



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 06:18 PM UTC

PDB ID : 4NHG / pdb_00004nhg
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:

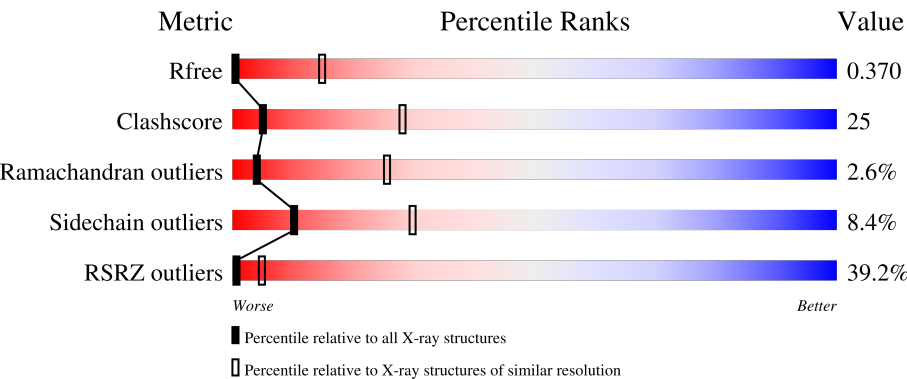
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1168 (11.50-4.00)
Clashscore	190562	1001 (11.50-4.06)
Ramachandran outliers	187476	1055 (11.50-4.00)
Sidechain outliers	187428	1018 (11.50-4.00)
RSRZ outliers	180081	1162 (11.50-4.00)

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	28% 47% 35% 6% 12%
1	D	243	28% 47% 34% 7% 12%
1	E	243	42% 48% 33% 7% 12%
1	H	243	22% 46% 37% 6% 12%
1	I	243	33% 45% 37% 6% 12%

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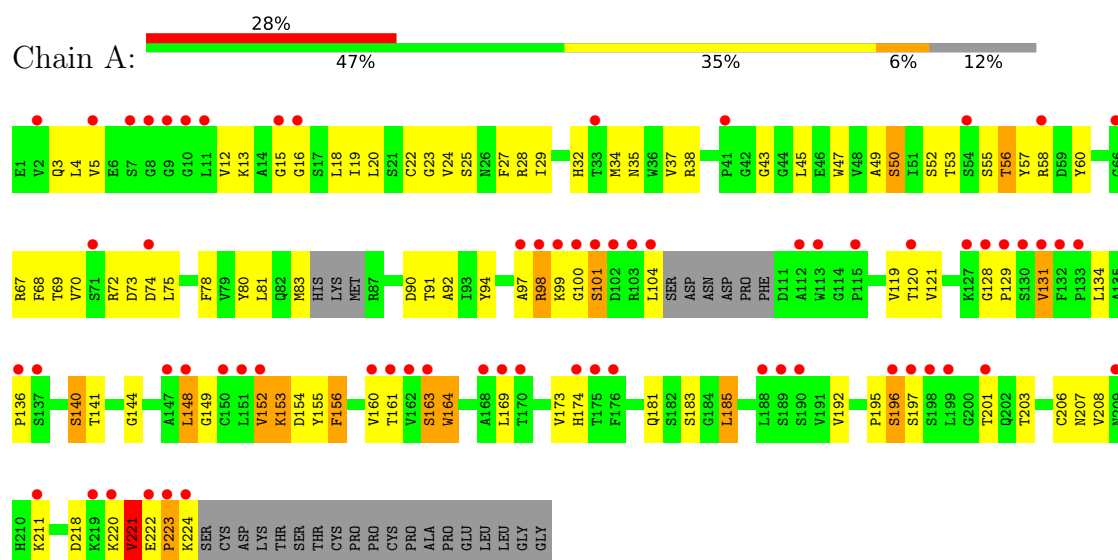
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Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	conflict	UNP Q6PYX1
O	448	GLY	-	expression tag	UNP Q6PYX1
P	272	GLN	GLU	conflict	UNP Q6PYX1
P	283	GLN	GLU	conflict	UNP Q6PYX1
P	294	GLN	GLU	conflict	UNP Q6PYX1
P	312	ASN	ASP	conflict	UNP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

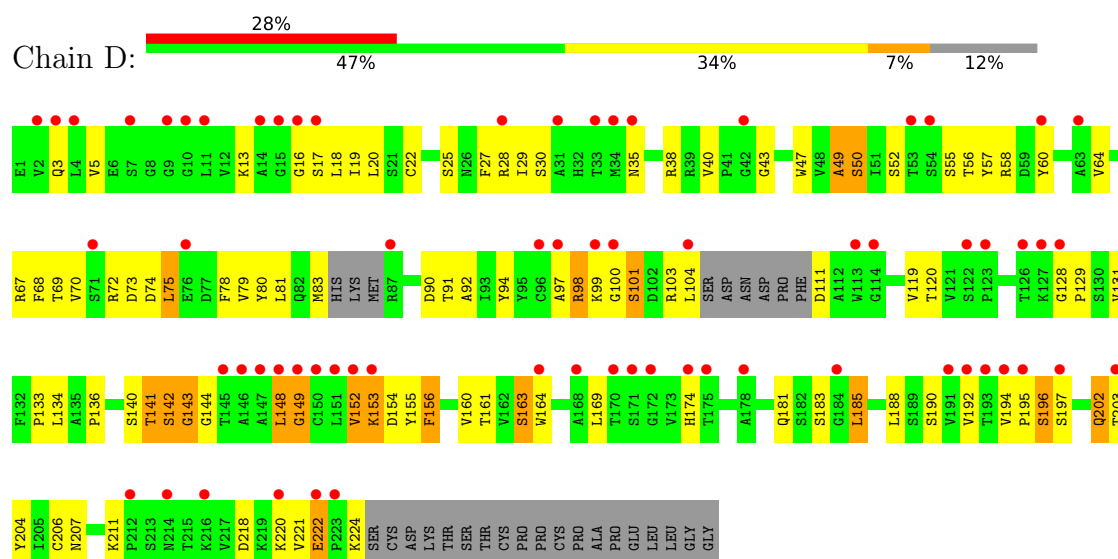
3 Residue-property plots [i](#)

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.

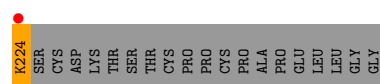
- Molecule 1: 2G12 IgG dimer heavy chain



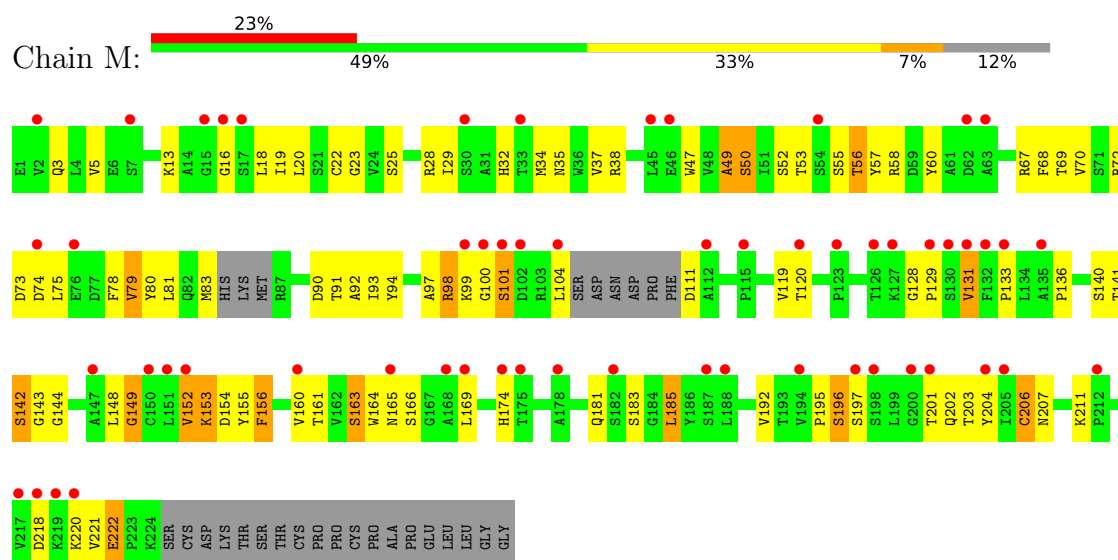
- Molecule 1: 2G12 IgG dimer heavy chain



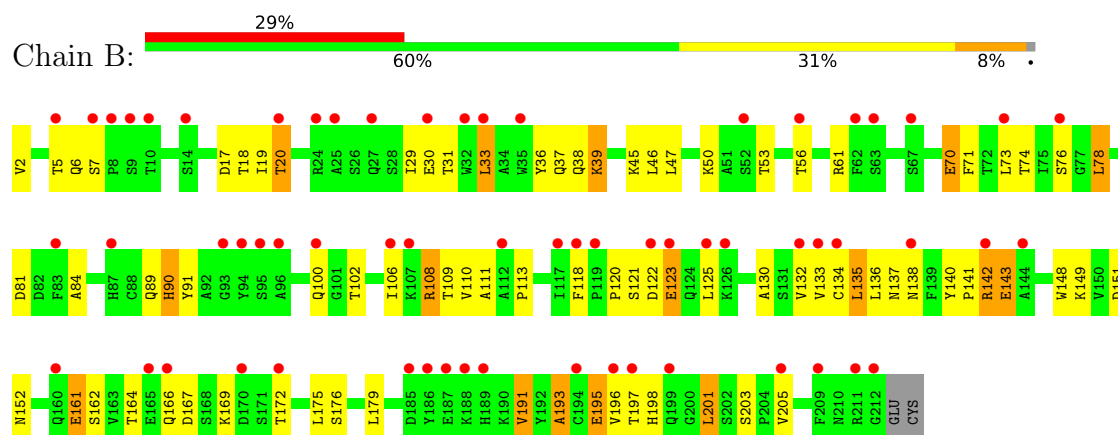
- Molecule 1: 2G12 IgG dimer heavy chain



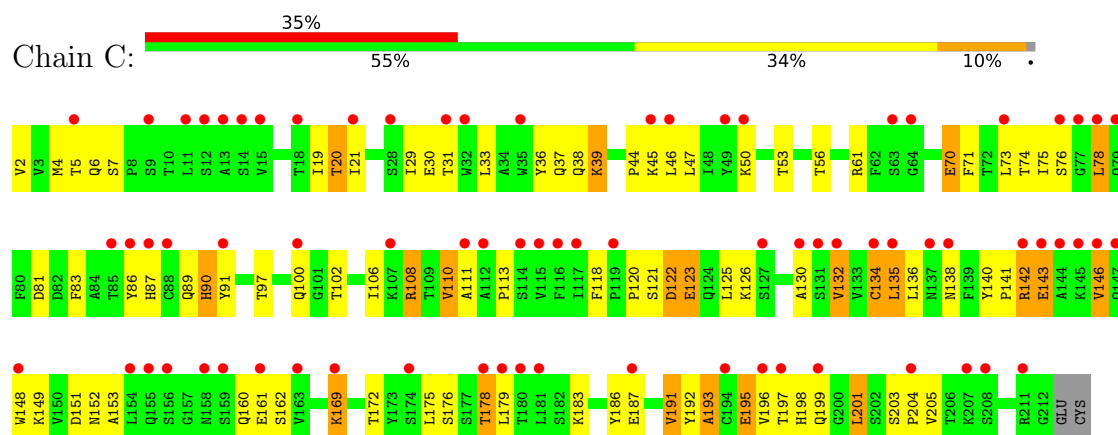
• Molecule 1: 2G12 IgG dimer heavy chain



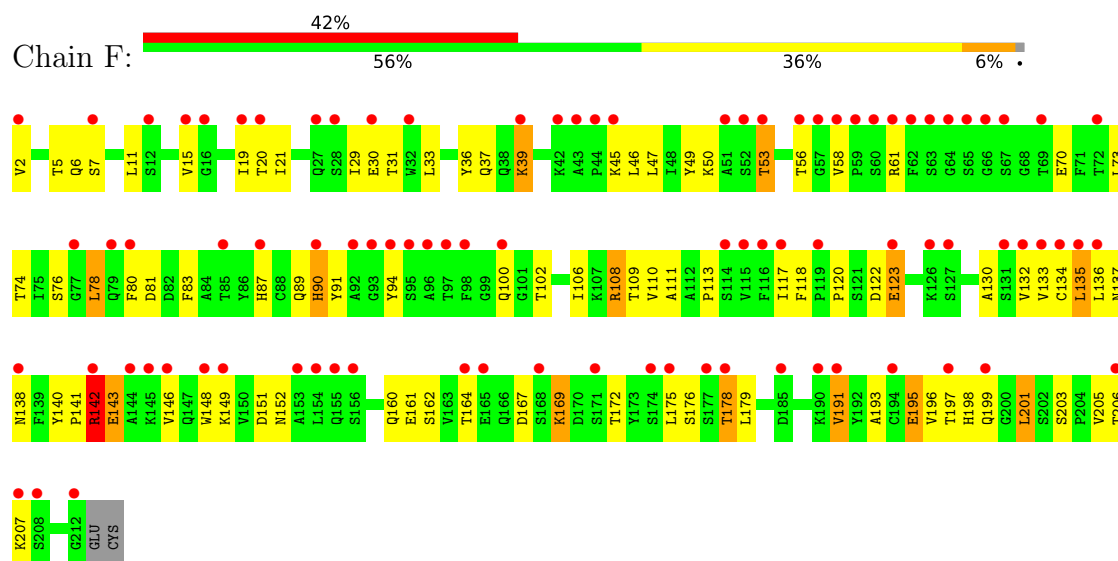
• Molecule 2: 2G12 IgG dimer light chain



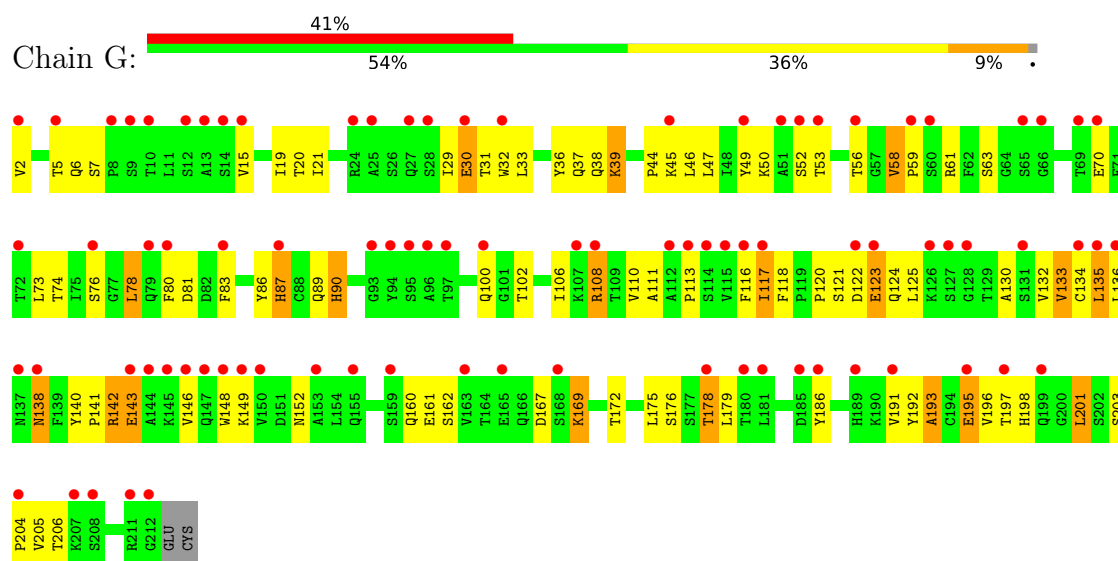
• Molecule 2: 2G12 IgG dimer light chain



