



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2014 – 11:30 PM EDT

PDB ID : 4NHG  
Title : Crystal Structure of 2G12 IgG Dimer  
Authors : Wu, Y.; West Jr., A.P.; Kim, H.J.; Thornton, M.E.; Ward, A.B.; Bjorkman, P.J.  
Deposited on : 2013-11-05  
Resolution : 8.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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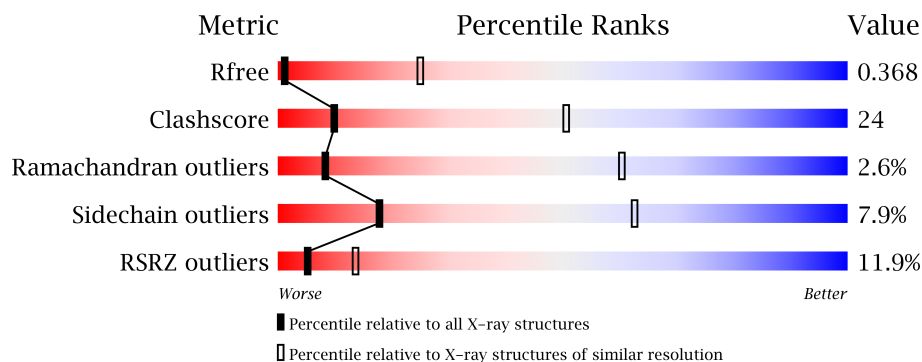
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable24103  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.1.3  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable24103

# 1 Overall quality at a glance

The reported resolution of this entry is 8.00 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))
$R_{free}$	66092	1106 (11.50-3.50)
Clashscore	79885	1007 (12.20-3.54)
Ramachandran outliers	78287	1302 (12.20-3.50)
Sidechain outliers	78261	1276 (12.20-3.50)
RSRZ outliers	66119	1105 (11.50-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	243	
1	D	243	
1	E	243	
1	H	243	
1	I	243	
1	M	243	
2	B	213	
2	C	213	
2	F	213	
2	G	213	
2	K	213	
2	L	213	
3	J	211	
3	N	211	

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Mol	Chain	Length	Quality of chain
3	O	211	
3	P	211	
3	X	211	
3	Y	211	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 29250 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2G12 IgG dimer heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	D	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	E	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	I	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			
1	H	215	Total	C	N	O	S	38	0	0
			1600	1007	273	314	6			
1	M	215	Total	C	N	O	S	51	0	0
			1600	1007	273	314	6			

- Molecule 2 is a protein called 2G12 IgG dimer light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	C	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	F	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	G	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	K	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			
2	L	211	Total	C	N	O	S	0	0	0
			1618	1018	272	323	5			

- Molecule 3 is a protein called Hepatitis B virus receptor binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	N	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	X	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	Y	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			
3	O	207	Total	C	N	O	S	0	0	0
			1660	1057	282	314	7			
3	P	206	Total	C	N	O	S	0	0	0
			1654	1054	280	313	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	272	GLN	GLU	CONFLICT	UNP Q6PYX1
X	283	GLN	GLU	CONFLICT	UNP Q6PYX1
X	294	GLN	GLU	CONFLICT	UNP Q6PYX1
X	312	ASN	ASP	CONFLICT	UNP Q6PYX1
X	315	ASP	ASN	CONFLICT	UNP Q6PYX1
X	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
Y	272	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	283	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	294	GLN	GLU	CONFLICT	UNP Q6PYX1
Y	312	ASN	ASP	CONFLICT	UNP Q6PYX1
Y	315	ASP	ASN	CONFLICT	UNP Q6PYX1
Y	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
J	272	GLN	GLU	CONFLICT	UNP Q6PYX1
J	283	GLN	GLU	CONFLICT	UNP Q6PYX1
J	294	GLN	GLU	CONFLICT	UNP Q6PYX1
J	312	ASN	ASP	CONFLICT	UNP Q6PYX1
J	315	ASP	ASN	CONFLICT	UNP Q6PYX1
J	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
N	272	GLN	GLU	CONFLICT	UNP Q6PYX1
N	283	GLN	GLU	CONFLICT	UNP Q6PYX1
N	294	GLN	GLU	CONFLICT	UNP Q6PYX1
N	312	ASN	ASP	CONFLICT	UNP Q6PYX1
N	315	ASP	ASN	CONFLICT	UNP Q6PYX1
N	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
O	272	GLN	GLU	CONFLICT	UNP Q6PYX1
O	283	GLN	GLU	CONFLICT	UNP Q6PYX1
O	294	GLN	GLU	CONFLICT	UNP Q6PYX1
O	312	ASN	ASP	CONFLICT	UNP Q6PYX1

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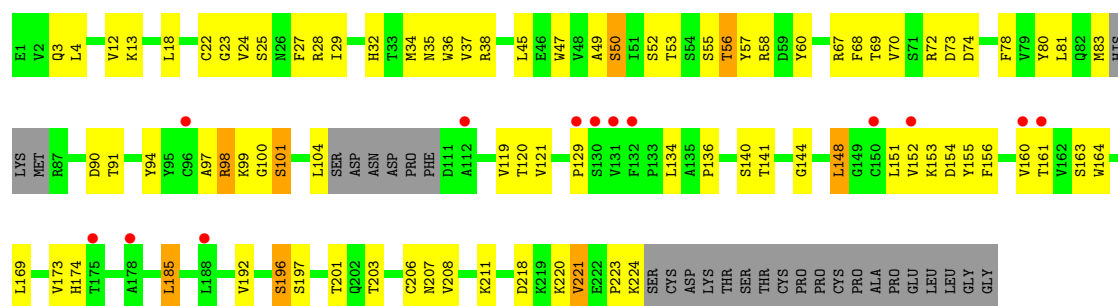
Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	CONFLICT	UNP Q6PYX1
O	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
P	272	GLN	GLU	CONFLICT	UNP Q6PYX1
P	283	GLN	GLU	CONFLICT	UNP Q6PYX1
P	294	GLN	GLU	CONFLICT	UNP Q6PYX1
P	312	ASN	ASP	CONFLICT	UNP Q6PYX1
P	315	ASP	ASN	CONFLICT	UNP Q6PYX1
P	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1

### 3 Residue-property plots

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

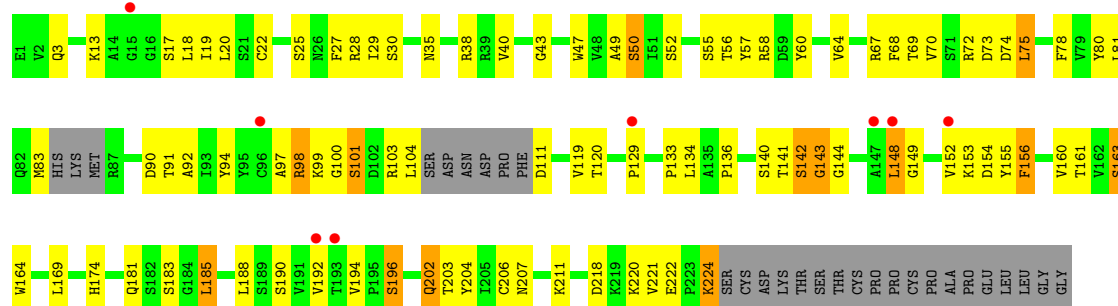
#### • Molecule 1: 2G12 IgG dimer heavy chain

Chain A: 



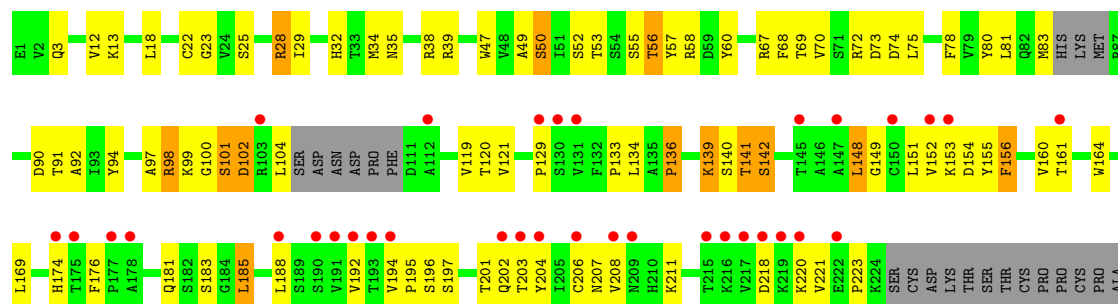
#### • Molecule 1: 2G12 IgG dimer heavy chain

Chain D: 



#### • Molecule 1: 2G12 IgG dimer heavy chain

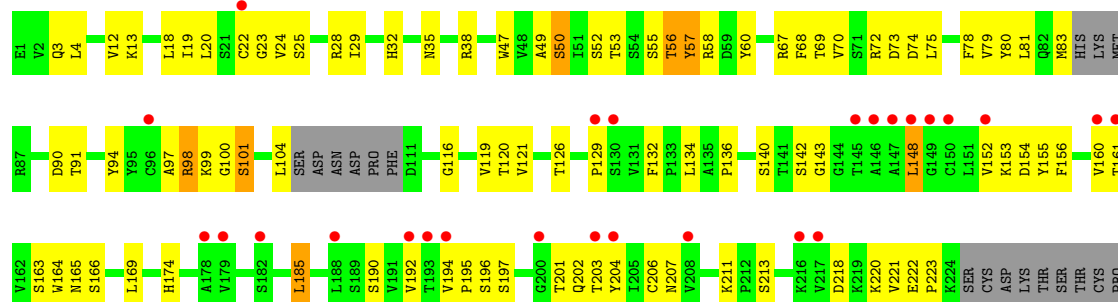
Chain E: 



PRO  
GLU  
LEU  
LEU  
GLY  
GLY

• Molecule 1: 2G12 IgG dimer heavy chain

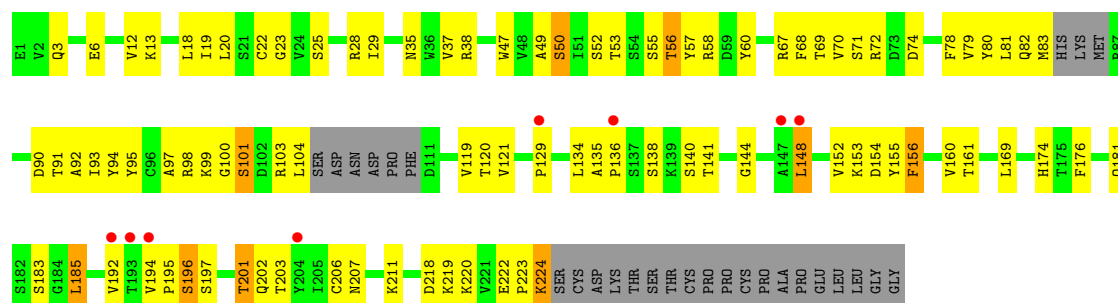
Chain I:



PRO  
CYS  
PRO  
ALA  
PRO  
GLU  
LEU  
LEU  
GLY  
GLY

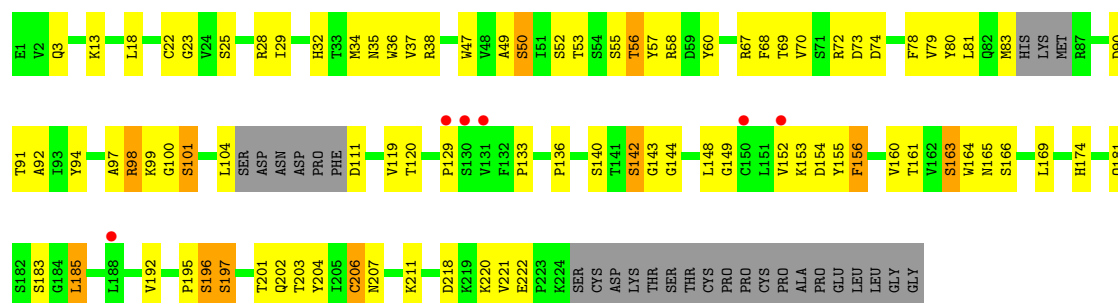
• Molecule 1: 2G12 IgG dimer heavy chain

Chain H:



• Molecule 1: 2G12 IgG dimer heavy chain

Chain M:

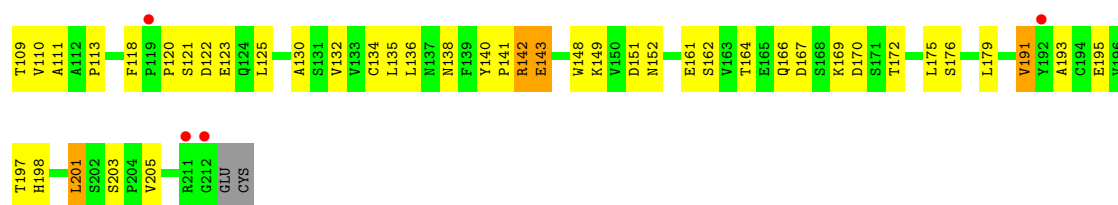


• Molecule 2: 2G12 IgG dimer light chain

Chain B:

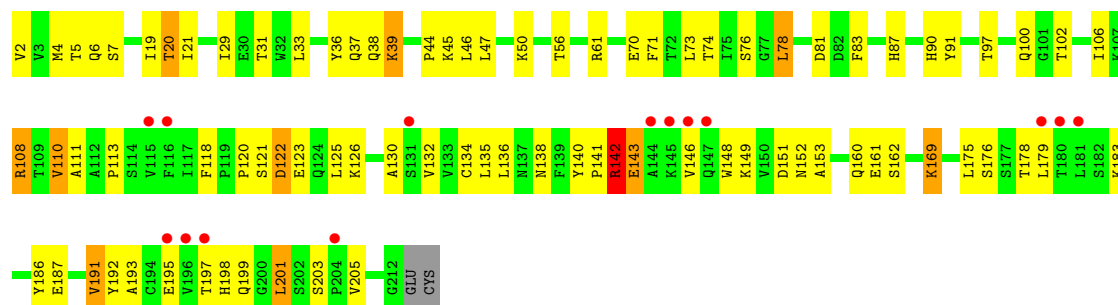






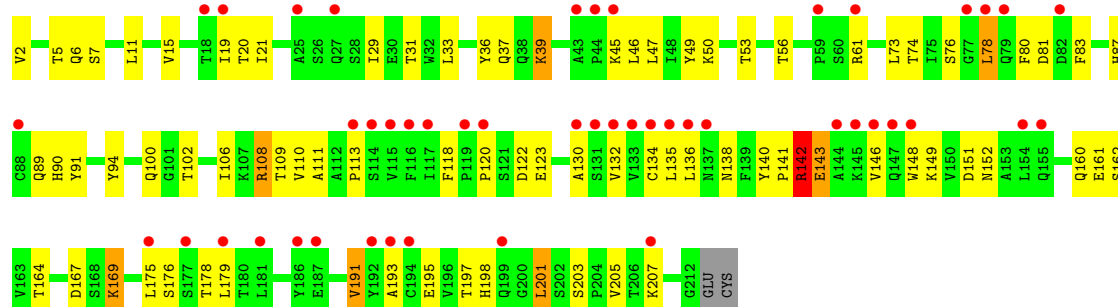
• Molecule 2: 2G12 IgG dimer light chain

Chain C:



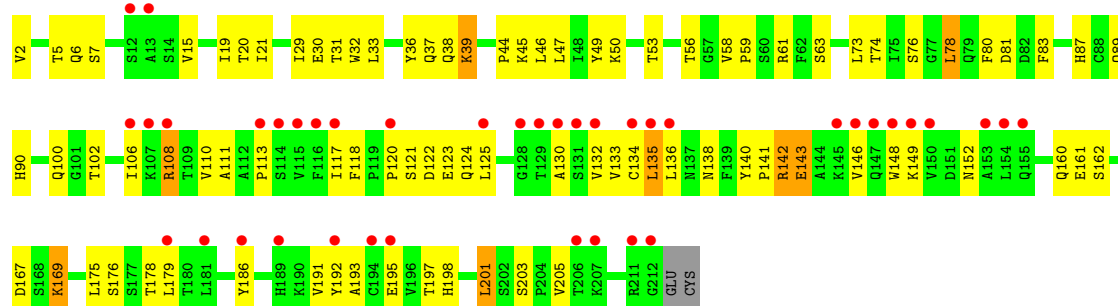
• Molecule 2: 2G12 IgG dimer light chain

Chain F:



• Molecule 2: 2G12 IgG dimer light chain

Chain G:

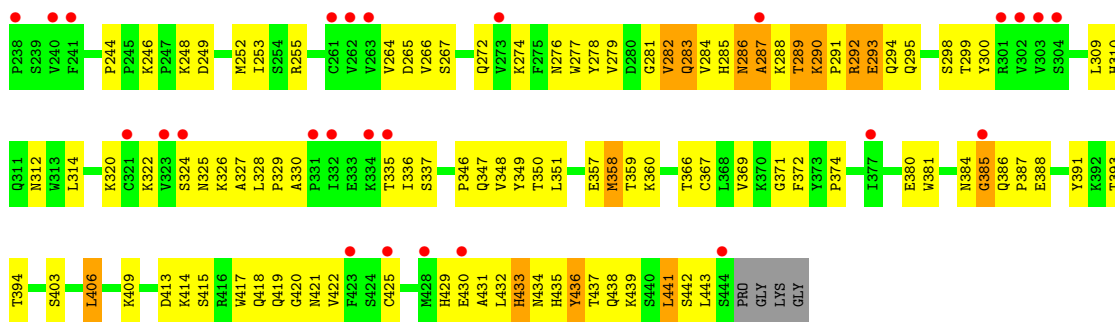


• Molecule 2: 2G12 IgG dimer light chain

Chain K:

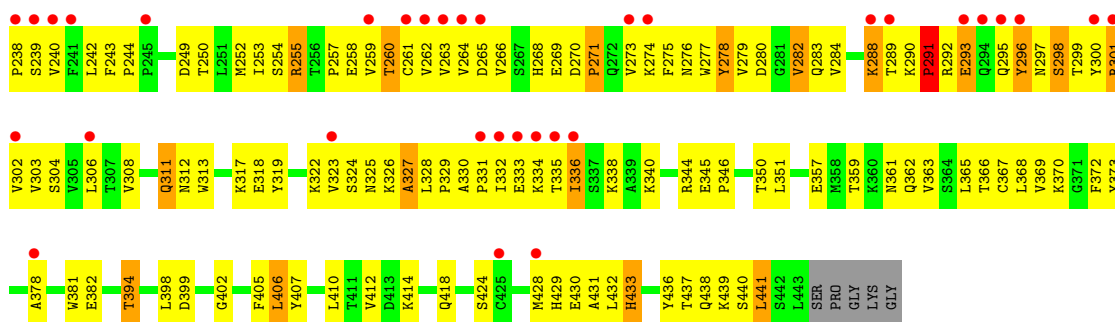


Chain X:



- Molecule 3: Hepatitis B virus receptor binding protein

Chain Y:



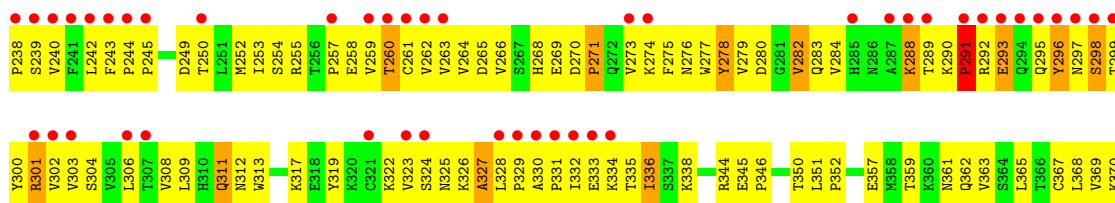
- Molecule 3: Hepatitis B virus receptor binding protein

Chain O:



