:ILE:HG12	2.05	0.57
1:C:252:VAL:HG12	1:C:255:ALA:HB2	1.84	0.57
1:D:333:PRO:O	1:D:334:ILE:HG12	2.03	0.57
1:G:333:PRO:O	1:G: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:HH11	1:E:360:ARG:HG2	1.70	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:K:283:LYS:O	1:K:287:LEU:HB2	2.05	0.57
1:F:287:LEU:HB3	1:F:315:PHE:CD2	2.39	0.57
1:F:360:ARG:HH11	1:F:360:ARG:HG2	1.70	0.57
1:J:164:PHE:HA	1:J:167:PHE:HB3	1.87	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: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: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:D:279:GLN:O	1:D:283:LYS:CB	2.53	0.57
1:D:360:ARG:HG2	1:D:360:ARG:HH11	1.70	0.57
1:D:164:PHE:HA	1:D:167:PHE:HB3	1.86	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:G:360:ARG:HH11	1:G:360:ARG:HG2	1.70	0.56
1:C:336:SER:HB3	1:C:339:THR:HG23	1.87	0.56
1:C:164:PHE:HA	1:C:167:PHE:HB3	1.87	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:HH11	1:J:360:ARG:HG2	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:F:288:THR:O	1:F:292:THR:HG23	2.06	0.56
1:B:164:PHE:HA	1:B:167:PHE:HB3	1.87	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:K:266:GLU:O	1:K:269:THR:CG2	2.45	0.55
1:K:49:ALA:CB	1:K:272:LEU:HD21	2.36	0.55
1:D:157:TYR:HB3	1:E:181:GLU:HB3	1.87	0.55
1:K:130:LEU:HB2	1:K:206:TYR:HB2	1.89	0.55
1:K:265:GLU:O	1:K:269:THR:HB	2.07	0.55
1:H:283:LYS:O	1:H:287:LEU:HG	2.06	0.55
1:D:130:LEU:HB2	1:D:206:TYR:HB2	1.89	0.55
1:C:429:LEU:O	1:C:433:THR:HG23	2.07	0.55
1:K:429:LEU:O	1:K:433:THR:HG23	2.08	0.54
1:I:130:LEU:HB2	1:I:206:TYR:HB2	1.89	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:H:336:SER:HB3	1:H:339:THR:HG23	1.87	0.54
1:D:284:GLN:O	1:D:288:THR:HG23	2.08	0.54
1:H:130:LEU:HB2	1:H:206:TYR:HB2	1.89	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:429:LEU:O	1:H:433:THR:HG23	2.08	0.54
1:B:429:LEU:O	1:B:433:THR:HG23	2.08	0.54
1:K:223:LEU:CD2	1:K:267:VAL:HG22	2.35	0.54
1:A:283:LYS:O	1:A:287:LEU:HG	2.08	0.54
1:H:286:LEU:HD13	1:H:290:VAL:HG21	1.90	0.54
1:D:358:GLN:CB	1:I:358:GLN:HB2	2.37	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:I:429:LEU:O	1:I:433:THR:HG23	2.08	0.53
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:G:130:LEU:HB2	1:G:206:TYR:HB2	1.89	0.53
1:D:418:MET:CG	1:I:416:ASN:HD22	2.21	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:K:359:ARG:NH1	1:K:415:TYR:O	2.39	0.53
1:H:288:THR:O	1:H:292:THR:HG23	2.07	0.53
1:G:201:ALA:HB3	1:G:202:PRO:HD3	1.90	0.53
1:L:429:LEU:O	1:L:433:THR:HG23	2.08	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: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:A:130:LEU:HB2	1:A:206:TYR:HB2	1.89	0.53
1:E:176:THR:HG22	1:E:177:ARG:N	2.24	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:F:176:THR:HG22	1:F:177:ARG:N	2.24	0.53
1:A:176:THR:HG22	1:A:177:ARG:N	2.24	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:A:201:ALA:HB3	1:A:202:PRO:HD3	1.90	0.53
1:I:215:ARG:HH22	1:K:299:PRO:CG	2.21	0.53
1:D:274:PHE:O	1:D:277:LYS:HG3	2.09	0.53
1:D:176:THR:HG22	1:D:177:ARG:N	2.24	0.53
1:G:176:THR:HG22	1:G:177:ARG:N	2.24	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:201:ALA:HB3	1:J:202:PRO:HD3	1.90	0.52
1:J:130:LEU:HB2	1:J:206:TYR:HB2	1.89	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:F:358:GLN:OE1	1:L:361:ARG:HB2	2.09	0.52
1:E:201:ALA:HB3	1:E:202:PRO:HD3	1.90	0.52
1:L:201:ALA:HB3	1:L:202:PRO:HD3	1.90	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: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: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:A:41:ARG:NH2	1:C:154:ALA:O	2.43	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:C:98:SER:HA	1:C:123:ALA:O	2.11	0.51
1:A:21:GLY:O	1:C:9:ASN:ND2	2.39	0.51
1:G:17:TYR:OH	1:I:11:THR:HG22	2.10	0.51
1:C:130:LEU:O	1:C:135:ASN:ND2	2.38	0.51
1:G:173:ASN:HD22	1:G:177:ARG:HG3	1.76	0.51
1:B:98:SER:HA	1:B:123:ALA:O	2.11	0.51
1:F:418:MET:O	1:L:371:GLY:HA2	2.10	0.51
1:J:157:TYR:HB3	1:K:181:GLU:HB3	1.92	0.51
1:L:297:ILE:HD11	1:L:434:CYS:O	2.11	0.51