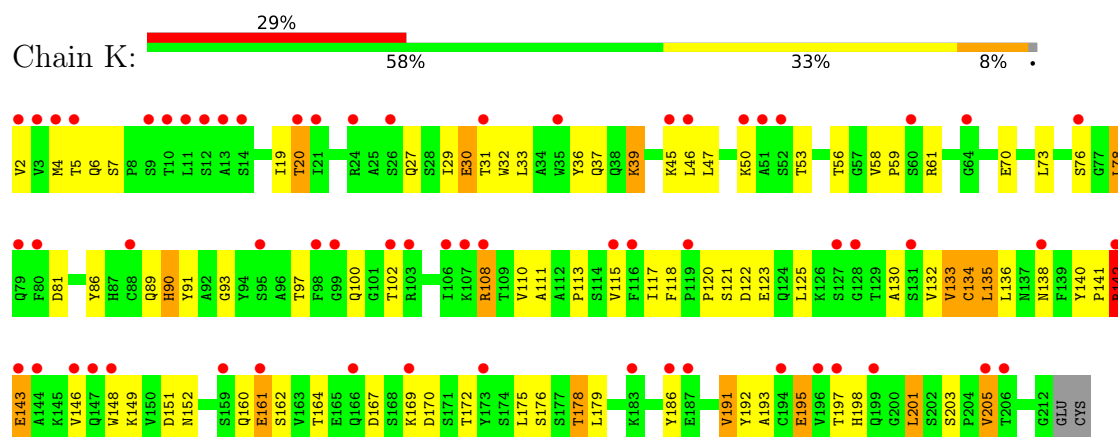
• Molecule 2: 2G12 IgG dimer light chain



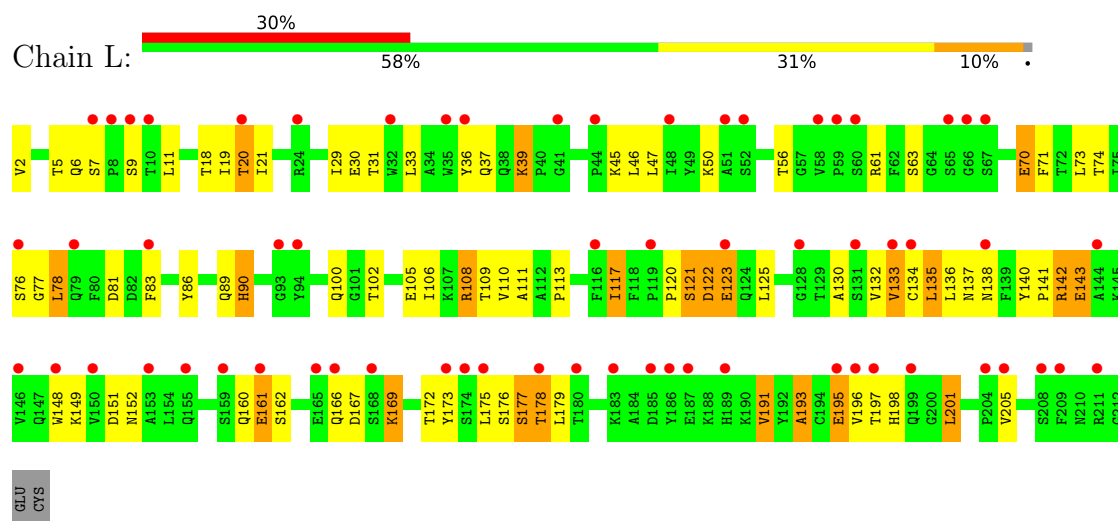
• Molecule 2: 2G12 IgG dimer light chain



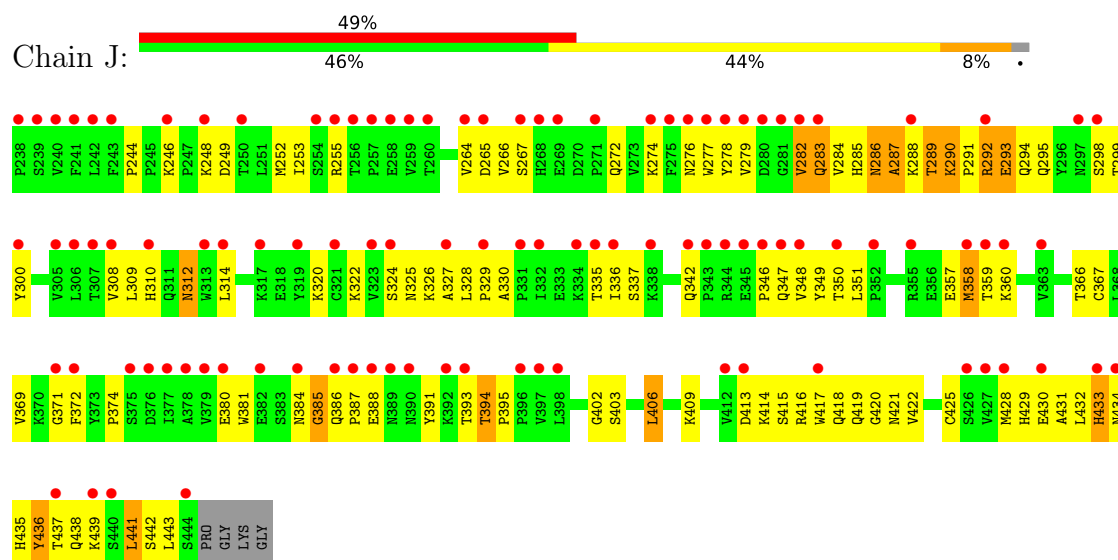
• Molecule 2: 2G12 IgG dimer light chain



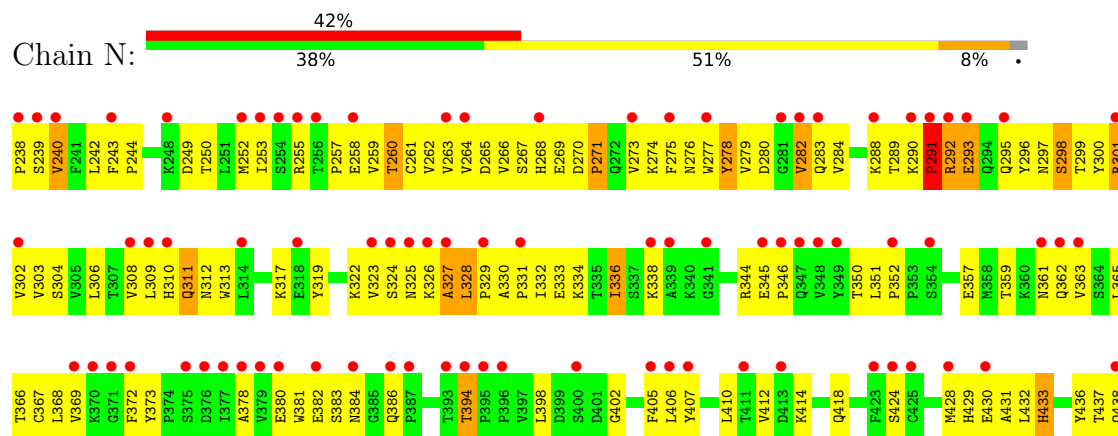
• Molecule 2: 2G12 IgG dimer light chain

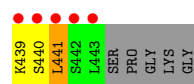


• Molecule 3: Hepatitis B virus receptor binding protein

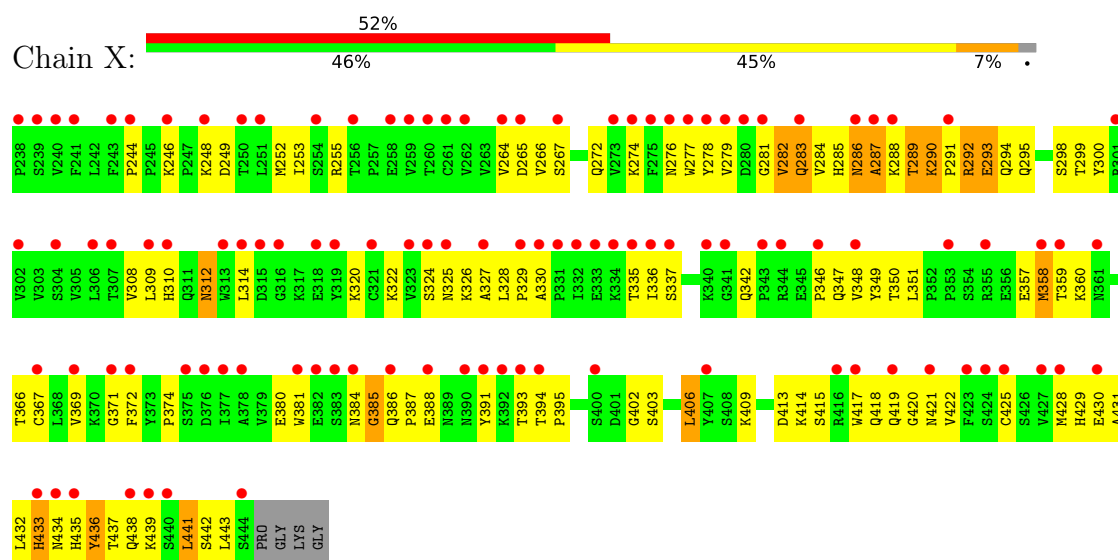


• Molecule 3: Hepatitis B virus receptor binding protein





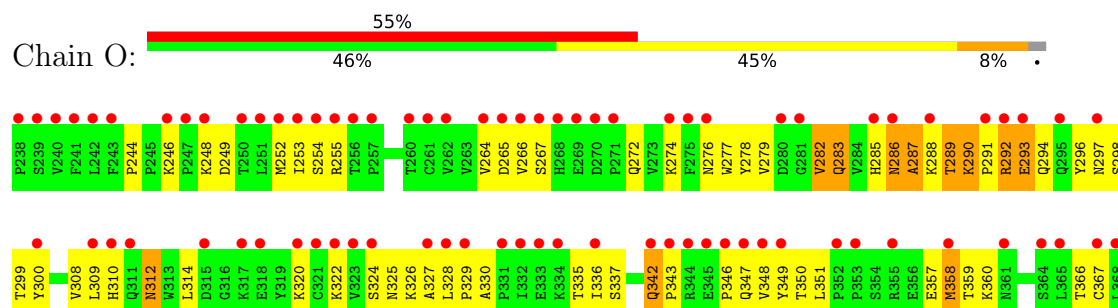
• Molecule 3: Hepatitis B virus receptor binding protein

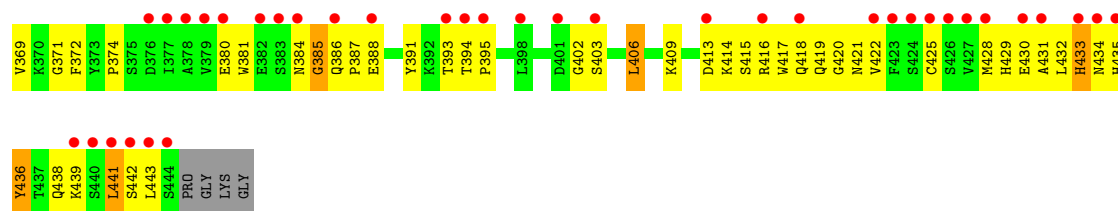


• Molecule 3: Hepatitis B virus receptor binding protein

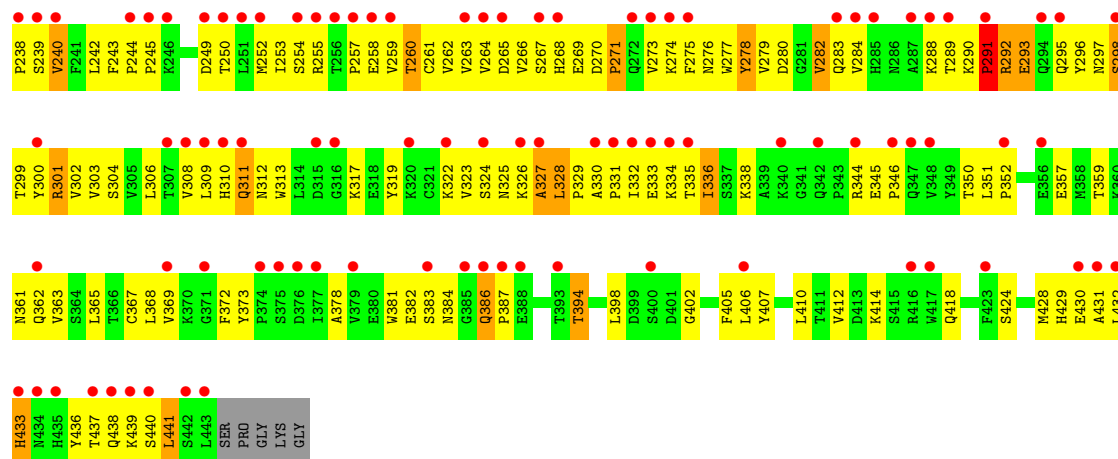


• Molecule 3: Hepatitis B virus receptor binding protein





● 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	1334 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	0.96	3/1633 (0.2%)	1.27	18/2220 (0.8%)
1	D	0.86	0/1631	1.20	11/2214 (0.5%)
1	E	0.95	2/1633 (0.1%)	1.25	13/2220 (0.6%)
1	H	0.88	3/1633 (0.2%)	1.22	14/2220 (0.6%)
1	I	0.95	0/1631	1.24	16/2214 (0.7%)
1	M	0.91	1/1631 (0.1%)	1.24	12/2214 (0.5%)
2	B	0.89	3/1654 (0.2%)	1.10	10/2246 (0.4%)
2	C	1.02	3/1654 (0.2%)	1.14	14/2246 (0.6%)
2	F	1.03	6/1654 (0.4%)	1.13	12/2246 (0.5%)
2	G	1.01	7/1654 (0.4%)	1.12	15/2246 (0.7%)
2	K	0.93	3/1654 (0.2%)	1.13	11/2246 (0.5%)
2	L	0.94	4/1654 (0.2%)	1.12	14/2246 (0.6%)
3	J	0.52	0/1706	1.02	8/2323 (0.3%)
3	N	0.73	2/1699 (0.1%)	1.02	9/2312 (0.4%)
3	O	0.52	0/1706	1.02	6/2323 (0.3%)
3	P	0.73	2/1699 (0.1%)	1.02	9/2312 (0.4%)
3	X	0.52	0/1706	1.02	6/2323 (0.3%)
3	Y	0.73	2/1699 (0.1%)	1.02	9/2312 (0.4%)
All	All	0.85	41/29931 (0.1%)	1.13	207/40683 (0.5%)