- Molecule 3: Hepatitis B virus receptor binding protein

Chain P:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	246.25Å 246.25Å 657.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.75 – 8.00 39.75 – 7.43	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.75-8.00) 82.2 (39.75-7.43)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 7.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.359 , 0.369 0.352 , 0.368	Depositor DCC
$R_{free}$ test set	1263 reflections (9.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	296.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 297.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 13337 reflections	Xtriage
$F_o, F_c$ correlation	0.60	EDS
Total number of atoms	29250	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.69	1/1633 (0.1%)	0.95	4/2220 (0.2%)
1	D	0.63	0/1631	0.85	3/2214 (0.1%)
1	E	0.67	0/1633	0.93	4/2220 (0.2%)
1	H	0.63	0/1633	0.92	3/2220 (0.1%)
1	I	0.68	0/1631	0.83	3/2214 (0.1%)
1	M	0.68	2/1631 (0.1%)	0.85	3/2214 (0.1%)
2	B	0.63	0/1654	0.75	1/2246 (0.0%)
2	C	0.70	1/1654 (0.1%)	0.78	2/2246 (0.1%)
2	F	0.69	0/1654	0.77	2/2246 (0.1%)
2	G	0.69	1/1654 (0.1%)	0.77	1/2246 (0.0%)
2	K	0.63	0/1654	0.77	3/2246 (0.1%)
2	L	0.67	1/1654 (0.1%)	0.78	1/2246 (0.0%)
3	J	0.43	0/1706	0.68	0/2323
3	N	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	O	0.43	0/1706	0.68	0/2323
3	P	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	X	0.43	0/1706	0.68	0/2323
3	Y	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
All	All	0.60	9/29931 (0.0%)	0.78	36/40683 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	3
3	N	0	1
3	P	0	1
3	Y	0	1
All	All	0	6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	433	HIS	CA-C	11.57	1.83	1.52
3	N	433	HIS	CA-C	11.50	1.82	1.52
3	P	433	HIS	CA-C	11.50	1.82	1.52
1	M	36	TRP	CB-CG	6.40	1.61	1.50
2	C	143	GLU	CB-CG	6.03	1.63	1.52
2	L	143	GLU	CB-CG	5.60	1.62	1.52
1	A	36	TRP	CB-CG	5.48	1.60	1.50
2	G	143	GLU	CB-CG	5.30	1.62	1.52
1	M	197	SER	CB-OG	-5.20	1.35	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	ARG	NE-CZ-NH1	-17.15	111.73	120.30
1	H	28	ARG	NE-CZ-NH1	-16.64	111.98	120.30
1	E	28	ARG	NE-CZ-NH1	-15.56	112.52	120.30
1	A	28	ARG	NE-CZ-NH2	14.53	127.56	120.30
1	E	28	ARG	NE-CZ-NH2	13.74	127.17	120.30
1	H	28	ARG	NE-CZ-NH2	12.48	126.54	120.30
1	D	28	ARG	NE-CZ-NH2	-12.04	114.28	120.30
1	M	28	ARG	NE-CZ-NH2	-11.26	114.67	120.30
2	G	135	LEU	CA-CB-CG	10.28	138.94	115.30
1	D	28	ARG	NE-CZ-NH1	10.17	125.38	120.30
2	F	135	LEU	CA-CB-CG	9.76	137.74	115.30
2	B	135	LEU	CA-CB-CG	9.65	137.50	115.30
1	I	28	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	C	135	LEU	CA-CB-CG	9.59	137.35	115.30
1	M	28	ARG	NE-CZ-NH1	9.35	124.98	120.30
2	K	135	LEU	CA-CB-CG	9.18	136.42	115.30
2	L	135	LEU	CA-CB-CG	9.13	136.30	115.30
1	I	28	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	E	28	ARG	CD-NE-CZ	8.21	135.09	123.60
1	A	28	ARG	CD-NE-CZ	7.90	134.66	123.60
1	H	28	ARG	CD-NE-CZ	7.30	133.82	123.60
3	N	433	HIS	CB-CA-C	-6.57	97.26	110.40
3	Y	433	HIS	CB-CA-C	-6.56	97.27	110.40
3	P	433	HIS	CB-CA-C	-6.54	97.33	110.40
3	Y	433	HIS	N-CA-C	-6.29	94.02	111.00
3	P	433	HIS	N-CA-C	-6.28	94.03	111.00
3	N	433	HIS	N-CA-C	-6.28	94.04	111.00
2	F	142	ARG	NE-CZ-NH1	6.25	123.43	120.30
2	K	142	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	M	28	ARG	CD-NE-CZ	5.53	131.34	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	151	LEU	CA-CB-CG	5.46	127.86	115.30
2	C	142	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	I	28	ARG	CD-NE-CZ	5.18	130.85	123.60
1	D	28	ARG	CD-NE-CZ	5.11	130.75	123.60
2	K	169	LYS	CD-CE-NZ	5.01	123.23	111.70
1	A	151	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	139	LYS	Peptide
1	E	140	SER	Peptide
1	E	142	SER	Peptide
3	N	373	TYR	Sidechain
3	P	373	TYR	Sidechain
3	Y	373	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1600	0	1581	73	0
1	D	1600	0	1579	96	11
1	E	1600	0	1581	72	0
1	H	1600	0	1580	78	2
1	I	1600	0	1578	78	0
1	M	1600	0	1579	85	0
2	B	1618	0	1580	49	23
2	C	1618	0	1580	54	0
2	F	1618	0	1580	69	0
2	G	1618	0	1580	58	2
2	K	1618	0	1580	54	0
2	L	1618	0	1580	57	19
3	J	1660	0	1632	99	60

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	N	1654	0	1627	114	37
3	O	1660	0	1630	93	19
3	P	1654	0	1624	123	37
3	X	1660	0	1632	98	56
3	Y	1654	0	1627	118	37
All	All	29250	0	28730	1381	174

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 24.

