



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 17, 2024 – 02:50 PM EST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

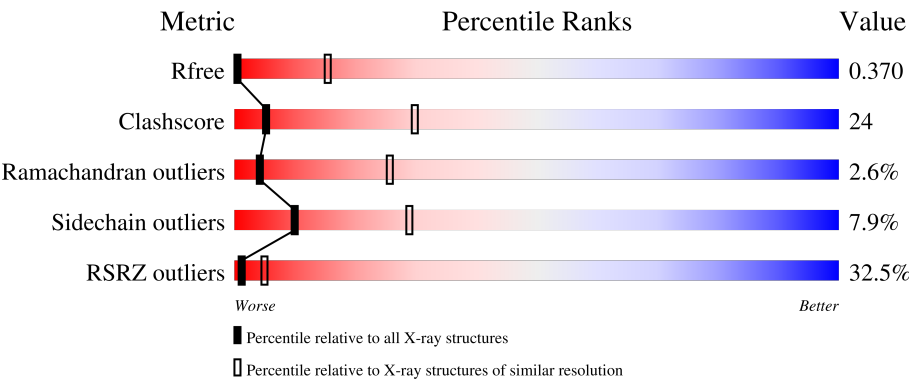
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance i

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

The reported resolution of this entry is 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}	164625	1107 (10.00-4.00)
Clashscore	180529	1146 (10.00-4.00)
Ramachandran outliers	177936	1014 (10.00-4.00)
Sidechain outliers	177891	1035 (10.00-3.96)
RSRZ outliers	164620	1102 (10.00-4.00)

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

Mol	Chain	Length	Quality of chain
1	A	243	<div><div>21%</div><div>53%33%•12%</div></div>
1	D	243	<div><div>21%</div><div>50%33%5%12%</div></div>
1	E	243	<div><div>35%</div><div>50%33%5%12%</div></div>
1	H	243	<div><div>19%</div><div>50%35%•12%</div></div>
1	I	243	<div><div>24%</div><div>50%36%•12%</div></div>

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Mol	Chain	Length	Quality of chain
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	
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 hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 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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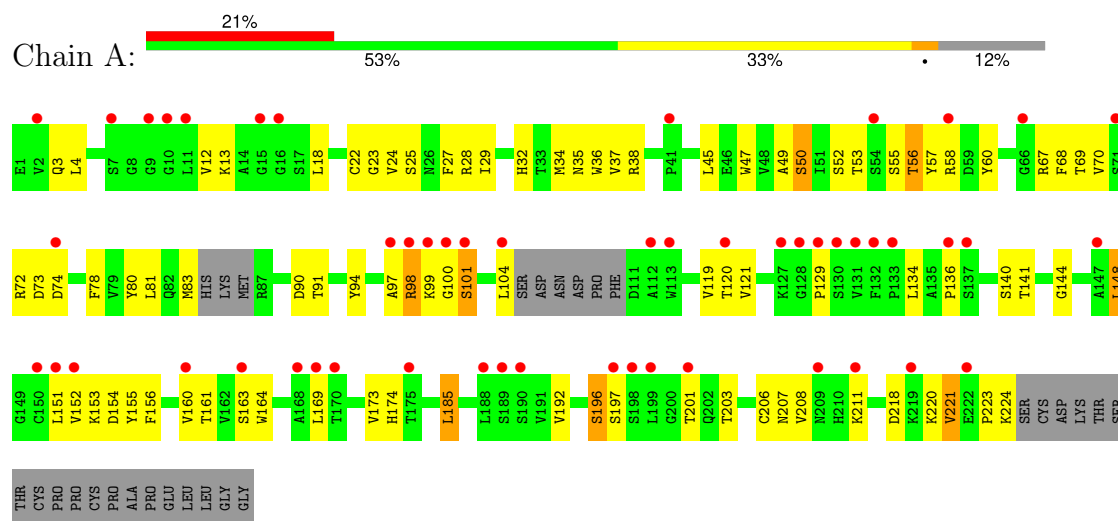
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Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	conflict	UNP Q6PYX1
O	448	GLY	-	expression tag	UNP Q6PYX1
P	272	GLN	GLU	conflict	UNP Q6PYX1
P	283	GLN	GLU	conflict	UNP Q6PYX1
P	294	GLN	GLU	conflict	UNP Q6PYX1
P	312	ASN	ASP	conflict	UNP Q6PYX1
P	315	ASP	ASN	conflict	UNP Q6PYX1
P	448	GLY	-	expression tag	UNP Q6PYX1

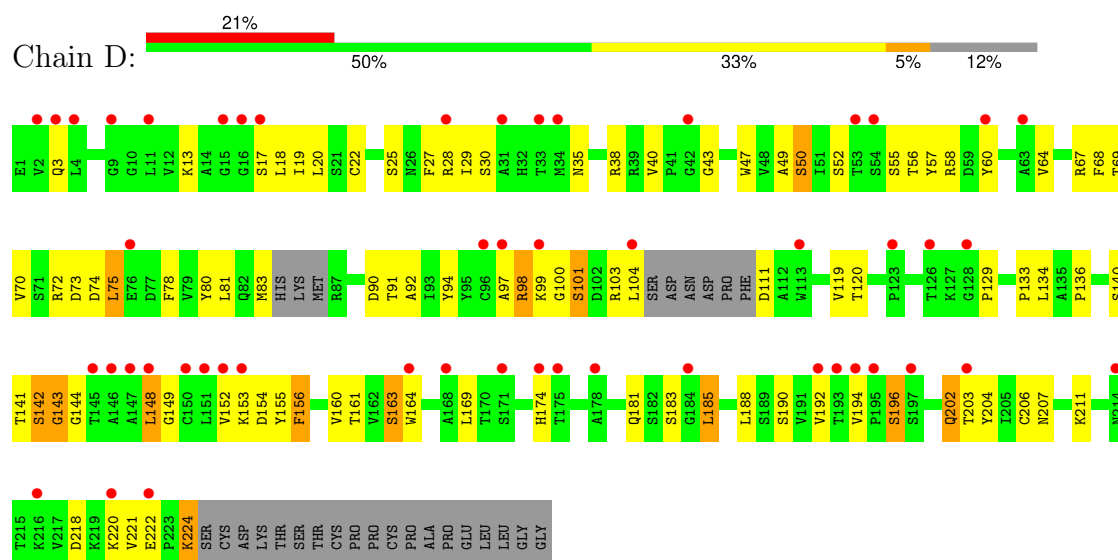
3 Residue-property plots [i](#)

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

• Molecule 1: 2G12 IgG dimer heavy chain

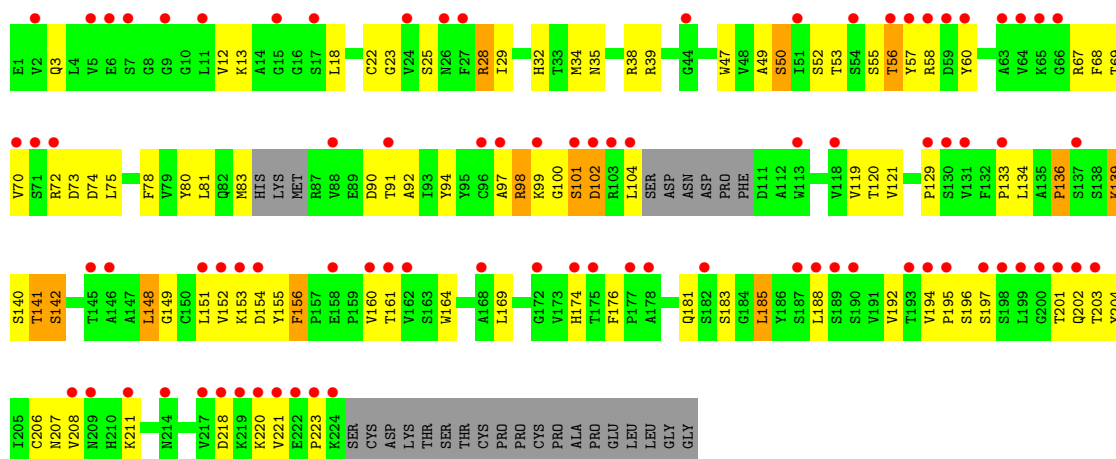


• Molecule 1: 2G12 IgG dimer heavy chain

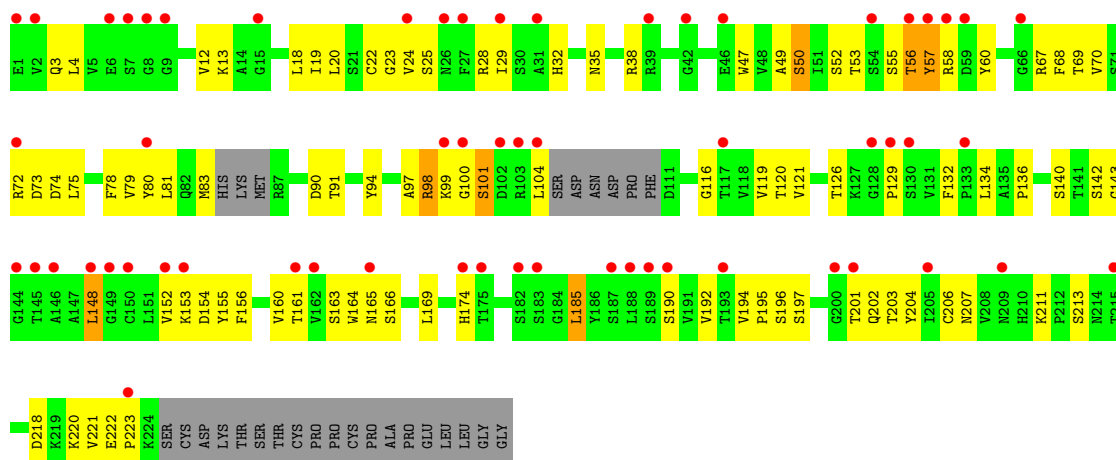


• Molecule 1: 2G12 IgG dimer heavy chain

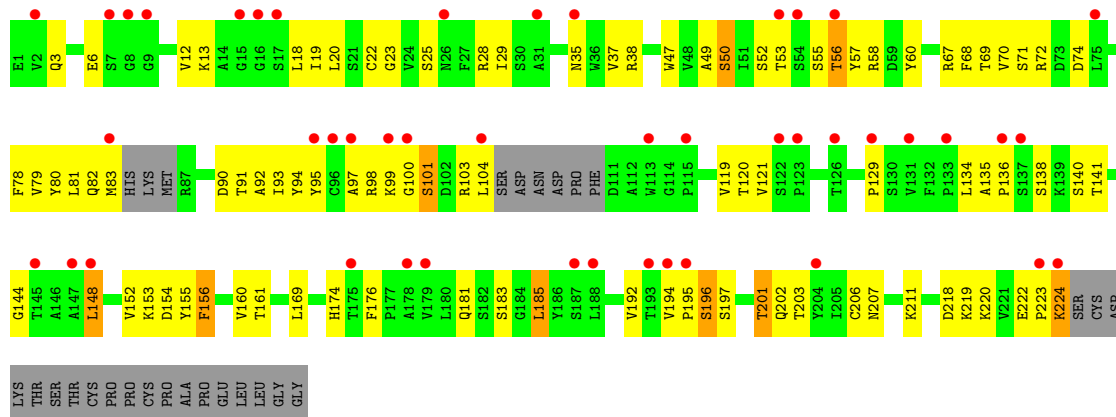




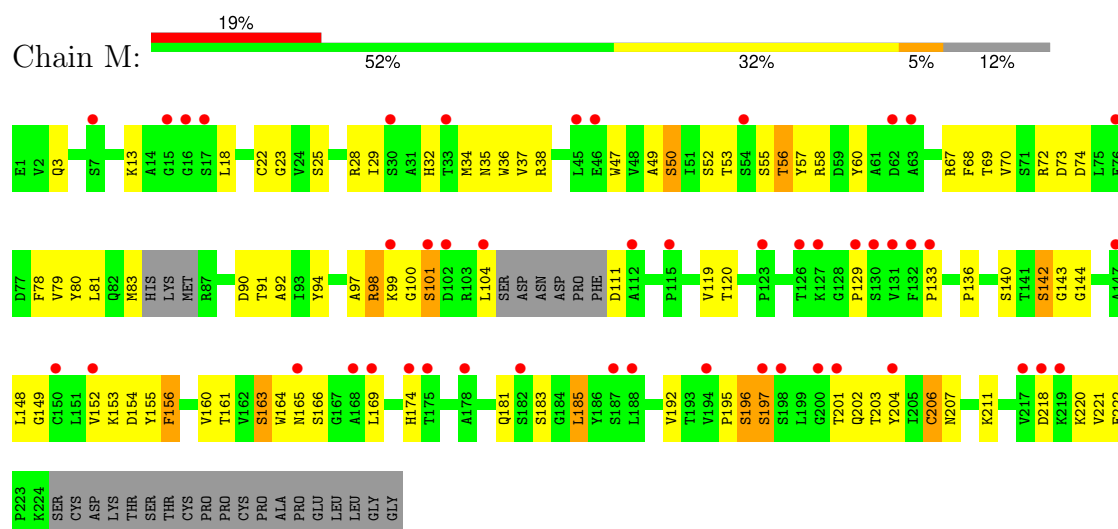
• Molecule 1: 2G12 IgG dimer heavy chain