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:LEU:CD2	1:K:223:LEU:HB3	2.43	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: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: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:I:297:ILE:HD11	1:I:437:ILE:HB	1.95	0.49
1:D:122:LEU:CD2	1:D:223:LEU:HB3	2.43	0.49
1:J:231:LEU:HD12	1:J:257:HIS:HE1	1.77	0.49
1:L:287:LEU:HB3	1:L:315:PHE:CD2	2.43	0.49
1:K:287:LEU:CD1	1:K:315:PHE:HB3	2.36	0.49
1:L:297:ILE:HD11	1:L:437:ILE:HB	1.95	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:H:130:LEU:O	1:H:135:ASN:ND2	2.38	0.49
1:K:297:ILE:HD11	1:K:437:ILE:HB	1.95	0.49
1:K:231:LEU:HD12	1:K:257:HIS:HE1	1.77	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:365:ASN:OD1	1:H:417:ARG:HD2	2.13	0.48
1:H:359:ARG:NH1	1:H:415:TYR:O	2.39	0.48
1:H:231:LEU:HD12	1:H:257:HIS:HE1	1.78	0.48
1:A:231:LEU:HD12	1:A:257:HIS:HE1	1.78	0.48
1:K:52:ARG:CZ	1:K:390:ILE:HD11	2.43	0.48
1:C:231:LEU:HD12	1:C:257:HIS:HE1	1.77	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:H:297:ILE:HD11	1:H:437:ILE:HB	1.95	0.48
1:E:122:LEU:CD2	1:E:223:LEU:HB3	2.43	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:L:288:THR:O	1:L:292:THR:HG23	2.13	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: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:K:307:ILE:HD11	1:K:335:LEU:HD11	1.97	0.47
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: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:L:347:PHE:O	1:L:351:VAL:HB	2.15	0.47
1:K:369:GLY:O	1:K:370:ASN:OD1	2.33	0.47
1:A:347:PHE:O	1:A:351:VAL:HB	2.14	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:C:347:PHE:O	1:C:351:VAL:HB	2.15	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:C:173:ASN:ND2	1:C:177:ARG:HG3	2.30	0.47
1:B:369:GLY:O	1:B:370:ASN:OD1	2.33	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:J:30:HIS:ND1	1:J:34:LEU:O	2.48	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:307:ILE:HD11	1:J:335:LEU:HD11	1.97	0.47
1:C:369:GLY:O	1:C:370:ASN:OD1	2.33	0.47
1:K:283:LYS:O	1:K:287:LEU:N	2.41	0.46
1:E:130:LEU:O	1:E:135:ASN:ND2	2.38	0.46
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: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:D:347:PHE:O	1:D:351:VAL:HB	2.15	0.46
1:J:303:LEU:HA	1:J:306:GLU:OE1	2.15	0.46
1:C:307:ILE:HD11	1:C:335:LEU:HD11	1.97	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:L:173:ASN:ND2	1:L:177:ARG:HG3	2.30	0.46
1:J:173:ASN:ND2	1:J:177:ARG:HG3	2.30	0.46
1:H:173:ASN:ND2	1:H: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:G:30:HIS:ND1	1:G:34:LEU:O	2.48	0.46
1:K:30:HIS:ND1	1:K:34:LEU:O	2.48	0.46
1:D:30:HIS:ND1	1:D:34:LEU:O	2.48	0.46
1:K:173:ASN:ND2	1:K:177:ARG:HG3	2.30	0.46
1:D:307:ILE:HD11	1:D:335:LEU:HD11	1.97	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:F:287:LEU:HD13	1:F:315:PHE:CG	2.50	0.46
1:B:173:ASN:ND2	1:B:177:ARG:HG3	2.30	0.46
1:F:303:LEU:HA	1:F:306:GLU:OE1	2.15	0.46
1:L:315:PHE:HE1	1:L:350:THR:HG21	1.81	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:287:LEU:HB3	1:L:315:PHE:CG	2.51	0.46
1:I:30:HIS:ND1	1:I:34:LEU:O	2.49	0.46
1:B:347:PHE:O	1:B:351:VAL:HB	2.15	0.46
1:L:284:GLN:CA	1:L:287:LEU:CD2	2.67	0.45
1:G:319:ASN:CA	1:G:352:PRO:HG2	2.46	0.45
1:F:307:ILE:HD11	1:F:335:LEU:HD11	1.97	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:L:30:HIS:ND1	1:L:34:LEU:O	2.49	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:A:141:PRO:O	1:A:144:PHE:HB3	2.17	0.45
1:A:365:ASN:OD1	1:H:417:ARG:CD	2.65	0.45
1:H:141:PRO:O	1:H:144:PHE:HB3	2.17	0.45
1:G:141:PRO:O	1:G:144:PHE:HB3	2.17	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:D:130:LEU:O	1:D:135:ASN:ND2	2.38	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: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:A:315:PHE:HE1	1:A:350:THR:HG21	1.81	0.45
1:A:30:HIS:ND1	1:A:34:LEU:O	2.48	0.45
1:B:130:LEU:O	1:B:135:ASN:ND2	2.38	0.45
1:L:369:GLY:O	1:L:370:ASN:OD1	2.33	0.45
1:F:141:PRO:O	1:F:144:PHE:HB3	2.17	0.45
1:H:315:PHE:HE1	1:H:350:THR:HG21	1.82	0.45
1:F:319:ASN:CA	1:F:352:PRO:HG2	2.46	0.45
1:E:141:PRO:O	1:E:144:PHE:HB3	2.17	0.45
1:G:315:PHE:HE1	1:G:350:THR:HG21	1.82	0.45
1:A:358:GLN:O	1:A:360:ARG:NH1	2.50	0.45
1:G:122:LEU:HD23	1:G:223:LEU:HB3	1.99	0.45