All (1381) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:103:ARG:C	2:F:50:LYS:HZ2	1.05	1.59
3:P:433:HIS:C	3:P:433:HIS:CA	1.82	1.45
3:N:433:HIS:C	3:N:433:HIS:CA	1.82	1.45
3:Y:433:HIS:C	3:Y:433:HIS:CA	1.83	1.45
1:D:103:ARG:CA	2:F:50:LYS:NZ	1.90	1.34
1:D:103:ARG:C	2:F:50:LYS:NZ	1.79	1.33
2:F:207:LYS:NZ	1:M:201:THR:HB	1.41	1.31
1:D:103:ARG:CA	2:F:50:LYS:HZ3	1.44	1.27
1:D:75:LEU:HD22	1:I:57:TYR:CZ	1.76	1.20
1:A:104:LEU:HD12	1:E:28:ARG:HG3	1.28	1.10
1:D:103:ARG:HA	2:F:50:LYS:NZ	1.53	1.09
3:P:266:VAL:HB	3:P:300:TYR:HB2	1.45	0.99
3:N:266:VAL:HB	3:N:300:TYR:HB2	1.45	0.99
3:Y:266:VAL:HB	3:Y:300:TYR:HB2	1.45	0.99
1:I:201:THR:HG1	1:I:202:GLN:N	1.62	0.96
1:H:174:HIS:NE2	2:K:138:ASN:OD1	1.99	0.96
1:A:174:HIS:NE2	2:B:138:ASN:OD1	2.00	0.94
1:D:103:ARG:HA	2:F:50:LYS:HZ3	0.76	0.92
3:X:272:GLN:HE22	3:X:326:LYS:HD2	1.35	0.92
3:O:272:GLN:HE22	3:O:326:LYS:HD2	1.35	0.91
2:F:207:LYS:HZ2	1:M:201:THR:HB	1.00	0.91
3:J:272:GLN:HE22	3:J:326:LYS:HD2	1.35	0.91
3:O:282:VAL:O	3:O:283:GLN:HB2	1.72	0.90
3:X:282:VAL:O	3:X:283:GLN:HB2	1.72	0.90
3:Y:311:GLN:H	3:Y:311:GLN:NE2	1.71	0.89
3:J:282:VAL:O	3:J:283:GLN:HB2	1.72	0.89
3:N:311:GLN:NE2	3:N:311:GLN:H	1.71	0.89
3:P:311:GLN:H	3:P:311:GLN:NE2	1.71	0.89
1:D:103:ARG:O	2:F:50:LYS:NZ	1.96	0.88
1:D:204:TYR:O	1:D:221:VAL:N	2.07	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:290:LYS:NZ	2:L:109:THR:HG21	1.90	0.86
1:E:174:HIS:NE2	2:F:138:ASN:OD1	2.08	0.85
3:N:328:LEU:HD21	3:N:332:ILE:HG13	1.59	0.84
1:A:197:SER:CB	3:X:295:GLN:HE22	1.90	0.84
2:F:207:LYS:NZ	1:M:201:THR:CB	2.35	0.84
3:Y:291:PRO:HB3	3:Y:304:SER:HA	1.60	0.84
1:I:148:LEU:HD13	1:I:221:VAL:HB	1.59	0.84
3:X:346:PRO:HB3	3:X:372:PHE:HB3	1.60	0.83
1:A:3:GLN:HB2	1:A:25:SER:HB2	1.58	0.83
3:P:328:LEU:HD21	3:P:332:ILE:HG13	1.59	0.83
3:P:243:PHE:HB2	3:P:260:THR:HG23	1.60	0.83
3:Y:328:LEU:HD21	3:Y:332:ILE:HG13	1.59	0.83
3:N:291:PRO:HB3	3:N:304:SER:HA	1.60	0.83
3:P:291:PRO:HB3	3:P:304:SER:HA	1.60	0.83
3:O:346:PRO:HB3	3:O:372:PHE:HB3	1.60	0.82
3:Y:243:PHE:HB2	3:Y:260:THR:HG23	1.60	0.82
2:F:207:LYS:HZ2	1:M:201:THR:CB	1.89	0.82
1:E:3:GLN:HB2	1:E:25:SER:HB2	1.61	0.82
1:D:3:GLN:HB2	1:D:25:SER:HB2	1.61	0.81
3:J:314:LEU:HD22	3:J:430:GLU:HG3	1.62	0.81
3:J:346:PRO:HB3	3:J:372:PHE:HB3	1.60	0.81
3:N:243:PHE:HB2	3:N:260:THR:HG23	1.60	0.81
1:H:90:ASP:O	1:H:94:TYR:OH	1.99	0.81
1:I:3:GLN:HB2	1:I:25:SER:HB2	1.60	0.81
3:O:314:LEU:HD22	3:O:430:GLU:HG3	1.62	0.81
1:M:3:GLN:HB2	1:M:25:SER:HB2	1.62	0.81
1:M:90:ASP:O	1:M:94:TYR:OH	1.99	0.80
1:E:90:ASP:O	1:E:94:TYR:OH	2.00	0.80
3:N:346:PRO:HB3	3:N:372:PHE:HB3	1.63	0.80
3:P:346:PRO:HB3	3:P:372:PHE:HB3	1.63	0.80
3:N:433:HIS:C	3:N:433:HIS:N	2.36	0.79
3:Y:429:HIS:HD2	3:Y:431:ALA:H	1.31	0.79
3:P:433:HIS:N	3:P:433:HIS:C	2.36	0.78
3:Y:346:PRO:HB3	3:Y:372:PHE:HB3	1.63	0.78
3:N:429:HIS:HD2	3:N:431:ALA:H	1.31	0.78
3:O:291:PRO:C	3:O:292:ARG:HD2	2.03	0.78
3:P:289:THR:HG22	3:P:290:LYS:H	1.48	0.78
1:E:207:ASN:ND2	1:E:218:ASP:OD2	2.17	0.78
3:X:291:PRO:C	3:X:292:ARG:HD2	2.03	0.78
3:Y:289:THR:HG22	3:Y:290:LYS:H	1.48	0.78
1:A:207:ASN:ND2	1:A:218:ASP:OD2	2.16	0.78
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:314:LEU:HD22	3:X:430:GLU:HG3	1.62	0.78
3:P:263:VAL:O	3:P:301:ARG:HA	1.84	0.78
1:E:39:ARG:HD2	2:G:38:GLN:HE22	1.47	0.78
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
3:Y:263:VAL:O	3:Y:301:ARG:HA	1.84	0.78
3:Y:433:HIS:C	3:Y:433:HIS:N	2.37	0.78
1:D:75:LEU:HD22	1:I:57:TYR:CE1	2.19	0.77
3:N:433:HIS:C	3:N:433:HIS:CB	2.53	0.77
3:O:292:ARG:O	3:O:293:GLU:HB3	1.84	0.77
3:P:429:HIS:HD2	3:P:431:ALA:H	1.31	0.77
1:H:101:SER:HB2	1:H:104:LEU:H	1.47	0.77
1:I:207:ASN:ND2	1:I:218:ASP:OD2	2.19	0.76
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.76
3:P:433:HIS:CB	3:P:433:HIS:C	2.53	0.76
3:X:292:ARG:O	3:X:293:GLU:HB3	1.85	0.76
3:N:263:VAL:O	3:N:301:ARG:HA	1.84	0.76
3:P:429:HIS:CD2	3:P:431:ALA:H	2.03	0.76
3:N:429:HIS:CD2	3:N:431:ALA:H	2.03	0.76
3:Y:429:HIS:CD2	3:Y:431:ALA:H	2.03	0.76
3:Y:433:HIS:CB	3:Y:433:HIS:C	2.53	0.76
1:D:90:ASP:O	1:D:94:TYR:OH	2.03	0.76
3:O:272:GLN:NE2	3:O:326:LYS:HD2	2.01	0.75
3:Y:266:VAL:HB	3:Y:300:TYR:CB	2.15	0.75
3:N:266:VAL:HB	3:N:300:TYR:CB	2.15	0.75
1:D:75:LEU:HD13	1:I:57:TYR:CE1	2.22	0.75
3:P:266:VAL:HB	3:P:300:TYR:CB	2.15	0.75
3:J:272:GLN:NE2	3:J:326:LYS:HD2	2.01	0.75
1:M:91:THR:HG23	1:M:120:THR:HA	1.68	0.75
1:D:91:THR:HG23	1:D:120:THR:HA	1.68	0.75
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.66	0.75
2:F:207:LYS:HZ3	1:M:201:THR:HB	1.46	0.75
3:X:429:HIS:CD2	3:X:431:ALA:H	2.05	0.75
1:D:75:LEU:HD22	1:I:57:TYR:CE2	2.20	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
3:N:328:LEU:HD12	3:N:329:PRO:HD2	1.69	0.74
1:H:207:ASN:ND2	1:H:218:ASP:OD2	2.20	0.74
3:P:365:LEU:HD12	3:P:410:LEU:HD23	1.69	0.74
1:H:224:LYS:HD2	1:H:224:LYS:N	2.03	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:O:429:HIS:CD2	3:O:431:ALA:H	2.05	0.74
3:X:272:GLN:NE2	3:X:326:LYS:HD2	2.01	0.74
1:I:152:VAL:HG11	1:I:160:VAL:HG11	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Y:365:LEU:HD12	3:Y:410:LEU:HD23	1.69	0.73
3:J:295:GLN:OE1	1:M:195:PRO:HB3	1.89	0.73
1:A:197:SER:HB2	3:X:295:GLN:HE22	1.53	0.72
1:M:153:LYS:HG2	1:M:154:ASP:CG	2.10	0.72
1:A:153:LYS:HG2	1:A:154:ASP:CG	2.09	0.72
2:B:142:ARG:HG2	2:B:142:ARG:HH11	1.54	0.72
1:E:101:SER:HB2	1:E:104:LEU:H	1.54	0.72
1:H:18:LEU:HB3	1:H:83:MET:HE3	1.70	0.72
3:Y:328:LEU:HD12	3:Y:329:PRO:HD2	1.69	0.72
3:J:290:LYS:HZ2	2:L:109:THR:HG21	1.54	0.72
1:D:220:LYS:HE2	1:D:222:GLU:CD	2.10	0.72
3:P:328:LEU:HD12	3:P:329:PRO:HD2	1.69	0.72
3:J:295:GLN:NE2	1:M:197:SER:OG	2.23	0.72
1:A:197:SER:HB3	3:X:295:GLN:NE2	2.04	0.71
2:L:39:LYS:NZ	2:L:81:ASP:O	2.22	0.71
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.71
1:H:91:THR:HG23	1:H:120:THR:HA	1.71	0.71
2:L:142:ARG:HH11	2:L:142:ARG:HG2	1.56	0.71
1:D:153:LYS:HG2	1:D:154:ASP:CG	2.10	0.71
3:Y:288:LYS:HD3	3:Y:288:LYS:H	1.54	0.71
1:D:18:LEU:HB3	1:D:83:MET:HE3	1.73	0.71
3:P:288:LYS:HD3	3:P:288:LYS:H	1.54	0.71
1:H:153:LYS:HG2	1:H:154:ASP:CG	2.11	0.71
1:I:90:ASP:O	1:I:94:TYR:OH	2.05	0.70
2:G:142:ARG:HG2	2:G:142:ARG:HH11	1.55	0.70
2:G:143:GLU:OE2	2:G:143:GLU:N	2.24	0.70
2:G:39:LYS:NZ	2:G:81:ASP:O	2.20	0.70
3:J:290:LYS:HZ2	2:L:109:THR:CG2	2.05	0.70
3:J:290:LYS:NZ	2:L:109:THR:CG2	2.53	0.70
1:E:153:LYS:HG2	1:E:154:ASP:CG	2.13	0.70
1:M:207:ASN:ND2	1:M:218:ASP:OD2	2.25	0.69
3:X:422:VAL:HG22	3:X:442:SER:OG	1.92	0.69
3:J:252:MET:HB2	3:J:255:ARG:HG3	1.75	0.69
1:A:197:SER:HB3	3:X:295:GLN:HE22	1.56	0.69
1:I:204:TYR:O	1:I:221:VAL:N	2.26	0.69
2:C:136:LEU:HD13	2:C:175:LEU:HD22	1.75	0.69
1:A:101:SER:HB2	1:A:104:LEU:H	1.57	0.68
2:L:143:GLU:N	2:L:143:GLU:OE2	2.26	0.68
3:O:422:VAL:HG22	3:O:442:SER:OG	1.92	0.68
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.68
3:X:252:MET:HB2	3:X:255:ARG:HG3	1.75	0.68
1:A:90:ASP:O	1:A:94:TYR:OH	2.06	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:143:GLU:N	2:C:143:GLU:OE2	2.27	0.68
1:E:152:VAL:HG11	1:E:160:VAL:HG11	1.76	0.68
1:M:152:VAL:HG11	1:M:160:VAL:HG11	1.75	0.68
3:X:325:ASN:HD21	3:X:327:ALA:HB3	1.58	0.68
1:D:152:VAL:HG11	1:D:160:VAL:HG11	1.75	0.68
3:P:270:ASP:N	3:P:271:PRO:HD3	2.09	0.68
1:I:153:LYS:HG2	1:I:154:ASP:CG	2.15	0.67
3:O:252:MET:HB2	3:O:255:ARG:HG3	1.75	0.67
3:J:325:ASN:HD21	3:J:327:ALA:HB3	1.58	0.67
1:I:91:THR:HG23	1:I:120:THR:HA	1.76	0.67
3:N:270:ASP:N	3:N:271:PRO:HD3	2.09	0.67
3:O:418:GLN:HA	3:O:443:LEU:CD2	2.24	0.67
3:X:418:GLN:HA	3:X:443:LEU:CD2	2.24	0.67
1:E:136:PRO:HD3	1:E:148:LEU:HB3	1.77	0.67
3:O:325:ASN:HD21	3:O:327:ALA:HB3	1.58	0.67
2:F:142:ARG:HH11	2:F:142:ARG:HG2	1.60	0.67
2:C:39:LYS:NZ	2:C:81:ASP:O	2.21	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.42	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
1:A:152:VAL:HG11	1:A:160:VAL:HG11	1.75	0.67
1:A:203:THR:HB	1:A:220:LYS:HE3	1.77	0.67
1:D:207:ASN:ND2	1:D:218:ASP:OD2	2.29	0.66
1:D:75:LEU:HD13	1:I:57:TYR:HE1	1.58	0.66
3:Y:270:ASP:N	3:Y:271:PRO:HD3	2.09	0.66
3:X:350:THR:HB	3:X:441:LEU:HG	1.77	0.66
3:O:325:ASN:ND2	3:O:327:ALA:HB3	2.10	0.66
3:O:350:THR:HB	3:O:441:LEU:HG	1.77	0.66
1:A:174:HIS:HE1	2:B:167:ASP:HB2	1.61	0.66
1:I:201:THR:OG1	1:I:202:GLN:N	2.28	0.66
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.66
3:J:350:THR:HB	3:J:441:LEU:HG	1.77	0.66
2:K:142:ARG:HH11	2:K:142:ARG:HG2	1.59	0.66
1:D:202:GLN:O	1:D:203:THR:HA	1.96	0.66
1:H:152:VAL:HG11	1:H:160:VAL:HG11	1.77	0.66
3:X:325:ASN:ND2	3:X:327:ALA:HB3	2.11	0.66
3:O:429:HIS:HD2	3:O:431:ALA:H	1.42	0.65
1:M:201:THR:HG1	1:M:202:GLN:N	1.94	0.65
3:P:290:LYS:HE3	3:P:292:ARG:HH22	1.61	0.65
2:F:143:GLU:OE2	2:F:143:GLU:N	2.30	0.65
2:F:149:LYS:NZ	2:F:195:GLU:OE1	2.27	0.65
1:D:154:ASP:HB3	1:D:185:LEU:HD23	1.79	0.65
1:A:136:PRO:HD3	1:A:148:LEU:HB3	1.79	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:143:GLU:N	2:B:143:GLU:OE2	2.29	0.64
3:J:279:VAL:O	3:J:282:VAL:HG13	1.97	0.64
3:O:328:LEU:HG	3:O:330:ALA:O	1.98	0.64
3:X:429:HIS:HD2	3:X:431:ALA:H	1.43	0.64
2:B:29:ILE:HG21	2:B:90:HIS:HD2	1.62	0.64
2:F:37:GLN:O	2:F:45:LYS:N	2.30	0.64
3:Y:332:ILE:HG22	3:Y:333:GLU:N	2.13	0.64
2:C:149:LYS:NZ	2:C:195:GLU:OE1	2.26	0.64
3:P:330:ALA:HB1	3:P:331:PRO:HD2	1.80	0.64
3:O:279:VAL:O	3:O:282:VAL:HG13	1.97	0.64
3:X:328:LEU:HG	3:X:330:ALA:O	1.98	0.64
3:Y:290:LYS:HE3	3:Y:292:ARG:HH22	1.61	0.64
2:G:149:LYS:NZ	2:G:195:GLU:OE1	2.26	0.64
3:X:288:LYS:HD2	3:X:288:LYS:H	1.63	0.64
3:J:288:LYS:H	3:J:288:LYS:HD2	1.63	0.63
3:O:288:LYS:HD2	3:O:288:LYS:H	1.63	0.63
1:E:174:HIS:HE1	2:F:167:ASP:HB2	1.62	0.63
1:I:101:SER:HB2	1:I:104:LEU:H	1.63	0.63
2:K:143:GLU:OE2	2:K:143:GLU:N	2.31	0.63
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.63
3:N:332:ILE:HG22	3:N:333:GLU:N	2.13	0.63
3:P:332:ILE:HG22	3:P:333:GLU:N	2.13	0.63
3:J:290:LYS:HZ3	2:L:109:THR:HG21	1.61	0.63
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.63
1:M:164:TRP:C	1:M:166:SER:H	2.02	0.63
1:M:204:TYR:O	1:M:221:VAL:N	2.32	0.63
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.79	0.63
1:A:154:ASP:HB3	1:A:185:LEU:HD23	1.80	0.63
1:E:201:THR:OG1	1:E:202:GLN:N	2.31	0.63
2:C:120:PRO:HG3	2:C:130:ALA:HB1	1.81	0.63
1:E:18:LEU:HB3	1:E:83:MET:HE3	1.79	0.63
3:J:290:LYS:NZ	2:L:109:THR:OG1	2.32	0.63
1:I:148:LEU:HB2	1:I:221:VAL:HG11	1.80	0.63
3:X:279:VAL:O	3:X:282:VAL:HG13	1.97	0.63
1:A:34:MET:SD	1:A:98:ARG:HB2	2.39	0.62
3:Y:330:ALA:HB1	3:Y:331:PRO:HD2	1.79	0.62
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.81	0.62
1:H:174:HIS:HE1	2:K:167:ASP:HB2	1.63	0.62
2:C:61:ARG:HB2	2:C:76:SER:O	1.99	0.62
2:C:142:ARG:HH11	2:C:142:ARG:HG2	1.63	0.62
1:E:203:THR:HB	1:E:220:LYS:HE3	1.81	0.62
1:H:154:ASP:HB3	1:H:185:LEU:HD23	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:75:LEU:CD2	1:I:57:TYR:CE1	2.82	0.62
3:O:384:ASN:O	3:O:386:GLN:N	2.31	0.62
2:K:136:LEU:HD13	2:K:175:LEU:HD22	1.82	0.62
2:C:29:ILE:HG21	2:C:90:HIS:HD2	1.64	0.62
2:G:136:LEU:HD13	2:G:175:LEU:HD22	1.80	0.62
1:I:18:LEU:HB3	1:I:83:MET:HE3	1.81	0.62
1:H:203:THR:HB	1:H:220:LYS:HE3	1.81	0.61
2:K:61:ARG:HB2	2:K:76:SER:O	2.00	0.61
2:G:37:GLN:O	2:G:45:LYS:N	2.29	0.61
2:G:29:ILE:HG21	2:G:90:HIS:HD2	1.64	0.61
1:M:163:SER:O	1:M:207:ASN:N	2.32	0.61
2:F:151:ASP:HA	2:F:191:VAL:HG12	1.81	0.61
1:M:99:LYS:HG2	1:M:100:GLY:N	2.14	0.61
2:C:37:GLN:O	2:C:45:LYS:N	2.31	0.61
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.32	0.61
3:P:394:THR:HG23	3:P:407:TYR:O	2.01	0.61
2:G:36:TYR:HB2	2:G:87:HIS:HB2	1.81	0.61
3:J:384:ASN:O	3:J:386:GLN:N	2.31	0.61
1:A:91:THR:HG23	1:A:120:THR:HA	1.83	0.60
2:F:136:LEU:HD13	2:F:175:LEU:HD22	1.82	0.60
2:G:120:PRO:HG3	2:G:130:ALA:HB1	1.83	0.60
1:A:99:LYS:HG2	1:A:100:GLY:N	2.16	0.60
3:N:406:LEU:HD12	3:N:406:LEU:C	2.22	0.60
1:D:99:LYS:HG2	1:D:100:GLY:N	2.16	0.60
1:D:203:THR:HB	1:D:220:LYS:HE3	1.83	0.60
3:X:417:TRP:CH2	3:X:441:LEU:HD22	2.37	0.60
3:J:417:TRP:CH2	3:J:441:LEU:HD22	2.37	0.60
3:J:421:ASN:N	3:J:421:ASN:HD22	2.00	0.60
1:M:18:LEU:HB3	1:M:83:MET:HE3	1.83	0.60
2:B:37:GLN:O	2:B:45:LYS:N	2.29	0.60
2:K:6:GLN:NE2	2:K:102:THR:OG1	2.35	0.60
3:P:406:LEU:HD12	3:P:406:LEU:C	2.22	0.60
3:X:384:ASN:O	3:X:386:GLN:N	2.31	0.60
3:Y:394:THR:HG23	3:Y:407:TYR:O	2.01	0.60
2:F:29:ILE:HG21	2:F:90:HIS:HD2	1.66	0.59
1:I:154:ASP:HB3	1:I:185:LEU:HD23	1.84	0.59
3:N:325:ASN:HD22	3:N:326:LYS:H	1.51	0.59
3:P:274:LYS:HE2	3:P:276:ASN:HD21	1.67	0.59
2:K:149:LYS:NZ	2:K:195:GLU:OE1	2.36	0.59
3:O:417:TRP:CH2	3:O:441:LEU:HD22	2.37	0.59
3:Y:406:LEU:C	3:Y:406:LEU:HD12	2.22	0.59
1:M:101:SER:HB2	1:M:104:LEU:H	1.66	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.84	0.59
1:A:197:SER:CB	3:X:295:GLN:NE2	2.62	0.59
1:A:129:PRO:HB3	1:A:155:TYR:HB3	1.83	0.59
1:I:60:TYR:OH	1:I:69:THR:HA	2.03	0.59
1:H:99:LYS:HG2	1:H:100:GLY:N	2.17	0.59
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.85	0.59
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	0.59
3:P:257:PRO:HB2	3:P:308:VAL:HB	1.84	0.59
1:D:72:ARG:NE	1:D:74:ASP:OD1	2.30	0.59
1:H:72:ARG:NE	1:H:74:ASP:OD1	2.31	0.59
3:Y:325:ASN:HD22	3:Y:326:LYS:H	1.51	0.59
1:E:154:ASP:HB3	1:E:185:LEU:HD23	1.84	0.59
1:D:148:LEU:HD13	1:D:221:VAL:HB	1.85	0.59
2:K:37:GLN:O	2:K:45:LYS:N	2.33	0.59
2:L:29:ILE:HG21	2:L:90:HIS:HD2	1.67	0.59
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	0.59
3:O:417:TRP:HH2	3:O:441:LEU:HD22	1.67	0.59
3:O:421:ASN:N	3:O:421:ASN:HD22	2.00	0.59
3:P:269:GLU:HG2	3:P:269:GLU:O	2.03	0.59
1:A:18:LEU:HB3	1:A:83:MET:HE3	1.83	0.59
3:P:296:TYR:CE1	3:P:301:ARG:HD3	2.38	0.59
1:D:75:LEU:CD2	1:I:57:TYR:CZ	2.69	0.58
3:J:417:TRP:HH2	3:J:441:LEU:HD22	1.67	0.58
3:P:279:VAL:O	3:P:279:VAL:HG23	2.03	0.58
3:X:433:HIS:ND1	3:X:434:ASN:OD1	2.36	0.58
1:M:133:PRO:HB3	1:M:221:VAL:HG22	1.85	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
3:O:276:ASN:HB2	3:O:322:LYS:HB3	1.86	0.58
3:Y:265:ASP:HA	3:Y:299:THR:HB	1.85	0.58
1:H:222:GLU:HB2	1:H:223:PRO:HD2	1.84	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
3:P:265:ASP:HA	3:P:299:THR:HB	1.86	0.58
3:X:421:ASN:N	3:X:421:ASN:HD22	2.00	0.58
3:Y:269:GLU:O	3:Y:269:GLU:HG2	2.03	0.58
2:G:201:LEU:HG	2:G:205:VAL:HG23	1.85	0.58
3:X:415:SER:O	3:X:419:GLN:HG3	2.04	0.58
3:Y:274:LYS:HE2	3:Y:276:ASN:HD21	1.67	0.58
3:Y:296:TYR:CE1	3:Y:301:ARG:HD3	2.38	0.58
2:B:136:LEU:HD13	2:B:175:LEU:HD22	1.83	0.58
3:J:286:ASN:O	3:J:287:ALA:HB2	2.03	0.58
3:Y:424:SER:OG	3:Y:438:GLN:HG2	2.04	0.58
2:F:201:LEU:HG	2:F:205:VAL:HG23	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:169:LEU:HD21	1:H:192:VAL:HG21	1.85	0.58
1:H:201:THR:OG1	1:H:202:GLN:N	2.33	0.58
3:N:288:LYS:HE2	3:N:306:LEU:HD11	1.86	0.58
3:X:417:TRP:HH2	3:X:441:LEU:HD22	1.67	0.58
1:E:91:THR:HG23	1:E:120:THR:HA	1.85	0.58
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.84	0.58
1:I:99:LYS:HG2	1:I:100:GLY:N	2.18	0.58
1:M:164:TRP:O	1:M:166:SER:N	2.37	0.58
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.58
3:O:286:ASN:O	3:O:287:ALA:HB2	2.03	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
2:B:39:LYS:NZ	2:B:81:ASP:O	2.27	0.58
2:C:201:LEU:HG	2:C:205:VAL:HG23	1.85	0.58
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.58
3:P:288:LYS:HE2	3:P:306:LEU:HD11	1.86	0.58
3:Y:257:PRO:HB2	3:Y:308:VAL:HB	1.85	0.57
3:Y:288:LYS:HE2	3:Y:306:LEU:HD11	1.86	0.57
2:C:19:ILE:HG12	2:C:78:LEU:HD11	1.86	0.57
2:G:118:PHE:CD2	1:I:134:LEU:HD13	2.39	0.57
1:I:203:THR:HB	1:I:220:LYS:HE3	1.85	0.57
1:M:73:ASP:N	1:M:78:PHE:O	2.37	0.57
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.57
3:P:325:ASN:HD22	3:P:326:LYS:H	1.51	0.57
2:L:136:LEU:HD13	2:L:175:LEU:HD22	1.86	0.57
1:M:154:ASP:HB3	1:M:185:LEU:HD23	1.86	0.57
2:K:91:TYR:HD1	1:M:99:LYS:NZ	2.03	0.57
3:N:265:ASP:HA	3:N:299:THR:HB	1.85	0.57
3:O:415:SER:O	3:O:419:GLN:HG3	2.04	0.57
3:X:286:ASN:O	3:X:287:ALA:HB2	2.03	0.57
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.33	0.57
3:O:433:HIS:ND1	3:O:434:ASN:OD1	2.35	0.57
1:D:35:ASN:O	1:D:97:ALA:N	2.37	0.57
3:Y:279:VAL:HG23	3:Y:279:VAL:O	2.03	0.57
1:D:52:SER:O	1:D:72:ARG:NH1	2.37	0.57
1:D:75:LEU:CD1	1:I:57:TYR:CE1	2.86	0.57
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.36	0.57
3:X:320:LYS:HG3	3:X:335:THR:HG22	1.87	0.57
2:K:29:ILE:HG21	2:K:90:HIS:HD2	1.69	0.57
3:O:320:LYS:HG3	3:O:335:THR:HG22	1.87	0.57
3:P:311:GLN:CD	3:P:311:GLN:H	2.08	0.57
3:P:424:SER:OG	3:P:438:GLN:HG2	2.04	0.57
3:N:328:LEU:HG	3:N:330:ALA:O	2.05	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.56
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
3:P:439:LYS:HE3	3:P:440:SER:O	2.05	0.56
1:D:144:GLY:O	1:D:196:SER:HB2	2.05	0.56
1:D:103:ARG:O	2:F:50:LYS:CE	2.53	0.56
1:A:153:LYS:HG2	1:A:154:ASP:OD2	2.06	0.56
2:G:6:GLN:NE2	2:G:102:THR:OG1	2.39	0.56
2:K:148:TRP:CE3	2:K:179:LEU:HD22	2.40	0.56
2:K:201:LEU:HG	2:K:205:VAL:HG23	1.87	0.56
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.87	0.56
3:X:276:ASN:HB2	3:X:322:LYS:HB3	1.86	0.56
2:C:6:GLN:NE2	2:C:102:THR:OG1	2.38	0.56
1:A:60:TYR:OH	1:A:69:THR:HA	2.04	0.56
2:G:19:ILE:HG12	2:G:78:LEU:HD11	1.88	0.56
1:H:136:PRO:HD3	1:H:148:LEU:HB3	1.87	0.56
3:N:311:GLN:CD	3:N:311:GLN:H	2.08	0.56
3:Y:325:ASN:ND2	3:Y:326:LYS:H	2.04	0.56
1:E:52:SER:O	1:E:72:ARG:NH1	2.37	0.56
3:N:301:ARG:HE	3:N:303:VAL:CG2	2.18	0.56
3:N:270:ASP:OD2	3:N:327:ALA:HB2	2.06	0.56
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	0.56
3:P:270:ASP:OD2	3:P:327:ALA:HB2	2.06	0.56
3:P:328:LEU:HG	3:P:330:ALA:O	2.05	0.56
3:X:288:LYS:O	3:X:289:THR:O	2.24	0.56
3:Y:301:ARG:HE	3:Y:303:VAL:CG2	2.18	0.56
2:B:6:GLN:NE2	2:B:102:THR:OG1	2.38	0.56
3:Y:328:LEU:HG	3:Y:330:ALA:O	2.05	0.56
1:H:35:ASN:OD1	1:H:50:SER:HB2	2.06	0.56
3:O:328:LEU:HD12	3:O:329:PRO:HD2	1.88	0.56
3:Y:311:GLN:H	3:Y:311:GLN:CD	2.08	0.56
1:A:104:LEU:HD12	1:E:28:ARG:CG	2.20	0.56
1:D:129:PRO:HB3	1:D:155:TYR:HB3	1.87	0.56
2:F:120:PRO:HG3	2:F:130:ALA:HB1	1.87	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
2:K:160:GLN:O	2:K:178:THR:N	2.36	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56
1:D:38:ARG:HB3	1:D:94:TYR:CE2	2.41	0.55
1:H:58:ARG:NH1	1:H:70:VAL:O	2.39	0.55
2:L:160:GLN:O	2:L:178:THR:N	2.38	0.55
3:J:289:THR:O	3:J:290:LYS:HB2	2.07	0.55
3:O:288:LYS:O	3:O:289:THR:O	2.24	0.55
3:O:289:THR:O	3:O:290:LYS:HB2	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:301:ARG:HE	3:P:303:VAL:CG2	2.18	0.55
1:A:70:VAL:HA	1:A:80:TYR:O	2.06	0.55
1:D:164:TRP:HZ2	1:D:190:SER:O	1.90	0.55
1:D:169:LEU:HD21	1:D:192:VAL:HG21	1.88	0.55
1:D:60:TYR:OH	1:D:69:THR:HA	2.06	0.55
2:F:142:ARG:HG2	2:F:142:ARG:NH1	2.22	0.55
3:J:328:LEU:HD12	3:J:329:PRO:HD2	1.88	0.55
3:Y:266:VAL:CB	3:Y:300:TYR:HB2	2.28	0.55
3:P:325:ASN:ND2	3:P:326:LYS:H	2.04	0.55
2:B:19:ILE:HG12	2:B:78:LEU:HD11	1.88	0.55
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.89	0.55
1:D:101:SER:H	1:D:104:LEU:HD23	1.71	0.55
2:F:39:LYS:NZ	2:F:81:ASP:O	2.30	0.55
1:H:70:VAL:HA	1:H:80:TYR:O	2.06	0.55
2:K:39:LYS:NZ	2:K:81:ASP:O	2.30	0.55
1:M:34:MET:SD	1:M:98:ARG:HB2	2.46	0.55
1:M:60:TYR:OH	1:M:69:THR:HA	2.06	0.55
1:I:29:ILE:O	1:I:72:ARG:NH2	2.39	0.55
3:Y:439:LYS:HE3	3:Y:440:SER:O	2.05	0.55
1:A:47:TRP:NE1	1:A:49:ALA:O	2.40	0.55
1:E:35:ASN:OD1	1:E:50:SER:HB2	2.07	0.55
2:L:167:ASP:HB2	1:M:174:HIS:HE1	1.71	0.55
3:X:289:THR:O	3:X:290:LYS:HB2	2.07	0.55
3:Y:270:ASP:OD2	3:Y:327:ALA:HB2	2.06	0.55
1:H:94:TYR:CE1	1:H:119:VAL:HB	2.42	0.55
1:M:94:TYR:CE1	1:M:119:VAL:HB	2.42	0.55
3:O:414:LYS:HE2	3:O:418:GLN:NE2	2.22	0.55
1:D:133:PRO:HG2	1:D:224:LYS:HZ1	1.72	0.55
2:F:2:VAL:HG11	2:F:90:HIS:CD2	2.42	0.55
2:K:142:ARG:NH1	2:K:142:ARG:HG2	2.22	0.55
3:P:238:PRO:CG	3:P:328:LEU:HD13	2.37	0.55
3:P:275:PHE:HE1	3:P:302:VAL:HG12	1.72	0.55
1:A:45:LEU:HG	2:C:87:HIS:CE1	2.43	0.54
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.89	0.54
2:L:37:GLN:O	2:L:45:LYS:N	2.37	0.54
1:M:70:VAL:HA	1:M:80:TYR:O	2.06	0.54
3:X:328:LEU:HD12	3:X:329:PRO:HD2	1.88	0.54
1:M:68:PHE:CD1	1:M:83:MET:HA	2.42	0.54
3:X:414:LYS:HE2	3:X:418:GLN:NE2	2.22	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:O:282:VAL:O	3:O:283:GLN:CB	2.52	0.54
3:Y:238:PRO:CG	3:Y:328:LEU:HD13	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Y:240:VAL:O	3:Y:334:LYS:HE3	2.08	0.54
2:B:91:TYR:HD1	1:D:99:LYS:NZ	2.04	0.54
1:H:135:ALA:HB3	1:H:224:LYS:HD3	1.89	0.54
2:K:162:SER:HB3	2:K:176:SER:OG	2.07	0.54
3:P:240:VAL:O	3:P:334:LYS:HE3	2.08	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.08	0.54
3:J:414:LYS:HE2	3:J:418:GLN:NE2	2.22	0.54
2:L:31:THR:OG1	2:L:50:LYS:HE2	2.07	0.54
3:N:275:PHE:HE1	3:N:302:VAL:HG12	1.72	0.54
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.54
3:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
3:O:414:LYS:O	3:O:418:GLN:HG3	2.08	0.54
1:D:103:ARG:O	2:F:50:LYS:CD	2.56	0.54
2:K:120:PRO:HG3	2:K:130:ALA:HB1	1.89	0.54
2:L:6:GLN:NE2	2:L:102:THR:OG1	2.40	0.54
3:O:285:HIS:O	3:O:286:ASN:HB2	2.08	0.54
3:O:418:GLN:HA	3:O:443:LEU:HD22	1.90	0.54
1:E:60:TYR:OH	1:E:69:THR:HA	2.08	0.54
1:E:99:LYS:HG2	1:E:100:GLY:N	2.23	0.54
3:P:351:LEU:C	3:P:441:LEU:HD11	2.28	0.54
3:X:418:GLN:HA	3:X:443:LEU:HD22	1.90	0.54
3:Y:289:THR:HG22	3:Y:290:LYS:N	2.22	0.54
1:I:169:LEU:HD21	1:I:192:VAL:HG21	1.90	0.54
2:L:162:SER:HB3	2:L:176:SER:OG	2.07	0.54
3:Y:275:PHE:HE1	3:Y:302:VAL:HG12	1.72	0.54
1:E:70:VAL:HA	1:E:80:TYR:O	2.07	0.53
1:H:153:LYS:HG2	1:H:154:ASP:OD2	2.08	0.53
1:H:69:THR:C	1:H:81:LEU:HD12	2.28	0.53
1:I:22:CYS:O	1:I:78:PHE:HA	2.08	0.53
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.90	0.53
1:M:47:TRP:NE1	1:M:49:ALA:O	2.41	0.53
3:X:414:LYS:O	3:X:418:GLN:HG3	2.08	0.53
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.18	0.53
3:N:351:LEU:C	3:N:441:LEU:HD11	2.28	0.53
3:X:285:HIS:O	3:X:286:ASN:HB2	2.08	0.53
3:Y:262:VAL:HG13	3:Y:303:VAL:HG22	1.90	0.53
3:Y:351:LEU:C	3:Y:441:LEU:HD11	2.28	0.53
1:D:35:ASN:OD1	1:D:50:SER:HB2	2.08	0.53
1:H:101:SER:H	1:H:104:LEU:CD2	2.21	0.53
3:P:322:LYS:HE3	3:P:333:GLU:OE2	2.08	0.53
3:P:266:VAL:CB	3:P:300:TYR:HB2	2.28	0.53
1:D:70:VAL:HA	1:D:80:TYR:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:285:HIS:O	3:J:286:ASN:HB2	2.08	0.53
2:L:142:ARG:CG	2:L:142:ARG:HH11	2.21	0.53
3:N:289:THR:HG22	3:N:290:LYS:N	2.21	0.53
3:Y:322:LYS:HE3	3:Y:333:GLU:OE2	2.08	0.53
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.90	0.53
1:M:220:LYS:C	1:M:221:VAL:HA	2.29	0.53
3:X:351:LEU:HB2	3:X:366:THR:HB	1.90	0.53
1:I:72:ARG:NE	1:I:74:ASP:OD1	2.34	0.53
2:F:160:GLN:O	2:F:178:THR:N	2.41	0.53
2:G:149:LYS:HB2	2:G:193:ALA:HB3	1.91	0.53
1:I:101:SER:OG	1:I:104:LEU:HA	2.09	0.53
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.53
1:A:22:CYS:O	1:A:78:PHE:HA	2.09	0.53
2:B:151:ASP:HA	2:B:191:VAL:HG12	1.90	0.53
3:O:351:LEU:HB2	3:O:366:THR:HB	1.90	0.53
2:F:140:TYR:CD2	2:F:141:PRO:HA	2.44	0.52
2:G:37:GLN:HB2	2:G:47:LEU:HD11	1.91	0.52
1:H:38:ARG:HB3	1:H:94:TYR:CE2	2.44	0.52
3:Y:297:ASN:O	3:Y:298:SER:HB3	2.09	0.52
2:B:201:LEU:HG	2:B:205:VAL:HG23	1.90	0.52
1:D:94:TYR:CE1	1:D:119:VAL:HB	2.44	0.52
3:J:418:GLN:HA	3:J:443:LEU:HD22	1.90	0.52
1:E:101:SER:H	1:E:104:LEU:HD23	1.75	0.52
1:H:29:ILE:O	1:H:72:ARG:NH2	2.43	0.52
1:M:35:ASN:O	1:M:97:ALA:N	2.42	0.52
3:P:262:VAL:HG13	3:P:303:VAL:HG22	1.90	0.52
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.52
3:N:312:ASN:ND2	3:N:317:LYS:HD2	2.24	0.52
1:A:164:TRP:CH2	1:A:221:VAL:HG21	2.45	0.52
1:A:73:ASP:N	1:A:78:PHE:O	2.40	0.52
1:D:101:SER:HB2	1:D:104:LEU:H	1.75	0.52
2:L:142:ARG:NH1	2:L:142:ARG:HG2	2.19	0.52
2:G:160:GLN:O	2:G:178:THR:N	2.40	0.52
3:X:283:GLN:C	3:X:285:HIS:N	2.62	0.52
1:A:52:SER:O	1:A:72:ARG:NH1	2.42	0.52
1:I:35:ASN:OD1	1:I:50:SER:HB2	2.10	0.52
3:Y:312:ASN:ND2	3:Y:317:LYS:HD2	2.24	0.52
1:A:134:LEU:HD13	2:B:118:PHE:CD2	2.45	0.52
2:C:138:ASN:OD1	1:D:174:HIS:NE2	2.43	0.52
1:E:47:TRP:NE1	1:E:49:ALA:O	2.43	0.52
2:F:148:TRP:CE3	2:F:179:LEU:HD22	2.44	0.52
2:F:149:LYS:HB2	2:F:193:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:G:148:TRP:CE3	2:G:179:LEU:HD22	2.45	0.52
1:M:129:PRO:HB3	1:M:155:TYR:HB3	1.90	0.52
1:M:203:THR:HG21	1:M:220:LYS:HZ1	1.75	0.52
1:M:35:ASN:OD1	1:M:50:SER:HB2	2.09	0.52
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.52
2:B:142:ARG:HH11	2:B:142:ARG:CG	2.21	0.52
2:C:186:TYR:HA	2:C:192:TYR:OH	2.10	0.52
2:G:21:ILE:HG12	2:G:102:THR:HG21	1.91	0.52
3:J:436:TYR:CD1	3:J:436:TYR:C	2.84	0.52
2:K:151:ASP:HA	2:K:191:VAL:HG12	1.91	0.52
3:X:384:ASN:OD1	3:X:385:GLY:N	2.41	0.52
1:D:153:LYS:HG2	1:D:154:ASP:OD1	2.10	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
3:J:393:THR:HG22	3:J:394:THR:O	2.10	0.51
3:P:312:ASN:ND2	3:P:317:LYS:HD2	2.24	0.51
3:X:393:THR:HG22	3:X:394:THR:O	2.10	0.51
3:Y:296:TYR:HE1	3:Y:301:ARG:HD3	1.74	0.51
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.91	0.51
1:D:153:LYS:HG2	1:D:154:ASP:OD2	2.10	0.51
1:D:149:GLY:O	1:D:221:VAL:HG21	2.10	0.51
1:D:69:THR:C	1:D:81:LEU:HD12	2.31	0.51
1:E:134:LEU:HD13	2:F:118:PHE:CD2	2.46	0.51
2:G:61:ARG:HB2	2:G:76:SER:O	2.10	0.51
1:I:101:SER:H	1:I:104:LEU:HD23	1.76	0.51
1:M:53:THR:O	1:M:56:THR:OG1	2.28	0.51
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
3:P:325:ASN:ND2	3:P:326:LYS:N	2.59	0.51
2:C:140:TYR:CD2	2:C:141:PRO:HA	2.45	0.51
1:D:58:ARG:NH1	1:D:70:VAL:O	2.43	0.51
1:E:164:TRP:CZ2	1:E:192:VAL:HG12	2.46	0.51
1:D:74:ASP:HB3	2:F:94:TYR:HE1	1.74	0.51
2:G:31:THR:OG1	2:G:50:LYS:HE2	2.10	0.51
1:H:35:ASN:O	1:H:97:ALA:N	2.41	0.51
2:L:5:THR:HG23	2:L:100:GLN:HE22	1.75	0.51
3:X:429:HIS:O	3:X:435:HIS:HA	2.11	0.51
2:G:167:ASP:HB2	1:I:174:HIS:HE1	1.75	0.51
1:I:94:TYR:CE1	1:I:119:VAL:HB	2.46	0.51
1:M:52:SER:O	1:M:72:ARG:NH1	2.43	0.51
3:P:291:PRO:CB	3:P:304:SER:HA	2.37	0.51
3:Y:291:PRO:CB	3:Y:304:SER:HA	2.37	0.51
1:A:35:ASN:O	1:A:97:ALA:N	2.44	0.51
1:D:202:GLN:HB2	1:D:204:TYR:CZ	2.45	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:297:ASN:O	3:P:298:SER:HB3	2.09	0.51
3:X:436:TYR:CD1	3:X:436:TYR:C	2.84	0.51
3:X:350:THR:HB	3:X:441:LEU:CG	2.40	0.51
3:Y:291:PRO:HB3	3:Y:304:SER:CA	2.37	0.51
3:Y:325:ASN:ND2	3:Y:326:LYS:N	2.59	0.51
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.93	0.51
1:E:72:ARG:NE	1:E:74:ASP:OD1	2.33	0.51
1:D:29:ILE:O	1:D:72:ARG:NH2	2.44	0.51
2:G:113:PRO:HD3	2:G:198:HIS:CG	2.46	0.51
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.51
3:O:393:THR:HG22	3:O:394:THR:O	2.10	0.51
3:O:429:HIS:O	3:O:435:HIS:HA	2.11	0.51
3:P:249:ASP:O	3:P:257:PRO:HG3	2.11	0.51
2:C:140:TYR:CG	2:C:141:PRO:HA	2.45	0.51
1:I:68:PHE:CD1	1:I:83:MET:HA	2.46	0.51
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.51
2:L:73:LEU:HD12	2:L:74:THR:H	1.76	0.51
2:L:19:ILE:HG12	2:L:78:LEU:HD11	1.91	0.51
3:O:350:THR:HB	3:O:441:LEU:CG	2.40	0.51
3:X:418:GLN:C	3:X:420:GLY:H	2.15	0.51
2:G:113:PRO:HD2	2:G:201:LEU:HD22	1.93	0.51
1:I:70:VAL:HA	1:I:80:TYR:O	2.10	0.51
1:H:134:LEU:HD13	2:K:118:PHE:CD2	2.46	0.51
3:O:384:ASN:OD1	3:O:385:GLY:N	2.41	0.51
3:Y:378:ALA:HB3	3:Y:428:MET:HB2	1.92	0.51
2:G:142:ARG:NH1	2:G:142:ARG:HG2	2.20	0.50
1:M:144:GLY:O	1:M:196:SER:HB2	2.10	0.50
3:O:443:LEU:HG	3:O:443:LEU:O	2.11	0.50
3:Y:261:CYS:HB2	3:Y:277:TRP:CZ2	2.47	0.50
1:A:35:ASN:OD1	1:A:50:SER:HB2	2.11	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.50
1:E:94:TYR:CE1	1:E:119:VAL:HB	2.46	0.50
1:M:23:GLY:HA2	1:M:78:PHE:CD2	2.46	0.50
3:X:360:LYS:O	3:X:414:LYS:HD2	2.11	0.50
1:H:68:PHE:CD1	1:H:83:MET:HA	2.47	0.50
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.50
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.50
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.50
2:F:36:TYR:HE2	2:F:89:GLN:HB3	1.76	0.50
2:G:36:TYR:CE1	2:G:46:LEU:HD13	2.46	0.50
3:X:294:GLN:O	3:X:300:TYR:CD1	2.65	0.50
3:Y:249:ASP:C	3:Y:257:PRO:HG3	2.32	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:38:ARG:HD3	1:D:94:TYR:CE2	2.46	0.50
1:I:220:LYS:HE2	1:I:222:GLU:HG3	1.93	0.50
1:M:153:LYS:HG2	1:M:154:ASP:OD1	2.11	0.50
1:M:195:PRO:C	1:M:197:SER:H	2.14	0.50
3:O:418:GLN:C	3:O:420:GLY:H	2.15	0.50
2:C:148:TRP:CE3	2:C:179:LEU:HD22	2.46	0.50
1:E:169:LEU:HD21	1:E:192:VAL:HG21	1.93	0.50
1:I:52:SER:O	1:I:72:ARG:NH1	2.44	0.50
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.47	0.50
1:M:169:LEU:HD21	1:M:192:VAL:HG21	1.94	0.50
1:M:133:PRO:HB2	1:M:221:VAL:HG13	1.92	0.50
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.50
3:O:360:LYS:O	3:O:414:LYS:HD2	2.11	0.50
3:P:249:ASP:C	3:P:257:PRO:HG3	2.32	0.50
3:P:278:TYR:CD1	3:P:278:TYR:N	2.79	0.50
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.92	0.50
3:J:283:GLN:C	3:J:285:HIS:N	2.63	0.50
3:N:291:PRO:HB3	3:N:304:SER:CA	2.37	0.50
3:O:294:GLN:O	3:O:300:TYR:CD1	2.65	0.50
1:A:67:ARG:C	1:A:68:PHE:HD1	2.15	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.50
3:P:332:ILE:CG2	3:P:333:GLU:N	2.74	0.50
3:P:406:LEU:HD12	3:P:406:LEU:O	2.12	0.50
3:P:432:LEU:CD1	3:P:437:THR:HG22	2.42	0.50
3:Y:249:ASP:O	3:Y:257:PRO:HG3	2.10	0.50
3:Y:292:ARG:O	3:Y:293:GLU:HB3	2.12	0.50
1:D:73:ASP:N	1:D:78:PHE:O	2.44	0.50
1:E:34:MET:SD	1:E:98:ARG:HB2	2.52	0.50
2:F:140:TYR:CG	2:F:141:PRO:HA	2.47	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
2:L:121:SER:O	2:L:125:LEU:HB2	2.11	0.50
3:O:436:TYR:C	3:O:436:TYR:CD1	2.84	0.50
3:P:250:THR:HG22	3:P:257:PRO:HB3	1.94	0.50
3:P:289:THR:HG22	3:P:290:LYS:N	2.21	0.50
1:H:38:ARG:NH1	1:H:90:ASP:HA	2.27	0.49
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.49
1:M:58:ARG:NH1	1:M:70:VAL:O	2.44	0.49
3:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	0.49
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	0.49
3:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
3:P:291:PRO:HB3	3:P:304:SER:CA	2.37	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Y:406:LEU:HD12	3:Y:406:LEU:O	2.12	0.49
3:X:409:LYS:HB2	3:Y:407:TYR:OH	2.12	0.49
1:D:92:ALA:N	1:D:119:VAL:O	2.44	0.49
3:J:443:LEU:HG	3:J:443:LEU:O	2.11	0.49
3:O:380:GLU:O	3:O:425:CYS:HA	2.12	0.49
3:P:378:ALA:HB3	3:P:428:MET:HB2	1.92	0.49
1:E:67:ARG:C	1:E:68:PHE:HD1	2.15	0.49
1:H:92:ALA:HB3	1:H:94:TYR:CE1	2.47	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:J:357:GLU:C	3:J:359:THR:H	2.15	0.49
3:O:292:ARG:O	3:O:293:GLU:CB	2.58	0.49
3:O:357:GLU:C	3:O:359:THR:H	2.15	0.49
3:Y:278:TYR:N	3:Y:278:TYR:CD1	2.79	0.49
3:Y:350:THR:HB	3:Y:441:LEU:HG	1.95	0.49
1:I:129:PRO:HB3	1:I:155:TYR:HB3	1.93	0.49
1:I:47:TRP:NE1	1:I:49:ALA:O	2.45	0.49
3:P:296:TYR:HE1	3:P:301:ARG:HD3	1.74	0.49
3:X:278:TYR:HB2	3:X:320:LYS:HB3	1.95	0.49
3:Y:332:ILE:CG2	3:Y:333:GLU:N	2.74	0.49
2:F:19:ILE:HG12	2:F:78:LEU:HD11	1.93	0.49
1:I:12:VAL:O	1:I:121:VAL:HA	2.13	0.49
1:M:164:TRP:CE2	1:M:206:CYS:HB2	2.47	0.49
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:O:246:LYS:HB2	3:O:249:ASP:OD2	2.12	0.49
3:X:357:GLU:C	3:X:359:THR:H	2.15	0.49
3:X:443:LEU:HG	3:X:443:LEU:O	2.11	0.49
2:B:5:THR:HG23	2:B:100:GLN:HE22	1.77	0.49
1:E:58:ARG:NH1	1:E:70:VAL:O	2.44	0.49
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.94	0.49
2:K:19:ILE:HG12	2:K:78:LEU:HD11	1.94	0.49
3:X:246:LYS:HB2	3:X:249:ASP:OD2	2.12	0.49
2:G:5:THR:HG23	2:G:100:GLN:HE22	1.77	0.49
2:G:138:ASN:OD1	1:I:174:HIS:NE2	2.45	0.49
2:G:142:ARG:CG	2:G:142:ARG:HH11	2.22	0.49
1:H:38:ARG:HD3	1:H:94:TYR:CE2	2.48	0.49
2:K:117:ILE:HG13	2:K:133:VAL:O	2.12	0.49
3:P:398:LEU:HD11	3:P:402:GLY:HA2	1.95	0.49
3:P:369:VAL:O	3:P:405:PHE:HA	2.12	0.49
3:X:380:GLU:O	3:X:425:CYS:HA	2.12	0.49
3:Y:369:VAL:O	3:Y:405:PHE:HA	2.13	0.49
3:Y:432:LEU:CD1	3:Y:437:THR:HG22	2.42	0.49
2:G:83:PHE:CE1	2:G:106:ILE:HG12	2.48	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.48	0.49
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
3:O:283:GLN:CD	3:O:287:ALA:HB2	2.33	0.49
1:E:23:GLY:HA2	1:E:78:PHE:CD2	2.48	0.49
1:I:101:SER:H	1:I:104:LEU:CD2	2.26	0.49
1:I:23:GLY:HA2	1:I:78:PHE:CD2	2.48	0.49
1:M:101:SER:H	1:M:104:LEU:HD23	1.77	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:O:409:LYS:HB2	3:P:407:TYR:OH	2.12	0.49
3:Y:250:THR:HG22	3:Y:257:PRO:HB3	1.94	0.49
1:A:53:THR:O	1:A:56:THR:OG1	2.31	0.49
1:H:60:TYR:OH	1:H:69:THR:HA	2.13	0.49
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.49
3:O:388:GLU:OE2	3:O:416:ARG:NH2	2.42	0.49
3:P:261:CYS:HB2	3:P:277:TRP:CZ2	2.47	0.49
3:X:283:GLN:CD	3:X:287:ALA:HB2	2.34	0.49
3:Y:398:LEU:HD11	3:Y:402:GLY:HA2	1.95	0.49
1:E:153:LYS:HG2	1:E:154:ASP:OD2	2.13	0.48
1:E:73:ASP:N	1:E:78:PHE:O	2.42	0.48
1:H:176:PHE:CD1	2:K:176:SER:HB3	2.48	0.48
1:H:69:THR:O	1:H:81:LEU:HD12	2.13	0.48
3:N:311:GLN:N	3:N:311:GLN:NE2	2.53	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48
3:O:248:LYS:O	3:O:255:ARG:HD3	2.13	0.48
2:G:31:THR:O	2:G:50:LYS:HA	2.13	0.48
1:H:202:GLN:O	1:H:203:THR:HA	2.12	0.48
2:L:201:LEU:HG	2:L:205:VAL:HG23	1.95	0.48
3:X:248:LYS:O	3:X:255:ARG:HD3	2.13	0.48
1:A:38:ARG:HB3	1:A:94:TYR:CE2	2.48	0.48
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.48
2:L:140:TYR:CG	2:L:141:PRO:HA	2.48	0.48
1:M:22:CYS:O	1:M:78:PHE:HA	2.12	0.48
3:X:277:TRP:O	3:X:283:GLN:HB3	2.13	0.48
1:A:69:THR:C	1:A:81:LEU:HD12	2.33	0.48
2:C:149:LYS:HB2	2:C:193:ALA:HB3	1.94	0.48
1:E:68:PHE:CD1	1:E:83:MET:HA	2.48	0.48
1:H:47:TRP:NE1	1:H:49:ALA:O	2.46	0.48
1:I:67:ARG:C	1:I:68:PHE:HD1	2.17	0.48
3:P:292:ARG:O	3:P:293:GLU:HB3	2.12	0.48
3:X:292:ARG:O	3:X:293:GLU:CB	2.58	0.48
1:A:197:SER:HB3	3:X:295:GLN:CD	2.34	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:266:VAL:O	3:X:300:TYR:HB2	2.13	0.48
2:G:2:VAL:HG11	2:G:90:HIS:CD2	2.48	0.48
1:I:35:ASN:O	1:I:97:ALA:N	2.45	0.48
1:M:29:ILE:O	1:M:72:ARG:NH2	2.46	0.48
1:A:32:HIS:ND1	1:A:98:ARG:HG3	2.29	0.48
2:B:20:THR:HG22	2:B:73:LEU:O	2.13	0.48
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	0.48
2:L:61:ARG:HB2	2:L:76:SER:O	2.14	0.48
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.48
3:O:266:VAL:O	3:O:300:TYR:HB2	2.13	0.48
2:F:108:ARG:NH1	2:F:111:ALA:HB2	2.28	0.48
1:I:153:LYS:HG2	1:I:154:ASP:OD2	2.13	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	0.48
1:M:72:ARG:NE	1:M:74:ASP:OD1	2.36	0.48
2:K:91:TYR:CD1	1:M:99:LYS:NZ	2.81	0.48
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
3:O:278:TYR:HB2	3:O:320:LYS:HB3	1.95	0.48
3:P:244:PRO:HB3	3:P:336:ILE:HD11	1.95	0.48
3:P:259:VAL:HG23	3:P:308:VAL:CG2	2.43	0.48
3:P:350:THR:HB	3:P:441:LEU:HG	1.95	0.48
2:B:140:TYR:CG	2:B:141:PRO:HA	2.49	0.48
2:G:118:PHE:CG	1:I:134:LEU:HB3	2.49	0.48
2:G:149:LYS:HZ1	2:G:195:GLU:CD	2.13	0.48
2:G:169:LYS:HB3	2:G:169:LYS:NZ	2.29	0.48
2:G:162:SER:HB3	2:G:176:SER:OG	2.13	0.48
1:I:101:SER:N	1:I:104:LEU:HD23	2.29	0.48
3:J:246:LYS:HB2	3:J:249:ASP:OD2	2.12	0.48
1:M:92:ALA:N	1:M:119:VAL:O	2.46	0.48
3:X:358:MET:O	3:X:414:LYS:HE3	2.14	0.48
3:O:277:TRP:O	3:O:283:GLN:HB3	2.13	0.48
3:X:371:GLY:HA2	3:X:403:SER:OG	2.14	0.48
2:C:142:ARG:HG2	2:C:142:ARG:NH1	2.28	0.48
3:J:388:GLU:OE1	3:J:388:GLU:HA	2.14	0.48
2:L:21:ILE:HG12	2:L:102:THR:HG21	1.95	0.48
1:M:149:GLY:O	1:M:221:VAL:HG21	2.14	0.48
3:O:283:GLN:C	3:O:285:HIS:N	2.63	0.48
3:P:312:ASN:HB3	3:P:319:TYR:OH	2.14	0.48
3:X:388:GLU:OE1	3:X:388:GLU:HA	2.14	0.48
3:Y:244:PRO:HB3	3:Y:336:ILE:HD11	1.95	0.48
3:Y:311:GLN:NE2	3:Y:311:GLN:N	2.53	0.48
2:C:201:LEU:HB3	2:C:203:SER:O	2.14	0.47
1:D:38:ARG:HB3	1:D:94:TYR:CD2	2.49	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:92:ALA:HB3	1:D:94:TYR:CE1	2.48	0.47
1:E:164:TRP:CH2	1:E:192:VAL:HG12	2.49	0.47
1:H:69:THR:O	1:H:81:LEU:HA	2.13	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	2.14	0.47
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47
3:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	0.47
3:O:358:MET:O	3:O:414:LYS:HE3	2.14	0.47
3:X:414:LYS:HG2	3:X:418:GLN:NE2	2.29	0.47
2:C:169:LYS:NZ	2:C:169:LYS:HB3	2.29	0.47
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.47
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.49	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:O:414:LYS:HG2	3:O:418:GLN:NE2	2.29	0.47
3:Y:312:ASN:HB3	3:Y:319:TYR:OH	2.14	0.47
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	0.47
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.47
2:L:169:LYS:NZ	2:L:169:LYS:HB3	2.29	0.47
2:L:151:ASP:HA	2:L:191:VAL:HG12	1.95	0.47
1:A:23:GLY:HA2	1:A:78:PHE:CD2	2.50	0.47
1:D:67:ARG:C	1:D:68:PHE:HD1	2.18	0.47
1:E:102:ASP:N	1:E:102:ASP:OD1	2.47	0.47
2:F:142:ARG:CG	2:F:142:ARG:HH11	2.26	0.47
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	0.47
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.47
3:X:282:VAL:O	3:X:283:GLN:CB	2.52	0.47
3:X:288:LYS:H	3:X:288:LYS:CD	2.27	0.47
3:Y:259:VAL:HG23	3:Y:308:VAL:CG2	2.43	0.47
2:C:113:PRO:HD3	2:C:198:HIS:CG	2.50	0.47
1:D:98:ARG:NH2	1:D:111:ASP:OD2	2.35	0.47
1:H:153:LYS:HG2	1:H:154:ASP:OD1	2.14	0.47
1:M:101:SER:OG	1:M:104:LEU:HA	2.14	0.47
1:M:203:THR:HG21	1:M:220:LYS:NZ	2.30	0.47
3:P:275:PHE:HZ	3:P:302:VAL:O	1.98	0.47
2:B:29:ILE:HG21	2:B:90:HIS:CD2	2.47	0.47
2:B:61:ARG:HB2	2:B:76:SER:O	2.15	0.47
2:C:162:SER:HB3	2:C:176:SER:OG	2.15	0.47
2:F:6:GLN:NE2	2:F:102:THR:OG1	2.48	0.47
1:H:174:HIS:HB3	2:K:164:THR:HG21	1.97	0.47
2:K:113:PRO:HD3	2:K:198:HIS:CG	2.49	0.47
2:K:121:SER:O	2:K:125:LEU:HB2	2.14	0.47
1:M:153:LYS:HG2	1:M:154:ASP:OD2	2.14	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:432:LEU:HD22	3:P:437:THR:HB	1.97	0.47
3:X:438:GLN:O	3:X:439:LYS:HD3	2.15	0.47
2:F:11:LEU:HD22	2:F:19:ILE:HD12	1.97	0.47
1:H:67:ARG:C	1:H:68:PHE:HD1	2.18	0.47
1:I:68:PHE:HB3	1:I:81:LEU:HD11	1.95	0.47
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.47
1:H:134:LEU:HB3	2:K:118:PHE:CG	2.49	0.47
2:K:4:MET:HG2	2:K:97:THR:HG23	1.95	0.47
3:N:244:PRO:HB3	3:N:336:ILE:HD11	1.95	0.47
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.47
3:P:308:VAL:HG11	3:P:313:TRP:HB2	1.97	0.47
2:C:31:THR:O	2:C:50:LYS:HA	2.14	0.47
2:F:167:ASP:OD2	2:F:169:LYS:HG3	2.15	0.47
2:L:20:THR:HG22	2:L:73:LEU:O	2.14	0.47
1:M:203:THR:HB	1:M:220:LYS:HE3	1.96	0.47
3:Y:322:LYS:HG3	3:Y:333:GLU:HG2	1.97	0.47
2:C:118:PHE:CD2	1:D:134:LEU:HD13	2.50	0.47
1:I:126:THR:HB	1:I:213:SER:HB3	1.97	0.47
1:I:53:THR:O	1:I:56:THR:OG1	2.32	0.47
3:O:289:THR:CG2	3:O:290:LYS:N	2.78	0.47
3:Y:275:PHE:HZ	3:Y:302:VAL:O	1.97	0.47
1:A:99:LYS:NZ	2:C:91:TYR:CD1	2.83	0.47
1:H:68:PHE:O	1:H:69:THR:OG1	2.31	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
1:M:164:TRP:C	1:M:166:SER:N	2.67	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:P:368:LEU:HD12	3:P:369:VAL:H	1.79	0.47
3:Y:279:VAL:O	3:Y:282:VAL:HG22	2.15	0.47
1:H:19:ILE:C	1:H:20:LEU:HD23	2.36	0.46
2:K:108:ARG:NH1	2:K:111:ALA:HB2	2.30	0.46
2:L:31:THR:O	2:L:50:LYS:HA	2.15	0.46
1:M:92:ALA:HB3	1:M:94:TYR:CE1	2.50	0.46
3:O:438:GLN:O	3:O:439:LYS:HD3	2.15	0.46
3:P:279:VAL:O	3:P:282:VAL:HG22	2.15	0.46
3:P:322:LYS:HG3	3:P:333:GLU:HG2	1.97	0.46
3:Y:308:VAL:HG11	3:Y:313:TRP:HB2	1.97	0.46
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.51	0.46
2:C:5:THR:HG23	2:C:100:GLN:HE22	1.80	0.46
2:K:36:TYR:HE2	2:K:89:GLN:HB3	1.81	0.46
1:M:101:SER:H	1:M:104:LEU:CD2	2.28	0.46
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
3:O:371:GLY:HA2	3:O:403:SER:OG	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:261:CYS:HB2	3:P:277:TRP:CH2	2.50	0.46
3:Y:300:TYR:HB3	3:Y:301:ARG:H	1.37	0.46
1:A:68:PHE:CD1	1:A:83:MET:HA	2.51	0.46
2:B:148:TRP:CE3	2:B:179:LEU:HD22	2.51	0.46
1:D:69:THR:O	1:D:81:LEU:HD12	2.15	0.46
2:G:146:VAL:HB	2:G:161:GLU:OE2	2.15	0.46
1:H:101:SER:OG	1:H:104:LEU:HA	2.15	0.46
1:I:220:LYS:HE2	1:I:222:GLU:CG	2.46	0.46
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.46
3:N:308:VAL:HG11	3:N:313:TRP:HB2	1.97	0.46
3:O:388:GLU:OE1	3:O:388:GLU:HA	2.14	0.46
3:O:421:ASN:N	3:O:421:ASN:ND2	2.64	0.46
2:B:201:LEU:HB3	2:B:203:SER:O	2.16	0.46
2:F:83:PHE:CE1	2:F:106:ILE:HG12	2.51	0.46
3:X:289:THR:CG2	3:X:290:LYS:N	2.78	0.46
3:X:421:ASN:N	3:X:421:ASN:ND2	2.64	0.46
3:Y:361:ASN:ND2	3:Y:362:GLN:HG3	2.31	0.46
2:B:140:TYR:CD2	2:B:141:PRO:HA	2.50	0.46
2:B:149:LYS:HB2	2:B:193:ALA:HB3	1.96	0.46
2:B:31:THR:O	2:B:50:LYS:HA	2.15	0.46
1:D:154:ASP:HA	1:D:185:LEU:HB3	1.97	0.46
1:E:29:ILE:O	1:E:72:ARG:NH2	2.48	0.46
2:G:36:TYR:HE2	2:G:89:GLN:HB3	1.81	0.46
1:H:103:ARG:O	1:H:104:LEU:HB2	2.15	0.46
1:I:52:SER:OG	1:I:56:THR:N	2.49	0.46
3:N:432:LEU:HD11	3:N:437:THR:HG22	1.98	0.46
3:P:278:TYR:CE2	3:P:284:VAL:HG22	2.50	0.46
3:P:300:TYR:O	3:P:301:ARG:HB2	2.16	0.46
3:X:286:ASN:O	3:X:287:ALA:CB	2.63	0.46
2:B:113:PRO:HD3	2:B:198:HIS:CG	2.50	0.46
2:B:162:SER:HB3	2:B:176:SER:OG	2.16	0.46
2:K:140:TYR:CG	2:K:141:PRO:HA	2.50	0.46
2:L:2:VAL:HG11	2:L:90:HIS:CD2	2.51	0.46
3:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.46
3:Y:261:CYS:HB2	3:Y:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD11	3:Y:437:THR:HG22	1.98	0.46
1:H:144:GLY:O	1:H:196:SER:HB2	2.15	0.46
1:M:22:CYS:N	1:M:79:VAL:O	2.48	0.46
3:O:265:ASP:HA	3:O:299:THR:HB	1.98	0.46
3:Y:278:TYR:CE2	3:Y:284:VAL:HG22	2.50	0.46
1:H:92:ALA:N	1:H:119:VAL:O	2.47	0.46
3:N:275:PHE:HZ	3:N:302:VAL:O	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:368:LEU:HD12	3:N:369:VAL:H	1.79	0.46
3:O:288:LYS:CD	3:O:288:LYS:H	2.27	0.46
1:E:153:LYS:HG2	1:E:154:ASP:OD1	2.15	0.46
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD22	3:Y:437:THR:HB	1.97	0.46
1:H:22:CYS:O	1:H:78:PHE:HA	2.15	0.46
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.46
2:K:146:VAL:HB	2:K:161:GLU:OE2	2.16	0.46
3:P:344:ARG:O	3:P:372:PHE:HA	2.16	0.46
3:P:432:LEU:HD11	3:P:437:THR:HG22	1.98	0.46
2:C:36:TYR:CE1	2:C:46:LEU:HD13	2.50	0.45
2:F:113:PRO:HD2	2:F:201:LEU:HD22	1.98	0.45
1:I:69:THR:C	1:I:81:LEU:HD12	2.36	0.45
2:L:106:ILE:O	2:L:166:GLN:NE2	2.46	0.45
3:N:300:TYR:O	3:N:301:ARG:CB	2.64	0.45
3:N:344:ARG:O	3:N:372:PHE:HA	2.16	0.45
3:P:439:LYS:HD2	3:P:439:LYS:HA	1.81	0.45
3:Y:368:LEU:HD12	3:Y:369:VAL:H	1.79	0.45
1:A:174:HIS:HB3	2:B:164:THR:HG21	1.98	0.45
2:C:121:SER:O	2:C:125:LEU:HB2	2.16	0.45
1:M:69:THR:C	1:M:81:LEU:HD12	2.36	0.45
1:A:94:TYR:CE1	1:A:119:VAL:HB	2.51	0.45
1:H:135:ALA:CB	1:H:224:LYS:HD3	2.47	0.45
2:L:83:PHE:CE1	2:L:106:ILE:HG12	2.52	0.45
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.98	0.45
3:P:433:HIS:CA	3:P:434:ASN:N	2.69	0.45
1:A:101:SER:H	1:A:104:LEU:HD23	1.82	0.45
2:G:124:GLN:NE2	1:I:132:PHE:CE2	2.85	0.45
2:K:142:ARG:HH11	2:K:142:ARG:CG	2.25	0.45
1:M:32:HIS:ND1	1:M:98:ARG:HG3	2.31	0.45
3:P:300:TYR:O	3:P:301:ARG:CB	2.65	0.45
3:P:311:GLN:N	3:P:311:GLN:NE2	2.53	0.45
3:P:361:ASN:ND2	3:P:362:GLN:HG3	2.31	0.45
3:Y:300:TYR:O	3:Y:301:ARG:HB2	2.16	0.45
1:A:29:ILE:O	1:A:72:ARG:NH2	2.49	0.45
1:E:69:THR:C	1:E:81:LEU:HD12	2.37	0.45
2:F:5:THR:HG23	2:F:100:GLN:HE22	1.81	0.45
2:F:162:SER:HB3	2:F:176:SER:OG	2.16	0.45
1:H:53:THR:O	1:H:56:THR:OG1	2.34	0.45
3:J:278:TYR:N	3:J:278:TYR:CD1	2.85	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:O:286:ASN:O	3:O:287:ALA:CB	2.63	0.45
3:X:265:ASP:HA	3:X:299:THR:HB	1.98	0.45
3:Y:279:VAL:O	3:Y:280:ASP:HB2	2.16	0.45
3:Y:242:LEU:HD13	3:Y:336:ILE:HG22	1.98	0.45
1:A:72:ARG:NE	1:A:74:ASP:OD1	2.38	0.45
2:C:146:VAL:HB	2:C:161:GLU:OE2	2.17	0.45
1:D:22:CYS:O	1:D:78:PHE:HA	2.16	0.45
1:E:32:HIS:ND1	1:E:98:ARG:HG3	2.31	0.45
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.45
3:O:342:GLN:HA	3:O:343:PRO:HD3	1.83	0.45
3:Y:290:LYS:HE3	3:Y:292:ARG:HH12	1.82	0.45
1:A:164:TRP:CZ3	1:A:221:VAL:HG21	2.52	0.45
1:D:101:SER:N	1:D:104:LEU:HD23	2.31	0.45
2:F:36:TYR:CE1	2:F:46:LEU:HD13	2.52	0.45
2:K:31:THR:O	2:K:50:LYS:HA	2.16	0.45
1:M:101:SER:N	1:M:104:LEU:HD23	2.31	0.45
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.45
3:N:279:VAL:O	3:N:280:ASP:HB2	2.17	0.45
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.45
3:P:406:LEU:CD1	3:P:406:LEU:C	2.85	0.45
3:Y:344:ARG:O	3:Y:372:PHE:HA	2.16	0.45
2:B:31:THR:OG1	2:B:50:LYS:HE2	2.15	0.45
2:C:113:PRO:HD2	2:C:201:LEU:HD22	1.99	0.45
1:D:101:SER:H	1:D:104:LEU:CD2	2.29	0.45
1:E:101:SER:N	1:E:104:LEU:HD23	2.32	0.45
1:E:101:SER:OG	1:E:104:LEU:HA	2.17	0.45
1:E:195:PRO:C	1:E:197:SER:H	2.20	0.45
2:G:108:ARG:NH1	2:G:111:ALA:HB2	2.32	0.45
1:I:164:TRP:HZ2	1:I:190:SER:O	1.99	0.45
2:K:140:TYR:CD2	2:K:141:PRO:HA	2.52	0.45
3:P:269:GLU:C	3:P:271:PRO:HD3	2.36	0.45
3:Y:406:LEU:C	3:Y:406:LEU:CD1	2.84	0.45
1:E:101:SER:H	1:E:104:LEU:CD2	2.29	0.45
2:F:113:PRO:HD3	2:F:198:HIS:CG	2.52	0.45
2:F:31:THR:OG1	2:F:50:LYS:HE2	2.15	0.45
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.45
3:P:279:VAL:O	3:P:280:ASP:HB2	2.17	0.45
3:Y:265:ASP:HA	3:Y:299:THR:CB	2.47	0.45
3:Y:300:TYR:O	3:Y:301:ARG:CB	2.65	0.45
3:Y:301:ARG:HG2	3:Y:303:VAL:HG23	1.99	0.45
3:Y:323:VAL:HG12	3:Y:324:SER:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:101:SER:H	1:A:104:LEU:CD2	2.30	0.45
1:E:133:PRO:HB3	1:E:221:VAL:HG22	1.99	0.45
1:E:3:GLN:HB2	1:E:25:SER:CB	2.41	0.45
2:F:31:THR:O	2:F:50:LYS:HA	2.16	0.45
3:N:323:VAL:HG12	3:N:324:SER:N	2.32	0.45
3:N:406:LEU:CD1	3:N:406:LEU:C	2.85	0.45
3:P:290:LYS:HE3	3:P:292:ARG:HH12	1.82	0.45
3:X:266:VAL:HB	3:X:300:TYR:HB2	1.98	0.45
1:D:91:THR:HG23	1:D:120:THR:HG22	1.99	0.44
1:E:38:ARG:HB3	1:E:94:TYR:CE2	2.52	0.44
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.98	0.44
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	0.44
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.44
3:O:346:PRO:CB	3:O:372:PHE:HB3	2.39	0.44
3:O:374:PRO:O	3:O:429:HIS:HE1	2.00	0.44
3:Y:345:GLU:HA	3:Y:431:ALA:HB3	1.99	0.44
1:E:148:LEU:HD12	1:E:164:TRP:CH2	2.53	0.44
2:F:61:ARG:HB2	2:F:76:SER:O	2.17	0.44
1:H:192:VAL:HG22	1:H:194:VAL:HG13	2.00	0.44
2:K:149:LYS:HB2	2:K:193:ALA:HB3	1.99	0.44
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.32	0.44
3:P:238:PRO:CB	3:P:328:LEU:HD13	2.47	0.44
3:X:244:PRO:HB3	3:X:336:ILE:HD13	1.99	0.44
1:A:12:VAL:O	1:A:121:VAL:HA	2.17	0.44
3:J:347:GLN:NE2	3:J:349:TYR:OH	2.51	0.44
3:P:242:LEU:HD13	3:P:336:ILE:HG22	1.98	0.44
3:P:239:SER:HB3	3:P:264:VAL:CG2	2.47	0.44
3:P:265:ASP:HA	3:P:299:THR:CB	2.47	0.44
3:X:291:PRO:O	3:X:292:ARG:HD2	2.17	0.44
3:Y:238:PRO:CB	3:Y:328:LEU:HD13	2.47	0.44
1:D:64:VAL:HB	1:D:68:PHE:CD2	2.53	0.44
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.44
2:K:27:GLN:O	2:K:29:ILE:HG23	2.17	0.44
3:P:345:GLU:HA	3:P:431:ALA:HB3	1.99	0.44
3:X:287:ALA:O	3:X:288:LYS:C	2.56	0.44
1:A:153:LYS:HG2	1:A:154:ASP:OD1	2.16	0.44
2:C:2:VAL:HG11	2:C:90:HIS:CD2	2.53	0.44
1:D:192:VAL:HG22	1:D:194:VAL:HG13	1.99	0.44
2:F:36:TYR:HB2	2:F:87:HIS:HB2	1.99	0.44
2:G:124:GLN:HB2	1:I:132:PHE:CD1	2.52	0.44
1:I:58:ARG:NH1	1:I:70:VAL:O	2.49	0.44
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	0.44
3:O:266:VAL:HB	3:O:300:TYR:HB2	1.98	0.44
3:O:347:GLN:NE2	3:O:349:TYR:OH	2.51	0.44
3:X:309:LEU:O	3:X:312:ASN:N	2.51	0.44
3:Y:269:GLU:C	3:Y:271:PRO:HD3	2.36	0.44
1:H:18:LEU:CB	1:H:83:MET:HE3	2.43	0.44
3:J:264:VAL:O	3:J:265:ASP:HB2	2.18	0.44
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.44
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.44
3:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	0.44
2:K:30:GLU:HB2	2:K:32:TRP:CD1	2.53	0.44
3:P:326:LYS:C	3:P:328:LEU:H	2.20	0.44
3:P:363:VAL:HG22	3:P:412:VAL:O	2.18	0.44
3:X:278:TYR:HA	3:X:282:VAL:O	2.18	0.44
3:Y:239:SER:HB3	3:Y:264:VAL:CG2	2.47	0.44
1:A:69:THR:O	1:A:81:LEU:HD12	2.18	0.44
1:D:188:LEU:O	1:D:188:LEU:HD12	2.17	0.44
1:D:69:THR:O	1:D:81:LEU:HA	2.18	0.44
1:D:92:ALA:HB3	1:D:94:TYR:CZ	2.53	0.44
1:E:174:HIS:HB3	2:F:164:THR:HG21	1.99	0.44
2:F:149:LYS:HZ1	2:F:195:GLU:CD	2.18	0.44
1:H:92:ALA:HB3	1:H:94:TYR:CZ	2.53	0.44
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:O:291:PRO:O	3:O:292:ARG:HD2	2.18	0.44
3:P:278:TYR:HE2	3:P:284:VAL:HG22	1.83	0.44
3:P:323:VAL:HG12	3:P:324:SER:N	2.32	0.44
3:X:278:TYR:N	3:X:278:TYR:CD1	2.85	0.44
3:Y:363:VAL:HG22	3:Y:412:VAL:O	2.18	0.44
1:E:12:VAL:O	1:E:121:VAL:HA	2.18	0.44
1:E:194:VAL:HG21	1:E:204:TYR:CZ	2.53	0.44
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.44
3:Y:278:TYR:HE2	3:Y:284:VAL:HG22	1.83	0.44
3:Y:439:LYS:HA	3:Y:439:LYS:HD2	1.82	0.44
2:B:108:ARG:NH1	2:B:111:ALA:HB2	2.33	0.44
1:H:23:GLY:HA2	1:H:78:PHE:CD2	2.52	0.44
2:L:117:ILE:HG13	2:L:133:VAL:O	2.17	0.44
1:M:185:LEU:HA	1:M:185:LEU:HD12	1.78	0.44
3:O:309:LEU:O	3:O:312:ASN:N	2.51	0.44
1:A:38:ARG:HD3	1:A:94:TYR:CE2	2.53	0.43
1:E:35:ASN:O	1:E:97:ALA:N	2.48	0.43
1:H:22:CYS:N	1:H:79:VAL:O	2.51	0.43
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
3:O:296:TYR:HB3	3:O:297:ASN:H	1.56	0.43
3:O:244:PRO:HB3	3:O:336:ILE:HD13	1.99	0.43
2:L:70:GLU:HG3	2:L:71:PHE:N	2.32	0.43
1:M:68:PHE:HB3	1:M:81:LEU:HD11	2.00	0.43
3:O:278:TYR:CD1	3:O:278:TYR:N	2.85	0.43
3:P:242:LEU:HA	3:P:242:LEU:HD23	1.86	0.43
1:A:69:THR:O	1:A:81:LEU:HA	2.18	0.43
1:E:136:PRO:HG2	1:E:223:PRO:HG3	1.99	0.43
1:I:22:CYS:N	1:I:79:VAL:O	2.47	0.43
2:K:170:ASP:OD1	2:K:172:THR:OG1	2.19	0.43
2:K:186:TYR:HA	2:K:192:TYR:OH	2.18	0.43
3:O:278:TYR:HA	3:O:282:VAL:O	2.18	0.43
3:X:347:GLN:NE2	3:X:349:TYR:OH	2.50	0.43
3:Y:326:LYS:C	3:Y:328:LEU:H	2.20	0.43
2:C:136:LEU:HB2	2:C:175:LEU:HB3	1.99	0.43
1:E:22:CYS:O	1:E:78:PHE:HA	2.18	0.43
1:E:68:PHE:HB3	1:E:81:LEU:HD11	2.00	0.43
2:F:207:LYS:HZ3	1:M:201:THR:CB	2.17	0.43
2:G:121:SER:O	2:G:125:LEU:HB2	2.19	0.43
2:L:113:PRO:HD3	2:L:198:HIS:CG	2.52	0.43
1:M:98:ARG:NH2	1:M:111:ASP:OD2	2.37	0.43
3:O:264:VAL:O	3:O:265:ASP:HB2	2.18	0.43
3:X:374:PRO:O	3:X:429:HIS:HE1	2.00	0.43
1:H:101:SER:H	1:H:104:LEU:HD22	1.83	0.43
1:I:60:TYR:CE2	1:I:69:THR:HA	2.54	0.43
2:K:20:THR:HG22	2:K:73:LEU:O	2.19	0.43
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	0.43
3:N:351:LEU:HA	3:N:352:PRO:HD3	1.91	0.43
3:P:258:GLU:HA	3:P:308:VAL:HG23	1.99	0.43
3:P:338:LYS:NZ	3:P:430:GLU:OE2	2.52	0.43
3:X:348:VAL:O	3:X:439:LYS:HG3	2.19	0.43
3:Y:338:LYS:NZ	3:Y:430:GLU:OE2	2.52	0.43
1:A:154:ASP:HA	1:A:185:LEU:HB3	2.01	0.43
2:B:36:TYR:HE2	2:B:89:GLN:HB3	1.83	0.43
1:D:156:PHE:HB3	1:D:185:LEU:HD12	2.00	0.43
1:E:181:GLN:C	1:E:183:SER:H	2.21	0.43
2:K:2:VAL:HG11	2:K:90:HIS:CD2	2.53	0.43
2:K:31:THR:OG1	2:K:50:LYS:HE2	2.18	0.43
2:L:63:SER:O	2:L:74:THR:N	2.52	0.43
3:P:325:ASN:HD22	3:P:326:LYS:N	2.15	0.43
3:P:414:LYS:O	3:P:418:GLN:HG3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Y:252:MET:SD	3:Y:428:MET:HE3	2.58	0.43
2:B:121:SER:O	2:B:125:LEU:HB2	2.18	0.43
2:C:83:PHE:CE1	2:C:106:ILE:HG12	2.53	0.43
2:G:161:GLU:HA	2:G:176:SER:O	2.18	0.43
1:I:194:VAL:HG21	1:I:204:TYR:CZ	2.54	0.43
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.43
3:N:414:LYS:O	3:N:418:GLN:HG3	2.19	0.43
1:A:27:PHE:CE1	1:A:29:ILE:HG22	2.53	0.43
1:A:3:GLN:HB2	1:A:25:SER:CB	2.41	0.43
2:C:20:THR:HG22	2:C:73:LEU:O	2.18	0.43
1:I:163:SER:O	1:I:164:TRP:CD1	2.71	0.43
1:I:222:GLU:HA	1:I:223:PRO:HD3	1.86	0.43
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	0.43
1:M:38:ARG:HB3	1:M:94:TYR:CE2	2.54	0.43
1:M:67:ARG:C	1:M:68:PHE:HD1	2.22	0.43
2:C:4:MET:HG2	2:C:97:THR:HG23	1.99	0.43
2:F:146:VAL:HB	2:F:161:GLU:OE2	2.18	0.43
2:G:201:LEU:HB3	2:G:203:SER:O	2.19	0.43
2:G:49:TYR:CE2	2:G:53:THR:HB	2.54	0.43
1:H:60:TYR:CE2	1:H:69:THR:HA	2.53	0.43
2:L:149:LYS:HB2	2:L:193:ALA:HB3	2.00	0.43
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	0.43
3:X:346:PRO:CB	3:X:372:PHE:HB3	2.39	0.43
1:A:144:GLY:O	1:A:196:SER:HB2	2.19	0.43
2:B:70:GLU:HG3	2:B:71:PHE:N	2.33	0.43
2:C:108:ARG:NH1	2:C:111:ALA:HB2	2.34	0.43
2:C:186:TYR:HA	2:C:192:TYR:HH	1.83	0.43
1:D:18:LEU:CB	1:D:83:MET:HE3	2.47	0.43
1:D:103:ARG:N	2:F:50:LYS:NZ	2.60	0.43
2:L:161:GLU:HA	2:L:176:SER:O	2.18	0.43
3:O:287:ALA:O	3:O:288:LYS:C	2.56	0.43
3:P:386:GLN:HA	3:P:387:PRO:HD3	1.76	0.43
3:X:264:VAL:O	3:X:265:ASP:HB2	2.18	0.43
3:Y:291:PRO:O	3:Y:292:ARG:HB3	2.19	0.43
3:Y:258:GLU:HA	3:Y:308:VAL:HG23	1.99	0.43
1:D:194:VAL:HG21	1:D:204:TYR:CZ	2.54	0.42
1:D:19:ILE:C	1:D:20:LEU:HD23	2.39	0.42
2:K:161:GLU:HA	2:K:176:SER:O	2.19	0.42
2:L:167:ASP:CB	1:M:174:HIS:HE1	2.32	0.42
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	0.42
3:P:266:VAL:HB	3:P:300:TYR:CD2	2.54	0.42
3:P:301:ARG:HG2	3:P:303:VAL:HG23	1.99	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:161:GLU:HA	2:B:176:SER:O	2.19	0.42
1:D:149:GLY:O	1:D:221:VAL:HG11	2.18	0.42
2:F:161:GLU:HA	2:F:176:SER:O	2.19	0.42
2:F:201:LEU:HB3	2:F:203:SER:O	2.19	0.42
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
3:P:368:LEU:HD12	3:P:369:VAL:N	2.34	0.42
2:B:38:GLN:O	2:B:84:ALA:HB1	2.20	0.42
2:G:29:ILE:HG21	2:G:90:HIS:CD2	2.50	0.42
1:H:156:PHE:CD1	1:H:156:PHE:C	2.92	0.42
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.42
2:L:36:TYR:HE2	2:L:89:GLN:HB3	1.85	0.42
1:M:37:VAL:HG22	1:M:47:TRP:HA	2.01	0.42
1:M:69:THR:O	1:M:81:LEU:HD12	2.20	0.42
3:O:274:LYS:HE2	3:O:324:SER:HB2	2.02	0.42
3:O:348:VAL:O	3:O:439:LYS:HG3	2.19	0.42
3:P:291:PRO:O	3:P:292:ARG:HB3	2.19	0.42
3:Y:266:VAL:HB	3:Y:300:TYR:CD2	2.54	0.42
1:A:58:ARG:NH1	1:A:70:VAL:O	2.52	0.42
1:I:164:TRP:O	1:I:166:SER:N	2.53	0.42
2:K:91:TYR:HD1	1:M:99:LYS:HZ3	1.66	0.42
3:Y:296:TYR:OH	3:Y:301:ARG:NH1	2.46	0.42
1:A:101:SER:N	1:A:104:LEU:HD23	2.34	0.42
1:D:153:LYS:NZ	1:D:181:GLN:OE1	2.23	0.42
2:F:29:ILE:HG21	2:F:90:HIS:CD2	2.52	0.42
1:H:68:PHE:HB3	1:H:81:LEU:HD11	2.01	0.42
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.42
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.42
3:O:336:ILE:HG12	3:O:337:SER:N	2.35	0.42
3:X:336:ILE:HG12	3:X:337:SER:N	2.35	0.42
3:Y:357:GLU:C	3:Y:359:THR:H	2.23	0.42
3:Y:368:LEU:HD12	3:Y:369:VAL:N	2.34	0.42
3:Y:414:LYS:O	3:Y:418:GLN:HG3	2.18	0.42
1:A:185:LEU:HA	1:A:185:LEU:HD12	1.78	0.42
1:A:38:ARG:NH1	1:A:90:ASP:HA	2.34	0.42
2:C:160:GLN:O	2:C:178:THR:N	2.44	0.42
1:D:185:LEU:HA	1:D:185:LEU:HD12	1.76	0.42
1:D:74:ASP:HB3	2:F:94:TYR:CE1	2.54	0.42
1:E:38:ARG:HD3	1:E:94:TYR:CE2	2.55	0.42
2:F:91:TYR:HD1	1:I:99:LYS:NZ	2.17	0.42
2:G:63:SER:O	2:G:74:THR:N	2.50	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
3:O:369:VAL:HB	3:O:406:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:P:296:TYR:OH	3:P:301:ARG:NH1	2.46	0.42
3:X:283:GLN:C	3:X:285:HIS:H	2.23	0.42
1:A:197:SER:HB3	3:X:295:GLN:OE1	2.20	0.42
3:X:384:ASN:CG	3:X:385:GLY:H	2.22	0.42
2:C:21:ILE:HG12	2:C:102:THR:HG21	2.02	0.42
1:E:152:VAL:HG22	1:E:208:VAL:HG21	2.01	0.42
1:I:153:LYS:HG2	1:I:154:ASP:OD1	2.20	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
1:E:149:GLY:HA2	1:E:164:TRP:CH2	2.55	0.42
1:E:53:THR:O	1:E:56:THR:OG1	2.38	0.42
1:E:60:TYR:CE2	1:E:69:THR:HA	2.54	0.42
1:H:38:ARG:HA	1:H:93:ILE:O	2.19	0.42
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.42
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	0.42
1:M:38:ARG:HD3	1:M:94:TYR:CE2	2.55	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
3:P:238:PRO:HB2	3:P:328:LEU:HD13	2.01	0.42
3:Y:238:PRO:HB2	3:Y:328:LEU:HD13	2.01	0.42
1:D:220:LYS:HE2	1:D:222:GLU:OE1	2.19	0.42
1:H:101:SER:N	1:H:104:LEU:HD22	2.35	0.42
1:I:32:HIS:ND1	1:I:98:ARG:HG3	2.35	0.42
3:X:369:VAL:HB	3:X:406:LEU:HD12	2.02	0.42
3:Y:328:LEU:HD12	3:Y:329:PRO:CD	2.47	0.42
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.55	0.42
1:H:6:GLU:OE1	1:H:95:TYR:HA	2.20	0.42
1:I:195:PRO:C	1:I:197:SER:H	2.23	0.42
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.01	0.42
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.42
2:K:58:VAL:HA	2:K:59:PRO:HD3	1.91	0.42
2:L:29:ILE:HG21	2:L:90:HIS:CD2	2.53	0.42
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.42
3:X:391:TYR:C	3:X:391:TYR:CD2	2.92	0.42
2:C:4:MET:SD	2:C:90:HIS:HB2	2.59	0.41
1:D:40:VAL:O	1:D:43:GLY:N	2.45	0.41
2:L:138:ASN:OD1	1:M:174:HIS:NE2	2.52	0.41
2:L:161:GLU:HG2	2:L:177:SER:HB2	2.02	0.41
3:O:367:CYS:HB2	3:O:381:TRP:CH2	2.55	0.41
3:Y:276:ASN:HB3	3:Y:278:TYR:CE1	2.56	0.41
2:C:183:LYS:HE2	2:C:187:GLU:OE1	2.20	0.41
1:D:181:GLN:C	1:D:183:SER:H	2.23	0.41
1:D:163:SER:OG	1:D:207:ASN:HB2	2.20	0.41
1:D:47:TRP:NE1	1:D:49:ALA:O	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:38:ARG:NH1	1:E:90:ASP:HA	2.35	0.41
2:F:49:TYR:CE2	2:F:53:THR:HB	2.55	0.41
2:G:133:VAL:HG21	1:I:134:LEU:HD21	2.01	0.41
2:G:58:VAL:HA	2:G:59:PRO:HD3	1.97	0.41
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	0.41
3:N:268:HIS:O	3:N:271:PRO:CG	2.68	0.41
3:P:296:TYR:HB3	3:P:297:ASN:H	1.34	0.41
3:P:350:THR:HB	3:P:441:LEU:CD1	2.50	0.41
3:X:314:LEU:HD23	3:X:314:LEU:HA	1.87	0.41
3:Y:268:HIS:O	3:Y:271:PRO:CG	2.68	0.41
1:A:173:VAL:HG22	1:A:192:VAL:HB	2.01	0.41
1:A:99:LYS:HZ3	2:C:91:TYR:HD1	1.68	0.41
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
1:H:176:PHE:CE1	2:K:176:SER:HB3	2.55	0.41
2:L:11:LEU:HD22	2:L:19:ILE:HD12	2.02	0.41
1:M:23:GLY:HA2	1:M:78:PHE:CE2	2.54	0.41
1:M:38:ARG:HB3	1:M:94:TYR:CD2	2.55	0.41
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.41
3:O:391:TYR:C	3:O:391:TYR:CD2	2.92	0.41
3:P:276:ASN:HB3	3:P:278:TYR:CE1	2.55	0.41
1:D:30:SER:HB3	1:D:74:ASP:HB3	2.01	0.41
1:E:188:LEU:HD12	1:E:188:LEU:O	2.20	0.41
1:I:4:LEU:HG	1:I:24:VAL:HG12	2.02	0.41
2:K:36:TYR:CE1	2:K:46:LEU:HD13	2.55	0.41
3:O:328:LEU:HD12	3:O:329:PRO:CD	2.50	0.41
2:B:138:ASN:C	2:B:172:THR:HB	2.41	0.41
2:B:113:PRO:HD2	2:B:201:LEU:HD22	2.03	0.41
2:G:38:GLN:HA	2:G:44:PRO:HA	2.02	0.41
2:G:73:LEU:HD12	2:G:74:THR:H	1.84	0.41
1:H:68:PHE:HA	1:H:82:GLN:O	2.20	0.41
3:O:386:GLN:HA	3:O:387:PRO:HD3	1.88	0.41
3:P:268:HIS:O	3:P:271:PRO:CG	2.68	0.41
3:X:386:GLN:HG3	3:X:387:PRO:HD2	2.02	0.41
3:Y:350:THR:HB	3:Y:441:LEU:CD1	2.50	0.41
1:A:160:VAL:HG13	1:A:208:VAL:HG13	2.02	0.41
2:C:110:VAL:HG13	2:C:199:GLN:HG2	2.02	0.41
2:G:167:ASP:CG	1:I:174:HIS:HE1	2.23	0.41
1:H:219:LYS:HE2	1:H:219:LYS:HB2	1.91	0.41
1:M:181:GLN:C	1:M:183:SER:H	2.24	0.41
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
3:O:283:GLN:C	3:O:285:HIS:H	2.23	0.41
3:O:384:ASN:CG	3:O:385:GLY:H	2.22	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:367:CYS:HB2	3:X:381:TRP:CH2	2.55	0.41
2:B:106:ILE:O	2:B:166:GLN:NE2	2.48	0.41
2:C:38:GLN:HA	2:C:44:PRO:HA	2.03	0.41
2:G:15:VAL:HG21	2:G:80:PHE:CZ	2.56	0.41
2:L:5:THR:CG2	2:L:100:GLN:HE22	2.33	0.41
3:X:274:LYS:HE2	3:X:324:SER:HB2	2.02	0.41
3:Y:335:THR:O	3:Y:336:ILE:HB	2.21	0.41
2:B:2:VAL:HG11	2:B:90:HIS:CD2	2.56	0.41
2:C:151:ASP:HA	2:C:191:VAL:HG12	2.02	0.41
2:G:140:TYR:CG	2:G:141:PRO:HA	2.56	0.41
2:L:100:GLN:N	2:L:100:GLN:OE1	2.44	0.41
3:Y:367:CYS:HB2	3:Y:381:TRP:CZ2	2.56	0.41
2:C:149:LYS:HA	2:C:153:ALA:O	2.21	0.41
1:E:34:MET:O	1:E:50:SER:HA	2.21	0.41
2:G:30:GLU:HB2	2:G:32:TRP:CD1	2.56	0.41
1:H:160:VAL:HG12	1:H:160:VAL:O	2.20	0.41
1:H:195:PRO:C	1:H:197:SER:H	2.23	0.41
1:I:94:TYR:O	1:I:116:GLY:HA2	2.20	0.41
3:J:386:GLN:HG3	3:J:387:PRO:HD2	2.02	0.41
2:K:201:LEU:HB3	2:K:203:SER:O	2.20	0.41
2:L:167:ASP:CG	1:M:174:HIS:CE1	2.94	0.41
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.41
3:O:252:MET:HB2	3:O:255:ARG:CG	2.49	0.41
3:O:386:GLN:HG3	3:O:387:PRO:HD2	2.02	0.41
3:P:273:VAL:HB	3:P:302:VAL:HG21	2.03	0.41
3:P:357:GLU:C	3:P:359:THR:H	2.23	0.41
3:P:350:THR:HB	3:P:441:LEU:CG	2.51	0.41
2:C:70:GLU:HG3	2:C:71:PHE:N	2.35	0.41
1:H:12:VAL:O	1:H:121:VAL:HA	2.20	0.41
2:K:4:MET:SD	2:K:90:HIS:HB2	2.61	0.41
1:M:34:MET:O	1:M:50:SER:HA	2.19	0.41
3:N:273:VAL:HB	3:N:302:VAL:HG21	2.03	0.41
3:X:386:GLN:HA	3:X:387:PRO:HD3	1.88	0.41
3:Y:351:LEU:HB2	3:Y:366:THR:HB	2.03	0.41
2:B:33:LEU:HA	2:B:89:GLN:O	2.21	0.41
1:D:17:SER:HA	1:D:83:MET:O	2.21	0.41
2:F:73:LEU:HD12	2:F:74:THR:H	1.85	0.41
2:G:186:TYR:HA	2:G:192:TYR:OH	2.20	0.41
1:I:73:ASP:N	1:I:78:PHE:O	2.50	0.41
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
2:L:122:ASP:HA	2:L:125:LEU:HB3	2.03	0.41
3:P:308:VAL:HG12	3:P:309:LEU:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:X:328:LEU:HD12	3:X:329:PRO:CD	2.50	0.41
3:Y:273:VAL:HB	3:Y:302:VAL:HG21	2.03	0.41
1:A:152:VAL:HG22	1:A:208:VAL:HG21	2.03	0.40
1:A:4:LEU:HG	1:A:24:VAL:HG12	2.02	0.40
2:C:122:ASP:O	2:C:126:LYS:HB2	2.20	0.40
1:D:164:TRP:HH2	1:D:221:VAL:HG21	1.85	0.40
1:D:27:PHE:CE1	1:D:29:ILE:HG22	2.57	0.40
1:M:38:ARG:NH1	1:M:90:ASP:HA	2.35	0.40
3:N:351:LEU:HB2	3:N:366:THR:HB	2.03	0.40
3:P:245:PRO:HB3	3:P:258:GLU:H	1.87	0.40
2:C:61:ARG:O	2:C:76:SER:N	2.36	0.40
2:C:73:LEU:HD12	2:C:74:THR:H	1.86	0.40
1:D:156:PHE:C	1:D:156:PHE:CD1	2.94	0.40
1:E:156:PHE:C	1:E:156:PHE:CD1	2.94	0.40
2:F:108:ARG:HD3	2:F:109:THR:N	2.35	0.40
1:E:176:PHE:CD2	2:F:164:THR:HG23	2.56	0.40
2:G:117:ILE:HG13	2:G:133:VAL:O	2.21	0.40
2:L:36:TYR:CE1	2:L:46:LEU:HD13	2.56	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.37	0.40
3:O:289:THR:HG22	3:O:290:LYS:N	2.36	0.40
3:X:289:THR:HG22	3:X:290:LYS:N	2.37	0.40
3:Y:242:LEU:HD23	3:Y:242:LEU:HA	1.85	0.40
2:B:108:ARG:HD3	2:B:109:THR:N	2.36	0.40
2:B:73:LEU:HD12	2:B:74:THR:H	1.86	0.40
2:C:149:LYS:HZ1	2:C:195:GLU:CD	2.18	0.40
3:J:328:LEU:HA	3:J:329:PRO:HD3	1.94	0.40
3:P:335:THR:O	3:P:336:ILE:HB	2.21	0.40
3:P:367:CYS:HB2	3:P:381:TRP:CZ2	2.56	0.40
3:P:350:THR:HB	3:P:441:LEU:HD12	2.03	0.40
2:B:91:TYR:CD1	1:D:99:LYS:NZ	2.86	0.40
1:E:101:SER:CB	1:E:104:LEU:H	2.29	0.40
1:E:181:GLN:C	1:E:183:SER:N	2.75	0.40
1:H:181:GLN:C	1:H:183:SER:H	2.24	0.40
1:H:58:ARG:NH1	1:H:71:SER:OG	2.52	0.40
1:M:69:THR:O	1:M:81:LEU:HA	2.20	0.40
3:X:432:LEU:HD22	3:X:437:THR:HB	2.04	0.40
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.23	0.40
1:D:220:LYS:HE2	1:D:222:GLU:OE2	2.21	0.40
1:E:38:ARG:HB2	1:E:92:ALA:CB	2.52	0.40
2:F:15:VAL:HG21	2:F:80:PHE:CZ	2.56	0.40
2:G:167:ASP:CG	1:I:174:HIS:CE1	2.95	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:19:ILE:C	1:I:20:LEU:HD23	2.41	0.40
1:I:38:ARG:NH1	1:I:90:ASP:HA	2.37	0.40
3:J:432:LEU:HD22	3:J:437:THR:HB	2.04	0.40
2:K:29:ILE:HG21	2:K:90:HIS:CD2	2.54	0.40
2:K:5:THR:HG23	2:K:100:GLN:HE22	1.86	0.40
1:M:156:PHE:CD1	1:M:156:PHE:C	2.94	0.40
3:P:351:LEU:HA	3:P:352:PRO:HD3	1.91	0.40