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 (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	433	HIS	CA-C	22.71	1.83	1.52
3	N	433	HIS	CA-C	22.58	1.82	1.52
3	P	433	HIS	CA-C	22.58	1.82	1.52
2	F	58	VAL	CA-C	9.34	1.59	1.52
2	L	133	VAL	CA-C	8.40	1.62	1.52
2	K	53	THR	CA-CB	8.12	1.63	1.53
2	C	53	THR	CA-CB	7.44	1.62	1.53
2	B	133	VAL	CA-C	7.22	1.60	1.52
1	A	163	SER	CA-C	6.32	1.60	1.52
3	N	433	HIS	N-CA	-6.32	1.38	1.46
2	G	87	HIS	CE1-NE2	-6.29	1.26	1.32
3	Y	433	HIS	N-CA	-6.17	1.38	1.46
3	P	433	HIS	N-CA	-6.14	1.38	1.46
2	F	133	VAL	CA-C	6.03	1.59	1.52
2	L	134	CYS	CA-C	6.01	1.59	1.53
2	G	133	VAL	CA-C	6.00	1.60	1.52
1	M	152	VAL	CA-CB	5.94	1.60	1.53
2	F	53	THR	CA-CB	5.83	1.60	1.53
1	H	132	PHE	CA-C	5.72	1.58	1.52
2	B	134	CYS	CA-C	5.70	1.58	1.53
2	C	75	ILE	CA-C	-5.68	1.45	1.52
2	K	133	VAL	CA-C	5.65	1.59	1.52
2	G	206	THR	CA-CB	5.65	1.62	1.53
1	E	193	THR	CA-CB	5.61	1.60	1.53
2	G	134	CYS	CA-C	5.58	1.58	1.53
2	B	53	THR	CA-CB	5.51	1.60	1.53
2	K	205	VAL	CA-CB	5.41	1.60	1.54
2	G	116	PHE	CA-C	5.36	1.59	1.52
2	G	133	VAL	CA-CB	5.29	1.61	1.54
1	H	152	VAL	CA-CB	5.22	1.59	1.53
2	L	133	VAL	CA-CB	5.20	1.63	1.54
1	E	64	VAL	CA-C	5.20	1.57	1.52
2	F	58	VAL	CA-CB	5.18	1.58	1.54
1	A	221	VAL	CA-CB	-5.09	1.47	1.53
2	C	134	CYS	CA-C	5.09	1.58	1.53
2	F	134	CYS	CA-C	5.08	1.58	1.53
2	L	178	THR	CA-CB	5.05	1.60	1.53
2	G	204	PRO	CA-C	5.05	1.57	1.52
1	H	152	VAL	CA-C	5.03	1.57	1.53
1	A	223	PRO	CA-C	5.02	1.59	1.52
2	F	206	THR	CA-CB	5.01	1.61	1.53

All (207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	433	HIS	N-CA-C	-10.63	94.02	109.96
3	P	433	HIS	N-CA-C	-10.62	94.03	109.96
3	N	433	HIS	N-CA-C	-10.62	94.04	109.96
1	A	28	ARG	NE-CZ-NH1	-9.77	111.73	121.50
1	H	28	ARG	NE-CZ-NH1	-9.52	111.98	121.50
1	A	28	ARG	NE-CZ-NH2	9.29	127.56	119.20
1	I	222	GLU	CA-C-N	9.25	130.71	119.98
1	I	222	GLU	C-N-CA	9.25	130.71	119.98
1	E	28	ARG	NE-CZ-NH1	-8.98	112.52	121.50
1	E	149	GLY	N-CA-C	8.93	124.09	110.88
1	E	28	ARG	NE-CZ-NH2	8.86	127.17	119.20
1	D	222	GLU	CA-C-N	8.72	130.74	119.84
1	D	222	GLU	C-N-CA	8.72	130.74	119.84
1	I	149	GLY	N-CA-C	8.48	123.43	110.88
1	A	222	GLU	CA-C-N	8.17	130.05	119.84
1	A	222	GLU	C-N-CA	8.17	130.05	119.84
1	H	28	ARG	NE-CZ-NH2	8.15	126.54	119.20
1	H	149	GLY	N-CA-C	7.95	122.64	110.88
3	N	433	HIS	CB-CA-C	-7.89	97.26	109.89
3	Y	433	HIS	CB-CA-C	-7.88	97.27	109.89
3	P	433	HIS	CB-CA-C	-7.85	97.33	109.89
1	E	28	ARG	CD-NE-CZ	7.64	135.09	124.40
3	X	402	GLY	N-CA-C	-7.63	104.51	115.27
1	D	141	THR	N-CA-C	7.59	120.11	110.24
3	J	402	GLY	N-CA-C	-7.59	104.57	115.27
3	O	402	GLY	N-CA-C	-7.57	104.59	115.27
1	D	149	GLY	N-CA-C	7.57	122.08	110.88
1	A	149	GLY	N-CA-C	7.52	122.01	110.88
1	M	141	THR	N-CA-C	7.33	120.62	110.35
1	A	28	ARG	CD-NE-CZ	7.33	134.66	124.40
1	A	16	GLY	N-CA-C	7.31	120.37	112.33
1	M	149	GLY	N-CA-C	7.22	121.56	110.88
1	E	16	GLY	N-CA-C	7.07	120.10	112.33
1	I	141	THR	N-CA-C	6.96	120.05	110.24
1	I	153	LYS	N-CA-C	6.83	120.58	109.59
1	H	28	ARG	CD-NE-CZ	6.73	133.82	124.40
1	I	16	GLY	N-CA-C	6.70	121.12	112.54
1	M	16	GLY	N-CA-C	6.61	119.60	112.33
2	L	134	CYS	N-CA-C	6.58	118.21	107.23
1	A	153	LYS	N-CA-C	6.54	120.11	109.59
2	G	70	GLU	N-CA-C	6.52	119.04	108.34
1	E	153	LYS	N-CA-C	6.51	120.07	109.59
3	Y	386	GLN	CA-C-N	6.47	126.39	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Y	386	GLN	C-N-CA	6.47	126.39	119.85
2	G	135	LEU	CA-CB-CG	6.47	138.94	116.30
3	N	386	GLN	CA-C-N	6.46	126.38	119.85
3	N	386	GLN	C-N-CA	6.46	126.38	119.85
3	P	386	GLN	CA-C-N	6.44	126.35	119.85
3	P	386	GLN	C-N-CA	6.44	126.35	119.85
1	H	153	LYS	N-CA-C	6.37	119.85	109.59
1	H	16	GLY	N-CA-C	6.32	119.29	112.33
1	I	128	GLY	CA-C-N	6.21	128.34	120.51
1	I	128	GLY	C-N-CA	6.21	128.34	120.51
2	F	196	VAL	N-CA-C	6.21	117.73	108.23
3	P	240	VAL	N-CA-C	6.21	117.96	108.71
1	D	153	LYS	N-CA-C	6.21	119.59	109.59
3	Y	240	VAL	N-CA-C	6.21	117.96	108.71
3	N	240	VAL	N-CA-C	6.20	117.94	108.71
2	L	195	GLU	N-CA-C	6.18	119.79	107.62
2	F	135	LEU	CA-CB-CG	6.12	137.74	116.30
2	G	196	VAL	N-CA-C	6.12	117.60	108.23
2	C	75	ILE	CB-CA-C	-6.07	103.39	110.91
2	C	123	GLU	N-CA-C	-6.07	105.88	113.28
2	B	135	LEU	CA-CB-CG	6.06	137.50	116.30
2	C	196	VAL	N-CA-C	6.05	117.49	108.23
1	E	140	SER	N-CA-C	6.05	123.70	110.80
2	C	135	LEU	CA-CB-CG	6.01	137.35	116.30
2	C	178	THR	N-CA-C	6.00	118.43	109.25
1	A	128	GLY	CA-C-N	5.97	128.03	120.51
1	A	128	GLY	C-N-CA	5.97	128.03	120.51
1	A	223	PRO	N-CA-C	5.97	124.77	112.47
2	L	70	GLU	N-CA-C	5.97	118.85	108.76
2	B	134	CYS	N-CA-C	5.94	117.15	107.23
2	K	70	GLU	N-CA-C	5.89	118.00	108.34
1	M	49	ALA	N-CA-C	5.89	116.33	108.38
2	G	134	CYS	N-CA-C	5.84	116.98	107.23
1	A	164	TRP	N-CA-C	5.82	118.72	109.24
1	M	153	LYS	N-CA-C	5.82	118.95	109.59
2	F	134	CYS	N-CA-C	5.81	116.94	107.23
2	L	193	ALA	N-CA-C	5.81	119.10	109.46
1	M	222	GLU	CA-C-N	5.78	126.12	119.93
1	M	222	GLU	C-N-CA	5.78	126.12	119.93
1	H	152	VAL	N-CA-C	5.77	114.92	106.55
2	L	117	ILE	N-CA-C	5.76	116.58	108.17
2	K	135	LEU	CA-CB-CG	5.75	136.42	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	195	GLU	N-CA-C	5.72	118.90	107.62
1	M	93	ILE	CB-CA-C	-5.71	103.82	110.91
2	L	135	LEU	CA-CB-CG	5.71	136.30	116.30
1	M	128	GLY	CA-C-N	5.71	127.71	120.51
1	M	128	GLY	C-N-CA	5.71	127.71	120.51
1	D	152	VAL	N-CA-C	5.67	114.78	106.55
1	H	128	GLY	CA-C-N	5.66	127.64	120.51
1	H	128	GLY	C-N-CA	5.66	127.64	120.51
3	X	342	GLN	CA-C-N	5.60	127.12	120.23
3	X	342	GLN	C-N-CA	5.60	127.12	120.23
2	G	193	ALA	N-CA-C	5.59	118.74	109.46
2	L	30	GLU	CB-CA-C	-5.59	109.63	117.23
1	D	128	GLY	CA-C-N	5.57	127.52	120.51
1	D	128	GLY	C-N-CA	5.57	127.52	120.51
2	K	30	GLU	CB-CA-C	-5.56	109.67	117.23
2	F	195	GLU	N-CA-C	5.56	118.57	107.62
2	K	195	GLU	N-CA-C	5.56	118.57	107.62
1	E	152	VAL	N-CA-C	5.55	114.59	106.55
2	K	134	CYS	N-CA-C	5.54	116.48	107.23
2	K	93	GLY	N-CA-C	-5.53	105.80	112.49
2	F	199	GLN	N-CA-C	5.52	118.06	111.71
3	O	342	GLN	CA-C-N	5.52	127.02	120.23
3	O	342	GLN	C-N-CA	5.52	127.02	120.23
1	I	223	PRO	N-CA-C	5.52	119.89	110.95
2	B	30	GLU	CB-CA-C	-5.50	109.75	117.23
2	C	86	TYR	N-CA-C	5.49	117.36	108.41
2	K	115	VAL	N-CA-C	5.49	116.63	108.23
2	K	86	TYR	N-CA-C	5.48	118.02	108.76
2	B	70	GLU	N-CA-C	5.47	118.01	108.76
3	J	342	GLN	CA-C-N	5.47	126.96	120.23
3	J	342	GLN	C-N-CA	5.47	126.96	120.23
1	D	28	ARG	NE-CZ-NH2	-5.47	114.28	119.20
2	F	178	THR	N-CA-C	5.46	117.14	108.67
2	G	117	ILE	N-CA-C	5.46	116.15	108.17
1	M	131	VAL	N-CA-C	5.45	115.63	107.51
2	F	137	ASN	N-CA-C	5.45	117.11	108.67
2	B	196	VAL	N-CA-C	5.42	116.53	108.23
1	I	176	PHE	CA-C-N	5.42	125.35	119.76
1	I	176	PHE	C-N-CA	5.42	125.35	119.76
2	K	178	THR	N-CA-C	5.42	117.54	109.25
1	E	141	THR	N-CA-C	5.41	122.33	110.80
2	L	86	TYR	N-CA-C	5.40	117.21	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	15	GLY	N-CA-C	-5.39	107.91	114.92
2	L	177	SER	N-CA-C	5.38	118.27	107.41
2	G	178	THR	N-CA-C	5.37	117.47	109.25
2	C	70	GLU	N-CA-C	5.37	117.83	108.76
1	D	16	GLY	N-CA-C	5.36	119.40	112.54
1	E	128	GLY	CA-C-N	5.36	127.26	120.51
1	E	128	GLY	C-N-CA	5.36	127.26	120.51
2	G	30	GLU	CB-CA-C	-5.35	109.96	117.23
2	L	178	THR	N-CA-C	5.34	117.42	109.25
1	I	49	ALA	N-CA-C	5.34	115.58	108.38
1	E	164	TRP	N-CA-C	5.33	117.43	107.99
1	A	152	VAL	N-CA-C	5.32	114.27	106.55
2	B	123	GLU	N-CA-C	-5.32	106.79	113.28
1	A	15	GLY	N-CA-C	-5.31	108.02	114.92
1	H	122	SER	CA-C-N	5.31	124.82	119.19
1	H	122	SER	C-N-CA	5.31	124.82	119.19
2	G	58	VAL	CA-C-N	5.31	125.25	119.78
2	G	58	VAL	C-N-CA	5.31	125.25	119.78
1	I	208	VAL	N-CA-C	5.30	114.89	107.37
2	C	132	VAL	N-CA-C	5.29	115.25	107.15
2	C	134	CYS	N-CA-C	5.28	116.05	107.23
2	B	161	GLU	N-CA-C	5.27	117.89	110.14
2	F	142	ARG	N-CA-C	5.26	117.09	111.36
2	G	86	TYR	N-CA-C	5.25	116.97	108.41
2	L	123	GLU	N-CA-C	-5.25	106.88	113.28
2	F	30	GLU	CB-CA-C	-5.22	110.13	117.23
2	C	30	GLU	CB-CA-C	-5.22	110.14	117.23
3	Y	292	ARG	N-CA-C	5.20	116.33	108.07
1	A	43	GLY	N-CA-C	-5.19	108.90	115.08
3	P	292	ARG	N-CA-C	5.19	116.33	108.07
1	I	92	ALA	N-CA-C	5.19	116.03	108.14
2	L	161	GLU	N-CA-C	5.19	117.77	110.14
3	J	395	PRO	CA-C-N	-5.19	114.44	119.78
3	J	395	PRO	C-N-CA	-5.19	114.44	119.78
2	K	161	GLU	N-CA-C	5.18	117.75	110.14
1	A	92	ALA	N-CA-C	5.17	116.00	108.14
3	N	292	ARG	N-CA-C	5.17	116.29	108.07
2	C	204	PRO	N-CA-C	5.16	118.61	110.50
2	C	195	GLU	N-CA-C	5.16	117.78	107.62
2	F	70	GLU	N-CA-C	5.16	116.80	108.34
3	O	312	ASN	N-CA-C	-5.15	105.75	111.36
2	B	137	ASN	N-CA-C	5.12	116.61	108.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	138	ASN	N-CA-C	5.11	118.18	111.28
2	F	117	ILE	N-CA-C	5.11	115.63	108.17
3	O	395	PRO	CA-C-N	-5.11	114.52	119.78
3	O	395	PRO	C-N-CA	-5.11	114.52	119.78
3	J	312	ASN	N-CA-C	-5.11	105.79	111.36
3	X	395	PRO	CA-C-N	-5.11	114.52	119.78
3	X	395	PRO	C-N-CA	-5.11	114.52	119.78
2	C	146	VAL	N-CA-C	5.10	115.19	107.80
2	G	52	SER	N-CA-C	5.10	121.66	110.80
1	H	223	PRO	N-CA-C	5.10	119.31	111.21
2	G	123	GLU	N-CA-C	-5.09	107.07	113.28
1	D	49	ALA	N-CA-C	5.09	115.25	108.38
3	X	312	ASN	N-CA-C	-5.09	105.81	111.36
3	N	328	LEU	CA-C-N	5.08	124.53	119.24
3	N	328	LEU	C-N-CA	5.08	124.53	119.24
1	I	152	VAL	N-CA-C	5.08	113.91	106.55
2	L	137	ASN	N-CA-C	5.07	116.53	108.67
2	G	195	GLU	N-CA-C	5.06	117.60	107.62
3	Y	267	SER	N-CA-C	5.06	117.21	110.53
3	Y	328	LEU	CA-C-N	5.06	124.50	119.24
3	Y	328	LEU	C-N-CA	5.06	124.50	119.24
3	N	267	SER	N-CA-C	5.06	117.20	110.53
2	C	193	ALA	N-CA-C	5.05	117.84	109.46
2	L	196	VAL	N-CA-C	5.05	115.96	108.23
2	K	142	ARG	N-CA-C	5.05	116.86	111.36
3	P	267	SER	N-CA-C	5.04	117.19	110.53
2	B	193	ALA	N-CA-C	5.04	117.83	109.46
2	F	123	GLU	N-CA-C	-5.04	107.13	113.28
1	I	188	LEU	N-CA-C	5.04	117.11	108.90
1	A	131	VAL	N-CA-C	5.03	115.01	107.51
1	M	28	ARG	NE-CZ-NH2	-5.03	114.67	119.20
1	A	140	SER	N-CA-C	5.03	121.50	110.80
1	H	140	SER	N-CA-C	5.02	121.48	110.80
3	P	328	LEU	CA-C-N	5.02	124.46	119.24
3	P	328	LEU	C-N-CA	5.02	124.46	119.24
3	J	394	THR	CA-C-N	-5.01	115.22	120.38
3	J	394	THR	C-N-CA	-5.01	115.22	120.38
1	E	3	GLN	N-CA-C	5.00	117.40	109.50