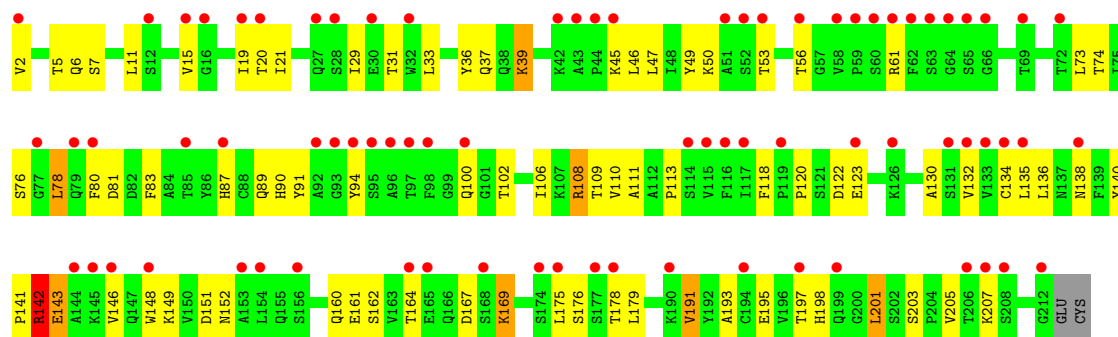


• Molecule 1: 2G12 IgG dimer heavy chain

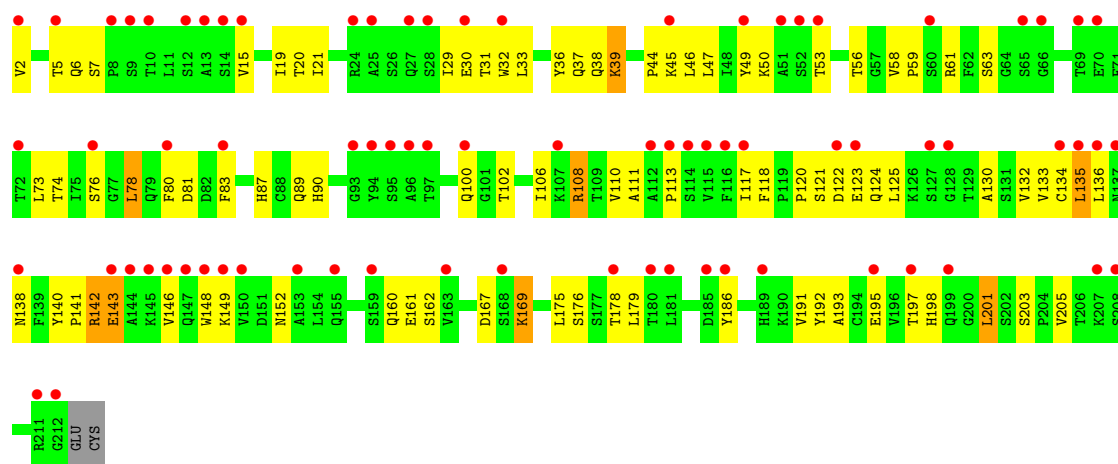


• Molecule 1: 2G12 IgG dimer heavy chain

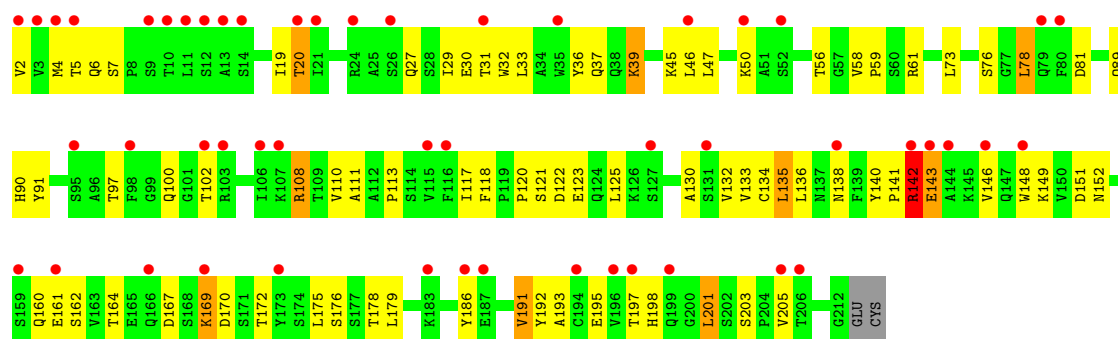




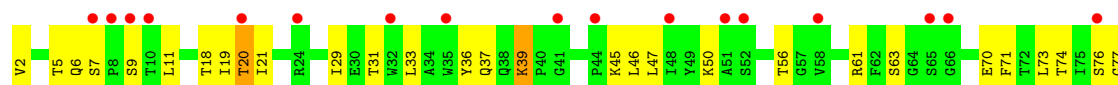
- Molecule 2: 2G12 IgG dimer light chain

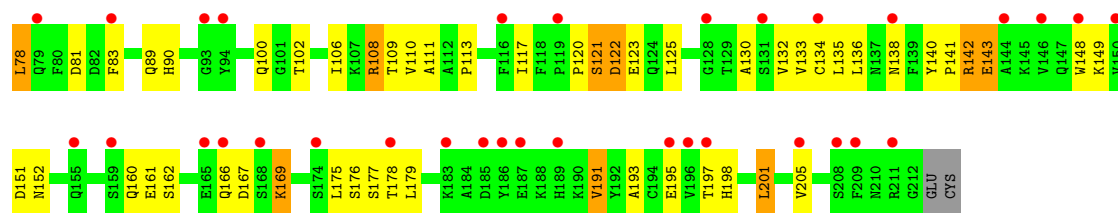


- Molecule 2: 2G12 IgG dimer light chain

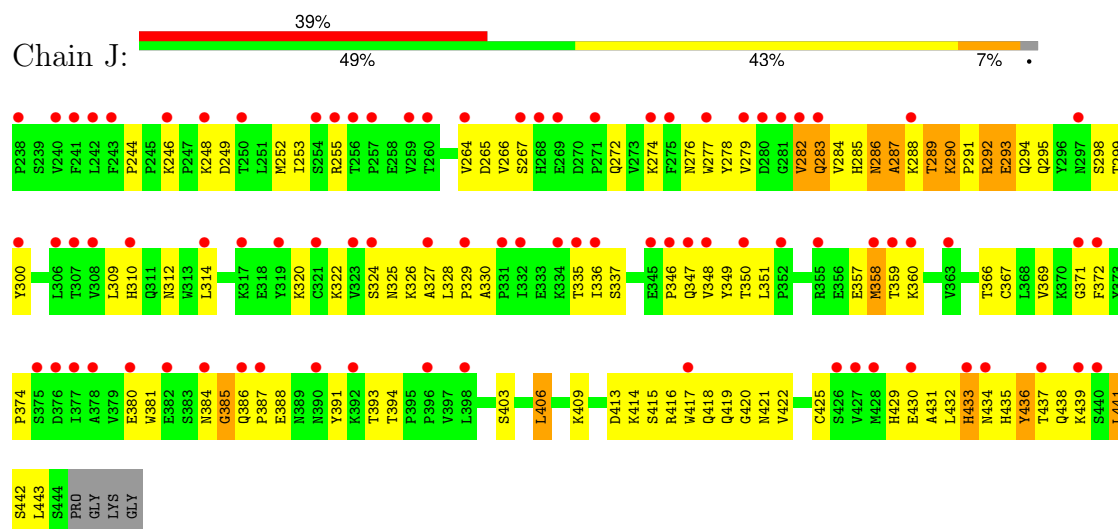


- Molecule 2: 2G12 IgG dimer light chain

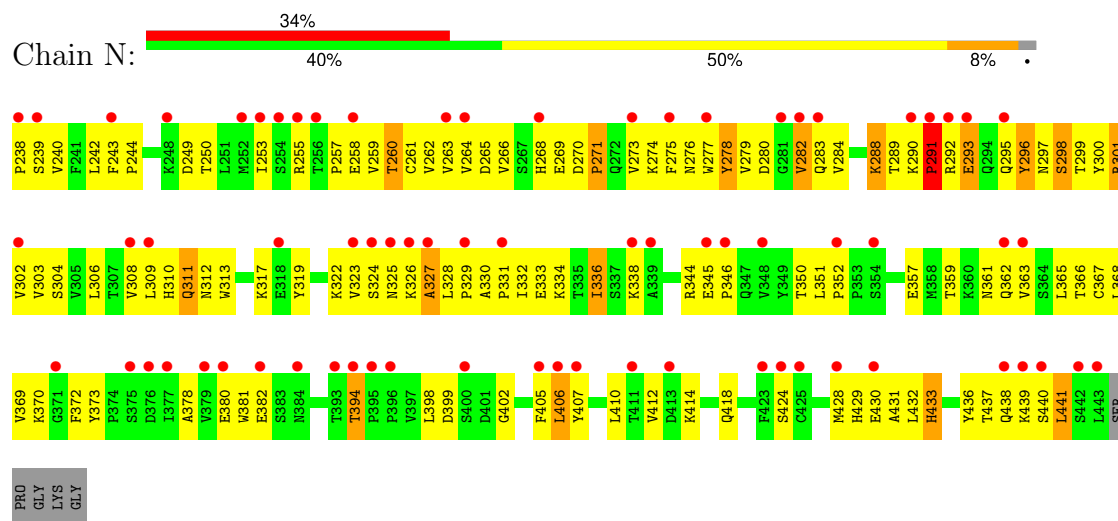




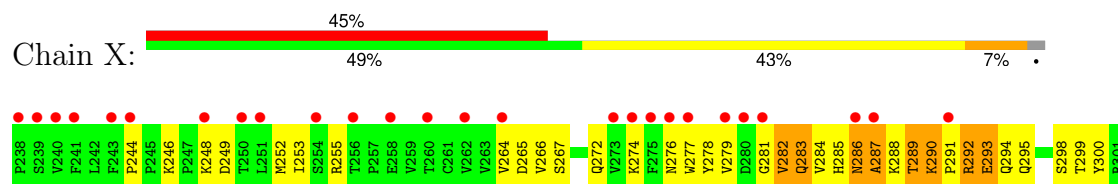
• Molecule 3: Hepatitis B virus receptor binding protein