All (174) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:Y:252:MET:O	3:Y:253:ILE:CG1[12_555]	0.41	1.79
3:J:252:MET:O	3:X:253:ILE:CD1[12_545]	0.48	1.72
3:O:253:ILE:CA	3:O:253:ILE:CB[10_444]	0.59	1.61
3:J:253:ILE:CD1	3:X:252:MET:O[12_545]	0.66	1.54
3:Y:253:ILE:CA	3:Y:253:ILE:CA[12_555]	0.70	1.50
2:B:18:THR:CA	3:J:285:HIS:ND1[12_545]	0.71	1.49
2:B:18:THR:CA	3:J:285:HIS:CE1[12_545]	0.71	1.49
3:J:253:ILE:CG1	3:X:252:MET:C[12_545]	0.73	1.47
3:X:284:VAL:CG1	2:L:18:THR:CG2[12_545]	0.86	1.34
3:J:253:ILE:CG1	3:X:253:ILE:N[12_545]	0.87	1.33
3:Y:253:ILE:CA	3:Y:253:ILE:C[12_555]	0.87	1.33
3:O:253:ILE:CB	3:O:253:ILE:CB[10_444]	0.96	1.24
3:N:310:HIS:CD2	3:P:253:ILE:CD1[6_445]	1.05	1.15
3:N:380:GLU:OE1	3:P:433:HIS:NE2[6_445]	1.05	1.15
3:X:285:HIS:CG	2:L:18:THR:OG1[12_545]	1.10	1.10
3:J:253:ILE:CD1	3:X:252:MET:C[12_545]	1.17	1.03
3:Y:382:GLU:OE2	3:Y:433:HIS:CG[12_555]	1.19	1.01
3:Y:253:ILE:CG2	3:Y:255:ARG:N[12_555]	1.20	1.00
3:J:253:ILE:CB	3:X:253:ILE:N[12_545]	1.20	1.00
3:O:253:ILE:CD1	3:O:254:SER:N[10_444]	1.22	0.98
2:B:18:THR:C	3:J:285:HIS:ND1[12_545]	1.25	0.95
3:N:253:ILE:CG2	3:P:253:ILE:C[6_445]	1.25	0.95
2:B:18:THR:N	3:J:285:HIS:CG[12_545]	1.25	0.95
3:N:253:ILE:N	3:P:253:ILE:N[6_445]	1.28	0.92
3:N:380:GLU:OE1	3:P:433:HIS:CE1[6_445]	1.30	0.90
3:X:285:HIS:ND1	2:L:18:THR:OG1[12_545]	1.30	0.90
1:D:143:GLY:O	3:Y:280:ASP:CG[8_555]	1.31	0.89
2:B:18:THR:OG1	3:J:285:HIS:CD2[12_545]	1.32	0.88
3:Y:382:GLU:OE2	3:Y:433:HIS:CB[12_555]	1.32	0.88
2:B:18:THR:N	3:J:285:HIS:ND1[12_545]	1.33	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:253:ILE:CG2	3:P:253:ILE:CA[6_445]	1.34	0.86
3:N:433:HIS:CG	3:P:382:GLU:OE2[6_445]	1.35	0.85
3:X:283:GLN:N	2:L:18:THR:O[12_545]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD1[8_555]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD2[8_555]	1.35	0.85
1:D:143:GLY:C	3:Y:280:ASP:OD2[8_555]	1.35	0.85
3:J:253:ILE:N	3:X:253:ILE:CG1[12_545]	1.36	0.84
3:N:253:ILE:CB	3:P:253:ILE:CA[6_445]	1.37	0.83
3:Y:253:ILE:N	3:Y:253:ILE:N[12_555]	1.37	0.83
1:D:144:GLY:N	3:Y:280:ASP:OD2[8_555]	1.37	0.83
3:J:253:ILE:CA	3:X:253:ILE:CG1[12_545]	1.39	0.81
3:O:253:ILE:CA	3:O:253:ILE:CG2[10_444]	1.40	0.80
3:O:253:ILE:CG1	3:O:254:SER:N[10_444]	1.41	0.79
3:N:253:ILE:CA	3:P:253:ILE:N[6_445]	1.41	0.79
3:J:252:MET:C	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CA	3:P:253:ILE:CA[6_445]	1.42	0.78
3:J:252:MET:O	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CG1	3:P:252:MET:C[6_445]	1.44	0.76
3:Y:253:ILE:CG2	3:Y:254:SER:C[12_555]	1.45	0.75
3:X:281:GLY:O	2:L:20:THR:OG1[12_545]	1.45	0.75
3:J:253:ILE:CA	3:X:253:ILE:CA[12_545]	1.46	0.74
3:J:310:HIS:NE2	3:X:253:ILE:CG2[12_545]	1.46	0.74
3:O:253:ILE:C	3:O:253:ILE:CG2[10_444]	1.47	0.73
1:D:144:GLY:CA	3:Y:280:ASP:OD2[8_555]	1.48	0.72
3:O:253:ILE:O	3:O:253:ILE:CG2[10_444]	1.48	0.72
3:Y:253:ILE:C	3:Y:253:ILE:CB[12_555]	1.48	0.72
3:Y:436:TYR:CD1	3:Y:436:TYR:CD1[12_555]	1.48	0.72
3:J:253:ILE:CB	3:X:253:ILE:CA[12_545]	1.49	0.71
3:J:253:ILE:CG1	3:X:252:MET:O[12_545]	1.50	0.70
3:N:310:HIS:CD2	3:P:253:ILE:CG1[6_445]	1.50	0.70
3:N:253:ILE:CB	3:P:253:ILE:N[6_445]	1.51	0.69
3:O:253:ILE:C	3:O:253:ILE:CG1[10_444]	1.51	0.69
2:B:18:THR:CA	3:J:285:HIS:NE2[12_545]	1.51	0.69
3:N:310:HIS:NE2	3:P:253:ILE:CD1[6_445]	1.51	0.69
3:O:253:ILE:CA	3:O:253:ILE:CG1[10_444]	1.54	0.66
3:J:253:ILE:CA	3:X:253:ILE:CB[12_545]	1.55	0.65
2:B:18:THR:CA	3:J:285:HIS:CG[12_545]	1.57	0.63
3:Y:252:MET:C	3:Y:253:ILE:CG1[12_555]	1.58	0.62
3:X:285:HIS:NE2	2:L:77:GLY:N[12_545]	1.58	0.62
3:Y:253:ILE:N	3:Y:254:SER:N[12_555]	1.60	0.60
3:Y:382:GLU:OE2	3:Y:433:HIS:CD2[12_555]	1.60	0.60
3:J:436:TYR:CD1	3:X:436:TYR:CE1[12_545]	1.61	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:142:SER:CB	3:Y:318:GLU:OE2[8_555]	1.62	0.58
3:N:436:TYR:CD1	3:P:436:TYR:CD1[6_445]	1.62	0.58
3:N:433:HIS:CD2	3:P:382:GLU:OE2[6_445]	1.65	0.55
3:N:253:ILE:C	3:P:253:ILE:CG2[6_445]	1.65	0.55
3:N:253:ILE:CG1	3:P:252:MET:O[6_445]	1.66	0.54
3:J:252:MET:C	3:X:253:ILE:CD1[12_545]	1.67	0.53
3:X:285:HIS:CB	2:L:18:THR:OG1[12_545]	1.67	0.53
3:J:310:HIS:CE1	3:X:253:ILE:CG2[12_545]	1.68	0.52
3:J:253:ILE:CB	3:X:252:MET:C[12_545]	1.69	0.51
2:B:18:THR:CB	3:J:285:HIS:CG[12_545]	1.69	0.51
2:B:18:THR:N	3:J:285:HIS:CD2[12_545]	1.71	0.49
3:J:380:GLU:OE1	3:X:433:HIS:NE2[12_545]	1.71	0.49
3:X:285:HIS:ND1	2:L:18:THR:CB[12_545]	1.71	0.49
3:Y:253:ILE:N	3:Y:253:ILE:CA[12_555]	1.71	0.49
3:N:253:ILE:CA	3:P:253:ILE:CB[6_445]	1.72	0.48
3:J:253:ILE:CA	3:X:253:ILE:N[12_545]	1.72	0.48
2:B:18:THR:C	3:J:285:HIS:CE1[12_545]	1.73	0.47
3:N:253:ILE:CA	3:P:253:ILE:CG2[6_445]	1.73	0.47
3:O:253:ILE:C	3:O:253:ILE:CB[10_444]	1.73	0.47
3:J:436:TYR:CD1	3:X:436:TYR:CD1[12_545]	1.74	0.46
3:O:253:ILE:C	3:O:253:ILE:CD1[10_444]	1.75	0.45
3:N:253:ILE:CG2	3:P:252:MET:O[6_445]	1.75	0.45
3:Y:252:MET:O	3:Y:253:ILE:CD1[12_555]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CB[10_444]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CG1[10_444]	1.75	0.45
3:N:253:ILE:O	3:P:253:ILE:CG2[6_445]	1.76	0.44
3:N:253:ILE:CD1	3:P:252:MET:O[6_445]	1.77	0.43
3:X:285:HIS:ND1	2:L:18:THR:CA[12_545]	1.77	0.43
3:X:284:VAL:CB	2:L:18:THR:CG2[12_545]	1.78	0.42
3:Y:253:ILE:CA	3:Y:254:SER:N[12_555]	1.78	0.42
3:X:281:GLY:O	2:L:20:THR:N[12_545]	1.78	0.42
2:B:18:THR:CB	3:J:285:HIS:ND1[12_545]	1.79	0.41
3:Y:252:MET:O	3:Y:253:ILE:CB[12_555]	1.79	0.41
1:D:143:GLY:C	3:Y:280:ASP:CG[8_555]	1.80	0.40
3:J:253:ILE:CG2	3:X:310:HIS:NE2[12_545]	1.80	0.40
2:B:18:THR:N	3:J:285:HIS:CE1[12_545]	1.81	0.39
3:J:253:ILE:C	3:X:253:ILE:CG1[12_545]	1.83	0.37
3:J:253:ILE:CG1	3:X:253:ILE:CA[12_545]	1.84	0.36
2:B:18:THR:O	3:J:285:HIS:ND1[12_545]	1.84	0.36
3:X:285:HIS:N	2:L:18:THR:CB[12_545]	1.84	0.36
2:B:18:THR:CB	3:J:285:HIS:CD2[12_545]	1.85	0.35
3:N:253:ILE:CB	3:P:252:MET:C[6_445]	1.85	0.35