1:B:122:LEU:HD23	1:B:223:LEU:HB3	1.99	0.45
1:E:358:GLN:O	1:E:360:ARG:NH1	2.50	0.44
1:D:122:LEU:HD23	1:D:223:LEU:HB3	1.99	0.44
1:H:122:LEU:HD23	1:H:223:LEU:HB3	1.99	0.44
1:L:287:LEU:HD12	1:L:288:THR:CA	2.47	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: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: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:B:286:LEU:O	1:B:290:VAL:HG23	2.18	0.44
1:F:358:GLN:O	1:F:360:ARG:NH1	2.50	0.44
1:J:358:GLN:O	1:J:360:ARG:NH1	2.50	0.44
1:J:315:PHE:HE1	1:J:350:THR:HG21	1.81	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:A:285:LYS:O	1:A:289:GLU:HG3	2.18	0.44
1:D:358:GLN:O	1:D:360:ARG:NH1	2.51	0.44
1:D:155:ASP:OD2	1:E:179:SER:OG	2.25	0.44
1:L:284:GLN:CA	1:L:287:LEU:HD21	2.39	0.43
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:D:315:PHE:HE1	1:D:350:THR:HG21	1.83	0.43
1:A:122:LEU:HD23	1:A:223:LEU:HB3	2.00	0.43
1:K:42:GLN:O	1:K:46:LEU:HG	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:122:LEU:HD23	1:J:223:LEU:HB3	1.99	0.43
1:E:122:LEU:HD23	1:E:223:LEU:HB3	1.99	0.43
1:I:122:LEU:HD23	1:I:223:LEU:HB3	1.99	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:I:130:LEU:O	1:I:135:ASN:ND2	2.38	0.43
1:G:169:ASN:HA	1:G:229:ARG:NH1	2.33	0.43
1:D:90:GLN:HB3	1:D:390:ILE:HD11	1.92	0.43
1:L:284:GLN:HA	1:L:287:LEU:CG	2.41	0.43
1:K:130:LEU:O	1:K:135:ASN:ND2	2.38	0.43
1:F:130:LEU:O	1:F:135:ASN:ND2	2.38	0.43
1:L:122:LEU:HD23	1:L:223:LEU:HB3	1.99	0.43
1:J:11:THR:HG21	1:K:1:PRO:HG2	2.01	0.43
1:J:319:ASN:CA	1:J:352:PRO:HG2	2.46	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:C:283:LYS:O	1:C:287:LEU:HG	2.19	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:169:ASN:HA	1:A:229:ARG:NH1	2.35	0.42
1:A:416:ASN:O	1:H:368:ASN:ND2	2.53	0.42
1:E:202:PRO:HA	1:E:205:TRP:CD2	2.55	0.42
1:D:144:PHE:CZ	1:D:148:ILE:HD11	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:H:286:LEU:HD21	1:H:392:PHE:CD1	2.55	0.42
1:C:202:PRO:HA	1:C:205:TRP:CD2	2.55	0.42
1:L:202:PRO:HA	1:L:205:TRP:CD2	2.54	0.42
1:B:169:ASN:HA	1:B:229:ARG:NH1	2.35	0.42
1:E:134:ASP:C	1:E:136:PRO:HD3	2.40	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:F:202:PRO:HA	1:F:205:TRP:CD2	2.55	0.42
1:I:202:PRO:HA	1:I:205:TRP:CD2	2.54	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:G:360:ARG:NH1	1:G:360:ARG:HG2	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:K:202:PRO:HA	1:K:205:TRP:CD2	2.55	0.42
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: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:H:144:PHE:CZ	1:H:148:ILE:HD11	2.55	0.41
1:G:144:PHE:CZ	1:G:148:ILE:HD11	2.55	0.41
1:K:144:PHE:CZ	1:K:148:ILE:HD11	2.55	0.41
1:H:134:ASP:C	1:H:136:PRO:HD3	2.41	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:A:418:MET:HG2	1:H:368:ASN:CG	2.40	0.41
1:G:252:VAL:CG1	1:G:255:ALA:HB2	2.49	0.41
1:J:202:PRO:HA	1:J:205:TRP:CD2	2.54	0.41
1:B:144:PHE:CZ	1:B:148:ILE:HD11	2.55	0.41
1:I:169:ASN:HA	1:I:229:ARG:NH1	2.35	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:H:11:THR:HG23	1:I:19:ASP:HB3	2.02	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:G:202:PRO:HA	1:G:205:TRP:CD2	2.55	0.41
1:L:297:ILE:CD1	1:L:437:ILE:HB	2.51	0.41
1:J:323:GLU:HB2	1:J:357:LEU:HD11	2.02	0.41
1:G:323:GLU:HB2	1:G:357:LEU:HD11	2.02	0.41
1:K:52:ARG:NH1	1:K:390:ILE:HD11	2.36	0.41
1:A:144:PHE:CZ	1:A:148:ILE:HD11	2.55	0.41
1:I:144:PHE:CZ	1:I:148:ILE:HD11	2.56	0.41
1:L:134:ASP:C	1:L:136:PRO:HD3	2.41	0.41
1:K:263:HIS:O	1:K:266:GLU:HB2	2.21	0.41
1:B:177:ARG:HD3	1:B:262:THR:O	2.21	0.41
1:H:202:PRO:HA	1:H:205:TRP:CD2	2.54	0.41
1:C:297:ILE:CD1	1:C:437:ILE:HB	2.50	0.41
1:J:252:VAL:CG1	1:J:255:ALA:HB2	2.49	0.41
1:C:94:LEU:HG	1:C:116:ILE:HD12	2.03	0.41
1:K:94:LEU:HG	1:K:116:ILE:HD12	2.02	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:LEU:HG	1:H:116:ILE:HD12	2.03	0.41
1:A:134:ASP:C	1:A:136:PRO:HD3	2.40	0.41
1:J:360:ARG:HH11	1:J:360:ARG:CG	2.34	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: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:D:134:ASP:C	1:D:136:PRO:HD3	2.41	0.41
1:D:130:LEU:HD12	1:D:130:LEU:HA	1.95	0.41