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	78	0
1	D	1600	0	1579	99	11
1	E	1600	0	1581	72	0
1	H	1600	0	1580	80	2
1	I	1600	0	1578	84	0
1	M	1600	0	1579	88	0
2	B	1618	0	1580	49	23
2	C	1618	0	1580	55	0
2	F	1618	0	1580	70	0
2	G	1618	0	1580	59	2
2	K	1618	0	1580	56	0
2	L	1618	0	1580	61	19
3	J	1660	0	1632	102	60
3	N	1654	0	1627	118	37
3	O	1660	0	1630	96	19
3	P	1654	0	1624	126	37
3	X	1660	0	1632	102	56
3	Y	1654	0	1627	122	37
All	All	29250	0	28730	1428	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 25.

All (1428) 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	1.63
3:Y:433:HIS:C	3:Y:433:HIS:CA	1.83	1.50
3:P:433:HIS:C	3:P:433:HIS:CA	1.82	1.49
3:N:433:HIS:C	3:N:433:HIS:CA	1.82	1.49
1:D:103:ARG:C	2:F:50:LYS:NZ	1.79	1.37
1:D:103:ARG:CA	2:F:50:LYS:NZ	1.90	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
1:I:201:THR:HG1	1:I:202:GLN:N	1.58	0.99
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: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:204:TYR:O	1:D:221:VAL:N	2.07	0.87
3:J:290:LYS:HZ2	2:L:109:THR:HG21	1.39	0.86
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:N:433:HIS:C	3:N:433:HIS:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:433:HIS:C	3:P:433:HIS:N	2.36	0.83
3:Y:328:LEU:HD21	3:Y:332:ILE:HG13	1.59	0.83
3:O:291:PRO:C	3:O:292:ARG:HD2	2.03	0.83
3:X:291:PRO:C	3:X:292:ARG:HD2	2.03	0.83
3:Y:433:HIS:C	3:Y:433:HIS:N	2.37	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:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.82
3:N:433:HIS:C	3:N:433:HIS:CB	2.53	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
3:P:433:HIS:C	3:P:433:HIS:CB	2.53	0.81
3:Y:433:HIS:C	3:Y:433:HIS:CB	2.53	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: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:N:429:HIS:HD2	3:N:431:ALA:H	1.31	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:Y:289:THR:HG22	3:Y:290:LYS:H	1.48	0.78
1:A:207:ASN:ND2	1:A:218:ASP:OD2	2.16	0.78
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78
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:Y:263:VAL:O	3:Y:301:ARG:HA	1.84	0.78
1:D:75:LEU:HD22	1:I:57:TYR:CE1	2.19	0.77
3:O:292:ARG:O	3:O:293:GLU:HB3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:153:LYS:HG2	1:M:154:ASP:CG	2.10	0.77
1:A:153:LYS:HG2	1:A:154:ASP:CG	2.09	0.77
1:D:220:LYS:HE2	1:D:222:GLU:CD	2.10	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
1:D:103:ARG:O	2:F:50:LYS:NZ	1.96	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
1:D:153:LYS:HG2	1:D:154:ASP:CG	2.10	0.76
3:J:290:LYS:HZ2	2:L:109:THR:CG2	1.98	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
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
1:H:153:LYS:HG2	1:H:154:ASP:CG	2.11	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
3:N:252:MET:SD	3:N:428:MET:HE1	2.26	0.75
3:Y:252:MET:SD	3:Y:428:MET:HE1	2.26	0.75
1:M:91:THR:HG23	1:M:120:THR:HA	1.68	0.75
3:P:252:MET:SD	3:P:428:MET:HE1	2.26	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
1:E:153:LYS:HG2	1:E:154:ASP:CG	2.13	0.74
3:P:365:LEU:HD12	3:P:410:LEU:HD23	1.69	0.74
1:H:224:LYS:HD2	1:H:224:LYS:N	2.03	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:O:429:HIS:CD2	3:O:431:ALA:H	2.05	0.74
3:X:272:GLN:NE2	3:X:326:LYS:HD2	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:153:LYS:HG2	1:I:154:ASP:CG	2.15	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
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
3:Y:288:LYS:H	3:Y:288:LYS:HD3	1.54	0.71
3:P:288:LYS:HD3	3:P:288:LYS:H	1.54	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:L:39:LYS:NZ	2:L:81:ASP:O	2.22	0.70
2:G:39:LYS:NZ	2:G:81:ASP:O	2.20	0.70
3:J:290:LYS:NZ	2:L:109:THR:CG2	2.53	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
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:M:164:TRP:C	1:M:166:SER:H	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:290:LYS:HE3	3:P:292:ARG:HH22	1.61	0.65
3:Y:406:LEU:HD12	3:Y:406:LEU:C	2.22	0.65
3:N:406:LEU:C	3:N:406:LEU:HD12	2.22	0.65
2:F:143:GLU:OE2	2:F:143:GLU:N	2.30	0.65
2:F:149:LYS:NZ	2:F:195:GLU:OE1	2.27	0.65
1:D:154:ASP:HB3	1:D:185:LEU:HD23	1.79	0.65
1:A:136:PRO:HD3	1:A:148:LEU:HB3	1.79	0.64
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
3:P:406:LEU:HD12	3:P:406:LEU:C	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
2:C:120:PRO:HG3	2:C:130:ALA:HB1	1.81	0.63
3:J:290:LYS:NZ	2:L:109:THR:OG1	2.32	0.63
1:I:148:LEU:HB2	1:I:221:VAL:HG11	1.80	0.63
3:X:279:VAL:O	3:X:282:VAL:HG13	1.97	0.63
1:A:34:MET:SD	1:A:98:ARG:HB2	2.39	0.62
3:Y:330:ALA:HB1	3:Y:331:PRO:HD2	1.79	0.62
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.81	0.62
1:H:174:HIS:HE1	2:K:167:ASP:HB2	1.63	0.62
2:C:61:ARG:HB2	2:C:76:SER:O	1.99	0.62
3:Y:332:ILE:HG22	3:Y:333:GLU:N	2.13	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:311:GLN:H	3:P:311:GLN:CD	2.08	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:N:311:GLN:H	3:N:311:GLN:CD	2.08	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:L:149:LYS:NZ	2:L:195:GLU:OE1	2.33	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
3:Y:311:GLN:H	3:Y:311:GLN:CD	2.08	0.60
1:A:99:LYS:HG2	1:A: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:201:THR:HG1	1:M:202:GLN:N	1.99	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
2:F:29:ILE:HG21	2:F:90:HIS:HD2	1.66	0.59
1:I:154:ASP:HB3	1:I:185:LEU:HD23	1.84	0.59
3:N:325:ASN:HD22	3:N:326:LYS:H	1.51	0.59
3:P:274:LYS:HE2	3:P:276:ASN:HD21	1.67	0.59
1:D:99:LYS:HG2	1:D:100:GLY:N	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:351:LEU:C	3:N:441:LEU:HD11	2.28	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:269:GLU:HG2	3:P:269:GLU:O	2.03	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:P:351:LEU:C	3:P:441:LEU:HD11	2.28	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
3:Y:351:LEU:C	3:Y:441:LEU:HD11	2.28	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:91:THR:HG23	1:E:120:THR:HA	1.85	0.58
1:H:69:THR:C	1:H:81:LEU:HD12	2.28	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
1:M:220:LYS:C	1:M:221:VAL:HA	2.29	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
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
3:O:433:HIS:ND1	3:O:434:ASN:OD1	2.35	0.57
1:D:35:ASN:O	1:D:97:ALA:N	2.37	0.57
3:Y:279:VAL:HG23	3:Y:279:VAL:O	2.03	0.57
1:D:52:SER:O	1:D:72:ARG:NH1	2.37	0.57
1:D:75:LEU:CD1	1:I:57:TYR:CE1	2.86	0.57
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.36	0.57
3:X:286:ASN:O	3:X:287:ALA:HB2	2.03	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:436:TYR:CD1	3:J:436:TYR:C	2.84	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
1:D:69:THR:C	1:D:81:LEU:HD12	2.31	0.56
2:G:19:ILE:HG12	2:G:78:LEU:HD11	1.88	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:X:436:TYR:CD1	3:X:436:TYR:C	2.84	0.56
3:Y:328:LEU:HG	3:Y:330:ALA:O	2.05	0.56
1:H:35:ASN:OD1	1:H:50:SER:HB2	2.06	0.56
3:O:328:LEU:HD12	3:O:329:PRO:HD2	1.88	0.56
1:A:104:LEU:HD12	1:E:28:ARG:CG	2.20	0.56
1:D:129:PRO:HB3	1:D:155:TYR:HB3	1.87	0.56
2:F:120:PRO:HG3	2:F:130:ALA:HB1	1.87	0.56
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
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
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.55
3:X:418:GLN:C	3:X:420:GLY:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:K:39:LYS:NZ	2:K:81:ASP:O	2.30	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
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:249:ASP:C	3:Y:257:PRO:HG3	2.32	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:M:195:PRO:C	1:M:197:SER:H	2.14	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
3:O:418:GLN:C	3:O:420:GLY:H	2.15	0.55
3:P:249:ASP:C	3:P:257:PRO:HG3	2.32	0.55
2:F:2:VAL:HG11	2:F:90:HIS:CD2	2.42	0.55
3:J:283:GLN:C	3:J:285:HIS:N	2.63	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
1:A:45:LEU:HG	2:C:87:HIS:CE1	2.43	0.54
1:A:67:ARG:C	1:A:68:PHE:HD1	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:436:TYR:CD1	3:O:436:TYR:C	2.84	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
1:E:67:ARG:C	1:E:68:PHE:HD1	2.15	0.54
3:J:357:GLU:C	3:J:359:THR:H	2.15	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:357:GLU:C	3:O:359:THR:H	2.15	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: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
1:I:169:LEU:HD21	1:I:192:VAL:HG21	1.90	0.54
3:X:357:GLU:C	3:X:359:THR:H	2.15	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
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.54
3:X:283:GLN:C	3:X:285:HIS:N	2.62	0.54
3:O:283:GLN:CD	3:O:287:ALA:HB2	2.33	0.54
3:O:285:HIS:O	3:O:286:ASN:HB2	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:414:LYS:O	3:X:418:GLN:HG3	2.08	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
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:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.53
3:X:283:GLN:CD	3:X:287:ALA:HB2	2.34	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
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: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
1:A:69:THR:C	1:A:81:LEU:HD12	2.33	0.53
1:A:197:SER:HB3	3:X:295:GLN:CD	2.34	0.53
1:I:67:ARG:C	1:I:68:PHE:HD1	2.17	0.53
3:X:351:LEU:HB2	3:X:366:THR:HB	1.90	0.53
1:I:72:ARG:NE	1:I:74:ASP:OD1	2.34	0.53
2:F:160:GLN:O	2:F:178:THR:N	2.41	0.53
2:G:149:LYS:HB2	2:G:193:ALA:HB3	1.91	0.53
1:I:101:SER:OG	1:I:104:LEU:HA	2.09	0.53
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.53
1:A:22:CYS:O	1:A:78:PHE:HA	2.09	0.53
2:B:151:ASP:HA	2:B:191:VAL:HG12	1.90	0.53
3:O:351:LEU:HB2	3:O:366:THR:HB	1.90	0.53
2:G:149:LYS:HZ1	2:G:195:GLU:CD	2.13	0.53
2:F:140:TYR:CD2	2:F:141:PRO:HA	2.44	0.52
2:G:37:GLN:HB2	2:G:47:LEU:HD11	1.91	0.52
1:H:38:ARG:HB3	1:H:94:TYR:CE2	2.44	0.52
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:18:LEU:HB3	1:H:83:MET:HE3	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:101:SER:HB2	1:D:104:LEU:H	1.75	0.52
3:J:285:HIS:O	3:J:286:ASN:HB2	2.08	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
1:A:52:SER:O	1:A:72:ARG:NH1	2.42	0.52
1:D:67:ARG:C	1:D:68:PHE:HD1	2.18	0.52
1:E:201:THR:OG1	1:E:202:GLN:N	2.31	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
3:Y:297:ASN:O	3:Y:298:SER:HB3	2.09	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
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: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
1:H:67:ARG:C	1:H:68:PHE:HD1	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O:283:GLN:C	3:O:285:HIS:N	2.63	0.51
3:P:325:ASN:ND2	3:P:326:LYS:N	2.59	0.51
2:C:140:TYR:CD2	2:C:141:PRO:HA	2.45	0.51
1:D:58:ARG:NH1	1:D:70:VAL:O	2.43	0.51
1: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
1:E:18:LEU:HB3	1:E:83:MET:HE3	1.93	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:H:19:ILE:C	1:H:20:LEU:HD23	2.36	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:I:69:THR:C	1:I:81:LEU:HD12	2.36	0.50
3:X:294:GLN:O	3:X:300:TYR:CD1	2.65	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:69:THR:C	1:M:81:LEU:HD12	2.36	0.50
1:M:153:LYS:HG2	1:M:154:ASP:OD1	2.11	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
1:H:177:PRO:O	2:K:162:SER:OG	2.26	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:278:TYR:N	3:P:278:TYR:CD1	2.79	0.50
1:E:69:THR:C	1:E:81:LEU:HD12	2.37	0.50
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.92	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
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:73:ASP:N	1:D:78:PHE:O	2.44	0.50
1:D:133:PRO:HG2	1:D:224:LYS:HZ1	1.76	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:443:LEU:HG	3:O:443:LEU:O	2.11	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
3:P:406:LEU:C	3:P:406:LEU:CD1	2.85	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:269:GLU:C	3:P:271:PRO:HD3	2.36	0.49
3:P:378:ALA:HB3	3:P:428:MET:HB2	1.92	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:N:326:LYS:C	3:N:328:LEU:H	2.20	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
3:Y:406:LEU:C	3:Y:406:LEU:CD1	2.84	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
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:N:406:LEU:C	3:N:406:LEU:CD1	2.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:E:195:PRO:C	1:E:197:SER:H	2.20	0.49
2:G:83:PHE:CE1	2:G:106:ILE:HG12	2.48	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
3:X:287:ALA:O	3:X:288:LYS:C	2.56	0.49
3:Y:326:LYS:C	3:Y:328:LEU:H	2.20	0.49
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.48	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:287:ALA:O	3:J:288:LYS:C	2.56	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
3:Y:269:GLU:C	3:Y:271:PRO:HD3	2.36	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: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
3:P:326:LYS:C	3:P:328:LEU:H	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:149:LYS:HZ1	2:F:195:GLU:CD	2.18	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
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:18:LEU:HB3	1:A:83:MET:HE3	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
2:C:149:LYS:HB2	2:C:193:ALA:HB3	1.94	0.48
1:D:18:LEU:O	1:D:83:MET:HE3	2.13	0.48
1:E:68:PHE:CD1	1:E:83:MET:HA	2.48	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
1:I:18:LEU:HB3	1:I:83:MET:HE3	1.96	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
3:X:443:LEU:O	3:X:443:LEU:HG	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:162:SER:HB3	2:G:176:SER:OG	2.13	0.48
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
2:K:91:TYR:HD1	1:M:99:LYS:HZ3	1.60	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
1:M:18:LEU:HB3	1:M:83:MET:HE3	1.96	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: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
1:M:67:ARG:C	1:M:68:PHE:HD1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.49	0.47
3:O:287:ALA:O	3:O:288:LYS:C	2.56	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
1:D:19:ILE:C	1:D:20:LEU:HD23	2.39	0.47
3:J:290:LYS:HZ3	2:L:109:THR:HG21	1.77	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: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
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.47
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.47
3:X:282:VAL:O	3:X:283:GLN:CB	2.52	0.47
3:X:288:LYS:H	3:X:288:LYS:CD	2.27	0.47
3:Y:259:VAL:HG23	3:Y:308:VAL:CG2	2.43	0.47
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	0.47
1:H:156:PHE:C	1:H:156:PHE:CD1	2.92	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
1:E:181:GLN:C	1:E:183:SER:H	2.21	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
3:Y:357:GLU:C	3:Y:359:THR:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:X:283:GLN:C	3:X:285:HIS:H	2.23	0.47
3:X:384:ASN:CG	3:X:385:GLY:H	2.22	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
2:G:167:ASP:CG	1:I:174:HIS:HE1	2.23	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:J:391:TYR:C	3:J:391:TYR:CD2	2.93	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
1:D:181:GLN:C	1:D:183:SER:H	2.23	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
3:N:357:GLU:C	3:N:359:THR:H	2.23	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:I:195:PRO:C	1:I:197:SER:H	2.23	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:18:LEU:HB3	1:D:83:MET:HE3	1.97	0.46
1:D:154:ASP:HA	1:D:185:LEU:HB3	1.97	0.46
1:E:29:ILE:O	1:E:72:ARG:NH2	2.48	0.46
2:G:36:TYR:HE2	2:G:89:GLN:HB3	1.81	0.46
1: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
3:X:391:TYR:C	3:X:391:TYR:CD2	2.92	0.46
1:H:103:ARG:O	1:H:104:LEU:HB2	2.15	0.46
3:O:391:TYR:C	3:O:391:TYR:CD2	2.92	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
1:H:201:THR:OG1	1:H:202:GLN:N	2.33	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
2:B:138:ASN:C	2:B:172:THR:HB	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:O:384:ASN:CG	3:O:385:GLY:H	2.22	0.46
1:E:153:LYS:HG2	1:E:154:ASP:OD1	2.15	0.46
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD22	3:Y:437:THR:HB	1.97	0.46
1:M:181:GLN:C	1:M:183:SER:H	2.24	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
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
2:L:167:ASP:CG	1:M:174:HIS:CE1	2.94	0.45
3:P:357:GLU:C	3:P:359:THR:H	2.23	0.45
3:P:439:LYS:HD2	3:P:439:LYS:HA	1.81	0.45
1:A:174:HIS:HB3	2:B:164:THR:HG21	1.98	0.45
2:C:121:SER:O	2:C:125:LEU:HB2	2.16	0.45
1: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
1:H:181:GLN:C	1:H:183:SER:H	2.24	0.45
2:L:83:PHE:CE1	2:L:106:ILE:HG12	2.52	0.45
3:O:388:GLU:HA	3:O:388:GLU:OE1	2.14	0.45
1:A:101:SER:H	1:A:104:LEU:HD23	1.82	0.45
1:E:156:PHE:CD1	1:E:156:PHE:C	2.94	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
1:H:18:LEU:O	1:H:83:MET:HE3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:156:PHE:CD1	1:D:156:PHE:C	2.94	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:432:LEU:C	3:N:433:HIS:C	2.85	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
3:P:432:LEU:C	3:P:433:HIS:C	2.85	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
2:C:149:LYS:HZ1	2:C:195:GLU:CD	2.18	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
1:I:220:LYS:HE2	1:I:222:GLU:CD	2.42	0.45
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.45
3:X:252:MET:SD	3:X:428:MET:HE1	2.57	0.45
3:Y:290:LYS:HE3	3:Y:292:ARG:HH12	1.82	0.45
3:O:283:GLN:C	3:O:285:HIS:H	2.23	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
1:E:181:GLN:C	1:E:183:SER:N	2.75	0.45
2:F:36:TYR:CE1	2:F:46:LEU:HD13	2.52	0.45
1:I:19:ILE:C	1:I:20:LEU:HD23	2.41	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:Y:344:ARG:O	3:Y:372:PHE:HA	2.16	0.45
2:K:31:THR:O	2:K:50:LYS:HA	2.16	0.45
1:M:101:SER:N	1:M:104:LEU:HD23	2.31	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:195:PRO:C	1:H:197:SER:H	2.23	0.45
2:K:140:TYR:CD2	2:K:141:PRO:HA	2.52	0.45
1:M:156:PHE:C	1:M:156:PHE:CD1	2.94	0.45
1:M:164:TRP:C	1:M:166:SER:N	2.67	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:J:252:MET:SD	3:J:428:MET:HE1	2.57	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:O:252:MET:SD	3:O:428:MET:HE1	2.57	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:A:181:GLN:C	1:A:183:SER:H	2.25	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: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
2:G:167:ASP:CG	1:I:174:HIS:CE1	2.95	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:89:GLN:CD	2:C:91:TYR:HB3	2.43	0.44
1:D:64:VAL:HB	1:D:68:PHE:CD2	2.53	0.44
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.44
2:K:27:GLN:O	2:K:29:ILE:HG23	2.17	0.44
3:P:345:GLU:HA	3:P:431:ALA:HB3	1.99	0.44
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:283:GLN:C	3:J:285:HIS:H	2.23	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:309:LEU:O	3:Y:310:HIS:C	2.61	0.44
3:Y:432:LEU:C	3:Y:433:HIS:C	2.85	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:264:VAL:O	3:J:265:ASP:HB2	2.18	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
2:K:30:GLU:HB2	2:K:32:TRP:CD1	2.53	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
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
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
2:L:167:ASP:CG	1:M:174:HIS:HE1	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:195:PRO:C	1:A:197:SER:H	2.24	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:I:181:GLN:C	1:I:183:SER:H	2.25	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:264:VAL:O	3:O:265:ASP:HB2	2.18	0.43
1:D:220:LYS:C	1:D:221:VAL:HA	2.43	0.43
1:I:60:TYR:CE2	1:I:69:THR:HA	2.54	0.43
1:I:181:GLN:C	1:I:183:SER:N	2.77	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
1:H:181:GLN:C	1:H:183:SER:N	2.76	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
3:N:309:LEU:O	3:N:310:HIS:C	2.61	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
1:M:19:ILE:C	1:M:20:LEU:HD23	2.43	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
1:A:181:GLN:C	1:A:183:SER:N	2.77	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
1:D:195:PRO:C	1:D:197:SER:H	2.24	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
3:X:309:LEU:O	3:X:310:HIS:C	2.62	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
3:P:309:LEU:O	3:P:310:HIS:C	2.61	0.43
1:A:156:PHE:C	1:A:156:PHE:CD1	2.97	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
3:O:309:LEU:O	3:O:310:HIS:C	2.62	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
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:P:386:GLN:HA	3:P:387:PRO:HD3	1.76	0.43
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:O:432:LEU:O	3:O:433:HIS:C	2.62	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
1:A:99:LYS:HZ3	2:C:91:TYR:HD1	1.67	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:432:LEU:O	3:J:433:HIS:C	2.62	0.42
3:X:418:GLN:C	3:X:420:GLY:N	2.77	0.42
3:Y:266:VAL:HB	3:Y:300:TYR:CD2	2.54	0.42
2:L:36:TYR:HE2	2:L:89:GLN:HB3	1.85	0.42
1:M:37:VAL:HG22	1:M:47:TRP:HA	2.01	0.42
1:M:69:THR:O	1:M:81:LEU:HD12	2.20	0.42
3:O:274:LYS:HE2	3:O:324:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:89:GLN:CD	2:K:91:TYR:HB3	2.44	0.42
2:L:105:GLU:OE2	2:L:173:TYR:OH	2.32	0.42
1:M:181:GLN:C	1:M:183:SER:N	2.77	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
1:D:181:GLN:C	1:D:183:SER:N	2.77	0.42
2:F:29:ILE:HG21	2:F:90:HIS:CD2	2.52	0.42
1:I:156:PHE:CD1	1:I:156:PHE:C	2.97	0.42
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.42
3:J:418:GLN:C	3:J:420:GLY:N	2.77	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: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:432:LEU:O	3:X:433:HIS:C	2.62	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:369:VAL:HB	3:J:406:LEU:HD12	2.02	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:A:19:ILE:C	1:A:20:LEU:HD23	2.44	0.42
1:D:220:LYS:HE2	1:D:222:GLU:OE1	2.19	0.42
2:F:138:ASN:C	2:F:172:THR:HB	2.44	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:68:PHE:O	1:H:69:THR:OG1	2.31	0.42
1:H:101:SER:N	1:H:104:LEU:HD22	2.35	0.42
1:M:195:PRO:C	1:M:197:SER:N	2.77	0.42
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.55	0.42
1:I:103:ARG:C	1:I:104:LEU:HG	2.45	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
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:J:309:LEU:O	3:J:310:HIS:C	2.62	0.41
3:Y:276:ASN:HB3	3:Y:278:TYR:CE1	2.56	0.41
3:Y:383:SER:O	3:Y:384:ASN:C	2.63	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: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
1:I:164:TRP:C	1:I:166:SER:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:173:VAL:HG22	1:A:192:VAL:HB	2.01	0.41
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:P:276:ASN:HB3	3:P:278:TYR:CE1	2.55	0.41
3:P:383:SER:O	3:P:384:ASN:C	2.63	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: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:C:138:ASN:C	2:C:172:THR:HB	2.45	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
2:L:138:ASN:C	2:L:172:THR:HB	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:383:SER:O	3:N:384:ASN:C	2.63	0.41
3:Y:367:CYS:HB2	3:Y:381:TRP:CZ2	2.56	0.41
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:291:PRO:O	3:X:292:ARG:HD2	2.17	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
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
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
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:138:ASN:C	2:G:172:THR:HB	2.46	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: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:90:HIS:ND1	2:L:90:HIS:C	2.79	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:B:89:GLN:CD	2:B:91:TYR:HB3	2.46	0.40
2:C:61:ARG:O	2:C:76:SER:N	2.36	0.40
2:C:73:LEU:HD12	2:C:74:THR:H	1.86	0.40
1: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
1:H:160:VAL:O	1:H:160:VAL:HG12	2.20	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
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
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:M:69:THR:O	1:M:81:LEU:HA	2.20	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
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
3:Y:320:LYS:HZ1	3:Y:322:LYS:HE3	1.86	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:253:ILE:CA	3:P:253:ILE:N[6_445]	1.41	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:380:GLU:OE1	3:X:433:HIS:NE2[12_545]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:253:ILE:CG2	3:P:254:SER:N[6_445]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:J:253:ILE:CG2	3:X:310:HIS:CD2[12_545]	2.12	0.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	31
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	9	40
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%)	24	63
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	24	63
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	24	63
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	24	63
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	24	63
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	12	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%)	1	16
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	1	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	1	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%)	1	16
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	4	25