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:N:253:ILE:CG2	3:P:253:ILE:N[6_445]	1.86	0.34
3:N:310:HIS:NE2	3:P:253:ILE:CB[6_445]	1.86	0.34
3:Y:253:ILE:N	3:Y:253:ILE:C[12_555]	1.87	0.33
3:N:433:HIS:CB	3:P:382:GLU:OE2[6_445]	1.87	0.33
2:B:18:THR:CA	3:J:285:HIS:CD2[12_545]	1.89	0.31
2:B:18:THR:CG2	3:J:284:VAL:CG1[12_545]	1.90	0.30
3:J:253:ILE:CG2	3:X:253:ILE:CA[12_545]	1.91	0.29
3:Y:253:ILE:C	3:Y:253:ILE:CG2[12_555]	1.91	0.29
3:Y:253:ILE:O	3:Y:253:ILE:CB[12_555]	1.92	0.28
3:Y:253:ILE:CA	3:Y:253:ILE:O[12_555]	1.93	0.27
3:N:253:ILE:CG2	3:P:254:SER:N[6_445]	1.93	0.27
3:N:310:HIS:NE2	3:P:253:ILE:CG1[6_445]	1.93	0.27
3:J:253:ILE:N	3:X:253:ILE:N[12_545]	1.93	0.27
3:Y:436:TYR:CD1	3:Y:436:TYR:CE1[12_555]	1.93	0.27
1:D:143:GLY:C	3:Y:280:ASP:OD1[8_555]	1.95	0.25
3:X:283:GLN:CA	2:L:18:THR:O[12_545]	1.96	0.24
3:N:253:ILE:CD1	3:P:249:ASP:O[6_445]	1.96	0.24
3:O:253:ILE:N	3:O:253:ILE:CD1[10_444]	1.97	0.23
3:X:285:HIS:N	2:L:18:THR:OG1[12_545]	1.97	0.23
3:Y:253:ILE:CA	3:Y:253:ILE:CB[12_555]	1.97	0.23
2:B:18:THR:N	3:J:285:HIS:NE2[12_545]	1.98	0.22
1:D:141:THR:CG2	3:Y:340:LYS:NZ[8_555]	1.99	0.21
3:Y:253:ILE:O	3:Y:253:ILE:CG2[12_555]	2.00	0.20
2:B:18:THR:OG1	3:J:285:HIS:NE2[12_545]	2.00	0.20
3:J:252:MET:SD	3:X:434:ASN:ND2[12_545]	2.00	0.20
3:N:253:ILE:CG2	3:P:252:MET:C[6_445]	2.01	0.19
2:B:18:THR:CB	3:J:285:HIS:CE1[12_545]	2.01	0.19
3:N:253:ILE:CB	3:P:252:MET:O[6_445]	2.01	0.19
2:B:18:THR:OG1	3:J:285:HIS:CG[12_545]	2.03	0.17
3:O:253:ILE:CG2	3:O:253:ILE:CG2[10_444]	2.03	0.17
2:B:18:THR:CB	3:J:285:HIS:NE2[12_545]	2.04	0.16
3:N:253:ILE:CG1	3:P:253:ILE:N[6_445]	2.04	0.16
3:J:253:ILE:CD1	3:X:252:MET:CA[12_545]	2.04	0.16
3:O:252:MET:CE	3:O:434:ASN:ND2[10_444]	2.04	0.16
3:O:253:ILE:CB	3:O:253:ILE:CG2[10_444]	2.05	0.15
3:X:285:HIS:CE1	2:L:77:GLY:N[12_545]	2.06	0.14
3:J:436:TYR:CE1	3:X:436:TYR:CD1[12_545]	2.06	0.14
3:X:281:GLY:O	2:L:20:THR:CB[12_545]	2.06	0.14
3:X:285:HIS:CA	2:L:18:THR:OG1[12_545]	2.07	0.13
3:N:253:ILE:CG2	3:P:253:ILE:O[6_445]	2.07	0.13
3:J:253:ILE:N	3:X:253:ILE:CB[12_545]	2.08	0.12
1:D:142:SER:CA	3:Y:318:GLU:OE2[8_555]	2.08	0.12