1:I:286:LEU:HD13	1:I:290:VAL:CG2	2.51	0.41
1:E:144:PHE:CZ	1:E:148:ILE:HD11	2.55	0.41
1:E:94:LEU:HG	1:E:116:ILE:HD12	2.03	0.41
1:E:169:ASN:HA	1:E:229:ARG:NH1	2.35	0.41
1:A:94:LEU:HG	1:A:116:ILE:HD12	2.03	0.41
1:D:286:LEU:HD21	1:D:424:GLU:CG	2.49	0.41
1:A:361:ARG:HD2	1:H:417:ARG:NH1	2.36	0.41
1:E:360:ARG:NH1	1:E:360:ARG:HG2	2.34	0.41
1:A:177:ARG:HD3	1:A:262:THR:O	2.21	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:C:144:PHE:CZ	1:C:148:ILE:HD11	2.55	0.41
1:L:144:PHE:CZ	1:L:148:ILE:HD11	2.55	0.41
1:G:380:VAL:HG21	1:K:380:VAL:HG21	2.03	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:K:263:HIS:O	1:K:266:GLU:N	2.54	0.40
1:K:177:ARG:HD3	1:K:262:THR:O	2.21	0.40
1:H:297:ILE:CD1	1:H:437:ILE:HB	2.51	0.40
1:D:323:GLU:HB2	1:D:357:LEU:HD11	2.02	0.40
1:K:52:ARG:CZ	1:K:390:ILE:CD1	3.00	0.40
1:F:326:MET:CE	1:F:347:PHE:HB2	2.51	0.40
1:F:144:PHE:CZ	1:F:148:ILE:HD11	2.55	0.40
1:A:358:GLN:OE1	1:H:361:ARG:CB	2.69	0.40
1:L:177:ARG:HD3	1:L:262:THR:O	2.21	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:C:90:GLN:NE2	1:C:90:GLN:HA	2.37	0.40
1:L:286:LEU:HD22	1:L:427:PHE:CD2	2.56	0.40
1:G:283:LYS:O	1:G:287:LEU:HB2	2.22	0.40
1:E:177:ARG:HD3	1:E:262:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:LEU:HA	1:C:130:LEU:HD12	1.95	0.40
1:D:11:THR:HB	1:E:1:PRO:HG3	2.03	0.40
1:C:134:ASP:C	1:C:136:PRO:HD3	2.40	0.40
1:B:94:LEU:HG	1:B:116:ILE:HD12	2.03	0.40
1:D:360:ARG:HG2	1:D:360:ARG:NH1	2.34	0.40
1:F:360:ARG:HH11	1:F:360:ARG:CG	2.34	0.40
1:C:177:ARG:HD3	1:C:262:THR:O	2.21	0.40
1:F:177:ARG:HD3	1:F:262:THR:O	2.21	0.40
1:K:297:ILE:CD1	1:K:437:ILE:HB	2.51	0.40
1:F:94:LEU:HG	1:F:116:ILE:HD12	2.03	0.40
1:J:90:GLN:HA	1:J:90:GLN:NE2	2.37	0.40
1:E:287:LEU:HD13	1:E:315:PHE:CA	2.50	0.40
1:A:326:MET:CE	1:A:347:PHE:HB2	2.51	0.40
1:E:90:GLN:HA	1:E:90:GLN:NE2	2.37	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%)	52	86
1	B	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	52	86
1	C	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	52	86
1	D	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	52	86
1	E	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	52	86
1	F	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	52	86
1	G	439/456 (96%)	428 (98%)	10 (2%)	1 (0%)	52	86
1	H	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	52	86
1	I	439/456 (96%)	425 (97%)	13 (3%)	1 (0%)	52	86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	439/456 (96%)	427 (97%)	11 (2%)	1 (0%)	52	86
1	K	439/456 (96%)	424 (97%)	14 (3%)	1 (0%)	52	86
1	L	439/456 (96%)	426 (97%)	12 (3%)	1 (0%)	52	86
All	All	5268/5472 (96%)	5118 (97%)	138 (3%)	12 (0%)	52	86

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%)	44	75
1	B	348/369 (94%)	337 (97%)	11 (3%)	46	76
1	C	348/369 (94%)	336 (97%)	12 (3%)	44	75
1	D	348/369 (94%)	336 (97%)	12 (3%)	44	75
1	E	348/369 (94%)	336 (97%)	12 (3%)	44	75
1	F	348/369 (94%)	337 (97%)	11 (3%)	46	76
1	G	348/369 (94%)	336 (97%)	12 (3%)	44	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	348/369 (94%)	337 (97%)	11 (3%)	46	76
1	I	348/369 (94%)	337 (97%)	11 (3%)	46	76
1	J	348/369 (94%)	336 (97%)	12 (3%)	44	75
1	K	348/369 (94%)	336 (97%)	12 (3%)	44	75
1	L	348/369 (94%)	337 (97%)	11 (3%)	46	76
All	All	4176/4428 (94%)	4037 (97%)	139 (3%)	45	76

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

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	441/456 (96%)	0.96	57 (12%) 5 11	120, 209, 300, 386	0
1	B	441/456 (96%)	0.92	56 (12%) 5 11	93, 191, 267, 346	0
1	C	441/456 (96%)	0.97	62 (14%) 4 10	114, 196, 263, 325	0
1	D	441/456 (96%)	0.93	55 (12%) 5 11	110, 223, 370, 443	0
1	E	441/456 (96%)	0.96	59 (13%) 4 10	122, 196, 275, 336	0
1	F	441/456 (96%)	0.85	52 (11%) 6 12	117, 208, 305, 393	0
1	G	441/456 (96%)	1.42	127 (28%) 1 5	142, 284, 420, 498	0
1	H	441/456 (96%)	0.95	55 (12%) 5 11	130, 228, 310, 365	0
1	I	441/456 (96%)	1.06	75 (17%) 2 8	179, 269, 364, 453	0
1	J	441/456 (96%)	1.09	74 (16%) 2 8	127, 225, 323, 448	0
1	K	441/456 (96%)	1.51	142 (32%) 1 5	194, 329, 412, 474	0
1	L	441/456 (96%)	1.48	134 (30%) 1 5	179, 305, 412, 500	0
All	All	5292/5472 (96%)	1.09	948 (17%) 2 7	93, 233, 368, 500	0