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
3	O	433	HIS

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Mol	Chain	Res	Type
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
3	O	286	ASN

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Mol	Chain	Res	Type
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%)	160 (89%)	20 (11%)	6	20
1	D	180/205 (88%)	160 (89%)	20 (11%)	6	20
1	E	180/205 (88%)	159 (88%)	21 (12%)	5	18
1	H	180/205 (88%)	161 (89%)	19 (11%)	6	21
1	I	180/205 (88%)	161 (89%)	19 (11%)	6	21
1	M	180/205 (88%)	159 (88%)	21 (12%)	5	18
2	B	182/184 (99%)	163 (90%)	19 (10%)	7	22
2	C	182/184 (99%)	162 (89%)	20 (11%)	6	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	182/184 (99%)	163 (90%)	19 (10%)	7	22
2	G	182/184 (99%)	163 (90%)	19 (10%)	7	22
2	K	182/184 (99%)	162 (89%)	20 (11%)	6	20
2	L	182/184 (99%)	162 (89%)	20 (11%)	6	20
3	J	193/196 (98%)	186 (96%)	7 (4%)	31	52
3	N	192/196 (98%)	185 (96%)	7 (4%)	31	52
3	O	193/196 (98%)	186 (96%)	7 (4%)	31	52
3	P	192/196 (98%)	185 (96%)	7 (4%)	31	52
3	X	193/196 (98%)	186 (96%)	7 (4%)	31	52
3	Y	192/196 (98%)	185 (96%)	7 (4%)	31	52
All	All	3327/3510 (95%)	3048 (92%)	279 (8%)	10	30

All (279) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	13	LYS
1	A	50	SER
1	A	55	SER
1	A	56	THR
1	A	57	TYR
1	A	75	LEU
1	A	98	ARG
1	A	101	SER
1	A	131	VAL
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

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Mol	Chain	Res	Type
2	B	39	LYS
2	B	56	THR
2	B	78	LEU
2	B	90	HIS
2	B	108	ARG
2	B	122	ASP
2	B	123	GLU
2	B	132	VAL
2	B	135	LEU
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	90	HIS
2	C	108	ARG
2	C	122	ASP
2	C	123	GLU
2	C	132	VAL
2	C	134	CYS
2	C	135	LEU
2	C	142	ARG
2	C	143	GLU
2	C	152	ASN
2	C	169	LYS
2	C	191	VAL
2	C	197	THR
2	C	201	LEU
1	D	5	VAL
1	D	13	LYS
1	D	50	SER
1	D	55	SER
1	D	56	THR
1	D	57	TYR

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Mol	Chain	Res	Type
1	D	75	LEU
1	D	79	VAL
1	D	98	ARG
1	D	101	SER
1	D	131	VAL
1	D	148	LEU
1	D	156	PHE
1	D	161	THR
1	D	163	SER
1	D	185	LEU
1	D	196	SER
1	D	202	GLN
1	D	206	CYS
1	D	211	LYS
1	E	5	VAL
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	79	VAL
1	E	98	ARG
1	E	101	SER
1	E	102	ASP
1	E	131	VAL
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	90	HIS