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:J:310:HIS:CD2	3:X:253:ILE:CG2[12_545]	2.08	0.12
3:Y:249:ASP:O	3:Y:253:ILE:CD1[12_555]	2.09	0.11
3:X:285:HIS:NE2	2:L:76:SER:C[12_545]	2.09	0.11
3:N:382:GLU:OE2	3:P:433:HIS:CB[6_445]	2.10	0.10
2:B:17:ASP:O	3:J:285:HIS:NE2[12_545]	2.10	0.10
3:J:253:ILE:CG1	3:X:252:MET:CA[12_545]	2.10	0.10
3:J:436:TYR:CE1	3:X:436:TYR:CE1[12_545]	2.11	0.09
3:O:253:ILE:CB	3:O:253:ILE:CG1[10_444]	2.11	0.09
3:O:253:ILE:CA	3:O:253:ILE:CA[10_444]	2.11	0.09
3:J:253:ILE:CG2	3:X:310:HIS:CD2[12_545]	2.12	0.08
3:J:380:GLU:OE1	3:X:433:HIS:CE1[12_545]	2.12	0.08
3:N:380:GLU:CD	3:P:433:HIS:NE2[6_445]	2.14	0.06
2:G:50:LYS:NZ	1:H:103:ARG:C[8_445]	2.15	0.05
2:G:50:LYS:NZ	1:H:103:ARG:CA[8_445]	2.16	0.04
3:N:436:TYR:CE1	3:P:436:TYR:O[6_445]	2.17	0.03
3:Y:382:GLU:CD	3:Y:433:HIS:CD2[12_555]	2.17	0.03
3:J:253:ILE:CB	3:X:252:MET:O[12_545]	2.18	0.02
3:X:284:VAL:CA	2:L:18:THR:CG2[12_545]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/243 (85%)	184 (89%)	19 (9%)	4 (2%)	12	68
1	D	204/243 (84%)	185 (91%)	15 (7%)	4 (2%)	11	67
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	16	73
1	H	207/243 (85%)	187 (90%)	16 (8%)	4 (2%)	12	68
1	I	204/243 (84%)	182 (89%)	17 (8%)	5 (2%)	9	61
1	M	204/243 (84%)	186 (91%)	13 (6%)	5 (2%)	9	61
2	B	209/213 (98%)	187 (90%)	21 (10%)	1 (0%)	38	88
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	38	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	38	88
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	38	88
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	38	88
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	22	80
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	3	41
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	43
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	3	41
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	43
3	X	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	3	41
3	Y	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	3	43
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	8	60