All (948) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	120	ALA	7.7
1	A	66	GLN	7.6
1	K	359	ARG	7.1
1	L	119	VAL	7.1
1	A	33	PRO	6.6
1	K	32	PHE	6.5
1	F	359	ARG	6.2
1	H	67	PRO	6.1
1	L	212	ASP	6.1
1	B	33	PRO	6.0
1	L	123	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	I	211	ALA	6.0
1	G	357	LEU	5.9
1	K	33	PRO	5.9
1	L	223	LEU	5.8
1	J	420	ALA	5.8
1	K	357	LEU	5.4
1	L	213	ILE	5.4
1	J	419	GLY	5.4
1	L	320	THR	5.4
1	L	94	LEU	5.3
1	L	211	ALA	5.3
1	C	33	PRO	5.3
1	G	381	LYS	5.2
1	C	178	ILE	5.2
1	F	377	ASP	5.2
1	L	59	ARG	5.2
1	G	59	ARG	5.2
1	K	379	ALA	5.1
1	J	33	PRO	5.1
1	G	307	ILE	5.1
1	L	178	ILE	5.1
1	H	261	TRP	5.1
1	G	380	VAL	5.0
1	L	359	ARG	5.0
1	L	214	PRO	5.0
1	K	3	ILE	5.0
1	K	358	GLN	5.0
1	K	59	ARG	4.9
1	L	124	SER	4.9
1	L	121	PHE	4.9
1	B	67	PRO	4.9
1	J	13	ILE	4.9
1	L	215	ARG	4.8
1	L	55	THR	4.8
1	H	178	ILE	4.8
1	I	33	PRO	4.8
1	L	216	ILE	4.8
1	K	382	LEU	4.7
1	I	418	MET	4.7
1	C	125	LEU	4.7
1	L	122	LEU	4.7
1	L	222	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	I	416	ASN	4.6
1	L	5	VAL	4.6
1	A	67	PRO	4.6
1	I	419	GLY	4.6
1	H	65	SER	4.6
1	K	5	VAL	4.5
1	L	357	LEU	4.5
1	G	198	ALA	4.5
1	G	382	LEU	4.4
1	K	79	ASP	4.4
1	L	118	ALA	4.4
1	F	33	PRO	4.4
1	L	257	HIS	4.4
1	J	421	VAL	4.4
1	L	420	ALA	4.4
1	G	377	ASP	4.4
1	K	198	ALA	4.3
1	I	213	ILE	4.3
1	I	67	PRO	4.3
1	L	258	GLY	4.3
1	C	124	SER	4.3
1	G	403	SER	4.3
1	G	376	MET	4.3
1	G	197	ALA	4.3
1	G	359	ARG	4.3
1	J	65	SER	4.2
1	J	126	GLU	4.2
1	H	33	PRO	4.2
1	C	359	ARG	4.2
1	G	354	GLU	4.2
1	K	94	LEU	4.2
1	A	419	GLY	4.2
1	A	251	GLU	4.2
1	A	60	GLY	4.2
1	E	18	GLU	4.2
1	K	69	THR	4.2
1	D	359	ARG	4.2
1	G	338	LEU	4.2
1	K	406	ALA	4.2
1	J	124	SER	4.1
1	G	333	PRO	4.1
1	C	179	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	194	GLY	4.1
1	F	380	VAL	4.1
1	B	65	SER	4.1
1	L	56	TYR	4.1
1	G	1	PRO	4.1
1	F	379	ALA	4.1
1	G	385	LYS	4.1
1	K	204	THR	4.1
1	D	368	ASN	4.1
1	E	33	PRO	4.0
1	J	185	ASN	4.0
1	G	404	ALA	4.0
1	G	223	LEU	4.0
1	G	402	TYR	4.0
1	L	224	HIS	4.0
1	G	17	TYR	4.0
1	K	67	PRO	4.0
1	G	120	ALA	4.0
1	H	251	GLU	4.0
1	C	261	TRP	4.0
1	G	399	SER	3.9
1	K	399	SER	3.9
1	C	67	PRO	3.9
1	B	32	PHE	3.9
1	K	195	PHE	3.9
1	D	251	GLU	3.9
1	C	68	THR	3.9
1	C	126	GLU	3.9
1	H	69	THR	3.9
1	B	66	GLN	3.9
1	J	14	ASP	3.9
1	C	224	HIS	3.9
1	K	80	LEU	3.9
1	I	413	LEU	3.8
1	F	178	ILE	3.8
1	L	54	ILE	3.8
1	L	108	VAL	3.8
1	F	224	HIS	3.8
1	G	384	ARG	3.8
1	L	43	SER	3.8
1	L	18	GLU	3.8
1	K	376	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	380	VAL	3.8
1	L	416	ASN	3.8
1	L	79	ASP	3.8
1	L	126	GLU	3.8
1	H	59	ARG	3.8
1	I	178	ILE	3.8
1	I	212	ASP	3.8
1	I	252	VAL	3.7
1	K	212	ASP	3.7
1	K	385	LYS	3.7
1	G	19	ASP	3.7
1	B	59	ARG	3.7
1	G	33	PRO	3.7
1	I	414	ILE	3.7
1	G	358	GLN	3.7
1	A	230	THR	3.7
1	A	421	VAL	3.7
1	H	224	HIS	3.7
1	A	103	GLU	3.7
1	L	321	ASP	3.7
1	I	318	LYS	3.7
1	K	11	THR	3.7
1	C	77	ALA	3.7
1	L	262	THR	3.7
1	H	104	VAL	3.6
1	I	59	ARG	3.6
1	G	339	THR	3.6
1	F	126	GLU	3.6
1	C	376	MET	3.6
1	E	178	ILE	3.6
1	E	32	PHE	3.6
1	K	120	ALA	3.6
1	C	225	GLY	3.6
1	G	56	TYR	3.6
1	H	377	ASP	3.6
1	K	354	GLU	3.6
1	K	398	ILE	3.6
1	K	13	ILE	3.6
1	G	375	ASN	3.6
1	B	359	ARG	3.6
1	J	186	SER	3.6
1	L	209	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	178	ILE	3.6
1	J	238	ARG	3.5
1	H	126	GLU	3.5
1	I	10	SER	3.5
1	B	225	GLY	3.5
1	G	390	ILE	3.5
1	G	212	ASP	3.5
1	A	193	GLY	3.5
1	F	381	LYS	3.5
1	J	251	GLU	3.5
1	F	358	GLN	3.5
1	E	410	CYS	3.5
1	K	386	LEU	3.5
1	E	419	GLY	3.5
1	I	379	ALA	3.5
1	H	68	THR	3.5
1	K	60	GLY	3.5
1	F	378	LYS	3.5
1	J	299	PRO	3.5
1	L	434	CYS	3.5
1	I	198	ALA	3.5
1	L	107	TYR	3.5
1	I	359	ARG	3.5
1	L	70	GLY	3.5
1	D	252	VAL	3.5
1	K	222	ILE	3.4
1	D	65	SER	3.4
1	J	387	LYS	3.4
1	D	225	GLY	3.4
1	F	420	ALA	3.4
1	L	261	TRP	3.4
1	B	79	ASP	3.4
1	J	178	ILE	3.4
1	K	223	LEU	3.4
1	L	364	GLN	3.4
1	A	32	PHE	3.4
1	L	355	ARG	3.4
1	G	320	THR	3.4
1	J	183	VAL	3.4
1	K	410	CYS	3.4
1	G	383	TYR	3.4
1	J	383	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	224	HIS	3.4
1	A	59	ARG	3.4
1	I	420	ALA	3.4
1	G	18	GLU	3.4
1	G	119	VAL	3.4
1	L	386	LEU	3.4
1	G	356	GLY	3.4
1	L	253	GLU	3.4
1	E	212	ASP	3.4
1	I	415	TYR	3.4
1	C	354	GLU	3.4
1	J	5	VAL	3.3
1	L	354	GLU	3.4