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Mol	Chain	Res	Type
2	F	108	ARG
2	F	122	ASP
2	F	123	GLU
2	F	132	VAL
2	F	135	LEU
2	F	142	ARG
2	F	143	GLU
2	F	152	ASN
2	F	169	LYS
2	F	191	VAL
2	F	197	THR
2	F	201	LEU
2	G	7	SER
2	G	20	THR
2	G	33	LEU
2	G	39	LYS
2	G	56	THR
2	G	78	LEU
2	G	90	HIS
2	G	108	ARG
2	G	122	ASP
2	G	123	GLU
2	G	132	VAL
2	G	135	LEU
2	G	142	ARG
2	G	143	GLU
2	G	152	ASN
2	G	169	LYS
2	G	191	VAL
2	G	197	THR
2	G	201	LEU
1	I	5	VAL
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	79	VAL
1	I	98	ARG
1	I	101	SER
1	I	131	VAL

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Mol	Chain	Res	Type
1	I	142	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	308	VAL
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	291	PRO
3	N	311	GLN
3	N	394	THR
3	N	441	LEU
3	X	282	VAL
3	X	292	ARG
3	X	308	VAL
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	291	PRO
3	Y	311	GLN
3	Y	394	THR
3	Y	441	LEU
1	H	5	VAL
1	H	13	LYS
1	H	50	SER
1	H	55	SER
1	H	56	THR
1	H	57	TYR

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Mol	Chain	Res	Type
1	H	75	LEU
1	H	79	VAL
1	H	98	ARG
1	H	101	SER
1	H	131	VAL
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
2	K	20	THR
2	K	33	LEU
2	K	39	LYS
2	K	56	THR
2	K	78	LEU
2	K	90	HIS
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	90	HIS
2	L	108	ARG

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Mol	Chain	Res	Type
2	L	122	ASP
2	L	123	GLU
2	L	132	VAL
2	L	135	LEU
2	L	142	ARG
2	L	143	GLU
2	L	152	ASN
2	L	169	LYS
2	L	191	VAL
2	L	197	THR
2	L	201	LEU
1	M	5	VAL
1	M	13	LYS
1	M	50	SER
1	M	55	SER
1	M	56	THR
1	M	57	TYR
1	M	75	LEU
1	M	79	VAL
1	M	98	ARG
1	M	101	SER
1	M	131	VAL
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	308	VAL
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

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Mol	Chain	Res	Type
3	P	291	PRO
3	P	311	GLN
3	P	394	THR
3	P	441	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	207	ASN
2	B	90	HIS
2	B	137	ASN
2	C	87	HIS
2	C	90	HIS
2	C	160	GLN
2	C	189	HIS
1	D	207	ASN
1	E	207	ASN
2	F	90	HIS
2	F	137	ASN
2	F	160	GLN
2	G	6	GLN
2	G	38	GLN
2	G	87	HIS
2	G	90	HIS
1	I	207	ASN
3	J	272	GLN
3	J	276	ASN
3	J	283	GLN
3	J	295	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

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Mol	Chain	Res	Type
3	N	311	GLN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	384	ASN
3	N	389	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN
3	X	272	GLN
3	X	276	ASN
3	X	283	GLN
3	X	295	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
3	Y	312	ASN
3	Y	325	ASN
3	Y	342	GLN
3	Y	361	ASN
3	Y	384	ASN
3	Y	389	ASN
3	Y	419	GLN
3	Y	429	HIS
3	Y	434	ASN
3	Y	438	GLN
1	H	207	ASN
2	K	87	HIS
2	K	90	HIS

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Mol	Chain	Res	Type
2	K	137	ASN
2	L	90	HIS
2	L	138	ASN
2	L	160	GLN
2	L	189	HIS
1	M	207	ASN
3	O	272	GLN
3	O	276	ASN
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	384	ASN
3	P	389	ASN
3	P	419	GLN
3	P	429	HIS
3	P	434	ASN
3	P	438	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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
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%)	1.63	67 (32%) 1 6	114, 118, 126, 134	0
1	D	207/243 (85%)	1.67	67 (32%) 1 6	113, 118, 125, 139	0
1	E	209/243 (86%)	2.20	101 (48%) 0 3	178, 182, 190, 198	0
1	H	209/243 (86%)	1.41	54 (25%) 1 8	96, 100, 107, 115	0
1	I	207/243 (85%)	1.80	81 (39%) 1 5	177, 182, 189, 203	0
1	M	207/243 (85%)	1.47	57 (27%) 1 8	94, 100, 107, 121	0
2	B	211/213 (99%)	1.54	62 (29%) 1 7	113, 118, 124, 139	0
2	C	211/213 (99%)	1.86	75 (35%) 1 6	113, 118, 123, 143	0
2	F	211/213 (99%)	2.04	90 (42%) 0 4	177, 182, 188, 203	0
2	G	211/213 (99%)	1.94	87 (41%) 0 4	177, 182, 187, 207	0
2	K	211/213 (99%)	1.46	62 (29%) 1 7	94, 100, 105, 120	0
2	L	211/213 (99%)	1.61	63 (29%) 1 7	94, 100, 105, 124	0
3	J	207/211 (98%)	2.39	104 (50%) 0 3	176, 176, 176, 176	0
3	N	206/211 (97%)	2.05	88 (42%) 0 4	179, 179, 179, 179	0
3	O	207/211 (98%)	2.35	115 (55%) 0 3	274, 274, 274, 274	0
3	P	206/211 (97%)	2.21	93 (45%) 0 4	277, 277, 277, 277	0
3	X	207/211 (98%)	2.29	110 (53%) 0 3	167, 167, 167, 167	0
3	Y	206/211 (97%)	2.08	97 (47%) 0 4	171, 171, 171, 171	0
All	All	3753/4002 (93%)	1.89	1473 (39%) 1 5	94, 167, 277, 277	0

All (1473) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	22.2
1	D	147	ALA	14.1
1	M	131	VAL	12.6

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Mol	Chain	Res	Type	RSRZ
3	O	332	ILE	12.1
3	Y	288	LYS	11.2
3	Y	268	HIS	10.0
1	E	193	THR	9.7
2	L	187	GLU	9.5
1	E	130	SER	9.4
2	G	52	SER	9.3
3	J	428	MET	9.3
2	L	93	GLY	9.0
2	C	13	ALA	9.0
1	H	31	ALA	8.7
1	D	31	ALA	8.6
2	F	45	LYS	8.5
2	C	146	VAL	8.4
3	P	250	THR	8.3
3	J	377	ILE	8.3
1	E	175	THR	8.3
2	F	95	SER	8.2
3	P	332	ILE	8.2
1	E	190	SER	8.1
2	B	93	GLY	8.1
2	B	94	TYR	8.0
1	M	130	SER	7.7
3	J	378	ALA	7.7
3	J	280	ASP	7.7
1	H	147	ALA	7.7
3	O	425	CYS	7.6
2	L	131	SER	7.5
1	I	130	SER	7.4
3	N	254	SER	7.4
2	F	100	GLN	7.3
3	X	434	ASN	7.3
1	A	131	VAL	7.3
3	O	430	GLU	7.2
1	I	200	GLY	7.1
1	D	148	LEU	7.1
3	Y	264	VAL	7.1
3	P	374	PRO	6.9
1	E	58	ARG	6.9
1	E	153	LYS	6.9
2	G	146	VAL	6.8
2	K	205	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
3	O	238	PRO	6.7
3	P	238	PRO	6.7
3	J	336	ILE	6.7
2	F	59	PRO	6.7
3	O	265	ASP	6.6
3	N	376	ASP	6.6
1	E	131	VAL	6.6
3	N	302	VAL	6.6
2	C	207	LYS	6.5
3	X	324	SER	6.5
2	F	94	TYR	6.5
2	L	52	SER	6.4
2	K	11	LEU	6.4
2	B	76	SER	6.4
2	B	212	GLY	6.3
1	A	175	THR	6.3
1	D	152	VAL	6.3
3	N	394	THR	6.2
3	P	434	ASN	6.2
3	O	444	SER	6.2
2	F	165	GLU	6.2
2	C	14	SER	6.2
2	C	131	SER	6.2
3	Y	417	TRP	6.1
3	P	256	THR	6.1
2	F	96	ALA	6.1
2	C	76	SER	6.1
1	H	175	THR	6.1
1	E	129	PRO	6.1
3	X	377	ILE	6.0
3	X	433	HIS	6.0
3	J	281	GLY	6.0
2	F	87	HIS	6.0
2	C	180	THR	6.0
1	A	188	LEU	6.0
3	P	433	HIS	6.0
3	X	335	THR	6.0
1	M	150	CYS	5.9
1	I	99	LYS	5.9
1	I	162	VAL	5.9
3	X	332	ILE	5.9
2	K	146	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	I	66	GLY	5.9
3	J	240	VAL	5.9
1	A	137	SER	5.9
3	O	274	LYS	5.8
1	A	130	SER	5.8
3	J	248	LYS	5.8
3	Y	377	ILE	5.8
2	C	187	GLU	5.8
3	P	442	SER	5.8
2	C	197	THR	5.7
1	E	209	ASN	5.7
3	Y	239	SER	5.7
3	J	355	ARG	5.7
3	Y	240	VAL	5.7
3	N	281	GLY	5.7
1	A	11	LEU	5.7
1	A	151	LEU	5.7
3	J	437	THR	5.7
3	Y	281	GLY	5.7
3	O	310	HIS	5.7
3	O	260	THR	5.7
3	J	434	ASN	5.6
3	P	346	PRO	5.6
1	A	136	PRO	5.6
3	P	348	VAL	5.5
2	C	138	ASN	5.5
3	N	380	GLU	5.5
2	B	7	SER	5.4
3	Y	392	LYS	5.4
3	J	332	ILE	5.4
2	K	187	GLU	5.4
3	X	384	ASN	5.4
1	I	7	SER	5.3
3	P	435	HIS	5.3
3	J	375	SER	5.3
3	J	256	THR	5.3
2	C	116	PHE	5.3
3	Y	423	PHE	5.3
3	P	347	GLN	5.3
1	E	70	VAL	5.3
3	J	329	PRO	5.3
3	N	268	HIS	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	132	VAL	5.2
2	K	186	TYR	5.2
2	C	114	SER	5.2
2	C	127	SER	5.2
3	X	258	GLU	5.2
3	P	310	HIS	5.2
3	N	282	VAL	5.2
3	N	348	VAL	5.2
3	O	376	ASP	5.2
1	I	104	LEU	5.2
3	O	275	PHE	5.2
3	O	393	THR	5.2
2	G	13	ALA	5.2
2	G	134	CYS	5.2
2	G	51	ALA	5.1
2	C	12	SER	5.1
1	A	99	LYS	5.1
2	K	3	VAL	5.1
3	X	346	PRO	5.1
3	X	241	PHE	5.1
3	X	382	GLU	5.1
1	E	104	LEU	5.1
2	C	119	PRO	5.1
2	G	28	SER	5.1
1	H	104	LEU	5.1
3	O	440	SER	5.0
2	L	209	PHE	5.0
3	P	430	GLU	5.0
3	X	275	PHE	5.0
3	N	423	PHE	5.0
1	E	202	GLN	5.0
1	A	189	SER	4.9
3	J	254	SER	4.9
3	X	239	SER	4.9
3	P	268	HIS	4.9
3	J	308	VAL	4.9
2	L	116	PHE	4.9
1	E	154	ASP	4.9
2	F	30	GLU	4.9
3	Y	254	SER	4.9
1	H	136	PRO	4.9
1	H	15	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
3	N	377	ILE	4.9
3	X	343	PRO	4.9
2	B	205	VAL	4.9
3	N	411	THR	4.9
1	I	103	ARG	4.9
1	E	152	VAL	4.9
3	O	241	PHE	4.9
3	N	238	PRO	4.9
1	M	152	VAL	4.9
3	P	431	ALA	4.8
2	B	166	GLN	4.8
3	X	440	SER	4.8
1	H	178	ALA	4.8
3	O	266	VAL	4.8
1	M	168	ALA	4.8
3	O	281	GLY	4.8
1	A	133	PRO	4.8
1	E	189	SER	4.8
2	F	114	SER	4.8
1	I	27	PHE	4.7
1	A	10	GLY	4.7
2	G	135	LEU	4.7
1	I	182	SER	4.7
3	X	430	GLU	4.7
3	X	286	ASN	4.7
3	X	238	PRO	4.7
2	C	45	LYS	4.7
1	A	15	GLY	4.7
1	A	120	THR	4.7
3	J	268	HIS	4.6
1	E	160	VAL	4.6
2	K	116	PHE	4.6
1	E	99	LYS	4.6
1	H	7	SER	4.6
2	F	208	SER	4.6
2	L	208	SER	4.6
3	X	329	PRO	4.6
3	P	251	LEU	4.6
2	G	137	ASN	4.6
2	F	115	VAL	4.6
1	E	223	PRO	4.6
2	G	136	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
3	J	430	GLU	4.6
3	P	344	ARG	4.6
2	C	144	ALA	4.6
3	J	323	VAL	4.6
1	E	133	PRO	4.6
3	P	258	GLU	4.6
1	I	102	ASP	4.6
1	D	192	VAL	4.6
3	J	282	VAL	4.6
1	H	99	LYS	4.6
3	P	340	LYS	4.6
2	L	183	LYS	4.5
2	F	44	PRO	4.5
3	N	248	LYS	4.5
2	B	20	THR	4.5
2	G	197	THR	4.5
3	O	243	PHE	4.5
2	G	45	LYS	4.5
3	N	407	TYR	4.5
1	H	193	THR	4.5
1	H	148	LEU	4.5
3	X	336	ILE	4.5
3	P	246	LYS	4.4
3	P	288	LYS	4.4
1	A	160	VAL	4.4
1	D	220	LYS	4.4
3	X	280	ASP	4.4
1	E	188	LEU	4.4
3	J	433	HIS	4.4
2	F	133	VAL	4.4
3	X	428	MET	4.4
1	D	197	SER	4.4
2	F	131	SER	4.4
1	A	112	ALA	4.4
2	B	83	PHE	4.4
3	J	277	TRP	4.4
2	B	144	ALA	4.4
1	D	15	GLY	4.4
1	D	184	GLY	4.4
2	F	146	VAL	4.4
3	P	273	VAL	4.4
3	J	390	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	Y	295	GLN	4.4
2	L	51	ALA	4.3
1	E	57	TYR	4.3
2	F	85	THR	4.3
3	O	334	LYS	4.3
2	G	27	GLN	4.3
1	A	163	SER	4.3
1	E	17	SER	4.3
3	Y	378	ALA	4.3
3	N	308	VAL	4.3
2	G	14	SER	4.3
1	D	104	LEU	4.3
1	E	151	LEU	4.3
1	A	98	ARG	4.3
3	X	393	THR	4.3
2	G	144	ALA	4.3
3	N	375	SER	4.3
3	N	430	GLU	4.3
3	Y	430	GLU	4.3
2	L	185	ASP	4.3
3	P	265	ASP	4.3
3	Y	412	VAL	4.3
3	O	264	VAL	4.3
1	I	9	GLY	4.3
3	X	423	PHE	4.3
1	H	194	VAL	4.3
3	X	358	MET	4.3
3	P	315	ASP	4.3
3	O	386	GLN	4.3
3	X	291	PRO	4.2
3	X	277	TRP	4.2
3	O	382	GLU	4.2
2	B	107	LYS	4.2
1	I	175	THR	4.2
1	I	193	THR	4.2
1	I	2	VAL	4.2
2	G	116	PHE	4.2
1	I	133	PRO	4.2
1	I	149	GLY	4.2
3	X	375	SER	4.2
2	F	53	THR	4.2
2	G	147	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	194	VAL	4.2
2	C	87	HIS	4.2
3	P	443	LEU	4.2
3	Y	302	VAL	4.2
3	P	331	PRO	4.2
1	D	174	HIS	4.1
3	J	380	GLU	4.1
1	A	150	CYS	4.1
1	E	161	THR	4.1
3	J	275	PHE	4.1
3	X	318	GLU	4.1
3	O	379	VAL	4.1
1	A	197	SER	4.1
2	G	155	GLN	4.1
1	H	53	THR	4.1
3	Y	256	THR	4.1
3	O	394	THR	4.1
1	M	99	LYS	4.1
2	K	138	ASN	4.1
1	E	44	GLY	4.1
1	I	144	GLY	4.1
1	D	2	VAL	4.1
1	A	129	PRO	4.1
1	A	7	SER	4.1
2	F	60	SER	4.1
2	G	107	LYS	4.1
1	I	39	ARG	4.1
3	N	382	GLU	4.1
3	J	238	PRO	4.1
2	F	168	SER	4.1
2	K	159	SER	4.1
3	Y	290	LYS	4.1
3	O	239	SER	4.1
3	P	320	LYS	4.1
1	H	179	VAL	4.1
2	C	49	TYR	4.1
3	Y	293	GLU	4.0
1	I	146	ALA	4.0
3	O	431	ALA	4.0
2	B	138	ASN	4.0
2	C	147	GLN	4.0
3	O	267	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	56	THR	4.0
2	B	185	ASP	4.0
2	L	155	GLN	4.0
2	G	212	GLY	4.0
3	Y	300	TYR	4.0
1	E	103	ARG	4.0
1	A	152	VAL	4.0
3	P	371	GLY	4.0
2	F	52	SER	4.0
2	C	18	THR	4.0
3	N	256	THR	4.0
3	N	338	LYS	4.0
3	N	339	ALA	4.0
2	C	134	CYS	4.0
2	C	46	LEU	4.0
2	C	130	ALA	4.0
3	N	273	VAL	4.0
1	E	66	GLY	4.0
3	J	246	LYS	4.0
2	G	32	TRP	4.0
3	O	377	ILE	4.0
2	G	189	HIS	4.0
2	F	132	VAL	4.0
3	X	348	VAL	3.9
3	J	241	PHE	3.9
1	A	128	GLY	3.9
3	O	250	THR	3.9
2	F	2	VAL	3.9
3	X	262	VAL	3.9
3	O	323	VAL	3.9
3	J	267	SER	3.9
1	D	222	GLU	3.9
3	Y	263	VAL	3.9
2	C	145	LYS	3.9
2	F	93	GLY	3.9
2	G	138	ASN	3.9
1	I	57	TYR	3.9
2	B	142	ARG	3.9
3	J	346	PRO	3.9
3	J	319	TYR	3.9
3	P	379	VAL	3.9
3	Y	248	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
3	O	352	PRO	3.9
1	H	54	SER	3.9
3	Y	379	VAL	3.9
3	J	334	LYS	3.8
3	J	359	THR	3.8
3	J	392	LYS	3.8
3	J	321	CYS	3.8
3	N	371	GLY	3.8
1	H	204	TYR	3.8
1	I	152	VAL	3.8
2	L	83	PHE	3.8
2	G	153	ALA	3.8
2	G	207	LYS	3.8
2	L	9	SER	3.8
3	O	364	SER	3.8
2	B	199	GLN	3.8
2	K	166	GLN	3.8
1	M	129	PRO	3.8
3	Y	244	PRO	3.8
1	I	15	GLY	3.8
1	M	132	PHE	3.8
1	A	97	ALA	3.8
1	E	97	ALA	3.8
1	D	3	GLN	3.8
1	H	9	GLY	3.8
2	B	119	PRO	3.8
2	C	77	GLY	3.8
1	D	150	CYS	3.8
3	X	319	TYR	3.8
3	N	291	PRO	3.8
3	X	250	THR	3.8
2	F	207	LYS	3.8
3	X	248	LYS	3.8
2	C	137	ASN	3.8
2	L	166	GLN	3.8
1	E	201	THR	3.8
3	O	256	THR	3.8
1	E	60	TYR	3.8
2	L	189	HIS	3.8
3	J	242	LEU	3.8
1	A	198	SER	3.8
3	J	255	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
3	N	396	PRO	3.8
3	Y	282	VAL	3.8
1	M	188	LEU	3.8
3	P	356	GLU	3.8
2	K	183	LYS	3.7
3	O	331	PRO	3.7
1	D	17	SER	3.7
2	K	131	SER	3.7
1	H	95	TYR	3.7
3	X	256	THR	3.7
3	X	376	ASP	3.7
3	J	317	LYS	3.7
1	D	195	PRO	3.7
3	X	276	ASN	3.7
3	P	342	GLN	3.7
1	A	170	THR	3.7
2	F	135	LEU	3.7
1	E	220	LYS	3.7
3	O	285	HIS	3.7
3	O	433	HIS	3.7
2	G	159	SER	3.7
3	Y	390	ASN	3.7
2	K	106	ILE	3.7
2	L	20	THR	3.7
1	A	2	VAL	3.7
3	P	291	PRO	3.7
2	F	28	SER	3.7
2	L	65	SER	3.7
3	J	307	THR	3.7
3	Y	289	THR	3.7
1	E	211	LYS	3.7
2	C	50	LYS	3.7
2	G	9	SER	3.7
2	G	12	SER	3.7
2	G	53	THR	3.7
1	I	24	VAL	3.7
3	Y	336	ILE	3.7
3	O	300	TYR	3.7
3	P	330	ALA	3.7
1	E	217	VAL	3.7
1	E	221	VAL	3.7
2	G	208	SER	3.7