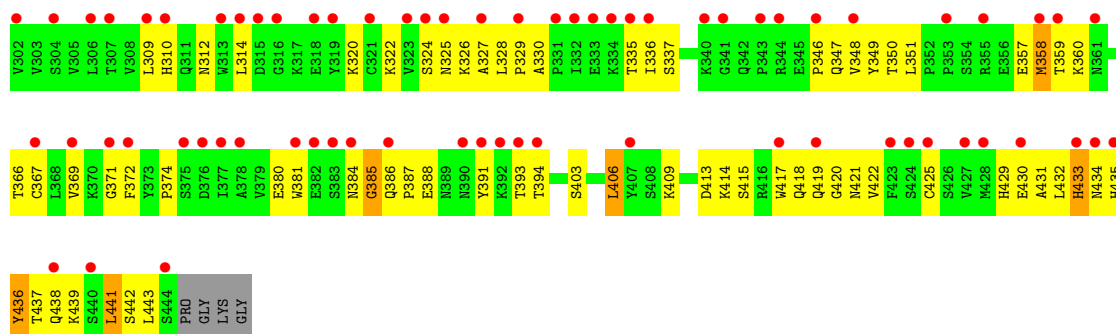


• Molecule 3: Hepatitis B virus receptor binding protein

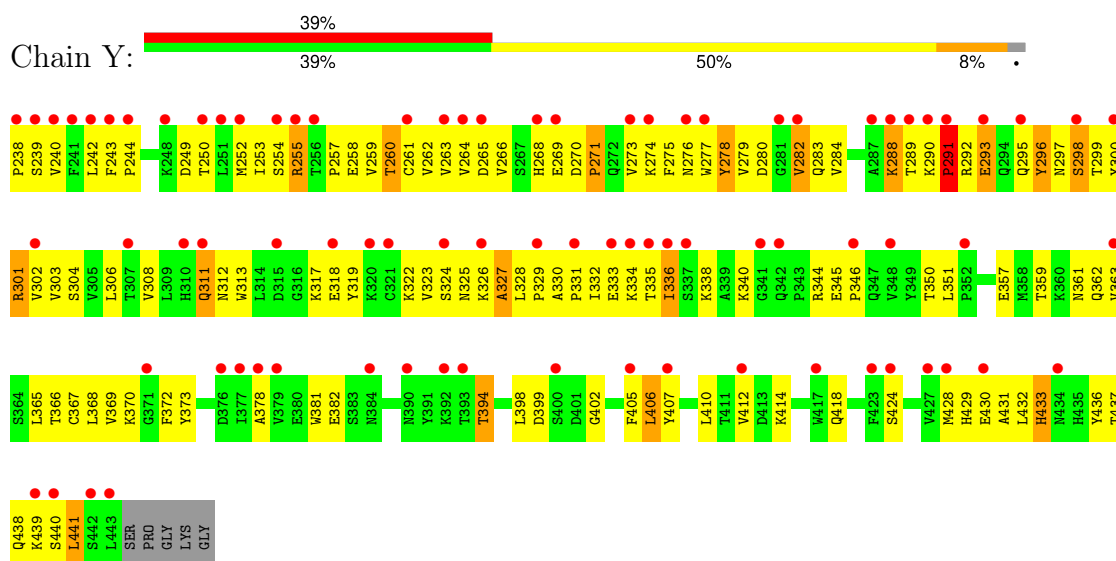


• Molecule 3: Hepatitis B virus receptor binding protein

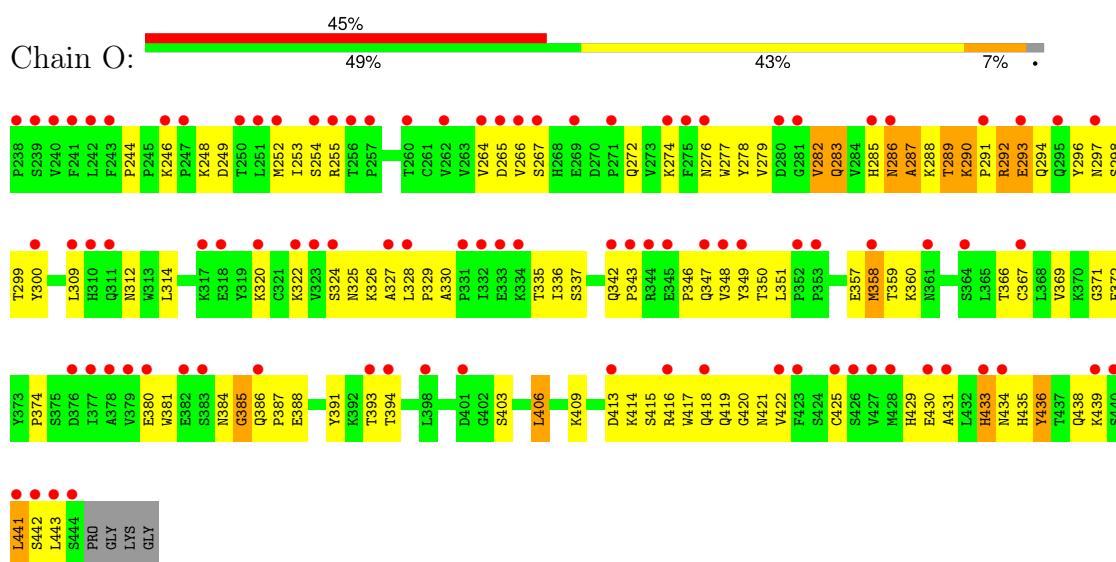




• Molecule 3: Hepatitis B virus receptor binding protein

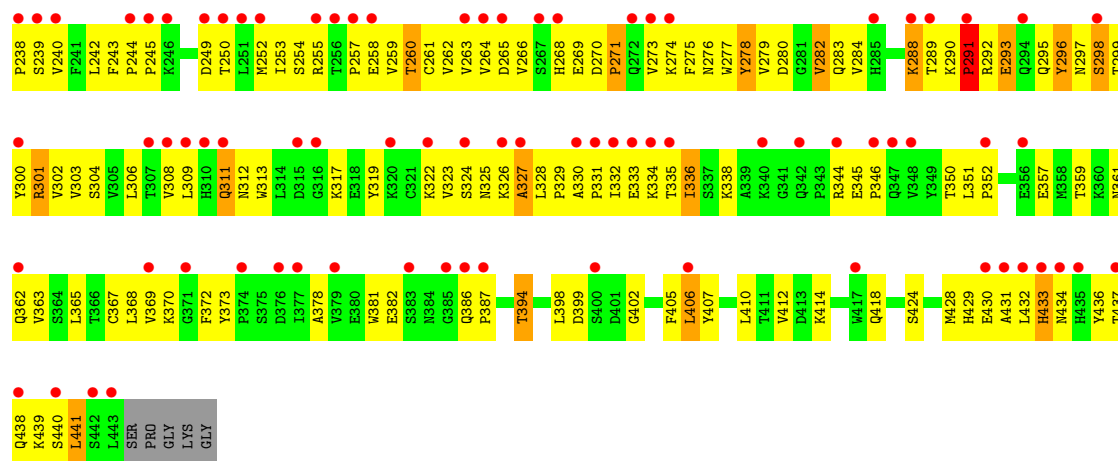


• Molecule 3: Hepatitis B virus receptor binding protein



• Molecule 3: Hepatitis B virus receptor binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	246.25Å 246.25Å 657.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.75 – 8.00 39.75 – 8.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.75-8.00) 95.8 (39.75-8.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 7.33Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, R_{free}	0.359 , 0.369 0.356 , 0.370	Depositor DCC
R_{free} test set	1265 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	296.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 365.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.59	EDS
Total number of atoms	29250	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	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 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
3	N	1654	0	1627	114	37
3	O	1660	0	1630	93	19