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	A	141	THR
1	A	223	PRO
1	D	136	PRO
1	D	140	SER
1	D	142	SER
1	E	141	THR
1	I	136	PRO
1	I	140	SER
1	I	142	SER
3	J	283	GLN
3	J	287	ALA
3	J	289	THR
3	J	433	HIS
3	N	298	SER
3	N	301	ARG
3	X	283	GLN
3	X	287	ALA
3	X	289	THR
3	X	433	HIS
3	Y	298	SER
3	Y	301	ARG
1	H	138	SER

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Mol	Chain	Res	Type
1	H	140	SER
1	H	141	THR
1	M	136	PRO
1	M	140	SER
1	M	142	SER
1	M	165	ASN
3	O	283	GLN
3	O	287	ALA
3	O	289	THR
3	O	433	HIS
3	P	298	SER
3	P	301	ARG
1	E	142	SER
2	F	110	VAL
2	G	110	VAL
1	I	165	ASN
3	J	267	SER
3	J	298	SER
3	N	271	PRO
3	X	267	SER
3	X	298	SER
3	Y	271	PRO
1	H	201	THR
3	O	267	SER
3	O	298	SER
3	P	271	PRO
3	J	293	GLU
3	N	282	VAL
3	N	291	PRO
3	N	293	GLU
3	X	293	GLU
3	Y	282	VAL
3	Y	291	PRO
3	Y	293	GLU
2	K	110	VAL
3	O	293	GLU
3	P	282	VAL
3	P	291	PRO
3	P	293	GLU
2	B	110	VAL
2	C	110	VAL
3	J	286	ASN

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Mol	Chain	Res	Type
3	J	358	MET
3	J	385	GLY
3	N	283	GLN
3	N	295	GLN
3	X	286	ASN
3	X	358	MET
3	X	385	GLY
3	Y	283	GLN
3	Y	295	GLN
3	O	286	ASN
3	O	358	MET
3	O	385	GLY
3	P	283	GLN
3	P	295	GLN
1	A	201	THR
1	E	136	PRO
1	I	143	GLY
3	N	336	ILE
3	Y	336	ILE
2	L	110	VAL
2	L	121	SER
3	P	327	ALA
3	P	336	ILE
3	N	327	ALA
3	Y	327	ALA
1	D	143	GLY
3	J	290	LYS
3	X	290	LYS
3	O	290	LYS
1	M	143	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/205 (88%)	163 (91%)	17 (9%)	13	53
1	D	180/205 (88%)	162 (90%)	18 (10%)	11	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	180/205 (88%)	162 (90%)	18 (10%)	11	50
1	H	180/205 (88%)	165 (92%)	15 (8%)	16	60
1	I	180/205 (88%)	165 (92%)	15 (8%)	16	60
1	M	180/205 (88%)	163 (91%)	17 (9%)	13	53
2	B	182/184 (99%)	164 (90%)	18 (10%)	11	50
2	C	182/184 (99%)	165 (91%)	17 (9%)	13	54
2	F	182/184 (99%)	164 (90%)	18 (10%)	11	50
2	G	182/184 (99%)	164 (90%)	18 (10%)	11	50
2	K	182/184 (99%)	163 (90%)	19 (10%)	10	48
2	L	182/184 (99%)	164 (90%)	18 (10%)	11	50
3	J	193/196 (98%)	187 (97%)	6 (3%)	52	88
3	N	192/196 (98%)	180 (94%)	12 (6%)	25	72
3	O	193/196 (98%)	187 (97%)	6 (3%)	52	88
3	P	192/196 (98%)	180 (94%)	12 (6%)	25	72
3	X	193/196 (98%)	187 (97%)	6 (3%)	52	88
3	Y	192/196 (98%)	180 (94%)	12 (6%)	25	72
All	All	3327/3510 (95%)	3065 (92%)	262 (8%)	18	62

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	50	SER
1	A	55	SER
1	A	56	THR
1	A	57	TYR
1	A	98	ARG
1	A	101	SER
1	A	148	LEU
1	A	156	PHE
1	A	161	THR
1	A	163	SER
1	A	185	LEU
1	A	196	SER
1	A	206	CYS
1	A	211	LYS

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Mol	Chain	Res	Type
1	A	221	VAL
1	A	224	LYS
2	B	7	SER
2	B	20	THR
2	B	33	LEU
2	B	39	LYS
2	B	56	THR
2	B	78	LEU
2	B	108	ARG
2	B	122	ASP
2	B	123	GLU
2	B	132	VAL
2	B	134	CYS
2	B	142	ARG
2	B	143	GLU
2	B	152	ASN
2	B	169	LYS
2	B	191	VAL
2	B	197	THR
2	B	201	LEU
2	C	7	SER
2	C	20	THR
2	C	33	LEU
2	C	39	LYS
2	C	56	THR
2	C	78	LEU
2	C	108	ARG
2	C	122	ASP
2	C	123	GLU
2	C	132	VAL
2	C	134	CYS
2	C	142	ARG
2	C	152	ASN
2	C	169	LYS
2	C	191	VAL
2	C	197	THR
2	C	201	LEU
1	D	13	LYS
1	D	50	SER
1	D	55	SER
1	D	56	THR
1	D	57	TYR

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Mol	Chain	Res	Type
1	D	75	LEU
1	D	98	ARG
1	D	101	SER
1	D	148	LEU
1	D	156	PHE
1	D	161	THR
1	D	163	SER
1	D	185	LEU
1	D	196	SER
1	D	202	GLN
1	D	206	CYS
1	D	211	LYS
1	D	224	LYS
1	E	13	LYS
1	E	50	SER
1	E	55	SER
1	E	56	THR
1	E	57	TYR
1	E	75	LEU
1	E	98	ARG
1	E	101	SER
1	E	102	ASP
1	E	139	LYS
1	E	141	THR
1	E	148	LEU
1	E	156	PHE
1	E	161	THR
1	E	185	LEU
1	E	196	SER
1	E	206	CYS
1	E	211	LYS
2	F	7	SER
2	F	20	THR
2	F	33	LEU
2	F	39	LYS
2	F	56	THR
2	F	78	LEU
2	F	108	ARG
2	F	122	ASP
2	F	123	GLU
2	F	132	VAL
2	F	134	CYS

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Mol	Chain	Res	Type
2	F	142	ARG
2	F	143	GLU
2	F	152	ASN
2	F	169	LYS
2	F	191	VAL
2	F	197	THR
2	F	201	LEU
2	G	7	SER
2	G	20	THR
2	G	33	LEU
2	G	39	LYS
2	G	56	THR
2	G	78	LEU
2	G	108	ARG
2	G	122	ASP
2	G	123	GLU
2	G	132	VAL
2	G	134	CYS
2	G	135	LEU
2	G	142	ARG
2	G	152	ASN
2	G	169	LYS
2	G	191	VAL
2	G	197	THR
2	G	201	LEU
1	I	13	LYS
1	I	50	SER
1	I	55	SER
1	I	56	THR
1	I	57	TYR
1	I	75	LEU
1	I	98	ARG
1	I	101	SER
1	I	148	LEU
1	I	156	PHE
1	I	161	THR
1	I	185	LEU
1	I	196	SER
1	I	206	CYS
1	I	211	LYS
3	J	282	VAL
3	J	292	ARG