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Mol	Chain	Res	Type	RSRZ
3	J	384	ASN	3.7
2	B	9	SER	3.6
2	F	177	SER	3.6
3	N	384	ASN	3.6
2	L	44	PRO	3.6
3	N	258	GLU	3.6
1	D	63	ALA	3.6
1	E	88	VAL	3.6
1	M	182	SER	3.6
1	E	219	LYS	3.6
3	O	247	PRO	3.6
3	X	302	VAL	3.6
1	A	101	SER	3.6
2	F	206	THR	3.6
3	P	285	HIS	3.6
1	I	188	LEU	3.6
3	Y	443	LEU	3.6
1	I	187	SER	3.6
3	O	434	ASN	3.6
3	Y	241	PHE	3.6
3	P	264	VAL	3.6
3	N	252	MET	3.6
3	X	251	LEU	3.6
3	X	321	CYS	3.6
2	F	145	LYS	3.6
2	B	8	PRO	3.6
3	P	335	THR	3.6
2	K	199	GLN	3.6
3	N	329	PRO	3.6
1	D	28	ARG	3.6
3	J	398	LEU	3.6
3	P	300	TYR	3.6
1	M	175	THR	3.6
3	O	269	GLU	3.6
2	C	15	VAL	3.5
2	G	80	PHE	3.5
3	O	344	ARG	3.5
3	O	378	ALA	3.5
1	E	137	SER	3.5
2	L	138	ASN	3.5
3	X	310	HIS	3.5
3	Y	384	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	219	LYS	3.5
2	F	119	PRO	3.5
1	D	99	LYS	3.5
3	J	335	THR	3.5
2	B	209	PHE	3.5
2	F	116	PHE	3.5
3	P	369	VAL	3.5
3	O	320	LYS	3.5
1	I	174	HIS	3.5
2	K	197	THR	3.5
3	N	295	GLN	3.5
3	J	427	VAL	3.5
3	O	255	ARG	3.5
2	K	144	ALA	3.5
2	K	21	ILE	3.5
3	X	383	SER	3.5
2	G	180	THR	3.5
2	K	5	THR	3.5
3	J	306	LEU	3.5
3	P	307	THR	3.5
1	H	131	VAL	3.5
2	L	205	VAL	3.5
2	K	143	GLU	3.5
3	Y	242	LEU	3.5
1	M	165	ASN	3.5
3	N	443	LEU	3.5
1	E	72	ARG	3.5
3	P	417	TRP	3.5
2	F	79	GLN	3.5
3	Y	346	PRO	3.5
2	K	169	LYS	3.4
1	H	188	LEU	3.4
2	B	123	GLU	3.4
3	P	377	ILE	3.4
1	M	17	SER	3.4
2	B	67	SER	3.4
2	C	112	ALA	3.4
2	F	97	THR	3.4
3	J	260	THR	3.4
1	D	60	TYR	3.4
3	Y	371	GLY	3.4
3	O	262	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
3	X	424	SER	3.4
2	C	107	LYS	3.4
2	C	117	ILE	3.4
2	B	187	GLU	3.4
3	P	362	GLN	3.4
3	N	264	VAL	3.4
3	J	358	MET	3.4
1	D	97	ALA	3.4
1	M	133	PRO	3.4
2	F	27	GLN	3.4
3	P	326	LYS	3.4
1	E	198	SER	3.4
3	J	348	VAL	3.4
3	J	345	GLU	3.4
2	L	211	ARG	3.4
3	Y	342	GLN	3.4
1	A	71	SER	3.4
3	J	440	SER	3.4
3	N	275	PHE	3.3
2	K	196	VAL	3.3
3	P	289	THR	3.3
1	A	168	ALA	3.3
1	E	174	HIS	3.3
3	O	291	PRO	3.3
1	H	2	VAL	3.3
3	Y	318	GLU	3.3
1	H	16	GLY	3.3
2	G	114	SER	3.3
1	A	222	GLU	3.3
1	E	222	GLU	3.3
2	G	123	GLU	3.3
3	X	281	GLY	3.3
3	P	385	GLY	3.3
3	X	334	LYS	3.3
2	F	92	ALA	3.3
2	G	10	THR	3.3
3	O	423	PHE	3.3
3	Y	407	TYR	3.3
1	A	100	GLY	3.3
2	C	100	GLN	3.3
2	B	5	THR	3.3
3	J	352	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
3	O	251	LEU	3.3
3	O	398	LEU	3.3
2	G	195	GLU	3.3
3	J	382	GLU	3.3
1	M	200	GLY	3.3
1	I	31	ALA	3.3
3	J	243	PHE	3.3
3	O	413	ASP	3.3
3	X	264	VAL	3.3
3	O	254	SER	3.3
3	J	310	HIS	3.3
3	Y	334	LYS	3.3
1	E	162	VAL	3.3
1	I	161	THR	3.3
2	F	63	SER	3.3
2	K	14	SER	3.3
3	N	424	SER	3.3
3	N	326	LYS	3.2
3	O	345	GLU	3.2
2	G	199	GLN	3.2
2	L	79	GLN	3.2
1	E	24	VAL	3.2
2	F	153	ALA	3.2
3	X	240	VAL	3.2
2	K	31	THR	3.2
3	P	383	SER	3.2
1	H	8	GLY	3.2
1	M	16	GLY	3.2
3	N	425	CYS	3.2
3	P	438	GLN	3.2
2	K	142	ARG	3.2
1	I	117	THR	3.2
1	I	201	THR	3.2
1	H	145	THR	3.2
2	L	159	SER	3.2
3	X	444	SER	3.2
3	J	269	GLU	3.2
1	I	58	ARG	3.2
3	X	327	ALA	3.2
3	N	253	ILE	3.2
3	Y	439	LYS	3.2
3	P	249	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	193	THR	3.2
1	I	215	THR	3.2
1	E	2	VAL	3.2
2	C	196	VAL	3.2
2	F	199	GLN	3.2
3	O	342	GLN	3.2
3	O	418	GLN	3.2
2	L	119	PRO	3.2
2	B	118	PHE	3.2
1	I	190	SER	3.2
2	L	178	THR	3.2
2	L	196	VAL	3.2
3	N	393	THR	3.2
2	K	50	LYS	3.2
2	F	148	TRP	3.2
3	X	344	ARG	3.2
3	Y	310	HIS	3.2
1	E	187	SER	3.2
3	N	324	SER	3.2
1	I	46	GLU	3.2
2	G	94	TYR	3.2
3	N	292	ARG	3.2
3	X	323	VAL	3.2
1	A	74	ASP	3.2
1	H	137	SER	3.1
1	H	224	LYS	3.1
3	Y	274	LYS	3.1
3	Y	326	LYS	3.1
2	F	138	ASN	3.1
1	D	9	GLY	3.1
3	J	264	VAL	3.1
2	B	134	CYS	3.1
2	B	87	HIS	3.1
2	B	112	ALA	3.1
2	F	144	ALA	3.1
1	D	145	THR	3.1
1	E	71	SER	3.1
2	G	30	GLU	3.1
3	Y	376	ASP	3.1
2	G	178	THR	3.1
3	Y	250	THR	3.1
3	P	324	SER	3.1