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1381) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D: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	Interatomic distance (Å)	Clash overlap (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:Y:346:PRO:HB3	3:Y:372:PHE:HB3	1.63	0.78
3:P:433:HIS:C	3:P:433:HIS:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78
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:X:292:ARG:O	3:X:293:GLU:HB3	1.85	0.76
3:P:433:HIS:C	3:P:433:HIS:CB	2.53	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:C	3:Y:433:HIS:CB	2.53	0.76
1:D:90:ASP:O	1:D:94:TYR:OH	2.03	0.76
3:Y:266:VAL:HB	3:Y:300:TYR:CB	2.15	0.75
3:O:272:GLN:NE2	3:O:326:LYS:HD2	2.01	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
2:F:207:LYS:HZ3	1:M:201:THR:HB	1.46	0.75
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.66	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HH11	2:B:142:ARG:HG2	1.54	0.72
1:E:101:SER:HB2	1:E:104:LEU:H	1.54	0.72
3:Y:328:LEU:HD12	3:Y:329:PRO:HD2	1.69	0.72
1:H:18:LEU:HB3	1:H:83:MET:HE3	1.70	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
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.71
2:L:39:LYS:NZ	2:L:81:ASP:O	2.22	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:H	3:Y:288:LYS:HD3	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:HH11	2:G:142:ARG:HG2	1.55	0.70
2:G:143:GLU:N	2:G:143:GLU:OE2	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
3:X:422:VAL:HG22	3:X:442:SER:OG	1.92	0.69
1:M:207:ASN:ND2	1:M:218:ASP:OD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:143:GLU:OE2	2:C:143:GLU:N	2.27	0.68
1:E:152:VAL:HG11	1:E:160:VAL:HG11	1.76	0.68
3:X:325:ASN:HD21	3:X:327:ALA:HB3	1.58	0.68
1:M:152:VAL:HG11	1:M:160:VAL:HG11	1.75	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:HG2	2:F:142:ARG:HH11	1.60	0.67
2:C:39:LYS:NZ	2:C:81:ASP:O	2.21	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.42	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:75:LEU:HD13	1:I:57:TYR:HE1	1.58	0.66
1:D:207:ASN:ND2	1:D:218:ASP:OD2	2.29	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:HG2	2:K:142:ARG:HH11	1.59	0.66
1:D:202:GLN:O	1:D:203:THR:HA	1.96	0.66
3:X:325:ASN:ND2	3:X:327:ALA:HB3	2.11	0.66
1:H:152:VAL:HG11	1:H:160:VAL:HG11	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
3:O:279:VAL:O	3:O:282:VAL:HG13	1.97	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:H	3:O:288:LYS:HD2	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
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
2:K:143:GLU:OE2	2:K:143:GLU:N	2.31	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
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.79	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	2:C:142:ARG:HH11	1.63	0.62
1:D:75:LEU:CD2	1:I:57:TYR:CE1	2.82	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
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:29:ILE:HG21	2:G:90:HIS:HD2	1.64	0.61
2:G:37:GLN:O	2:G:45:LYS:N	2.29	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:C	3:N:406:LEU:HD12	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:Y:406:LEU:HD12	3:Y:406:LEU:C	2.22	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:N:257:PRO:HB2	3:N:308:VAL:HB	1.84	0.59
1:M:101:SER:HB2	1:M:104:LEU:H	1.66	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
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	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: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
3:Y:325:ASN:HD22	3:Y:326:LYS:H	1.51	0.59
1:H:72:ARG:NE	1:H:74:ASP:OD1	2.31	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
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	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: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:X:433:HIS:ND1	3:X:434:ASN:OD1	2.36	0.58
3:P:279:VAL:O	3:P:279:VAL:HG23	2.03	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
3:Y:265:ASP:HA	3:Y:299:THR:HB	1.85	0.58
1:M:133:PRO:HB3	1:M:221:VAL:HG22	1.85	0.58
3:O:276:ASN:HB2	3:O:322:LYS:HB3	1.86	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	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
1:H:222:GLU:HB2	1:H:223:PRO:HD2	1.84	0.58
3:P:265:ASP:HA	3:P:299:THR:HB	1.86	0.58
2:G:201:LEU:HG	2:G:205:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:E:91:THR:HG23	1:E:120:THR:HA	1.85	0.58
1:I:99:LYS:HG2	1:I:100:GLY:N	2.18	0.58
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.58
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.84	0.58
1:M:164:TRP:O	1:M:166:SER:N	2.37	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
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.57
1:M:73:ASP:N	1:M:78:PHE:O	2.37	0.57
3:P:325:ASN:HD22	3:P:326:LYS:H	1.51	0.57
3:N:265:ASP:HA	3:N:299:THR:HB	1.85	0.57
3:X:286:ASN:O	3:X:287:ALA:HB2	2.03	0.57
2:K:91:TYR:HD1	1:M:99:LYS:NZ	2.03	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
3:O:415:SER:O	3:O:419:GLN:HG3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:P:311:GLN:CD	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
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.56
3:P:439:LYS:HE3	3:P:440:SER:O	2.05	0.56
1:A:153:LYS:HG2	1:A:154:ASP:OD2	2.06	0.56
1:D:103:ARG:O	2:F:50:LYS:CE	2.53	0.56
1:D:144:GLY:O	1:D:196:SER:HB2	2.05	0.56
2:G:6:GLN:NE2	2:G:102:THR:OG1	2.39	0.56
3:X:276:ASN:HB2	3:X:322:LYS:HB3	1.86	0.56
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.87	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: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
3:N:311:GLN:H	3:N:311:GLN:CD	2.08	0.56
3:Y:325:ASN:ND2	3:Y:326:LYS:H	2.04	0.56
1:H:136:PRO:HD3	1:H:148:LEU:HB3	1.87	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: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
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
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
3:Y:311:GLN:H	3:Y:311:GLN:CD	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56
2:K:160:GLN:O	2:K:178:THR:N	2.36	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
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:60:TYR:OH	1:D:69:THR:HA	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
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
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
2:L:167:ASP:HB2	1:M:174:HIS:HE1	1.71	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:HG2	2:K:142:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:X:328:LEU:HD12	3:X:329:PRO:HD2	1.88	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:414:LYS:HE2	3:X:418:GLN:NE2	2.22	0.54
1:M:68:PHE:CD1	1:M:83:MET:HA	2.42	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:Y:238:PRO:CG	3:Y:328:LEU:HD13	2.37	0.54
3:Y:240:VAL:O	3:Y:334:LYS:HE3	2.08	0.54
3:O:282:VAL:O	3:O:283:GLN:CB	2.52	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
3:N:262:VAL:HG13	3:N:303:VAL:HG22	1.90	0.54
3:N:275:PHE:HE1	3:N:302:VAL:HG12	1.72	0.54
2:L:31:THR:OG1	2:L:50:LYS:HE2	2.07	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: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
3:P:351:LEU:C	3:P:441:LEU:HD11	2.28	0.54
1:I:169:LEU:HD21	1:I:192:VAL:HG21	1.90	0.54
3:Y:275:PHE:HE1	3:Y:302:VAL:HG12	1.72	0.54
2:L:162:SER:HB3	2:L:176:SER:OG	2.07	0.54
1:E:70:VAL:HA	1:E:80:TYR:O	2.07	0.53
1:I:22:CYS:O	1:I:78:PHE:HA	2.08	0.53
3:X:414:LYS:O	3:X:418:GLN:HG3	2.08	0.53
1:H:69:THR:C	1:H:81:LEU:HD12	2.28	0.53
1:H:153:LYS:HG2	1:H:154:ASP:OD2	2.08	0.53
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:47:TRP:NE1	1:M:49:ALA:O	2.41	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
3:J:285:HIS:O	3:J:286:ASN:HB2	2.08	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
2:L:142:ARG:HH11	2:L:142:ARG:CG	2.21	0.53
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.90	0.53
3:X:351:LEU:HB2	3:X:366:THR:HB	1.90	0.53
1:M:220:LYS:C	1:M:221:VAL:HA	2.29	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
3:Y:297:ASN:O	3:Y:298:SER:HB3	2.09	0.52
1:H:38:ARG:HB3	1:H:94:TYR:CE2	2.44	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:73:ASP:N	1:A:78:PHE:O	2.40	0.52
1:A:164:TRP:CH2	1:A:221:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:SER:HB2	1:D:104:LEU:H	1.75	0.52
2:L:142:ARG:HG2	2:L:142:ARG:NH1	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
2:G:148:TRP:CE3	2:G:179:LEU:HD22	2.45	0.52
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.52
1:M:35:ASN:OD1	1:M:50:SER:HB2	2.09	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
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
3:X:384:ASN:OD1	3:X:385:GLY:N	2.41	0.52
2:K:151:ASP:HA	2:K:191:VAL:HG12	1.91	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: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
3:P:312:ASN:ND2	3:P:317:LYS:HD2	2.24	0.51
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.91	0.51
1:D:69:THR:C	1:D:81:LEU:HD12	2.31	0.51
1:D:149:GLY:O	1:D:221:VAL:HG21	2.10	0.51
1:D:153:LYS:HG2	1:D:154:ASP:OD2	2.10	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
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
1:M:53:THR:O	1:M:56:THR:OG1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:ASP:HB3	2:F:94:TYR:HE1	1.74	0.51
1:E:164:TRP:CZ2	1:E:192:VAL:HG12	2.46	0.51
2:G:31:THR:OG1	2:G:50:LYS:HE2	2.10	0.51
3:X:429:HIS:O	3:X:435:HIS:HA	2.11	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
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
3:Y:291:PRO:CB	3:Y:304:SER:HA	2.37	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
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
3:X:350:THR:HB	3:X:441:LEU:CG	2.40	0.51
3:X:436:TYR:CD1	3:X:436:TYR:C	2.84	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
3:P:297:ASN:O	3:P:298:SER:HB3	2.09	0.51
1:E:72:ARG:NE	1:E:74:ASP:OD1	2.33	0.51
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.93	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
3:X:418:GLN:C	3:X:420:GLY:H	2.15	0.51
2:L:19:ILE:HG12	2:L:78:LEU:HD11	1.91	0.51
2:L:73:LEU:HD12	2:L:74:THR:H	1.76	0.51
3:O:350:THR:HB	3:O:441:LEU:CG	2.40	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
3:Y:378:ALA:HB3	3:Y:428:MET:HB2	1.92	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
2:G:142:ARG:HG2	2:G:142:ARG:NH1	2.20	0.50
3:Y:261:CYS:HB2	3:Y:277:TRP:CZ2	2.47	0.50
1:M:144:GLY:O	1:M:196:SER:HB2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:443:LEU:HG	3:O:443:LEU:O	2.11	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
3:X:360:LYS:O	3:X:414:LYS:HD2	2.11	0.50
1:M:23:GLY:HA2	1:M:78:PHE:CD2	2.46	0.50
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.50
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.50
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.50
1:H:68:PHE:CD1	1:H:83:MET:HA	2.47	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
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
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.50
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.47	0.50
1:M:133:PRO:HB2	1:M:221:VAL:HG13	1.92	0.50
1:M:169:LEU:HD21	1:M:192:VAL:HG21	1.94	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:N	3:P:278:TYR:CD1	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	3:O:436:TYR:C	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
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	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:X:409:LYS:HB2	3:Y:407:TYR:OH	2.12	0.49
3:Y:406:LEU:HD12	3:Y:406:LEU:O	2.12	0.49
1:H:38:ARG:NH1	1:H:90:ASP:HA	2.27	0.49
1:M:58:ARG:NH1	1:M:70:VAL:O	2.44	0.49
3:P:291:PRO:HB3	3:P:304:SER:CA	2.37	0.49
1:D:92:ALA:N	1:D:119:VAL:O	2.44	0.49
3:J:443:LEU:O	3:J:443:LEU:HG	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
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: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:H:92:ALA:HB3	1:H:94:TYR:CE1	2.47	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
1:I:47:TRP:NE1	1:I:49:ALA:O	2.45	0.49
1:I:129:PRO:HB3	1:I:155:TYR:HB3	1.93	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
3:P:296:TYR:HE1	3:P:301:ARG:HD3	1.74	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
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:X:357:GLU:C	3:X:359:THR:H	2.15	0.49
3:X:443:LEU:O	3:X:443:LEU:HG	2.11	0.49
1:M:164:TRP:CE2	1:M:206:CYS:HB2	2.47	0.49
3:O:246:LYS:HB2	3:O:249:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:X:246:LYS:HB2	3:X:249:ASP:OD2	2.12	0.49
2:K:19:ILE:HG12	2:K:78:LEU:HD11	1.94	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:HH11	2:G:142:ARG:CG	2.22	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
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:369:VAL:O	3:P:405:PHE:HA	2.12	0.49
3:P:398:LEU:HD11	3:P:402:GLY:HA2	1.95	0.49
2:G:83:PHE:CE1	2:G:106:ILE:HG12	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
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.48	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:23:GLY:HA2	1:I:78:PHE:CD2	2.48	0.49
1:I:101:SER:H	1:I:104:LEU:CD2	2.26	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	0.49
3:Y:250:THR:HG22	3:Y:257:PRO:HB3	1.94	0.49
1:M:101:SER:H	1:M:104:LEU:HD23	1.77	0.49
3:O:409:LYS:HB2	3:P:407:TYR:OH	2.12	0.49
1:A:53:THR:O	1:A:56:THR:OG1	2.31	0.49
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	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:H:60:TYR:OH	1:H:69:THR:HA	2.13	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
1:E:73:ASP:N	1:E:78:PHE:O	2.42	0.48
1:E:153:LYS:HG2	1:E:154:ASP:OD2	2.13	0.48
3:N:311:GLN:NE2	3:N:311:GLN:N	2.53	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48
1:H:69:THR:O	1:H:81:LEU:HD12	2.13	0.48
1:H:176:PHE:CD1	2:K:176:SER:HB3	2.48	0.48
3:O:248:LYS:O	3:O:255:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:31:THR:O	2:G:50:LYS:HA	2.13	0.48
3:X:248:LYS:O	3:X:255:ARG:HD3	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
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
3:X:277:TRP:O	3:X:283:GLN:HB3	2.13	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
1:A:69:THR:C	1:A:81:LEU:HD12	2.33	0.48
1:A:197:SER:HB3	3:X:295:GLN:CD	2.34	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:I:67:ARG:C	1:I:68:PHE:HD1	2.17	0.48
3:X:266:VAL:O	3:X:300:TYR:HB2	2.13	0.48
3:X:292:ARG:O	3:X:293:GLU:CB	2.58	0.48
1:H:47:TRP:NE1	1:H:49:ALA:O	2.46	0.48
3:P:292:ARG:O	3:P:293:GLU:HB3	2.12	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
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.48
2:L:61:ARG:HB2	2:L:76:SER:O	2.14	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
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
2:K:91:TYR:CD1	1:M:99:LYS:NZ	2.81	0.48
1:M:72:ARG:NE	1:M:74:ASP:OD1	2.36	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:162:SER:HB3	2:G:176:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:169:LYS:NZ	2:G:169:LYS:HB3	2.29	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
3:X:358:MET:O	3:X:414:LYS:HE3	2.14	0.48
1:M:92:ALA:N	1:M:119:VAL:O	2.46	0.48
3:X:371:GLY:HA2	3:X:403:SER:OG	2.14	0.48
3:O:277:TRP:O	3:O:283:GLN:HB3	2.13	0.48
2:C:142:ARG:HG2	2:C:142:ARG:NH1	2.28	0.48
3:J:388:GLU:HA	3:J:388:GLU:OE1	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: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
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
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
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	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:X:414:LYS:HG2	3:X:418:GLN:NE2	2.29	0.47
1:H:69:THR:O	1:H:81:LEU:HA	2.13	0.47
3:O:358:MET:O	3:O:414:LYS:HE3	2.14	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
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:Y:312:ASN:HB3	3:Y:319:TYR:OH	2.14	0.47
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.49	0.47
3:O:414:LYS:HG2	3:O:418:GLN:NE2	2.29	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:151:ASP:HA	2:L:191:VAL:HG12	1.95	0.47
2:L:169:LYS:NZ	2:L:169:LYS:HB3	2.29	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:OD1	1:E:102:ASP:N	2.47	0.47
2:F:142:ARG:HH11	2:F:142:ARG:CG	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	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
2:F:11:LEU:HD22	2:F:19:ILE:HD12	1.97	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
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:X:438:GLN:O	3:X:439:LYS:HD3	2.15	0.47
1:H:67:ARG:C	1:H:68:PHE:HD1	2.18	0.47
1:H:134:LEU:HB3	2:K:118:PHE:CG	2.49	0.47
1:H:174:HIS:HB3	2:K:164:THR:HG21	1.97	0.47
2:K:4:MET:HG2	2:K:97:THR:HG23	1.95	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
3:P:308:VAL:HG11	3:P:313:TRP:HB2	1.97	0.47
3:P:432:LEU:HD22	3:P:437:THR:HB	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
3:Y:322:LYS:HG3	3:Y:333:GLU:HG2	1.97	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
2:C:118:PHE:CD2	1:D:134:LEU:HD13	2.50	0.47
1:I:53:THR:O	1:I:56:THR:OG1	2.32	0.47
1:I:126:THR:HB	1:I:213:SER:HB3	1.97	0.47
3:Y:275:PHE:HZ	3:Y:302:VAL:O	1.97	0.47
3:O:289:THR:CG2	3:O:290:LYS:N	2.78	0.47
1:A:99:LYS:NZ	2:C:91:TYR:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:Y:279:VAL:O	3:Y:282:VAL:HG22	2.15	0.47
1:H:68:PHE:O	1:H:69:THR:OG1	2.31	0.47
1:M:164:TRP:C	1:M:166:SER:N	2.67	0.47
3:P:368:LEU:HD12	3:P:369:VAL:H	1.79	0.47
3:Y:308:VAL:HG11	3:Y:313:TRP:HB2	1.97	0.46
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
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
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
3:Y:300:TYR:HB3	3:Y:301:ARG:H	1.37	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:O:371:GLY:HA2	3:O:403:SER:OG	2.14	0.46