1	A	105	ALA	3.3
1	J	182	ALA	3.3
1	A	18	GLU	3.3
1	G	71	TYR	3.3
1	K	279	GLN	3.3
1	K	178	ILE	3.3
1	F	124	SER	3.3
1	K	261	TRP	3.3
1	L	42	GLN	3.3
1	A	223	LEU	3.3
1	K	121	PHE	3.3
1	G	303	LEU	3.3
1	J	354	GLU	3.3
1	L	32	PHE	3.3
1	H	320	THR	3.3
1	K	105	ALA	3.3
1	J	56	TYR	3.3
1	L	40	GLU	3.3
1	L	430	VAL	3.3
1	B	60	GLY	3.3
1	G	321	ASP	3.3
1	J	123	ALA	3.3
1	D	298	ILE	3.2
1	K	4	THR	3.2
1	L	358	GLN	3.2
1	L	112	GLY	3.2
1	L	429	LEU	3.2
1	L	433	THR	3.2
1	I	179	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	71	TYR	3.2
1	G	79	ASP	3.2
1	D	262	THR	3.2
1	D	419	GLY	3.2
1	L	210	ARG	3.2
1	E	209	PHE	3.2
1	L	263	HIS	3.2
1	E	224	HIS	3.2
1	L	259	LEU	3.2
1	F	416	ASN	3.2
1	J	59	ARG	3.2
1	J	32	PHE	3.2
1	A	357	LEU	3.2
1	F	105	ALA	3.2
1	K	197	ALA	3.2
1	D	59	ARG	3.2
1	D	370	ASN	3.2
1	H	105	ALA	3.2
1	G	94	LEU	3.1
1	K	402	TYR	3.1
1	A	217	ASP	3.1
1	E	408	ALA	3.1
1	J	353	SER	3.1
1	J	334	ILE	3.1
1	K	350	THR	3.1
1	A	68	THR	3.1
1	K	76	PHE	3.1
1	D	369	GLY	3.1
1	K	95	VAL	3.1
1	G	401	SER	3.1
1	L	58	ARG	3.1
1	B	236	THR	3.1
1	D	3	ILE	3.1
1	K	278	ALA	3.1
1	H	177	ARG	3.1
1	G	350	THR	3.1
1	D	430	VAL	3.1
1	G	325	LEU	3.1
1	E	334	ILE	3.1
1	F	198	ALA	3.1
1	G	398	ILE	3.0
1	L	421	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	K	106	ARG	3.0
1	K	179	SER	3.0
1	G	105	ALA	3.0
1	K	27	VAL	3.0
1	I	11	THR	3.0
1	E	213	ILE	3.0
1	F	433	THR	3.0
1	J	350	THR	3.0
1	C	73	TYR	3.0
1	B	419	GLY	3.0
1	I	356	GLY	3.0
1	B	68	THR	3.0
1	C	399	SER	3.0
1	F	360	ARG	3.0
1	I	223	LEU	3.0
1	L	426	ALA	3.0
1	G	336	SER	3.0
1	B	235	ASN	3.0
1	I	334	ILE	3.0
1	L	44	ALA	3.0
1	K	294	VAL	3.0
1	I	56	TYR	3.0
1	L	141	PRO	3.0
1	E	420	ALA	3.0
1	G	337	PRO	3.0
1	L	109	SER	3.0
1	D	10	SER	2.9
1	E	223	LEU	2.9
1	K	103	GLU	2.9
1	D	126	GLU	2.9
1	D	297	ILE	2.9
1	I	417	ARG	2.9
1	J	253	GLU	2.9
1	A	420	ALA	2.9
1	G	213	ILE	2.9
1	J	3	ILE	2.9
1	J	357	LEU	2.9
1	G	342	ILE	2.9
1	G	302	PRO	2.9
1	D	360	ARG	2.9
1	D	255	ALA	2.9
1	K	205	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	83	VAL	2.9
1	G	207	THR	2.9
1	I	65	SER	2.9
1	K	381	LYS	2.9
1	J	55	THR	2.9
1	K	248	GLU	2.9
1	E	411	MET	2.9
1	G	373	PRO	2.9
1	J	197	ALA	2.9
1	F	376	MET	2.9
1	K	388	ARG	2.9
1	C	103	GLU	2.9
1	I	358	GLN	2.9
1	I	68	THR	2.9
1	K	375	ASN	2.9
1	K	290	VAL	2.9
1	D	125	LEU	2.9
1	G	319	ASN	2.9
1	G	391	THR	2.9
1	I	216	ILE	2.9
1	C	417	ARG	2.9
1	G	62	GLY	2.8
1	E	202	PRO	2.8
1	F	236	THR	2.8
1	L	127	PRO	2.8
1	I	105	ALA	2.8
1	A	65	SER	2.8
1	D	198	ALA	2.8
1	L	13	ILE	2.8
1	B	416	ASN	2.8
1	J	352	PRO	2.8
1	F	334	ILE	2.8
1	C	32	PHE	2.8
1	G	405	GLY	2.8
1	K	416	ASN	2.8
1	G	335	LEU	2.8
1	G	261	TRP	2.8
1	K	378	LYS	2.8
1	K	15	LEU	2.8
1	L	46	LEU	2.8
1	B	356	GLY	2.8
1	E	406	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	10	SER	2.8
1	G	372	ASP	2.8
1	I	210	ARG	2.8
1	K	384	ARG	2.8
1	L	319	ASN	2.8
1	G	40	GLU	2.8
1	L	217	ASP	2.8
1	L	350	THR	2.8
1	I	108	VAL	2.8
1	I	66	GLN	2.8
1	I	195	PHE	2.8
1	L	384	ARG	2.8
1	G	341	GLY	2.8
1	G	379	ALA	2.8
1	K	270	ALA	2.8
1	B	103	GLU	2.8
1	F	34	LEU	2.8
1	E	205	TRP	2.8
1	I	124	SER	2.8
1	C	79	ASP	2.8
1	K	326	MET	2.8
1	H	399	SER	2.8
1	L	399	SER	2.8
1	H	168	TYR	2.8
1	E	103	GLU	2.8
1	B	83	VAL	2.8
1	H	71	TYR	2.8
1	G	433	THR	2.8
1	K	377	ASP	2.8
1	H	223	LEU	2.7
1	E	201	ALA	2.7
1	K	202	PRO	2.7
1	E	17	TYR	2.7
1	I	410	CYS	2.7
1	J	247	ALA	2.7
1	H	260	LEU	2.7
1	J	68	THR	2.7
1	G	216	ILE	2.7
1	D	354	GLU	2.7
1	C	223	LEU	2.7
1	E	19	ASP	2.7
1	J	433	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	124	SER	2.7
1	K	107	TYR	2.7
1	L	19	ASP	2.7
1	A	179	SER	2.7
1	B	34	LEU	2.7
1	E	389	GLU	2.7
1	C	177	ARG	2.7
1	D	14	ASP	2.7
1	L	356	GLY	2.7
1	A	216	ILE	2.7
1	H	233	ILE	2.7
1	L	383	TYR	2.7
1	H	124	SER	2.7
1	I	32	PHE	2.7
1	F	415	TYR	2.7
1	F	237	ALA	2.7
1	G	139	ALA	2.7
1	K	407	LEU	2.7
1	C	377	ASP	2.7
1	H	15	LEU	2.7
1	H	66	GLN	2.7
1	J	351	VAL	2.7
1	G	310	ARG	2.7
1	C	389	GLU	2.7
1	F	186	SER	2.7
1	A	257	HIS	2.7
1	G	202	PRO	2.7
1	G	83	VAL	2.7
1	K	77	ALA	2.7
1	K	404	ALA	2.7
1	K	405	GLY	2.7
1	A	383	TYR	2.7
1	B	223	LEU	2.7
1	K	68	THR	2.7
1	K	207	THR	2.7
1	G	360	ARG	2.7
1	L	98	SER	2.7
1	A	356	GLY	2.7
1	G	374	ASN	2.7
1	E	216	ILE	2.6
1	E	364	GLN	2.6
1	G	32	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	K	235	ASN	2.6