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Mol	Chain	Res	Type
3	J	406	LEU
3	J	413	ASP
3	J	436	TYR
3	J	441	LEU
3	N	255	ARG
3	N	260	THR
3	N	278	TYR
3	N	288	LYS
3	N	291	PRO
3	N	296	TYR
3	N	311	GLN
3	N	370	LYS
3	N	394	THR
3	N	399	ASP
3	N	406	LEU
3	N	441	LEU
3	X	282	VAL
3	X	292	ARG
3	X	406	LEU
3	X	413	ASP
3	X	436	TYR
3	X	441	LEU
3	Y	255	ARG
3	Y	260	THR
3	Y	278	TYR
3	Y	288	LYS
3	Y	291	PRO
3	Y	296	TYR
3	Y	311	GLN
3	Y	370	LYS
3	Y	394	THR
3	Y	399	ASP
3	Y	406	LEU
3	Y	441	LEU
1	H	13	LYS
1	H	50	SER
1	H	55	SER
1	H	56	THR
1	H	57	TYR
1	H	98	ARG
1	H	101	SER
1	H	148	LEU

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Mol	Chain	Res	Type
1	H	156	PHE
1	H	161	THR
1	H	185	LEU
1	H	196	SER
1	H	206	CYS
1	H	211	LYS
1	H	224	LYS
2	K	7	SER
2	K	20	THR
2	K	33	LEU
2	K	39	LYS
2	K	56	THR
2	K	78	LEU
2	K	108	ARG
2	K	122	ASP
2	K	123	GLU
2	K	132	VAL
2	K	134	CYS
2	K	135	LEU
2	K	142	ARG
2	K	143	GLU
2	K	152	ASN
2	K	169	LYS
2	K	191	VAL
2	K	197	THR
2	K	201	LEU
2	L	7	SER
2	L	9	SER
2	L	20	THR
2	L	33	LEU
2	L	39	LYS
2	L	56	THR
2	L	78	LEU
2	L	108	ARG
2	L	122	ASP
2	L	123	GLU
2	L	132	VAL
2	L	134	CYS
2	L	142	ARG
2	L	152	ASN
2	L	169	LYS
2	L	191	VAL

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Mol	Chain	Res	Type
2	L	197	THR
2	L	201	LEU
1	M	13	LYS
1	M	50	SER
1	M	55	SER
1	M	56	THR
1	M	57	TYR
1	M	98	ARG
1	M	101	SER
1	M	142	SER
1	M	148	LEU
1	M	156	PHE
1	M	161	THR
1	M	163	SER
1	M	185	LEU
1	M	196	SER
1	M	206	CYS
1	M	211	LYS
1	M	222	GLU
3	O	282	VAL
3	O	292	ARG
3	O	406	LEU
3	O	413	ASP
3	O	436	TYR
3	O	441	LEU
3	P	255	ARG
3	P	260	THR
3	P	278	TYR
3	P	288	LYS
3	P	291	PRO
3	P	296	TYR
3	P	311	GLN
3	P	370	LYS
3	P	394	THR
3	P	399	ASP
3	P	406	LEU
3	P	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	6	GLN

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Mol	Chain	Res	Type
2	B	90	HIS
2	C	87	HIS
2	C	90	HIS
2	F	90	HIS
2	G	6	GLN
2	G	38	GLN
2	G	87	HIS
2	G	90	HIS
3	J	272	GLN
3	J	283	GLN
3	J	311	GLN
3	J	325	ASN
3	J	347	GLN
3	J	361	ASN
3	J	390	ASN
3	J	418	GLN
3	J	419	GLN
3	J	421	ASN
3	J	429	HIS
3	N	272	GLN
3	N	276	ASN
3	N	283	GLN
3	N	286	ASN
3	N	311	GLN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	389	ASN
3	N	390	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN
3	X	272	GLN
3	X	283	GLN
3	X	311	GLN
3	X	325	ASN
3	X	347	GLN
3	X	361	ASN
3	X	390	ASN
3	X	418	GLN

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Mol	Chain	Res	Type
3	X	419	GLN
3	X	421	ASN
3	X	429	HIS
3	Y	272	GLN
3	Y	276	ASN
3	Y	283	GLN
3	Y	286	ASN
3	Y	311	GLN
3	Y	312	ASN
3	Y	325	ASN
3	Y	342	GLN
3	Y	361	ASN
3	Y	389	ASN
3	Y	390	ASN
3	Y	419	GLN
3	Y	429	HIS
3	Y	434	ASN
3	Y	438	GLN
2	K	87	HIS
2	K	90	HIS
2	K	137	ASN
2	L	90	HIS
2	L	199	GLN
3	O	272	GLN
3	O	283	GLN
3	O	311	GLN
3	O	325	ASN
3	O	347	GLN
3	O	361	ASN
3	O	390	ASN
3	O	418	GLN
3	O	419	GLN
3	O	421	ASN
3	O	429	HIS
3	P	272	GLN
3	P	276	ASN
3	P	283	GLN
3	P	286	ASN
3	P	311	GLN
3	P	312	ASN
3	P	325	ASN
3	P	342	GLN

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Mol	Chain	Res	Type
3	P	361	ASN
3	P	389	ASN
3	P	390	ASN
3	P	419	GLN
3	P	429	HIS
3	P	434	ASN
3	P	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	209/243 (86%)	0.74	13 (6%) 20 26	114, 118, 126, 134	0
1	D	207/243 (85%)	0.66	8 (3%) 37 36	113, 118, 125, 139	0
1	E	209/243 (86%)	1.12	34 (16%) 2 9	178, 182, 190, 198	0
1	H	209/243 (86%)	0.64	8 (3%) 38 37	96, 100, 107, 115	0
1	I	207/243 (85%)	0.96	26 (12%) 4 12	177, 182, 189, 203	0
1	M	207/243 (85%)	0.57	6 (2%) 49 44	94, 100, 107, 121	0
2	B	211/213 (99%)	0.52	6 (2%) 50 45	113, 118, 124, 139	0
2	C	211/213 (99%)	0.65	14 (6%) 18 25	113, 118, 123, 143	0
2	F	211/213 (99%)	1.34	47 (22%) 1 6	177, 182, 188, 203	0
2	G	211/213 (99%)	1.24	40 (18%) 2 7	177, 182, 187, 207	0
2	K	211/213 (99%)	0.72	10 (4%) 30 32	94, 100, 105, 120	0
2	L	211/213 (99%)	0.69	17 (8%) 12 20	94, 100, 105, 124	0
3	J	207/211 (98%)	1.03	22 (10%) 7 15	176, 176, 176, 176	0
3	N	206/211 (97%)	1.05	24 (11%) 5 14	179, 179, 179, 179	0
3	O	207/211 (98%)	1.39	57 (27%) 1 6	274, 274, 274, 274	0
3	P	206/211 (97%)	1.45	54 (26%) 1 6	277, 277, 277, 277	0
3	X	207/211 (98%)	0.96	26 (12%) 4 12	167, 167, 167, 167	0
3	Y	206/211 (97%)	1.04	33 (16%) 3 9	171, 171, 171, 171	0
All	All	3753/4002 (93%)	0.93	445 (11%) 5 13	94, 167, 277, 277	0

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	10.2
2	G	134	CYS	7.5
2	G	147	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
3	O	238	PRO	5.4
1	E	193	THR	5.1
3	Y	333	GLU	4.8
3	P	292	ARG	4.8
3	P	273	VAL	4.7
3	P	296	TYR	4.6
2	L	187	GLU	4.5
1	E	190	SER	4.4
3	P	330	ALA	4.4
2	F	135	LEU	4.3
2	F	116	PHE	4.3
3	Y	302	VAL	4.3
2	F	147	GLN	4.3
2	F	194	CYS	4.3
1	A	131	VAL	4.3
3	P	293	GLU	4.2
2	C	145	LYS	4.2
2	F	132	VAL	4.1
3	Y	238	PRO	4.1
3	J	321	CYS	4.1
1	E	152	VAL	4.0
3	O	332	ILE	4.0
1	E	150	CYS	4.0
2	C	197	THR	4.0
1	E	131	VAL	4.0
3	X	261	CYS	4.0
3	P	332	ILE	4.0
2	F	120	PRO	3.9
1	I	152	VAL	3.9
3	P	295	GLN	3.9
3	O	326	LYS	3.9
3	P	323	VAL	3.9
2	G	194	CYS	3.9
2	C	179	LEU	3.9
2	F	136	LEU	3.9
3	P	274	LYS	3.8
1	A	152	VAL	3.8
1	E	204	TYR	3.8
3	Y	239	SER	3.8
3	X	302	VAL	3.8
3	P	302	VAL	3.7
3	O	265	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
3	Y	332	ILE	3.7
2	G	107	LYS	3.7
1	D	152	VAL	3.7
1	I	129	PRO	3.7
1	E	161	THR	3.7
2	G	148	TRP	3.7
1	H	148	LEU	3.7
2	G	155	GLN	3.7
3	P	331	PRO	3.7
2	G	116	PHE	3.6
3	Y	240	VAL	3.6
3	J	428	MET	3.6
3	Y	301	ARG	3.5
2	F	79	GLN	3.5
3	P	244	PRO	3.5
1	E	175	THR	3.5
2	F	146	VAL	3.5
3	O	329	PRO	3.5
2	F	115	VAL	3.4
3	J	332	ILE	3.4
3	X	240	VAL	3.4
3	Y	264	VAL	3.4
3	P	294	GLN	3.4
2	G	130	ALA	3.4
3	N	394	THR	3.4
2	F	154	LEU	3.4
2	C	147	GLN	3.4
1	E	130	SER	3.4
1	I	149	GLY	3.4
3	P	407	TYR	3.4
3	Y	263	VAL	3.4
2	K	194	CYS	3.4
2	G	13	ALA	3.3
3	P	433	HIS	3.3
3	O	327	ALA	3.3
3	O	425	CYS	3.3
2	C	144	ALA	3.3
2	F	117	ILE	3.3
3	P	240	VAL	3.3
3	O	394	THR	3.3
1	E	206	CYS	3.3
2	G	154	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
3	P	301	ARG	3.2
1	D	147	ALA	3.2
2	F	119	PRO	3.2
3	O	331	PRO	3.2
3	J	240	VAL	3.2
3	Y	289	THR	3.2
3	Y	294	GLN	3.2
1	A	150	CYS	3.2
1	E	129	PRO	3.2
1	H	204	TYR	3.2
3	Y	378	ALA	3.2
1	E	208	VAL	3.1
1	E	222	GLU	3.1
1	E	188	LEU	3.1
2	F	145	LYS	3.1
1	I	147	ALA	3.1
3	Y	334	LYS	3.1
2	G	115	VAL	3.1
3	P	259	VAL	3.1
2	G	136	LEU	3.1
1	M	130	SER	3.1
2	G	146	VAL	3.1
3	O	328	LEU	3.1
2	F	77	GLY	3.1
3	P	245	PRO	3.1
2	G	153	ALA	3.1
3	O	239	SER	3.1
3	P	329	PRO	3.0
2	K	134	CYS	3.0
1	I	161	THR	3.0
3	X	321	CYS	3.0
3	O	293	GLU	3.0
2	F	199	GLN	3.0
3	O	266	VAL	3.0
2	L	186	TYR	3.0
3	P	328	LEU	3.0
3	N	338	LYS	3.0
3	O	264	VAL	3.0
2	K	192	TYR	3.0
1	E	219	LYS	3.0
1	E	178	ALA	3.0
3	O	393	THR	3.0

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Mol	Chain	Res	Type	RSRZ
3	P	238	PRO	3.0
3	O	243	PHE	3.0
3	O	318	GLU	3.0
3	P	306	LEU	3.0
3	O	319	TYR	3.0
3	P	291	PRO	3.0
3	X	263	VAL	3.0
1	D	148	LEU	3.0
3	O	378	ALA	3.0
2	G	212	GLY	2.9
1	I	148	LEU	2.9
3	Y	428	MET	2.9
2	F	175	LEU	2.9
3	O	241	PHE	2.9
2	L	88	CYS	2.9
3	P	243	PHE	2.9
3	X	334	LYS	2.9
2	G	145	LYS	2.9
2	G	113	PRO	2.9
2	G	117	ILE	2.9
3	P	297	ASN	2.9
3	P	263	VAL	2.9
1	I	96	CYS	2.9
3	P	257	PRO	2.9
1	A	112	ALA	2.9
3	X	238	PRO	2.8
3	P	324	SER	2.8
3	P	394	THR	2.8
2	F	45	LYS	2.8
3	O	251	LEU	2.8
2	C	196	VAL	2.8
2	F	113	PRO	2.8
2	F	148	TRP	2.8
2	L	211	ARG	2.8
2	F	59	PRO	2.8
3	O	261	CYS	2.8
3	O	269	GLU	2.8
3	X	241	PHE	2.8
2	G	135	LEU	2.8
3	P	285	HIS	2.8
3	J	323	VAL	2.8
3	N	339	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	182	SER	2.8
2	C	146	VAL	2.8
3	O	330	ALA	2.7
3	O	441	LEU	2.7
1	E	202	GLN	2.7
2	G	128	GLY	2.7
2	L	192	TYR	2.7
3	O	321	CYS	2.7
3	P	434	ASN	2.7
2	F	207	LYS	2.7
2	G	129	THR	2.7
1	I	200	GLY	2.7
1	A	132	PHE	2.7
3	P	262	VAL	2.7
2	F	133	VAL	2.7
3	O	260	THR	2.7
1	H	192	VAL	2.7
3	Y	300	TYR	2.7
3	P	242	LEU	2.7
3	N	329	PRO	2.7
1	H	193	THR	2.7
3	P	287	ALA	2.7
2	F	114	SER	2.7
3	X	323	VAL	2.7
3	Y	273	VAL	2.7
3	O	292	ARG	2.7
3	Y	336	ILE	2.6
1	I	208	VAL	2.6
3	Y	241	PHE	2.6
1	D	192	VAL	2.6
1	I	192	VAL	2.6
2	G	149	LYS	2.6
3	O	350	THR	2.6
2	F	144	ALA	2.6
2	F	131	SER	2.6
3	O	337	SER	2.6
2	L	195	GLU	2.6
1	A	160	VAL	2.6
2	K	4	MET	2.6
3	O	280	ASP	2.6
2	G	186	TYR	2.6
3	N	395	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	425	CYS	2.6
2	K	2	VAL	2.6
3	O	333	GLU	2.6
3	X	425	CYS	2.6
2	C	195	GLU	2.6
3	Y	425	CYS	2.6
2	F	44	PRO	2.6
3	X	287	ALA	2.6
2	F	61	ARG	2.6
2	G	207	LYS	2.6
3	X	332	ILE	2.6
3	Y	265	ASP	2.6
1	E	218	ASP	2.5
3	P	423	PHE	2.5
1	E	177	PRO	2.5
3	P	321	CYS	2.5
3	P	289	THR	2.5
1	M	131	VAL	2.5
3	X	444	SER	2.5
3	J	378	ALA	2.5
3	P	425	CYS	2.5
1	E	153	LYS	2.5
1	I	146	ALA	2.5
1	A	188	LEU	2.5
3	Y	245	PRO	2.5
1	A	130	SER	2.5
2	G	125	LEU	2.5
1	D	15	GLY	2.5
3	N	281	GLY	2.5
3	O	395	PRO	2.5
2	F	88	CYS	2.5
3	N	238	PRO	2.5
3	J	377	ILE	2.5
1	E	194	VAL	2.5
2	F	177	SER	2.5
1	M	152	VAL	2.4
3	J	238	PRO	2.4
3	J	334	LYS	2.4
3	Y	296	TYR	2.4
1	I	150	CYS	2.4
1	I	160	VAL	2.4
1	A	129	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	13	ALA	2.4
2	B	211	ARG	2.4
3	N	331	PRO	2.4
2	G	195	GLU	2.4
3	N	240	VAL	2.4
3	P	261	CYS	2.4
3	X	385	GLY	2.4
2	C	181	LEU	2.4
2	F	155	GLN	2.4
3	N	327	ALA	2.4
3	X	423	PHE	2.4
3	J	374	PRO	2.4
3	O	365	LEU	2.4
3	Y	323	VAL	2.4
3	P	250	THR	2.4
1	E	112	ALA	2.4
2	L	212	GLY	2.4
2	B	88	CYS	2.4
2	L	194	CYS	2.4
1	E	191	VAL	2.4
3	O	240	VAL	2.4
1	I	193	THR	2.4
1	H	129	PRO	2.4
1	M	188	LEU	2.4
1	E	217	VAL	2.4
3	J	350	THR	2.4
3	X	335	THR	2.4
1	E	103	ARG	2.4
3	P	288	LYS	2.4
3	J	275	PHE	2.4
2	F	130	ALA	2.4
3	Y	274	LYS	2.4
2	G	106	ILE	2.4
1	I	216	LYS	2.4
3	N	321	CYS	2.3
3	Y	331	PRO	2.3
2	L	147	GLN	2.3
3	X	428	MET	2.3
3	P	241	PHE	2.3
3	N	380	GLU	2.3
1	E	192	VAL	2.3
2	C	180	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	178	ALA	2.3
3	N	407	TYR	2.3
3	J	434	ASN	2.3
3	X	273	VAL	2.3
3	X	303	VAL	2.3
2	G	132	VAL	2.3
1	A	96	CYS	2.3
3	X	430	GLU	2.3
3	O	262	VAL	2.3
2	G	150	VAL	2.3
3	Y	259	VAL	2.3
1	A	178	ALA	2.3
2	G	131	SER	2.3
2	G	179	LEU	2.3
1	H	136	PRO	2.3
2	F	18	THR	2.3
3	O	270	ASP	2.3
3	O	428	MET	2.3
3	P	260	THR	2.3
3	X	262	VAL	2.3
1	D	193	THR	2.3
3	O	317	LYS	2.3
2	F	181	LEU	2.3
2	K	186	TYR	2.3
1	E	216	LYS	2.3
1	I	194	VAL	2.3
2	C	204	PRO	2.3
1	I	130	SER	2.3
3	X	301	ARG	2.3
3	J	376	ASP	2.3
2	L	155	GLN	2.3
3	N	393	THR	2.3
3	J	263	VAL	2.3
2	G	189	HIS	2.3
2	G	108	ARG	2.3
3	J	261	CYS	2.3
2	G	114	SER	2.3
1	I	188	LEU	2.2
3	O	374	PRO	2.2
2	F	192	TYR	2.2
3	P	442	SER	2.2
2	B	212	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	150	CYS	2.2
2	F	187	GLU	2.2
3	N	301	ARG	2.2
3	Y	288	LYS	2.2
2	G	192	TYR	2.2
3	N	319	TYR	2.2
2	F	82	ASP	2.2
3	O	273	VAL	2.2
2	F	27	GLN	2.2
3	J	333	GLU	2.2
3	P	333	GLU	2.2
2	C	115	VAL	2.2
2	G	181	LEU	2.2
3	N	333	GLU	2.2
3	O	272	GLN	2.2
2	F	43	ALA	2.2
2	F	78	LEU	2.2
3	X	304	SER	2.2
1	I	145	THR	2.2
3	J	281	GLY	2.2
2	L	204	PRO	2.2
3	O	364	SER	2.2
3	O	250	THR	2.2
2	L	145	LYS	2.2
3	O	385	GLY	2.2
3	N	334	LYS	2.2
1	I	203	THR	2.2
1	E	147	ALA	2.2
1	E	209	ASN	2.2
2	F	186	TYR	2.2
3	P	303	VAL	2.2
2	F	137	ASN	2.2
2	F	25	ALA	2.2
2	L	196	VAL	2.2
3	O	255	ARG	2.2
3	P	299	THR	2.2
3	P	307	THR	2.2
2	F	179	LEU	2.2
1	I	217	VAL	2.2
2	G	12	SER	2.2
3	J	339	ALA	2.2
3	O	430	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	116	PHE	2.2
3	Y	335	THR	2.2
3	X	331	PRO	2.1
3	O	271	PRO	2.1
2	L	134	CYS	2.1
3	O	377	ILE	2.1
1	I	179	VAL	2.1
1	H	194	VAL	2.1
3	P	379	VAL	2.1
2	C	131	SER	2.1
2	K	187	GLU	2.1
1	I	204	TYR	2.1
1	D	129	PRO	2.1
3	O	302	VAL	2.1
3	P	239	SER	2.1
3	Y	262	VAL	2.1
3	J	319	TYR	2.1
3	N	423	PHE	2.1
2	L	132	VAL	2.1
3	O	353	PRO	2.1
3	P	334	LYS	2.1
2	L	144	ALA	2.1
3	X	377	ILE	2.1
2	K	116	PHE	2.1
3	O	340	LYS	2.1
2	F	193	ALA	2.1
3	O	301	ARG	2.1
2	F	19	ILE	2.1
3	O	257	PRO	2.1
3	Y	306	LEU	2.1
3	N	439	LYS	2.1
1	E	220	LYS	2.1
2	B	93	GLY	2.1
2	K	147	GLN	2.1
1	A	175	THR	2.1
3	J	241	PHE	2.1
3	P	441	LEU	2.1
1	D	96	CYS	2.1
3	O	323	VAL	2.1
3	O	423	PHE	2.1
2	L	51	ALA	2.1
3	Y	261	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
3	X	324	SER	2.1
2	G	120	PRO	2.1
1	E	145	THR	2.1
1	M	129	PRO	2.1
3	P	298	SER	2.0
1	A	161	THR	2.0
1	I	22	CYS	2.0
3	Y	293	GLU	2.0
2	B	119	PRO	2.0
3	N	265	ASP	2.0
3	Y	295	GLN	2.0
1	E	215	THR	2.0
2	B	192	TYR	2.0
1	E	174	HIS	2.0
1	E	203	THR	2.0
3	O	418	GLN	2.0
2	G	211	ARG	2.0
3	N	367	CYS	2.0
3	J	291	PRO	2.0
1	H	147	ALA	2.0
2	G	206	THR	2.0
3	N	440	SER	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.