3:P:261:CYS:HB2	3:P:277:TRP:CH2	2.50	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: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
1:H:101:SER:OG	1:H:104:LEU:HA	2.15	0.46
3:O:388:GLU:HA	3:O:388:GLU:OE1	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:31:THR:O	2:B:50:LYS:HA	2.15	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
1:D:154:ASP:HA	1:D:185:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:X:286:ASN:O	3:X:287:ALA:CB	2.63	0.46
1:H:103:ARG:O	1:H:104:LEU:HB2	2.15	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
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
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
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:Y:278:TYR:CE2	3:Y:284:VAL:HG22	2.50	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:N:275:PHE:HZ	3:N:302:VAL:O	1.98	0.46
3:N:368:LEU:HD12	3:N:369:VAL:H	1.79	0.46
1:H:92:ALA:N	1:H:119:VAL:O	2.47	0.46
3:O:288:LYS:H	3:O:288:LYS:CD	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
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.46
1:H:22:CYS:O	1:H:78:PHE:HA	2.15	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
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:Y:368:LEU:HD12	3:Y:369:VAL:H	1.79	0.45
2:L:106:ILE:O	2:L:166:GLN:NE2	2.46	0.45
3:P:439:LYS:HD2	3:P:439:LYS:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.98	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: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
3:Y:300:TYR:O	3:Y:301:ARG:HB2	2.16	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:NE2	3:P:311:GLN:N	2.53	0.45
3:P:361:ASN:ND2	3:P:362:GLN:HG3	2.31	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
3:J:278:TYR:CD1	3:J:278:TYR:N	2.85	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:X:265:ASP:HA	3:X:299:THR:HB	1.98	0.45
3:Y:242:LEU:HD13	3:Y:336:ILE:HG22	1.98	0.45
3:Y:279:VAL:O	3:Y:280:ASP:HB2	2.16	0.45
1:H:53:THR:O	1:H:56:THR:OG1	2.34	0.45
3:O:286:ASN:O	3:O:287:ALA:CB	2.63	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:Y:290:LYS:HE3	3:Y:292:ARG:HH12	1.82	0.45
3:O:342:GLN:HA	3:O:343:PRO:HD3	1.83	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
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:Y:344:ARG:O	3:Y:372:PHE:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:P:406:LEU:C	3:P:406:LEU:CD1	2.85	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
3:Y:406:LEU:C	3:Y:406:LEU:CD1	2.84	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
1:E:101:SER:H	1:E:104:LEU:CD2	2.29	0.45
2:F:31:THR:OG1	2:F:50:LYS:HE2	2.15	0.45
2:F:113:PRO:HD3	2:F:198:HIS:CG	2.52	0.45
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	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
3:P:279:VAL:O	3:P:280:ASP:HB2	2.17	0.45
1:A:101:SER:H	1:A:104:LEU:CD2	2.30	0.45
1:E:3:GLN:HB2	1:E:25:SER:CB	2.41	0.45
1:E:133:PRO:HB3	1:E:221:VAL:HG22	1.99	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:C	3:N:406:LEU:CD1	2.85	0.45
3:X:266:VAL:HB	3:X:300:TYR:HB2	1.98	0.45
3:P:290:LYS:HE3	3:P:292:ARG:HH12	1.82	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
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:Y:345:GLU:HA	3:Y:431:ALA:HB3	1.99	0.44
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.98	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:244:PRO:HB3	3:X:336:ILE:HD13	1.99	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
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: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
3:P:239:SER:HB3	3:P:264:VAL:CG2	2.47	0.44
3:P:242:LEU:HD13	3:P:336:ILE:HG22	1.98	0.44
3:P:265:ASP:HA	3:P:299:THR:CB	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
3:X:287:ALA:O	3:X:288:LYS:C	2.56	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
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
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	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
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:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	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: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:H:18:LEU:CB	1:H:83:MET:HE3	2.43	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
1:A:69:THR:O	1:A:81:LEU:HD12	2.18	0.44
1:D:69:THR:O	1:D:81:LEU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ALA:HB3	1:D:94:TYR:CZ	2.53	0.44
1:D:188:LEU:HD12	1:D:188:LEU:O	2.17	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
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:X:278:TYR:CD1	3:X:278:TYR:N	2.85	0.44
3:Y:363:VAL:HG22	3:Y:412:VAL:O	2.18	0.44
1:H:92:ALA:HB3	1:H:94:TYR:CZ	2.53	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
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:HD12	1:M:185:LEU:HA	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
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
1:H:22:CYS:N	1:H:79:VAL:O	2.51	0.43
3:O:244:PRO:HB3	3:O:336:ILE:HD13	1.99	0.43
3:O:296:TYR:HB3	3:O:297:ASN:H	1.56	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:HD23	3:P:242:LEU:HA	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
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: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
2:C:136:LEU:HB2	2:C:175:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:X:374:PRO:O	3:X:429:HIS:HE1	2.00	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
1:I:60:TYR:CE2	1:I:69:THR:HA	2.54	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: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:H:101:SER:H	1:H:104:LEU:HD22	1.83	0.43
2:K:20:THR:HG22	2:K:73:LEU:O	2.19	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
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
3:Y:252:MET:SD	3:Y:428:MET:HE3	2.58	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
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:3:GLN:HB2	1:A:25:SER:CB	2.41	0.43
1:A:27:PHE:CE1	1:A:29:ILE:HG22	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:TYR:CE2	2:G:53:THR:HB	2.54	0.43
2:G:201:LEU:HB3	2:G:203:SER:O	2.19	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: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
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
3:X:264:VAL:O	3:X:265:ASP:HB2	2.18	0.43
3:Y:258:GLU:HA	3:Y:308:VAL:HG23	1.99	0.43
3:Y:291:PRO:O	3:Y:292:ARG:HB3	2.19	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
1:D:19:ILE:C	1:D:20:LEU:HD23	2.39	0.42
1:D:194:VAL:HG21	1:D:204:TYR:CZ	2.54	0.42
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	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: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
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
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.42
3:Y:266:VAL:HB	3:Y:300:TYR:CD2	2.54	0.42
1:H:156:PHE:CD1	1:H:156:PHE:C	2.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:Y:296:TYR:OH	3:Y:301:ARG:NH1	2.46	0.42
2:K:91:TYR:HD1	1:M:99:LYS:HZ3	1.66	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
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: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:H:68:PHE:HB3	1:H:81:LEU:HD11	2.01	0.42
3:O:336:ILE:HG12	3:O:337:SER:N	2.35	0.42
1:A:38:ARG:NH1	1:A:90:ASP:HA	2.34	0.42
1:A:185:LEU:HD12	1:A:185:LEU:HA	1.78	0.42
1:A:197:SER:HB3	3:X:295:GLN:OE1	2.20	0.42
2:C:160:GLN:O	2:C:178:THR:N	2.44	0.42
1:D:74:ASP:HB3	2:F:94:TYR:CE1	2.54	0.42
1:D:185:LEU:HD12	1:D:185:LEU:HA	1.76	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:X:283:GLN:C	3:X:285:HIS:H	2.23	0.42
3:X:384:ASN:CG	3:X:385:GLY:H	2.22	0.42
3:O:369:VAL:HB	3:O:406:LEU:HD12	2.02	0.42
3:P:296:TYR:OH	3:P:301:ARG:NH1	2.46	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: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:E:149:GLY:HA2	1:E:164:TRP:CH2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
3:Y:238:PRO:HB2	3:Y:328:LEU:HD13	2.01	0.42
1:H:38:ARG:HA	1:H:93:ILE:O	2.19	0.42
1:M:38:ARG:HD3	1:M:94:TYR:CE2	2.55	0.42
3:P:238:PRO:HB2	3:P:328:LEU:HD13	2.01	0.42
1:D:220:LYS:HE2	1:D:222:GLU:OE1	2.19	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:H:101:SER:N	1:H:104:LEU:HD22	2.35	0.42
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.55	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
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
1:H:6:GLU:OE1	1:H:95:TYR:HA	2.20	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
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
3:Y:276:ASN:HB3	3:Y:278:TYR:CE1	2.56	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
2:C:183:LYS:HE2	2:C:187:GLU:OE1	2.20	0.41
1:D:47:TRP:NE1	1:D:49:ALA:O	2.53	0.41
1:D:163:SER:OG	1:D:207:ASN:HB2	2.20	0.41
1:D:181:GLN:C	1:D:183:SER:H	2.23	0.41
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:58:VAL:HA	2:G:59:PRO:HD3	1.97	0.41
2:G:133:VAL:HG21	1:I:134:LEU:HD21	2.01	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: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
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
1:A:99:LYS:HZ3	2:C:91:TYR:HD1	1.68	0.41
1:A:173:VAL:HG22	1:A:192:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	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:O:391:TYR:CD2	3:O:391:TYR:C	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:O	1:E:188:LEU:HD12	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:113:PRO:HD2	2:B:201:LEU:HD22	2.03	0.41
2:B:138:ASN:C	2:B:172:THR:HB	2.41	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
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: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
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
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
3:X:367:CYS:HB2	3:X:381:TRP:CH2	2.55	0.41
1:H:219:LYS:HB2	1:H:219:LYS:HE2	1.91	0.41
1:M:181:GLN:C	1:M:183:SER:H	2.24	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
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
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:L:5:THR:CG2	2:L:100:GLN:HE22	2.33	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
3:Y:367:CYS:HB2	3:Y:381:TRP:CZ2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:100:GLN:OE1	2:L:100:GLN:N	2.44	0.41
2:C:70:GLU:HG3	2:C:71:PHE:N	2.35	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: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
3:N:273:VAL:HB	3:N:302:VAL:HG21	2.03	0.41
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	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
1:H:12:VAL:O	1:H:121:VAL:HA	2.20	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
2:K:4:MET:SD	2:K:90:HIS:HB2	2.61	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
1:M:34:MET:O	1:M:50:SER:HA	2.19	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:350:THR:HB	3:P:441:LEU:CG	2.51	0.41
3:P:357:GLU:C	3:P:359:THR:H	2.23	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
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
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
1:A:4:LEU:HG	1:A:24:VAL:HG12	2.02	0.40
1:A:152:VAL:HG22	1:A:208:VAL:HG21	2.03	0.40
2:C:122:ASP:O	2:C:126:LYS:HB2	2.20	0.40
1:D:27:PHE:CE1	1:D:29:ILE:HG22	2.57	0.40
1:D:164:TRP:HH2	1:D:221:VAL:HG21	1.85	0.40
3:N:351:LEU:HB2	3:N:366:THR:HB	2.03	0.40
1:M:38:ARG:NH1	1:M:90:ASP:HA	2.35	0.40
3:P:245:PRO:HB3	3:P:258:GLU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CD1	1:D:156:PHE:C	2.94	0.40
1:E:156:PHE:CD1	1:E:156:PHE:C	2.94	0.40
1:E:176:PHE:CD2	2:F:164:THR:HG23	2.56	0.40
2:F:108:ARG:HD3	2:F:109:THR:N	2.35	0.40
2:G:117:ILE:HG13	2:G:133:VAL:O	2.21	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: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:L:36:TYR:CE1	2:L:46:LEU:HD13	2.56	0.40
3:O:289:THR:HG22	3:O:290:LYS:N	2.36	0.40
2:B:73:LEU:HD12	2:B:74:THR:H	1.86	0.40
2:B:108:ARG:HD3	2:B:109:THR:N	2.36	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:350:THR:HB	3:P:441:LEU:HD12	2.03	0.40
3:P:367:CYS:HB2	3:P:381:TRP:CZ2	2.56	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
3:X:432:LEU:HD22	3:X:437:THR:HB	2.04	0.40
1:H:58:ARG:NH1	1:H:71:SER:OG	2.52	0.40
1:H:181:GLN:C	1:H:183:SER:H	2.24	0.40
1:M:69:THR:O	1:M:81:LEU:HA	2.20	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
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:5:THR:HG23	2:K:100:GLN:HE22	1.86	0.40
2:K:29:ILE:HG21	2:K:90:HIS:CD2	2.54	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	Interatomic distance (Å)	Clash overlap (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:J:253:ILE:CB	3:X:253:ILE:N[12_545]	1.20	1.00
3:Y:253:ILE:CG2	3:Y:255:ARG:N[12_555]	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
2:B:18:THR:N	3:J:285:HIS:CG[12_545]	1.25	0.95
3:N:253:ILE:CG2	3:P:253:ILE:C[6_445]	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
3:N:253:ILE:CG2	3:P:253:ILE:CA[6_445]	1.34	0.86
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: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
3:J:253:ILE:N	3:X:253:ILE:CG1[12_545]	1.36	0.84
1:D:144:GLY:N	3:Y:280:ASP:OD2[8_555]	1.37	0.83
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:253:ILE:CA	3:P:253:ILE:N[6_445]	1.41	0.79
3:O:253:ILE:CG1	3:O:254:SER:N[10_444]	1.41	0.79
3:J:252:MET:C	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:J:252:MET:O	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:N:253:ILE:CG1	3:P:252:MET:C[6_445]	1.44	0.76
3:X:281:GLY:O	2:L:20:THR:OG1[12_545]	1.45	0.75
3:Y:253:ILE:CG2	3:Y:254:SER:C[12_555]	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: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:O:253:ILE:O	3:O:253:ILE:CG2[10_444]	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
2:B:18:THR:CA	3:J:285:HIS:NE2[12_545]	1.51	0.69
3:N:253:ILE:CB	3:P:253:ILE:N[6_445]	1.51	0.69
3:N:310:HIS:NE2	3:P:253:ILE:CD1[6_445]	1.51	0.69
3:O:253:ILE:C	3:O:253:ILE:CG1[10_444]	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:X:285:HIS:NE2	2:L:77:GLY:N[12_545]	1.58	0.62
3:Y:252:MET:C	3:Y:253:ILE:CG1[12_555]	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
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:253:ILE:C	3:P:253:ILE:CG2[6_445]	1.65	0.55
3:N:433:HIS:CD2	3:P:382:GLU:OE2[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
2:B:18:THR:CB	3:J:285:HIS:CG[12_545]	1.69	0.51
3:J:253:ILE:CB	3:X:252:MET:C[12_545]	1.69	0.51
2:B:18:THR:N	3:J:285:HIS:CD2[12_545]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:253:ILE:CA	3:X:253:ILE:N[12_545]	1.72	0.48
3:N:253:ILE:CA	3:P:253:ILE:CB[6_445]	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: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:C	3:O:253:ILE:CD1[10_444]	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:281:GLY:O	2:L:20:THR:N[12_545]	1.78	0.42
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
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
2:B:18:THR:O	3:J:285:HIS:ND1[12_545]	1.84	0.36
3:J:253:ILE:CG1	3:X:253:ILE:CA[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
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:N:433:HIS:CB	3:P:382:GLU:OE2[6_445]	1.87	0.33
3:Y:253:ILE:N	3:Y:253:ILE:C[12_555]	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:J:253:ILE:N	3:X:253:ILE:N[12_545]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Y:253:ILE:CA	3:Y:253:ILE:O[12_555]	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:N:253:ILE:CD1	3:P:249:ASP:O[6_445]	1.96	0.24
3:X:283:GLN:CA	2:L:18:THR:O[12_545]	1.96	0.24
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
3:O:253:ILE:N	3:O:253:ILE:CD1[10_444]	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
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:Y:253:ILE:O	3:Y:253:ILE:CG2[12_555]	2.00	0.20
2:B:18:THR:CB	3:J:285:HIS:CE1[12_545]	2.01	0.19
3:N:253:ILE:CG2	3:P:252:MET:C[6_445]	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:J:253:ILE:CD1	3:X:252:MET:CA[12_545]	2.04	0.16
3:N:253:ILE:CG1	3:P:253:ILE:N[6_445]	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: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:CE1	2:L:77:GLY:N[12_545]	2.06	0.14
3:N:253:ILE:CG2	3:P:253:ILE:O[6_445]	2.07	0.13
3:X:285:HIS:CA	2:L:18:THR:OG1[12_545]	2.07	0.13
1:D:142:SER:CA	3:Y:318:GLU:OE2[8_555]	2.08	0.12
3:J:253:ILE:N	3:X:253:ILE:CB[12_545]	2.08	0.12
3:J:310:HIS:CD2	3:X:253:ILE:CG2[12_545]	2.08	0.12
3:X:285:HIS:NE2	2:L:76:SER:C[12_545]	2.09	0.11
3:Y:249:ASP:O	3:Y:253:ILE:CD1[12_555]	2.09	0.11
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:N:382:GLU:OE2	3:P:433:HIS:CB[6_445]	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	32
1	D	204/243 (84%)	185 (91%)	15 (7%)	4 (2%)	6	32
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	9	41
1	H	207/243 (85%)	187 (90%)	16 (8%)	4 (2%)	6	32
1	I	204/243 (84%)	182 (89%)	17 (8%)	5 (2%)	4	26
1	M	204/243 (84%)	186 (91%)	13 (6%)	5 (2%)	4	26
2	B	209/213 (98%)	187 (90%)	21 (10%)	1 (0%)	25	64
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	25	64
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	25	64
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	25	64
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	25	64
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	13	49
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16
3	X	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15
3	Y	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	16
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	4	26