1	B	178	ILE	2.6
1	C	69	THR	2.6
1	I	357	LEU	2.6
1	H	404	ALA	2.6
1	B	358	GLN	2.6
1	D	416	ASN	2.6
1	K	74	ASP	2.6
1	D	205	TRP	2.6
1	C	76	PHE	2.6
1	K	415	TYR	2.6
1	G	200	ALA	2.6
1	J	15	LEU	2.6
1	D	66	GLN	2.6
1	L	41	ARG	2.6
1	F	32	PHE	2.6
1	G	121	PHE	2.6
1	K	70	GLY	2.6
1	K	347	PHE	2.6
1	H	380	VAL	2.6
1	G	201	ALA	2.6
1	K	275	LEU	2.6
1	E	376	MET	2.6
1	G	34	LEU	2.6
1	L	53	VAL	2.6
1	E	1	PRO	2.6
1	A	108	VAL	2.6
1	D	224	HIS	2.6
1	L	431	CYS	2.6
1	A	126	GLU	2.6
1	J	198	ALA	2.6
1	K	441	GLN	2.6
1	D	410	CYS	2.6
1	H	125	LEU	2.6
1	J	63	GLN	2.6
1	L	208	ASP	2.6
1	L	93	VAL	2.6
1	B	129	LEU	2.6
1	I	126	GLU	2.6
1	K	122	LEU	2.6
1	I	261	TRP	2.6
1	L	360	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	199	ALA	2.6
1	L	294	VAL	2.6
1	I	376	MET	2.6
1	G	260	LEU	2.6
1	C	415	TYR	2.6
1	G	178	ILE	2.6
1	G	209	PHE	2.6
1	I	160	TYR	2.6
1	G	311	LEU	2.5
1	G	400	LEU	2.5
1	J	237	ALA	2.5
1	J	244	LEU	2.5
1	F	390	ILE	2.5
1	C	360	ARG	2.5
1	J	188	ASN	2.5
1	B	193	GLY	2.5
1	G	348	THR	2.5
1	L	418	MET	2.5
1	D	413	LEU	2.5
1	F	251	GLU	2.5
1	E	62	GLY	2.5
1	G	76	PHE	2.5
1	H	390	ILE	2.5
1	J	195	PHE	2.5
1	K	433	THR	2.5
1	L	436	GLN	2.5
1	I	335	LEU	2.5
1	D	427	PHE	2.5
1	K	360	ARG	2.5
1	L	67	PRO	2.5
1	L	198	ALA	2.5
1	G	306	GLU	2.5
1	D	202	PRO	2.5
1	L	140	ALA	2.5
1	G	378	LYS	2.5
1	E	125	LEU	2.5
1	K	126	GLU	2.5
1	L	377	ASP	2.5
1	J	356	GLY	2.5
1	K	403	SER	2.5
1	K	348	THR	2.5
1	I	180	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	56	TYR	2.5
1	J	418	MET	2.5
1	K	390	ILE	2.5
1	C	357	LEU	2.5
1	E	405	GLY	2.5
1	L	65	SER	2.5
1	G	193	GLY	2.5
1	G	386	LEU	2.5
1	D	411	MET	2.5
1	F	179	SER	2.4
1	L	197	ALA	2.4
1	J	66	GLN	2.4
1	G	315	PHE	2.4
1	D	364	GLN	2.4
1	C	205	TRP	2.4
1	K	177	ARG	2.4
1	E	198	ALA	2.4
1	I	94	LEU	2.4
1	K	276	ALA	2.4
1	J	216	ILE	2.4
1	K	383	TYR	2.4
1	C	129	LEU	2.4
1	C	358	GLN	2.4
1	C	251	GLU	2.4
1	L	251	GLU	2.4
1	A	34	LEU	2.4
1	C	348	THR	2.4
1	I	260	LEU	2.4
1	E	16	TYR	2.4
1	J	103	GLU	2.4
1	L	110	SER	2.4
1	G	322	LEU	2.4
1	F	364	GLN	2.4
1	G	66	GLN	2.4
1	A	139	ALA	2.4
1	E	333	PRO	2.4
1	A	104	VAL	2.4
1	H	301	GLY	2.4
1	I	204	THR	2.4
1	K	6	GLY	2.4
1	L	125	LEU	2.4
1	C	403	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	L	76	PHE	2.4
1	I	183	VAL	2.4
1	K	66	GLN	2.4
1	L	260	LEU	2.4
1	A	168	TYR	2.4
1	H	359	ARG	2.4
1	C	1	PRO	2.4
1	G	37	HIS	2.4
1	B	226	THR	2.4
1	L	27	VAL	2.4
1	E	403	SER	2.4
1	K	109	SER	2.4
1	K	247	ALA	2.4
1	G	205	TRP	2.4
1	I	354	GLU	2.4
1	L	419	GLY	2.4
1	B	139	ALA	2.4
1	L	380	VAL	2.4
1	C	371	GLY	2.4
1	J	320	THR	2.4
1	K	401	SER	2.4
1	D	33	PRO	2.4
1	G	389	GLU	2.4
1	B	418	MET	2.4
1	C	375	ASN	2.4
1	H	173	ASN	2.4
1	B	190	ALA	2.4
1	D	67	PRO	2.4
1	A	323	GLU	2.4
1	K	356	GLY	2.4
1	G	343	LEU	2.4
1	K	437	ILE	2.4
1	I	377	ASP	2.4
1	F	383	TYR	2.3
1	K	250	VAL	2.3
1	E	409	SER	2.3
1	K	49	ALA	2.3
1	D	415	TYR	2.3
1	G	416	ASN	2.3
1	B	18	GLU	2.3
1	B	376	MET	2.3
1	C	56	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	335	LEU	2.3
1	L	415	TYR	2.3
1	C	107	TYR	2.3
1	D	418	MET	2.3
1	C	207	THR	2.3
1	I	25	PRO	2.3
1	K	237	ALA	2.3
1	F	56	TYR	2.3
1	L	363	VAL	2.3
1	D	350	THR	2.3
1	I	177	ARG	2.3
1	H	420	ALA	2.3
1	L	80	LEU	2.3
1	A	195	PHE	2.3
1	D	253	GLU	2.3
1	K	297	ILE	2.3
1	I	175	GLY	2.3
1	K	104	VAL	2.3
1	E	56	TYR	2.3
1	E	67	PRO	2.3
1	H	430	VAL	2.3
1	H	249	TYR	2.3
1	G	126	GLU	2.3
1	H	302	PRO	2.3
1	K	7	GLN	2.3
1	B	198	ALA	2.3
1	G	305	ALA	2.3
1	I	214	PRO	2.3
1	H	60	GLY	2.3
1	C	233	ILE	2.3
1	D	263	HIS	2.3
1	A	250	VAL	2.3
1	B	335	LEU	2.3
1	G	15	LEU	2.3
1	K	373	PRO	2.3
1	I	262	THR	2.3
1	F	59	ARG	2.3
1	F	177	ARG	2.3
1	K	238	ARG	2.3
1	B	383	TYR	2.3
1	K	232	PRO	2.3
1	G	334	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	123	ALA	2.3
1	G	308	ALA	2.3
1	A	260	LEU	2.3
1	C	401	SER	2.3
1	E	335	LEU	2.3
1	G	314	VAL	2.3
1	A	342	ILE	2.3
1	B	357	LEU	2.3
1	G	60	GLY	2.3
1	L	381	LYS	2.3
1	H	403	SER	2.3
1	I	3	ILE	2.3
1	E	262	THR	2.3
1	J	184	ARG	2.3
1	E	385	LYS	2.3
1	K	389	GLU	2.3
1	J	240	PHE	2.3
1	B	373	PRO	2.3
1	D	380	VAL	2.3
1	L	177	ARG	2.3
1	K	352	PRO	2.3
1	G	351	VAL	2.3
1	I	399	SER	2.2
1	K	73	TYR	2.2
1	G	194	GLY	2.2
1	I	125	LEU	2.2
1	E	105	ALA	2.2
1	I	121	PHE	2.2
1	F	399	SER	2.2
1	D	355	ARG	2.2