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	7	23
1	D	180/205 (88%)	162 (90%)	18 (10%)	6	20
1	E	180/205 (88%)	162 (90%)	18 (10%)	6	20
1	H	180/205 (88%)	165 (92%)	15 (8%)	9	27
1	I	180/205 (88%)	165 (92%)	15 (8%)	9	27
1	M	180/205 (88%)	163 (91%)	17 (9%)	7	23
2	B	182/184 (99%)	164 (90%)	18 (10%)	6	21
2	C	182/184 (99%)	165 (91%)	17 (9%)	7	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	182/184 (99%)	164 (90%)	18 (10%)	6	21
2	G	182/184 (99%)	164 (90%)	18 (10%)	6	21
2	K	182/184 (99%)	163 (90%)	19 (10%)	5	19
2	L	182/184 (99%)	164 (90%)	18 (10%)	6	21
3	J	193/196 (98%)	187 (97%)	6 (3%)	35	54
3	N	192/196 (98%)	180 (94%)	12 (6%)	15	36
3	O	193/196 (98%)	187 (97%)	6 (3%)	35	54
3	P	192/196 (98%)	180 (94%)	12 (6%)	15	36
3	X	193/196 (98%)	187 (97%)	6 (3%)	35	54
3	Y	192/196 (98%)	180 (94%)	12 (6%)	15	36
All	All	3327/3510 (95%)	3065 (92%)	262 (8%)	10	29

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	I	3
1	D	3
1	M	3
1	A	1
1	E	1
1	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	202:GLN	C	203:THR	N	3.88
1	D	202:GLN	C	203:THR	N	3.77
1	M	202:GLN	C	203:THR	N	3.62
1	A	202:GLN	C	203:THR	N	3.50
1	E	202:GLN	C	203:THR	N	3.41
1	I	201:THR	C	202:GLN	N	3.34

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	220:LYS	C	221:VAL	N	3.17
1	H	202:GLN	C	203:THR	N	3.10
1	D	201:THR	C	202:GLN	N	3.07
1	I	220:LYS	C	221:VAL	N	3.04
1	M	201:THR	C	202:GLN	N	2.99
1	M	220:LYS	C	221:VAL	N	2.88

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	209/243 (86%)	1.37	52 (24%) 2 7	114, 118, 126, 134	0
1	D	207/243 (85%)	1.41	51 (24%) 2 7	113, 118, 125, 139	0
1	E	209/243 (86%)	1.90	85 (40%) 1 4	178, 182, 190, 198	0
1	H	209/243 (86%)	1.17	45 (21%) 3 8	96, 100, 107, 115	0
1	I	207/243 (85%)	1.53	59 (28%) 1 5	177, 182, 189, 203	0
1	M	207/243 (85%)	1.22	47 (22%) 3 7	94, 100, 107, 121	0
2	B	211/213 (99%)	1.29	52 (24%) 2 7	113, 118, 124, 139	0
2	C	211/213 (99%)	1.59	69 (32%) 1 5	113, 118, 123, 143	0
2	F	211/213 (99%)	1.76	77 (36%) 1 4	177, 182, 188, 203	0
2	G	211/213 (99%)	1.66	77 (36%) 1 4	177, 182, 187, 207	0
2	K	211/213 (99%)	1.22	51 (24%) 2 7	94, 100, 105, 120	0
2	L	211/213 (99%)	1.36	50 (23%) 2 7	94, 100, 105, 124	0
3	J	207/211 (98%)	2.07	83 (40%) 1 4	176, 176, 176, 176	0
3	N	206/211 (97%)	1.75	72 (34%) 1 5	179, 179, 179, 179	0
3	O	207/211 (98%)	2.04	94 (45%) 1 3	274, 274, 274, 274	0
3	P	206/211 (97%)	1.90	80 (38%) 1 4	277, 277, 277, 277	0
3	X	207/211 (98%)	1.98	94 (45%) 1 3	167, 167, 167, 167	0
3	Y	206/211 (97%)	1.79	82 (39%) 1 4	171, 171, 171, 171	0
All	All	3753/4002 (93%)	1.61	1220 (32%) 1 5	94, 167, 277, 277	0

All (1220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	21.4
1	D	147	ALA	12.8
1	M	131	VAL	11.5

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Mol	Chain	Res	Type	RSRZ
3	O	332	ILE	11.1
3	Y	288	LYS	10.0
3	Y	268	HIS	9.0
1	E	193	THR	8.7
3	J	428	MET	8.7
1	E	130	SER	8.7
2	L	187	GLU	8.6
2	G	52	SER	8.6
2	L	93	GLY	8.2
2	C	13	ALA	8.1
1	H	31	ALA	7.8
1	D	31	ALA	7.7
3	J	377	ILE	7.6
2	C	146	VAL	7.6
2	F	95	SER	7.6
2	F	45	LYS	7.5
1	E	190	SER	7.5
3	P	250	THR	7.5
3	P	332	ILE	7.5
1	E	175	THR	7.5
2	B	93	GLY	7.4
2	B	94	TYR	7.3
3	O	425	CYS	7.2
1	M	130	SER	7.1
3	J	378	ALA	6.9
1	H	147	ALA	6.9
2	L	131	SER	6.9
1	I	130	SER	6.8
3	N	254	SER	6.8
3	J	280	ASP	6.8
3	X	434	ASN	6.8
1	A	131	VAL	6.6
1	D	148	LEU	6.5
2	F	100	GLN	6.5
3	O	430	GLU	6.5
1	I	200	GLY	6.5
3	Y	264	VAL	6.4
3	P	374	PRO	6.2
2	G	146	VAL	6.1
3	J	336	ILE	6.1
2	K	205	VAL	6.1
1	E	153	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
3	O	238	PRO	6.0
3	P	238	PRO	6.0
1	E	58	ARG	6.0
3	X	324	SER	6.0
2	F	59	PRO	6.0
2	F	94	TYR	5.9
1	E	131	VAL	5.9
2	L	52	SER	5.9
3	N	302	VAL	5.9
3	O	265	ASP	5.8
2	B	76	SER	5.8
2	K	11	LEU	5.8
3	N	376	ASP	5.8
3	Y	417	TRP	5.7
2	C	207	LYS	5.7
3	P	434	ASN	5.7
2	B	212	GLY	5.7
3	O	444	SER	5.7
1	A	175	THR	5.7
1	M	150	CYS	5.7
1	D	152	VAL	5.6
2	C	14	SER	5.6
2	C	131	SER	5.6
2	C	76	SER	5.6
2	F	165	GLU	5.5
3	N	394	THR	5.5
3	X	377	ILE	5.5
1	A	188	LEU	5.4
3	P	256	THR	5.4
2	F	96	ALA	5.4
3	J	281	GLY	5.4
1	H	175	THR	5.4
1	E	129	PRO	5.4
3	X	433	HIS	5.4
3	X	332	ILE	5.4
1	A	137	SER	5.4
2	C	180	THR	5.4
2	F	87	HIS	5.4
1	A	130	SER	5.3
3	P	433	HIS	5.3
3	X	335	THR	5.3
1	I	162	VAL	5.3

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Mol	Chain	Res	Type	RSRZ
2	K	146	VAL	5.3
1	I	66	GLY	5.3
3	Y	377	ILE	5.3
3	P	442	SER	5.3
1	E	209	ASN	5.3
3	J	240	VAL	5.3
3	Y	239	SER	5.2
2	C	187	GLU	5.2
3	J	434	ASN	5.2
1	I	99	LYS	5.2
1	A	11	LEU	5.2
1	A	151	LEU	5.2
3	N	281	GLY	5.1
3	Y	240	VAL	5.1
3	O	274	LYS	5.1
2	C	197	THR	5.1
3	Y	281	GLY	5.1
3	J	248	LYS	5.1
2	C	138	ASN	5.1
3	J	437	THR	5.1
3	O	260	THR	5.0
3	O	310	HIS	5.0
3	P	346	PRO	5.0
1	A	136	PRO	5.0
3	P	348	VAL	5.0
2	B	7	SER	5.0
3	X	384	ASN	5.0
3	J	355	ARG	4.9
3	J	332	ILE	4.9
2	C	116	PHE	4.9
3	Y	423	PHE	4.9
3	N	380	GLU	4.9
2	G	134	CYS	4.9
1	I	7	SER	4.9
2	K	187	GLU	4.9
3	J	375	SER	4.8
3	O	275	PHE	4.8
2	C	114	SER	4.8
2	C	127	SER	4.8
2	K	186	TYR	4.8
3	Y	392	LYS	4.8
3	P	435	HIS	4.7

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Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	4.7
3	J	256	THR	4.7
3	X	241	PHE	4.7
1	I	104	LEU	4.7
2	C	132	VAL	4.7
3	J	329	PRO	4.7
3	X	258	GLU	4.7
2	C	12	SER	4.7
2	L	209	PHE	4.7
3	N	268	HIS	4.7
3	N	282	VAL	4.7
3	N	348	VAL	4.7
3	P	347	GLN	4.7
3	P	310	HIS	4.6
2	G	28	SER	4.6
3	X	275	PHE	4.6
3	O	440	SER	4.6
3	O	393	THR	4.6
3	N	423	PHE	4.6
1	E	104	LEU	4.6
2	G	13	ALA	4.6
1	H	104	LEU	4.6
2	L	116	PHE	4.6
2	G	51	ALA	4.6
2	K	3	VAL	4.6
3	O	376	ASP	4.5
3	X	382	GLU	4.5
3	X	346	PRO	4.5
1	A	189	SER	4.5
3	J	254	SER	4.5
3	X	239	SER	4.5
2	C	119	PRO	4.5
3	O	241	PHE	4.5
3	Y	254	SER	4.5
3	P	430	GLU	4.5
1	A	99	LYS	4.5
3	N	377	ILE	4.4
3	J	308	VAL	4.4
3	X	440	SER	4.4
1	I	27	PHE	4.4
2	F	30	GLU	4.4
3	P	268	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	H	15	GLY	4.4
2	B	205	VAL	4.4
1	E	202	GLN	4.4
1	H	136	PRO	4.4
1	E	152	VAL	4.3
1	M	152	VAL	4.3
3	X	343	PRO	4.3
1	E	189	SER	4.3
2	F	114	SER	4.3
3	N	411	THR	4.3
1	E	154	ASP	4.3
3	X	286	ASN	4.3
3	N	238	PRO	4.3
3	P	431	ALA	4.3
1	I	182	SER	4.3
2	G	135	LEU	4.3
2	K	116	PHE	4.3
3	O	281	GLY	4.3
3	O	266	VAL	4.3
1	H	178	ALA	4.3
2	B	166	GLN	4.3
1	M	168	ALA	4.2
1	A	10	GLY	4.2
1	A	133	PRO	4.2
2	G	137	ASN	4.2
3	X	430	GLU	4.2
1	I	103	ARG	4.2
1	H	7	SER	4.2
2	F	208	SER	4.2
2	L	208	SER	4.2
1	A	15	GLY	4.2
3	O	243	PHE	4.2
3	X	238	PRO	4.2
3	P	251	LEU	4.2
2	G	136	LEU	4.1
1	A	120	THR	4.1
1	E	160	VAL	4.1
3	J	268	HIS	4.1
2	F	115	VAL	4.1
3	J	430	GLU	4.1
3	J	323	VAL	4.1
3	X	329	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
2	C	45	LYS	4.1
3	P	258	GLU	4.1
1	D	192	VAL	4.1
3	J	282	VAL	4.1
3	N	407	TYR	4.1
1	E	223	PRO	4.1
3	J	277	TRP	4.1
2	C	144	ALA	4.1
1	E	133	PRO	4.1
1	H	148	LEU	4.0
3	X	428	MET	4.0
2	B	83	PHE	4.0
3	X	336	ILE	4.0
2	F	44	PRO	4.0
1	E	99	LYS	4.0
2	B	20	THR	4.0
2	G	197	THR	4.0
1	I	102	ASP	4.0
3	J	390	ASN	4.0
1	D	197	SER	4.0
2	F	131	SER	4.0
1	E	188	LEU	4.0
1	H	193	THR	4.0
1	H	99	LYS	4.0
3	P	340	LYS	4.0
1	A	160	VAL	3.9
2	L	183	LYS	3.9
3	X	423	PHE	3.9
3	X	277	TRP	3.9
1	E	57	TYR	3.9
3	N	248	LYS	3.9
3	P	344	ARG	3.9
1	A	163	SER	3.9
1	E	17	SER	3.9
2	G	14	SER	3.9
3	X	358	MET	3.9
2	F	133	VAL	3.9
1	A	150	CYS	3.9
2	G	45	LYS	3.9
1	D	15	GLY	3.9
1	D	184	GLY	3.9
1	D	104	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	E	151	LEU	3.9
3	N	375	SER	3.9
2	F	146	VAL	3.9
3	P	273	VAL	3.9
3	J	433	HIS	3.9
1	A	112	ALA	3.9
2	G	116	PHE	3.9
2	B	144	ALA	3.9
3	P	246	LYS	3.9
3	P	288	LYS	3.9
3	X	280	ASP	3.8
2	L	51	ALA	3.8
3	N	308	VAL	3.8
2	F	85	THR	3.8
1	D	220	LYS	3.8
3	J	275	PHE	3.8
3	Y	378	ALA	3.8
3	Y	295	GLN	3.8
1	I	9	GLY	3.8
3	N	430	GLU	3.8
3	Y	412	VAL	3.8
3	Y	430	GLU	3.8
3	O	264	VAL	3.8
2	G	27	GLN	3.8
3	X	393	THR	3.8
2	G	144	ALA	3.8
3	X	375	SER	3.8
1	H	194	VAL	3.8
3	O	382	GLU	3.8
2	C	134	CYS	3.8
3	O	334	LYS	3.8
2	K	138	ASN	3.8
3	X	291	PRO	3.8
3	P	443	LEU	3.7
1	A	197	SER	3.7
1	I	2	VAL	3.7
1	I	175	THR	3.7
1	I	149	GLY	3.7
2	L	185	ASP	3.7
3	O	386	GLN	3.7
3	P	265	ASP	3.7
1	I	193	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	7	SER	3.7
2	F	60	SER	3.7
3	P	315	ASP	3.7
1	E	194	VAL	3.7
1	I	133	PRO	3.7
3	Y	302	VAL	3.7
2	B	138	ASN	3.7
1	A	98	ARG	3.7
2	F	53	THR	3.7
3	J	380	GLU	3.7
2	F	168	SER	3.7
2	G	32	TRP	3.7
2	K	159	SER	3.7
3	O	239	SER	3.7
2	B	107	LYS	3.7
2	C	87	HIS	3.7
3	X	318	GLU	3.7
3	O	379	VAL	3.7
3	P	331	PRO	3.7
3	O	267	SER	3.7
2	C	49	TYR	3.7
1	D	174	HIS	3.7
1	E	44	GLY	3.7
1	I	144	GLY	3.7
1	E	161	THR	3.7
2	G	147	GLN	3.7
1	D	2	VAL	3.6
1	H	53	THR	3.6
3	Y	256	THR	3.6
3	O	394	THR	3.6
3	Y	300	TYR	3.6
2	F	52	SER	3.6
3	J	241	PHE	3.6
3	J	321	CYS	3.6
1	A	129	PRO	3.6
2	G	155	GLN	3.6
3	N	382	GLU	3.6
1	H	179	VAL	3.6
3	Y	293	GLU	3.6
2	C	46	LEU	3.6
2	G	212	GLY	3.6
3	J	238	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	150	CYS	3.6
3	O	377	ILE	3.6
3	P	371	GLY	3.6
1	I	146	ALA	3.6
3	O	431	ALA	3.6
1	A	152	VAL	3.6
1	E	56	THR	3.6
1	M	99	LYS	3.6
2	G	138	ASN	3.5
1	E	66	GLY	3.5
3	J	267	SER	3.5
2	C	147	GLN	3.5
3	N	273	VAL	3.5
2	L	83	PHE	3.5
2	C	18	THR	3.5
3	N	256	THR	3.5
3	N	339	ALA	3.5
2	G	107	LYS	3.5
2	L	155	GLN	3.5
1	M	132	PHE	3.5
2	C	130	ALA	3.5
2	B	185	ASP	3.5
2	F	132	VAL	3.5
3	Y	290	LYS	3.5
3	P	320	LYS	3.5
1	I	57	TYR	3.5
1	A	128	GLY	3.5
3	X	348	VAL	3.5
2	G	189	HIS	3.5
3	J	319	TYR	3.5
1	H	54	SER	3.5
1	I	39	ARG	3.5
2	F	2	VAL	3.5
3	X	262	VAL	3.5
2	L	9	SER	3.5
3	O	364	SER	3.5
3	O	323	VAL	3.5
3	O	250	THR	3.5
1	H	204	TYR	3.5
2	F	93	GLY	3.5
1	D	222	GLU	3.5
3	N	338	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
3	Y	263	VAL	3.5
2	C	137	ASN	3.4
1	E	103	ARG	3.4
3	J	246	LYS	3.4
3	X	319	TYR	3.4
3	P	379	VAL	3.4
3	N	371	GLY	3.4
3	Y	379	VAL	3.4
3	J	346	PRO	3.4
1	A	198	SER	3.4
1	I	15	GLY	3.4
1	E	60	TYR	3.4
1	I	152	VAL	3.4
3	X	276	ASN	3.4
3	O	352	PRO	3.4
1	D	17	SER	3.4
2	K	131	SER	3.4
1	H	9	GLY	3.4
2	C	77	GLY	3.4
3	J	359	THR	3.4
3	J	242	LEU	3.4
3	Y	390	ASN	3.4
2	G	153	ALA	3.4
1	H	95	TYR	3.4
1	M	188	LEU	3.4
1	M	129	PRO	3.4
3	Y	244	PRO	3.4
3	X	321	CYS	3.4
1	A	97	ALA	3.4
1	E	97	ALA	3.4
2	G	159	SER	3.4
2	C	145	LYS	3.4
2	B	119	PRO	3.4
2	F	28	SER	3.3
2	F	135	LEU	3.3
2	L	65	SER	3.3
2	B	199	GLN	3.3
2	K	166	GLN	3.3
3	N	291	PRO	3.3
3	X	250	THR	3.3
2	K	106	ILE	3.3
3	J	384	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
3	Y	282	VAL	3.3
3	Y	248	LYS	3.3
1	D	3	GLN	3.3
2	G	9	SER	3.3
2	G	12	SER	3.3
1	E	201	THR	3.3
3	O	256	THR	3.3
3	P	356	GLU	3.3
3	J	334	LYS	3.3
3	J	392	LYS	3.3
3	N	384	ASN	3.3
2	B	142	ARG	3.3
2	L	189	HIS	3.3
2	G	208	SER	3.3
3	N	396	PRO	3.3
2	G	207	LYS	3.3
3	O	300	TYR	3.3
2	L	166	GLN	3.3
3	Y	241	PHE	3.3
3	O	331	PRO	3.3
2	B	9	SER	3.3
2	F	177	SER	3.3
3	Y	336	ILE	3.3
3	X	256	THR	3.3
3	N	252	MET	3.3
1	D	195	PRO	3.3
1	A	2	VAL	3.3
1	M	182	SER	3.3
1	A	170	THR	3.3
3	O	285	HIS	3.3
3	O	433	HIS	3.3
3	O	434	ASN	3.3
2	F	207	LYS	3.3
3	X	248	LYS	3.3
1	A	101	SER	3.3
2	L	20	THR	3.3
2	G	80	PHE	3.3
1	I	24	VAL	3.3
3	P	291	PRO	3.3
3	P	342	GLN	3.3
1	I	187	SER	3.2
3	J	307	THR	3.2