1	E	320	THR	2.2
1	A	261	TRP	2.2
1	K	34	LEU	2.2
1	E	298	ILE	2.2
1	D	238	ARG	2.2
1	G	58	ARG	2.2
1	A	140	ALA	2.2
1	E	299	PRO	2.2
1	L	252	VAL	2.2
1	D	434	CYS	2.2
1	I	251	GLU	2.2
1	H	357	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	37	HIS	2.2
1	F	173	ASN	2.2
1	K	236	THR	2.2
1	L	339	THR	2.2
1	D	226	THR	2.2
1	B	354	GLU	2.2
1	E	261	TRP	2.2
1	H	216	ILE	2.2
1	L	3	ILE	2.2
1	K	234	GLU	2.2
1	A	322	LEU	2.2
1	L	353	SER	2.2
1	D	294	VAL	2.2
1	G	370	ASN	2.2
1	C	59	ARG	2.2
1	H	34	LEU	2.2
1	D	426	ALA	2.2
1	I	69	THR	2.2
1	C	402	TYR	2.2
1	B	333	PRO	2.2
1	C	105	ALA	2.2
1	L	342	ILE	2.2
1	F	223	LEU	2.2
1	C	426	ALA	2.2
1	L	33	PRO	2.2
1	G	347	PHE	2.2
1	L	427	PHE	2.2
1	F	60	GLY	2.2
1	G	127	PRO	2.2
1	C	378	LYS	2.2
1	H	391	THR	2.2
1	G	57	ASP	2.2
1	G	129	LEU	2.2
1	J	122	LEU	2.2
1	J	168	TYR	2.2
1	B	233	ILE	2.2
1	I	360	ARG	2.2
1	B	137	ASP	2.2
1	G	73	TYR	2.2
1	G	230	THR	2.2
1	A	380	VAL	2.2
1	K	252	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	438	ALA	2.2
1	E	59	ARG	2.2
1	G	215	ARG	2.2
1	H	32	PHE	2.2
1	J	62	GLY	2.2
1	K	58	ARG	2.2
1	L	69	THR	2.2
1	J	416	ASN	2.2
1	L	81	ASN	2.2
1	A	102	GLY	2.2
1	B	420	ALA	2.2
1	L	105	ALA	2.2
1	B	56	TYR	2.2
1	H	122	LEU	2.2
1	A	190	ALA	2.2
1	D	236	THR	2.2
1	J	98	SER	2.2
1	E	15	LEU	2.2
1	G	224	HIS	2.2
1	G	240	PHE	2.2
1	J	322	LEU	2.2
1	A	252	VAL	2.1
1	I	79	ASP	2.2
1	H	237	ALA	2.1
1	L	388	ARG	2.1
1	C	226	THR	2.1
1	I	202	PRO	2.1
1	L	82	THR	2.1
1	E	104	VAL	2.1
1	E	359	ARG	2.1
1	I	9	ASN	2.1
1	J	200	ALA	2.1
1	J	355	ARG	2.1
1	H	433	THR	2.1
1	K	254	GLY	2.1
1	B	80	LEU	2.1
1	F	411	MET	2.1
1	E	421	VAL	2.1
1	A	198	ALA	2.1
1	D	32	PHE	2.1
1	D	73	TYR	2.1
1	K	298	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	325	LEU	2.1
1	L	113	THR	2.1
1	L	390	ILE	2.1
1	K	211	ALA	2.1
1	E	383	TYR	2.1
1	K	413	LEU	2.1
1	J	226	THR	2.1
1	E	382	LEU	2.1
1	G	323	GLU	2.1
1	I	24	THR	2.1
1	K	91	ASP	2.1
1	B	5	VAL	2.1
1	D	13	ILE	2.1
1	J	125	LEU	2.1
1	A	376	MET	2.1
1	F	354	GLU	2.1
1	G	355	ARG	2.1
1	J	257	HIS	2.1
1	K	119	VAL	2.1
1	F	382	LEU	2.1
1	H	198	ALA	2.1
1	L	142	GLN	2.1
1	L	347	PHE	2.1
1	F	67	PRO	2.1
1	E	9	ASN	2.1
1	A	106	ARG	2.1
1	C	102	GLY	2.1
1	C	237	ALA	2.1
1	F	106	ARG	2.1
1	G	436	GLN	2.1
1	H	364	GLN	2.1
1	H	83	VAL	2.1
1	H	376	MET	2.1
1	L	191	ALA	2.1
1	F	363	VAL	2.1
1	E	79	ASP	2.1
1	B	123	ALA	2.1
1	B	379	ALA	2.1
1	C	396	LYS	2.1
1	K	21	GLY	2.1
1	A	386	LEU	2.1
1	K	221	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	377	ASP	2.1
1	G	107	TYR	2.1
1	K	439	ASP	2.1
1	A	232	PRO	2.1
1	B	76	PHE	2.1
1	B	319	ASN	2.1
1	D	259	LEU	2.1
1	G	140	ALA	2.1
1	F	175	GLY	2.1
1	G	225	GLY	2.1
1	I	226	THR	2.1
1	L	387	LYS	2.1
1	J	248	GLU	2.1
1	J	80	LEU	2.1
1	D	348	THR	2.1
1	F	199	ALA	2.1
1	L	298	ILE	2.1
1	D	367	LEU	2.1
1	K	409	SER	2.1
1	C	262	THR	2.1
1	A	228	ASP	2.1
1	F	373	PRO	2.1
1	J	127	PRO	2.1
1	L	173	ASN	2.1
1	E	249	TYR	2.1
1	E	380	VAL	2.1
1	J	249	TYR	2.1
1	A	237	ALA	2.1
1	G	118	ALA	2.1
1	K	61	PHE	2.1
1	A	294	VAL	2.1
1	A	377	ASP	2.1
1	C	380	VAL	2.1
1	I	112	GLY	2.1
1	I	205	TRP	2.1
1	K	251	GLU	2.1
1	L	17	TYR	2.1
1	J	386	LEU	2.1
1	K	47	LEU	2.1
1	B	216	ILE	2.1
1	B	378	LYS	2.1
1	K	344	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	104	VAL	2.0
1	L	389	GLU	2.0
1	B	125	LEU	2.0
1	H	360	ARG	2.0
1	H	61	PHE	2.0
1	K	168	TYR	2.0
1	A	335	LEU	2.0
1	I	197	ALA	2.0
1	L	45	ALA	2.0
1	I	320	THR	2.0
1	C	372	ASP	2.0
1	E	251	GLU	2.0
1	H	389	GLU	2.0
1	J	60	GLY	2.0
1	J	258	GLY	2.0
1	C	421	VAL	2.0
1	D	440	SER	2.0
1	I	355	ARG	2.0
1	K	114	ALA	2.0
1	K	201	ALA	2.0
1	H	262	THR	2.0
1	H	363	VAL	2.0
1	F	125	LEU	2.0
1	A	404	ALA	2.0
1	C	374	ASN	2.0
1	G	441	GLN	2.0
1	J	54	ILE	2.0
1	B	69	THR	2.0
1	K	176	THR	2.0
1	L	231	LEU	2.0
1	K	26	VAL	2.0
1	K	78	ALA	2.0
1	B	205	TRP	2.0
1	G	168	TYR	2.0
1	K	271	LEU	2.0
1	K	343	LEU	2.0
1	L	168	TYR	2.0
1	L	437	ILE	2.0
1	C	55	THR	2.0
1	C	123	ALA	2.0
1	F	182	ALA	2.0
1	F	404	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	74	ASP	2.0
1	L	84	LEU	2.0
1	B	20	HIS	2.0
1	C	236	THR	2.0
1	K	240	PHE	2.0
1	E	407	LEU	2.0
1	K	173	ASN	2.0
1	A	224	HIS	2.0
1	B	207	THR	2.0
1	G	108	VAL	2.0
1	L	97	PHE	2.0
1	J	358	GLN	2.0
1	K	289	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.