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Mol	Chain	Res	Type	RSRZ
3	Y	289	THR	3.2
3	X	376	ASP	3.2
1	E	217	VAL	3.2
1	E	221	VAL	3.2
2	G	53	THR	3.2
2	K	183	LYS	3.2
1	I	188	LEU	3.2
2	B	209	PHE	3.2
2	F	116	PHE	3.2
3	Y	443	LEU	3.2
3	P	330	ALA	3.2
2	L	138	ASN	3.2
3	Y	384	ASN	3.2
3	J	317	LYS	3.2
3	N	258	GLU	3.2
3	X	251	LEU	3.2
1	E	88	VAL	3.2
3	J	255	ARG	3.2
1	E	220	LYS	3.2
1	E	137	SER	3.2
3	X	302	VAL	3.2
3	P	300	TYR	3.2
2	L	44	PRO	3.2
1	D	63	ALA	3.2
3	P	417	TRP	3.2
3	J	398	LEU	3.2
3	O	247	PRO	3.2
3	P	264	VAL	3.2
2	F	206	THR	3.2
1	E	211	LYS	3.2
2	C	50	LYS	3.2
3	P	285	HIS	3.2
1	M	165	ASN	3.2
3	X	383	SER	3.2
3	O	269	GLU	3.1
2	B	8	PRO	3.1
3	P	335	THR	3.1
2	K	21	ILE	3.1
2	C	15	VAL	3.1
3	N	329	PRO	3.1
3	J	306	LEU	3.1
1	M	175	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	219	LYS	3.1
3	Y	242	LEU	3.1
3	O	378	ALA	3.1
3	P	369	VAL	3.1
2	K	199	GLN	3.1
3	X	310	HIS	3.1
2	F	119	PRO	3.1
3	N	443	LEU	3.1
3	J	358	MET	3.1
3	J	427	VAL	3.1
3	J	335	THR	3.1
1	M	17	SER	3.1
2	B	67	SER	3.1
1	H	131	VAL	3.1
2	L	205	VAL	3.1
2	F	145	LYS	3.1
1	I	174	HIS	3.1
2	K	197	THR	3.1
1	H	188	LEU	3.1
3	X	424	SER	3.1
2	K	144	ALA	3.1
1	D	60	TYR	3.1
2	K	143	GLU	3.1
3	P	377	ILE	3.1
3	N	275	PHE	3.1
2	G	180	THR	3.1
2	K	5	THR	3.1
3	P	307	THR	3.1
3	N	295	GLN	3.0
2	C	117	ILE	3.0
1	A	219	LYS	3.0
1	E	198	SER	3.0
1	D	28	ARG	3.0
1	D	99	LYS	3.0
3	Y	346	PRO	3.0
3	Y	371	GLY	3.0
1	A	71	SER	3.0
3	J	440	SER	3.0
2	B	123	GLU	3.0
3	N	425	CYS	3.0
3	O	423	PHE	3.0
3	O	320	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	O	344	ARG	3.0
3	O	262	VAL	3.0
2	C	112	ALA	3.0
2	F	79	GLN	3.0
2	F	97	THR	3.0
3	J	260	THR	3.0
3	J	243	PHE	3.0
2	B	187	GLU	3.0
2	G	114	SER	3.0
3	N	264	VAL	3.0
3	O	255	ARG	3.0
3	J	348	VAL	3.0
3	J	345	GLU	3.0
1	D	97	ALA	3.0
1	M	133	PRO	3.0
3	Y	407	TYR	3.0
2	K	169	LYS	3.0
2	K	196	VAL	2.9
3	O	254	SER	2.9
3	P	362	GLN	2.9
1	H	16	GLY	2.9
1	E	72	ARG	2.9
1	H	2	VAL	2.9
2	B	134	CYS	2.9
3	Y	318	GLU	2.9
3	O	251	LEU	2.9
3	O	398	LEU	2.9
2	F	27	GLN	2.9
2	F	63	SER	2.9
2	K	14	SER	2.9
3	N	424	SER	2.9
3	X	281	GLY	2.9
3	P	385	GLY	2.9
1	A	168	ALA	2.9
3	P	289	THR	2.9
1	A	222	GLU	2.9
1	E	222	GLU	2.9
2	G	123	GLU	2.9
2	F	148	TRP	2.9
2	C	107	LYS	2.9
2	L	134	CYS	2.9
1	A	100	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
3	Y	342	GLN	2.9
3	O	291	PRO	2.9
1	E	174	HIS	2.9
2	B	118	PHE	2.9
3	P	383	SER	2.9
1	M	200	GLY	2.9
2	L	159	SER	2.9
3	X	444	SER	2.9
2	F	92	ALA	2.9
3	P	326	LYS	2.9
2	G	10	THR	2.9
2	G	195	GLU	2.9
3	J	382	GLU	2.9
3	X	264	VAL	2.9
2	B	5	THR	2.9
3	J	352	PRO	2.9
1	E	162	VAL	2.9
3	N	253	ILE	2.9
1	I	190	SER	2.9
1	I	31	ALA	2.9
1	H	8	GLY	2.9
1	M	16	GLY	2.9
3	O	345	GLU	2.9
1	E	24	VAL	2.9
2	C	100	GLN	2.9
3	J	310	HIS	2.9
3	X	240	VAL	2.9
1	E	187	SER	2.8
2	L	211	ARG	2.8
3	N	324	SER	2.8
2	F	138	ASN	2.8
1	I	161	THR	2.8
2	B	32	TRP	2.8
2	F	153	ALA	2.8
1	H	137	SER	2.8
3	J	269	GLU	2.8
3	X	334	LYS	2.8
2	K	31	THR	2.8
2	G	94	TYR	2.8
3	O	413	ASP	2.8
1	E	71	SER	2.8
3	P	324	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	2	VAL	2.8
2	C	196	VAL	2.8
1	I	117	THR	2.8
1	I	201	THR	2.8
1	H	145	THR	2.8
2	G	199	GLN	2.8
2	L	79	GLN	2.8
3	X	327	ALA	2.8
2	G	168	SER	2.8
2	L	196	VAL	2.8
1	D	193	THR	2.8
1	I	215	THR	2.8
3	P	438	GLN	2.8
3	N	309	LEU	2.8
3	Y	334	LYS	2.8
2	L	119	PRO	2.8
1	I	46	GLU	2.8
2	L	178	THR	2.8
3	N	393	THR	2.8
3	N	326	LYS	2.8
1	D	9	GLY	2.8
3	X	323	VAL	2.8
2	G	127	SER	2.8
2	F	199	GLN	2.8
3	O	342	GLN	2.8
3	O	418	GLN	2.8
3	X	390	ASN	2.8
3	Y	310	HIS	2.8
2	B	125	LEU	2.8
3	J	264	VAL	2.8
3	P	249	ASP	2.8
2	G	30	GLU	2.8
3	N	354	SER	2.8
1	D	4	LEU	2.7
2	F	98	PHE	2.7
2	B	112	ALA	2.7
2	F	144	ALA	2.7
3	Y	439	LYS	2.7
1	E	199	LEU	2.7
1	E	5	VAL	2.7
2	B	87	HIS	2.7
1	D	128	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	145	THR	2.7
2	G	178	THR	2.7
3	Y	250	THR	2.7
2	K	142	ARG	2.7
3	O	271	PRO	2.7
3	N	406	LEU	2.7
3	O	380	GLU	2.7
1	E	182	SER	2.7
1	M	54	SER	2.7
2	B	52	SER	2.7
3	J	324	SER	2.7
1	M	174	HIS	2.7
1	I	58	ARG	2.7
2	F	77	GLY	2.7
1	A	74	ASP	2.7
1	H	129	PRO	2.7
3	X	331	PRO	2.7
3	O	276	ASN	2.7
2	K	50	LYS	2.7
3	X	309	LEU	2.7
2	G	150	VAL	2.7
3	P	294	GLN	2.7
2	K	95	SER	2.7
3	O	383	SER	2.7
2	L	66	GLY	2.7
1	E	177	PRO	2.7
2	G	5	THR	2.7
3	X	359	THR	2.7
2	K	194	CYS	2.7
3	X	306	LEU	2.7
3	Y	376	ASP	2.7
1	D	34	MET	2.7
2	L	186	TYR	2.7
2	F	62	PHE	2.7
2	L	165	GLU	2.7
3	Y	427	VAL	2.7
1	H	224	LYS	2.7
2	G	148	TRP	2.7
2	L	76	SER	2.7
3	Y	274	LYS	2.7
3	Y	326	LYS	2.7
2	C	204	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	11	LEU	2.7
3	X	344	ARG	2.7
3	O	349	TYR	2.7
3	X	419	GLN	2.7
2	C	78	LEU	2.7
3	X	244	PRO	2.7
3	X	254	SER	2.7
3	P	257	PRO	2.7
2	B	197	THR	2.7
1	I	26	ASN	2.7
1	I	165	ASN	2.7
3	N	292	ARG	2.7
1	I	150	CYS	2.7
3	P	274	LYS	2.7
2	B	33	LEU	2.7
1	D	54	SER	2.7
3	J	257	PRO	2.7
3	X	417	TRP	2.7
3	Y	324	SER	2.7
3	P	387	PRO	2.7
1	H	97	ALA	2.7
2	G	25	ALA	2.7
1	I	59	ASP	2.6
1	M	218	ASP	2.6
2	G	49	TYR	2.6
3	J	439	LYS	2.6
1	E	15	GLY	2.6
3	P	352	PRO	2.6
1	H	113	TRP	2.6
1	I	205	ILE	2.6
2	B	14	SER	2.6
2	G	60	SER	2.6
1	D	175	THR	2.6
1	E	203	THR	2.6
2	F	197	THR	2.6
1	M	62	ASP	2.6
2	G	186	TYR	2.6
1	E	9	GLY	2.6
3	J	331	PRO	2.6
2	B	63	SER	2.6
3	X	394	THR	2.6
3	X	314	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	P	376	ASP	2.6
1	A	16	GLY	2.6
2	C	79	GLN	2.6
2	C	155	GLN	2.6
3	J	386	GLN	2.6
1	E	146	ALA	2.6
3	N	428	MET	2.6
3	Y	238	PRO	2.6
3	P	245	PRO	2.6
2	C	163	VAL	2.6
3	Y	273	VAL	2.6
2	C	208	SER	2.6
2	K	12	SER	2.6
3	J	426	SER	2.6
2	K	102	THR	2.6
2	G	70	GLU	2.6
3	N	438	GLN	2.6
3	O	293	GLU	2.6
1	D	123	PRO	2.6
1	H	195	PRO	2.6
2	G	24	ARG	2.6
2	L	8	PRO	2.6
3	J	297	ASN	2.6
1	A	211	LYS	2.6
2	F	126	LYS	2.6
2	L	146	VAL	2.6
3	N	379	VAL	2.6
1	A	104	LEU	2.6
1	M	45	LEU	2.6
3	O	242	LEU	2.6
1	M	197	SER	2.6
2	K	52	SER	2.6
1	H	96	CYS	2.6
3	Y	255	ARG	2.6
1	D	216	LYS	2.6
2	G	145	LYS	2.6
3	O	246	LYS	2.6
2	L	148	TRP	2.6
3	Y	251	LEU	2.6
1	I	145	THR	2.6
2	G	76	SER	2.6
3	Y	298	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	G	117	ILE	2.6
1	E	178	ALA	2.6
3	O	257	PRO	2.6
2	F	32	TRP	2.6
1	M	15	GLY	2.6
2	L	94	TYR	2.6
1	A	190	SER	2.6
2	F	190	LYS	2.6
2	G	72	THR	2.6
2	L	10	THR	2.6
3	J	350	THR	2.6
3	N	442	SER	2.6
3	N	395	PRO	2.6
3	Y	311	GLN	2.6
2	K	80	PHE	2.6
1	A	209	ASN	2.5
1	D	113	TRP	2.5
2	C	35	TRP	2.5
2	L	32	TRP	2.5
2	L	144	ALA	2.5
1	E	59	ASP	2.5
3	Y	265	ASP	2.5
3	O	333	GLU	2.5
3	P	272	GLN	2.5
1	A	132	PHE	2.5
1	E	224	LYS	2.5
3	Y	320	LYS	2.5
3	P	334	LYS	2.5
2	F	64	GLY	2.5
3	O	427	VAL	2.5
2	K	4	MET	2.5
2	F	51	ALA	2.5
1	D	11	LEU	2.5
1	E	145	THR	2.5
1	I	148	LEU	2.5
1	H	17	SER	2.5
1	M	7	SER	2.5
3	J	250	THR	2.5
3	J	283	GLN	2.5
2	G	143	GLU	2.5
3	X	243	PHE	2.5
3	Y	269	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	96	CYS	2.5
3	N	363	VAL	2.5
1	D	203	THR	2.5
1	M	76	GLU	2.5
2	F	65	SER	2.5
2	L	7	SER	2.5
1	E	102	ASP	2.5
1	E	113	TRP	2.5
3	O	343	PRO	2.5
3	N	439	LYS	2.5
3	X	307	THR	2.5
3	P	440	SER	2.5
3	P	309	LEU	2.5
1	M	115	PRO	2.5
3	X	274	LYS	2.5
1	E	6	GLU	2.5
2	C	88	CYS	2.5
1	E	197	SER	2.5
3	N	413	ASP	2.5
3	O	426	SER	2.5
1	I	29	ILE	2.5
2	B	133	VAL	2.5
2	B	196	VAL	2.5
1	D	151	LEU	2.5
2	C	11	LEU	2.5
2	B	211	ARG	2.5
3	N	323	VAL	2.5
1	E	168	ALA	2.5
2	B	62	PHE	2.5
2	K	24	ARG	2.5
2	K	148	TRP	2.5
3	O	416	ARG	2.5
2	B	73	LEU	2.4
2	F	20	THR	2.4
1	H	83	MET	2.4
1	M	102	ASP	2.4
2	K	103	ARG	2.4
1	I	8	GLY	2.4
3	N	318	GLU	2.4
3	Y	341	GLY	2.4
2	B	10	THR	2.4
2	G	69	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	Y	287	ALA	2.4
2	G	83	PHE	2.4
1	E	195	PRO	2.4
3	Y	321	CYS	2.4
3	Y	329	PRO	2.4
2	K	107	LYS	2.4
3	O	252	MET	2.4
3	P	322	LYS	2.4
2	C	158	ASN	2.4
3	O	361	ASN	2.4
2	B	186	TYR	2.4
2	F	178	THR	2.4
2	K	20	THR	2.4
3	X	260	THR	2.4
3	O	327	ALA	2.4
1	E	7	SER	2.4
1	I	183	SER	2.4
2	C	63	SER	2.4
3	N	239	SER	2.4
3	J	387	PRO	2.4
2	C	115	VAL	2.4
3	J	417	TRP	2.4
2	C	169	LYS	2.4
3	N	290	LYS	2.4
1	M	112	ALA	2.4
2	B	24	ARG	2.4
3	N	405	PHE	2.4
1	E	54	SER	2.4
3	Y	352	PRO	2.4
2	K	2	VAL	2.4
2	G	93	GLY	2.4
3	X	341	GLY	2.4
2	K	13	ALA	2.4
3	N	327	ALA	2.4
3	X	325	ASN	2.4
3	P	437	THR	2.4
1	H	123	PRO	2.4
3	Y	315	ASP	2.4
2	F	15	VAL	2.4
3	O	240	VAL	2.4
3	O	348	VAL	2.4
1	E	65	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	M	187	SER	2.4
2	K	127	SER	2.4
2	C	211	ARG	2.4
2	L	41	GLY	2.4
1	I	1	GLU	2.4
1	M	63	ALA	2.4
1	D	53	THR	2.4
1	H	126	THR	2.4
2	K	35	TRP	2.4
3	J	314	LEU	2.4
3	P	432	LEU	2.4
1	M	217	VAL	2.4
3	Y	348	VAL	2.4
2	B	194	CYS	2.4
2	G	97	THR	2.4
2	B	122	ASP	2.4
1	H	187	SER	2.4
3	X	304	SER	2.4
3	X	313	TRP	2.3
1	E	118	VAL	2.3
1	I	80	TYR	2.3
3	O	439	LYS	2.3
3	P	240	VAL	2.3
3	P	244	PRO	2.3
2	F	61	ARG	2.3
1	E	26	ASN	2.3
1	I	42	GLY	2.3
1	H	100	GLY	2.3
2	C	194	CYS	2.3
2	G	66	GLY	2.3
2	G	128	GLY	2.3
3	X	425	CYS	2.3
3	O	367	CYS	2.3
2	L	174	SER	2.3
3	P	386	GLN	2.3
2	F	175	LEU	2.3
3	X	392	LYS	2.3
1	D	194	VAL	2.3
1	E	208	VAL	2.3
2	B	189	HIS	2.3
3	N	293	GLU	2.3
2	G	8	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
3	J	396	PRO	2.3
1	I	128	GLY	2.3
3	J	376	ASP	2.3
3	O	428	MET	2.3
3	X	369	VAL	2.3
1	M	204	TYR	2.3
3	N	352	PRO	2.3
1	E	200	GLY	2.3
2	C	179	LEU	2.3
3	Y	393	THR	2.3
3	O	322	LYS	2.3
1	E	214	ASN	2.3
1	H	26	ASN	2.3
3	N	243	PHE	2.3
3	X	361	ASN	2.3
3	X	386	GLN	2.3
3	Y	434	ASN	2.3
3	O	286	ASN	2.3
2	G	2	VAL	2.3
3	X	279	VAL	2.3
1	D	76	GLU	2.3
1	A	127	LYS	2.3
1	D	42	GLY	2.3
1	D	153	LYS	2.3
2	C	64	GLY	2.3
1	M	201	THR	2.3
2	G	96	ALA	2.3
2	F	80	PHE	2.3
2	L	58	VAL	2.3
3	J	363	VAL	2.3
3	N	263	VAL	2.3
1	M	30	SER	2.3
2	G	95	SER	2.3
2	K	9	SER	2.3
1	H	133	PRO	2.3
2	G	181	LEU	2.3
3	X	427	VAL	2.3
1	A	113	TRP	2.3
1	I	209	ASN	2.3
2	C	32	TRP	2.3
1	M	46	GLU	2.3
1	M	169	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	358	MET	2.3
3	Y	405	PHE	2.3
1	H	56	THR	2.3
2	G	211	ARG	2.3
2	L	197	THR	2.3
1	D	164	TRP	2.3
2	B	95	SER	2.3
3	N	345	GLU	2.3
3	Y	440	SER	2.3
3	P	333	GLU	2.3
1	D	178	ALA	2.3
3	X	287	ALA	2.3
2	B	160	GLN	2.2
2	G	122	ASP	2.2
2	C	86	TYR	2.2
2	F	154	LEU	2.2
1	H	35	ASN	2.2
1	E	172	GLY	2.2
2	L	168	SER	2.2
3	P	400	SER	2.2
3	P	327	ALA	2.2
1	E	51	ILE	2.2
1	D	33	THR	2.2
1	M	126	THR	2.2
2	G	113	PRO	2.2
3	N	346	PRO	2.2
3	Y	252	MET	2.2
2	C	143	GLU	2.2
1	D	168	ALA	2.2
3	N	440	SER	2.2
3	X	355	ARG	2.2
3	X	372	PHE	2.2
3	Y	276	ASN	2.2
1	I	72	ARG	2.2
2	G	65	SER	2.2
3	O	442	SER	2.2
2	F	42	LYS	2.2
2	G	149	LYS	2.2
3	O	311	GLN	2.2
1	I	223	PRO	2.2
3	Y	335	THR	2.2
3	X	367	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	Y	333	GLU	2.2
3	J	372	PHE	2.2
2	B	126	LYS	2.2
2	K	46	LEU	2.2
3	J	271	PRO	2.2
3	Y	428	MET	2.2
1	D	126	THR	2.2
3	O	280	ASP	2.2
1	E	64	VAL	2.2
1	I	100	GLY	2.2
3	X	378	ALA	2.2
3	J	288	LYS	2.2
1	A	169	LEU	2.2
1	H	75	LEU	2.2
3	Y	337	SER	2.2
1	I	129	PRO	2.2
1	A	201	THR	2.2
2	C	178	THR	2.2
3	O	317	LYS	2.2
1	A	54	SER	2.2
1	D	171	SER	2.2
1	I	54	SER	2.2
3	N	400	SER	2.2
3	P	267	SER	2.2
2	C	199	GLN	2.2
2	G	100	GLN	2.2
3	X	407	TYR	2.2
3	O	295	GLN	2.2
2	C	21	ILE	2.2
3	J	279	VAL	2.2
2	B	25	ALA	2.2
2	C	5	THR	2.2
3	N	277	TRP	2.2
3	Y	277	TRP	2.2
2	C	159	SER	2.2
2	K	115	VAL	2.2
3	P	255	ARG	2.2
1	M	127	LYS	2.2
2	B	117	ILE	2.2
1	A	9	GLY	2.2
3	O	328	LEU	2.2
1	E	158	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	O	318	GLU	2.2
2	G	15	VAL	2.1
3	J	259	VAL	2.1
2	K	79	GLN	2.1
2	L	128	GLY	2.1
3	P	406	LEU	2.1
2	F	72	THR	2.1
2	F	58	VAL	2.1
3	J	360	LYS	2.1
3	X	340	LYS	2.1
3	Y	331	PRO	2.1
1	D	214	ASN	2.1
1	I	189	SER	2.1
2	C	111	ALA	2.1
2	F	156	SER	2.1
3	P	239	SER	2.1
1	E	91	THR	2.1
2	F	69	THR	2.1
3	Y	307	THR	2.1
1	I	153	LYS	2.1
3	N	255	ARG	2.1
3	P	308	VAL	2.1
2	L	48	ILE	2.1
1	D	16	GLY	2.1
1	E	27	PHE	2.1
1	M	178	ALA	2.1
3	X	438	GLN	2.1
1	E	101	SER	2.1
1	H	122	SER	2.1
2	C	28	SER	2.1
2	F	174	SER	2.1
3	O	297	ASN	2.1
2	F	164	THR	2.1
3	X	333	GLU	2.1
2	G	115	VAL	2.1
2	L	150	VAL	2.1
1	A	41	PRO	2.1
2	K	98	PHE	2.1
3	Y	291	PRO	2.1
3	O	309	LEU	2.1
1	D	146	ALA	2.1
2	G	112	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	283	GLN	2.1
3	X	316	GLY	2.1
3	X	371	GLY	2.1
3	X	391	TYR	2.1
3	Y	400	SER	2.1
3	O	324	SER	2.1
2	B	35	TRP	2.1
1	I	56	THR	2.1
2	F	19	ILE	2.1
2	K	10	THR	2.1
3	O	422	VAL	2.1
1	A	199	LEU	2.1
1	M	104	LEU	2.1
1	E	63	ALA	2.1
2	K	173	TYR	2.1
3	J	327	ALA	2.1
3	J	371	GLY	2.1
3	P	298	SER	2.1
2	C	135	LEU	2.1
2	C	148	TRP	2.1
2	L	195	GLU	2.1
1	M	33	THR	2.1
2	G	185	ASP	2.1
1	A	147	ALA	2.1
2	F	194	CYS	2.1
1	M	194	VAL	2.1
1	M	198	SER	2.1
2	C	156	SER	2.1
2	F	12	SER	2.1
3	Y	363	VAL	2.1
3	Y	442	SER	2.1
3	P	252	MET	2.1
3	P	263	VAL	2.1
1	A	66	GLY	2.1
2	F	66	GLY	2.1
3	N	331	PRO	2.1
3	X	353	PRO	2.1
3	O	353	PRO	2.1
3	N	362	GLN	2.1
1	E	96	CYS	2.0
3	X	273	VAL	2.0
2	C	154	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	Y	261	CYS	2.0
1	M	101	SER	2.0
2	K	26	SER	2.0
3	X	435	HIS	2.0
1	E	218	ASP	2.0
1	H	115	PRO	2.0
1	M	123	PRO	2.0
2	F	16	GLY	2.0
2	K	206	THR	2.0
3	X	315	ASP	2.0
3	P	316	GLY	2.0
2	L	24	ARG	2.0
3	P	311	GLN	2.0
2	G	163	VAL	2.0
3	O	441	LEU	2.0
2	C	174	SER	2.0
2	K	161	GLU	2.0
3	Y	424	SER	2.0
1	H	223	PRO	2.0
2	F	43	ALA	2.0
2	L	35	TRP	2.0
3	X	381	TRP	2.0
3	N	325	ASN	2.0
2	C	85	THR	2.0
2	F	56	THR	2.0
3	O	401	ASP	2.0
3	J	347	GLN	2.0
3	O	347	GLN	2.0
2	C	181	LEU	2.0
2	F	117	ILE	2.0
3	O	443	LEU	2.0
1	M	219	LYS	2.0
3	Y	243	PHE	2.0
1	A	58	ARG	2.0
1	I	6	GLU	2.0
2	F	123	GLU	2.0
2	F	212	GLY	2.0
3	J	300	TYR	2.0
2	B	132	VAL	2.0
3	J	274	LYS	2.0
1	M	147	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.