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Mol	Chain	Res	Type	RSRZ
3	P	294	GLN	3.1
3	N	309	LEU	3.1
3	O	271	PRO	3.1
3	P	274	LYS	3.1
1	M	174	HIS	3.1
2	L	134	CYS	3.1
2	G	168	SER	3.1
1	H	129	PRO	3.1
3	X	331	PRO	3.1
1	E	5	VAL	3.1
3	J	439	LYS	3.1
2	B	125	LEU	3.1
3	O	380	GLU	3.1
1	E	177	PRO	3.1
2	G	5	THR	3.1
3	X	359	THR	3.1
3	X	419	GLN	3.1
1	D	128	GLY	3.1
2	B	32	TRP	3.1
1	D	4	LEU	3.1
1	I	59	ASP	3.1
1	M	218	ASP	3.1
2	C	204	PRO	3.1
2	G	24	ARG	3.1
2	G	127	SER	3.1
2	G	150	VAL	3.1
2	F	77	GLY	3.1
1	E	199	LEU	3.1
2	L	165	GLU	3.1
3	Y	255	ARG	3.1
3	Y	427	VAL	3.1
3	X	244	PRO	3.1
3	P	257	PRO	3.1
1	M	62	ASP	3.1
2	B	197	THR	3.1
2	L	66	GLY	3.1
3	N	354	SER	3.1
3	N	406	LEU	3.1
3	X	390	ASN	3.1
1	A	211	LYS	3.1
2	F	126	LYS	3.1
3	J	257	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	P	387	PRO	3.0
3	X	309	LEU	3.0
3	P	376	ASP	3.0
1	H	97	ALA	3.0
2	G	25	ALA	3.0
1	D	216	LYS	3.0
2	G	145	LYS	3.0
3	O	246	LYS	3.0
3	P	352	PRO	3.0
2	C	79	GLN	3.0
2	C	155	GLN	3.0
3	J	386	GLN	3.0
3	X	306	LEU	3.0
1	D	175	THR	3.0
1	E	182	SER	3.0
1	E	203	THR	3.0
1	M	54	SER	3.0
2	B	52	SER	3.0
2	F	197	THR	3.0
3	J	324	SER	3.0
1	E	11	LEU	3.0
2	L	186	TYR	3.0
3	J	331	PRO	3.0
3	N	438	GLN	3.0
2	F	98	PHE	3.0
2	K	95	SER	3.0
3	X	394	THR	3.0
3	O	383	SER	3.0
2	F	190	LYS	3.0
3	O	276	ASN	3.0
2	C	78	LEU	3.0
1	E	15	GLY	3.0
3	Y	238	PRO	3.0
3	O	349	TYR	3.0
3	P	245	PRO	3.0
1	E	146	ALA	3.0
2	K	102	THR	3.0
2	L	76	SER	3.0
2	B	33	LEU	3.0
1	D	123	PRO	3.0
1	E	9	GLY	3.0
1	H	195	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	8	PRO	3.0
1	E	224	LYS	3.0
3	Y	320	LYS	3.0
3	P	334	LYS	3.0
2	C	163	VAL	3.0
3	Y	273	VAL	3.0
3	X	254	SER	3.0
1	A	16	GLY	3.0
2	G	49	TYR	3.0
2	G	70	GLU	3.0
3	O	293	GLU	3.0
3	Y	311	GLN	3.0
2	L	146	VAL	3.0
3	N	379	VAL	3.0
1	D	34	MET	3.0
1	I	205	ILE	3.0
1	D	54	SER	3.0
1	E	59	ASP	3.0
1	I	145	THR	3.0
3	Y	265	ASP	3.0
3	Y	324	SER	3.0
2	G	186	TYR	3.0
3	O	257	PRO	3.0
1	I	26	ASN	3.0
1	I	165	ASN	3.0
1	E	178	ALA	3.0
2	F	62	PHE	3.0
3	P	272	GLN	3.0
3	X	314	LEU	2.9
2	B	14	SER	2.9
2	G	60	SER	2.9
2	G	72	THR	2.9
2	L	10	THR	2.9
3	J	350	THR	2.9
3	N	395	PRO	2.9
3	N	439	LYS	2.9
2	B	211	ARG	2.9
3	J	283	GLN	2.9
2	G	148	TRP	2.9
1	E	102	ASP	2.9
2	B	63	SER	2.9
3	X	274	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	144	ALA	2.9
1	A	104	LEU	2.9
1	M	45	LEU	2.9
2	K	24	ARG	2.9
3	O	242	LEU	2.9
3	O	416	ARG	2.9
1	M	15	GLY	2.9
1	E	145	THR	2.9
2	C	208	SER	2.9
2	K	12	SER	2.9
3	J	250	THR	2.9
3	J	426	SER	2.9
2	F	51	ALA	2.9
2	K	103	ARG	2.9
3	Y	251	LEU	2.9
3	O	333	GLU	2.9
3	X	417	TRP	2.9
2	K	194	CYS	2.9
1	D	203	THR	2.9
1	M	197	SER	2.9
2	G	117	ILE	2.9
2	K	52	SER	2.9
3	O	427	VAL	2.9
3	N	413	ASP	2.9
2	G	143	GLU	2.9
3	Y	269	GLU	2.9
3	J	297	ASN	2.9
1	H	113	TRP	2.9
2	F	64	GLY	2.9
2	L	94	TYR	2.9
3	N	363	VAL	2.9
3	O	343	PRO	2.9
3	N	428	MET	2.9
2	G	76	SER	2.9
3	X	307	THR	2.9
3	Y	298	SER	2.9
1	M	76	GLU	2.9
1	M	115	PRO	2.9
2	B	24	ARG	2.9
1	A	190	SER	2.9
1	I	150	CYS	2.9
3	N	442	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	M	102	ASP	2.9
2	K	107	LYS	2.9
3	P	322	LYS	2.9
1	D	11	LEU	2.9
1	I	148	LEU	2.9
2	C	169	LYS	2.8
3	N	290	LYS	2.8
1	E	6	GLU	2.8
1	A	209	ASN	2.8
2	B	133	VAL	2.8
2	B	196	VAL	2.8
2	C	211	ARG	2.8
1	E	168	ALA	2.8
1	H	17	SER	2.8
1	M	7	SER	2.8
2	F	20	THR	2.8
2	L	148	TRP	2.8
3	N	323	VAL	2.8
1	E	65	LYS	2.8
2	K	80	PHE	2.8
3	P	309	LEU	2.8
2	B	10	THR	2.8
2	F	65	SER	2.8
2	G	69	THR	2.8
2	L	7	SER	2.8
2	F	32	TRP	2.8
1	E	195	PRO	2.8
3	Y	287	ALA	2.8
3	Y	329	PRO	2.8
1	D	151	LEU	2.8
2	C	11	LEU	2.8
1	A	132	PHE	2.8
1	I	29	ILE	2.8
2	F	61	ARG	2.8
1	D	113	TRP	2.8
2	C	35	TRP	2.8
2	F	178	THR	2.8
2	K	4	MET	2.8
2	K	20	THR	2.8
2	L	32	TRP	2.8
3	N	318	GLU	2.8
3	X	260	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	P	440	SER	2.8
3	Y	315	ASP	2.8
3	J	387	PRO	2.8
3	O	327	ALA	2.8
1	H	96	CYS	2.8
3	X	243	PHE	2.8
1	I	8	GLY	2.8
3	Y	341	GLY	2.8
1	E	197	SER	2.8
3	O	426	SER	2.8
3	O	439	LYS	2.8
1	M	112	ALA	2.8
3	Y	352	PRO	2.8
2	B	73	LEU	2.8
2	C	115	VAL	2.8
3	X	392	LYS	2.8
2	K	13	ALA	2.8
3	N	327	ALA	2.8
3	P	437	THR	2.8
1	H	123	PRO	2.8
2	B	122	ASP	2.8
2	K	2	VAL	2.7
1	E	113	TRP	2.7
1	M	63	ALA	2.7
1	D	53	THR	2.7
1	H	126	THR	2.7
2	F	15	VAL	2.7
3	O	240	VAL	2.7
3	O	348	VAL	2.7
3	O	322	LYS	2.7
2	G	93	GLY	2.7
3	X	341	GLY	2.7
2	B	186	TYR	2.7
1	I	1	GLU	2.7
3	P	386	GLN	2.7
2	G	97	THR	2.7
3	J	376	ASP	2.7
1	A	127	LYS	2.7
1	D	153	LYS	2.7
2	L	41	GLY	2.7
1	D	96	CYS	2.7
2	B	62	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
3	P	244	PRO	2.7
1	E	7	SER	2.7
1	I	183	SER	2.7
1	M	217	VAL	2.7
2	C	63	SER	2.7
2	G	211	ARG	2.7
3	N	239	SER	2.7
3	Y	348	VAL	2.7
1	H	83	MET	2.7
2	C	158	ASN	2.7
3	O	361	ASN	2.7
2	B	189	HIS	2.7
2	K	148	TRP	2.7
2	G	8	PRO	2.7
3	J	396	PRO	2.7
3	X	386	GLN	2.7
1	E	118	VAL	2.7
3	P	240	VAL	2.7
1	E	54	SER	2.7
2	G	83	PHE	2.7
3	N	352	PRO	2.7
1	D	194	VAL	2.7
1	E	208	VAL	2.7
3	N	293	GLU	2.7
2	C	88	CYS	2.7
3	O	252	MET	2.7
3	J	314	LEU	2.7
3	Y	393	THR	2.7
3	P	432	LEU	2.7
1	M	187	SER	2.7
2	K	127	SER	2.7
1	I	42	GLY	2.7
1	H	100	GLY	2.7
2	G	66	GLY	2.7
2	G	128	GLY	2.7
3	X	325	ASN	2.7
1	I	72	ARG	2.7
3	X	355	ARG	2.7
3	X	369	VAL	2.7
1	M	201	THR	2.7
1	I	128	GLY	2.7
2	G	96	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	N	405	PHE	2.7
1	I	80	TYR	2.6
1	H	133	PRO	2.6
2	G	2	VAL	2.6
3	J	417	TRP	2.6
3	X	279	VAL	2.6
1	D	76	GLU	2.6
2	F	175	LEU	2.6
1	E	200	GLY	2.6
1	H	187	SER	2.6
3	X	304	SER	2.6
2	F	42	LYS	2.6
2	G	122	ASP	2.6
2	G	149	LYS	2.6
2	L	58	VAL	2.6
3	J	363	VAL	2.6
3	N	263	VAL	2.6
2	B	160	GLN	2.6
1	D	42	GLY	2.6
2	C	64	GLY	2.6
1	H	56	THR	2.6
2	B	126	LYS	2.6
2	L	197	THR	2.6
2	L	174	SER	2.6
1	M	204	TYR	2.6
3	X	427	VAL	2.6
3	Y	321	CYS	2.6
2	C	179	LEU	2.6
1	E	26	ASN	2.6
1	M	46	GLU	2.6
1	D	178	ALA	2.6
3	J	288	LYS	2.6
3	X	287	ALA	2.6
2	K	35	TRP	2.6
3	N	345	GLU	2.6
3	O	311	GLN	2.6
3	P	333	GLU	2.6
3	O	317	LYS	2.6
3	P	327	ALA	2.6
2	G	181	LEU	2.6
3	P	255	ARG	2.6
1	D	33	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	126	THR	2.6
2	G	113	PRO	2.6
3	N	346	PRO	2.6
3	X	313	TRP	2.6
3	O	280	ASP	2.6
1	E	214	ASN	2.6
1	H	26	ASN	2.6
3	X	361	ASN	2.6
3	Y	434	ASN	2.6
3	O	286	ASN	2.6
1	D	168	ALA	2.6
1	M	169	LEU	2.6
3	O	428	MET	2.6
1	I	223	PRO	2.6
3	Y	335	THR	2.6
1	M	30	SER	2.6
2	G	95	SER	2.6
2	K	9	SER	2.6
1	M	127	LYS	2.6
1	E	172	GLY	2.6
2	C	143	GLU	2.6
1	D	126	THR	2.6
3	J	271	PRO	2.6
3	N	243	PHE	2.5
2	F	154	LEU	2.5
2	C	199	GLN	2.5
2	G	100	GLN	2.5
3	N	255	ARG	2.5
3	X	378	ALA	2.5
3	Y	333	GLU	2.5
3	O	295	GLN	2.5
2	B	194	CYS	2.5
1	I	209	ASN	2.5
2	C	86	TYR	2.5
1	I	129	PRO	2.5
1	A	201	THR	2.5
2	C	178	THR	2.5
2	F	80	PHE	2.5
3	J	360	LYS	2.5
3	X	340	LYS	2.5
1	E	51	ILE	2.5
2	B	95	SER	2.5

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Mol	Chain	Res	Type	RSRZ
3	Y	440	SER	2.5
1	E	64	VAL	2.5
2	C	194	CYS	2.5
3	X	425	CYS	2.5
3	O	367	CYS	2.5
1	I	153	LYS	2.5
2	C	5	THR	2.5
1	I	100	GLY	2.5
2	L	168	SER	2.5
3	P	400	SER	2.5
2	B	25	ALA	2.5
3	O	358	MET	2.5
2	K	79	GLN	2.5
1	H	35	ASN	2.5
3	Y	405	PHE	2.5
2	K	46	LEU	2.5
1	A	113	TRP	2.5
2	C	32	TRP	2.5
3	J	279	VAL	2.5
2	G	65	SER	2.5
3	N	440	SER	2.5
3	O	442	SER	2.5
1	A	169	LEU	2.5
1	H	75	LEU	2.5
3	Y	276	ASN	2.5
1	D	164	TRP	2.5
2	K	115	VAL	2.5
2	F	72	THR	2.5
1	E	158	GLU	2.5
3	X	438	GLN	2.5
3	O	318	GLU	2.5
3	Y	331	PRO	2.5
2	G	15	VAL	2.5
3	J	259	VAL	2.5
1	A	9	GLY	2.5
3	Y	252	MET	2.5
2	C	111	ALA	2.5
1	E	91	THR	2.5
2	F	69	THR	2.5
3	Y	307	THR	2.5
3	Y	337	SER	2.5
3	N	283	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
3	X	372	PHE	2.5
3	X	407	TYR	2.5
2	C	21	ILE	2.5
2	F	58	VAL	2.5
2	L	24	ARG	2.5
2	L	128	GLY	2.5
1	M	178	ALA	2.5
2	F	164	THR	2.4
3	J	372	PHE	2.4
3	O	328	LEU	2.4
1	A	54	SER	2.4
1	D	171	SER	2.4
1	I	54	SER	2.4
2	B	117	ILE	2.4
3	N	400	SER	2.4
3	P	267	SER	2.4
1	A	41	PRO	2.4
3	Y	291	PRO	2.4
2	G	185	ASP	2.4
3	P	308	VAL	2.4
3	Y	428	MET	2.4
1	D	146	ALA	2.4
2	G	112	ALA	2.4
3	P	406	LEU	2.4
1	I	56	THR	2.4
2	K	10	THR	2.4
2	C	159	SER	2.4
3	X	333	GLU	2.4
1	A	58	ARG	2.4
2	G	115	VAL	2.4
2	L	150	VAL	2.4
1	D	16	GLY	2.4
1	E	63	ALA	2.4
3	J	327	ALA	2.4
1	M	33	THR	2.4
3	N	362	GLN	2.4
3	O	422	VAL	2.4
1	M	219	LYS	2.4
1	A	147	ALA	2.4
1	E	218	ASP	2.4
3	X	315	ASP	2.4
3	X	316	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
3	X	371	GLY	2.4
2	L	48	ILE	2.4
2	L	195	GLU	2.4
3	N	331	PRO	2.4
3	X	353	PRO	2.4
3	O	353	PRO	2.4
3	P	311	GLN	2.4
1	I	189	SER	2.4
2	F	156	SER	2.4
3	J	274	LYS	2.4
3	P	239	SER	2.4
3	J	371	GLY	2.4
3	X	367	CYS	2.4
3	O	309	LEU	2.4
3	N	277	TRP	2.4
3	Y	277	TRP	2.4
3	O	401	ASP	2.4
1	D	214	ASN	2.4
1	M	194	VAL	2.4
3	X	391	TYR	2.4
3	X	435	HIS	2.4
3	Y	363	VAL	2.4
3	P	263	VAL	2.4
1	H	115	PRO	2.4
1	M	123	PRO	2.4
2	K	206	THR	2.4
3	J	347	GLN	2.4
3	O	347	GLN	2.4
1	A	199	LEU	2.4
1	E	101	SER	2.4
1	H	122	SER	2.4
1	M	104	LEU	2.4
2	C	28	SER	2.4
2	F	174	SER	2.4
2	F	19	ILE	2.4
1	E	67	ARG	2.4
2	K	173	TYR	2.4
3	X	273	VAL	2.4
1	I	216	LYS	2.4
3	O	297	ASN	2.4
1	H	223	PRO	2.4
2	C	135	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	66	GLY	2.4
2	C	85	THR	2.4
2	F	56	THR	2.4
2	F	66	GLY	2.4
2	F	43	ALA	2.4
3	Y	400	SER	2.4
3	O	324	SER	2.4
2	G	163	VAL	2.4
1	A	224	LYS	2.4
1	E	82	GLN	2.3
1	E	27	PHE	2.3
2	F	16	GLY	2.3
2	G	79	GLN	2.3
2	K	161	GLU	2.3
3	P	316	GLY	2.3
3	P	298	SER	2.3
1	E	90	ASP	2.3
1	M	74	ASP	2.3
2	C	154	LEU	2.3
1	I	6	GLU	2.3
1	M	147	ALA	2.3
2	F	123	GLU	2.3
2	K	98	PHE	2.3
3	P	295	GLN	2.3
1	M	198	SER	2.3
2	B	132	VAL	2.3
2	C	156	SER	2.3
2	F	12	SER	2.3
3	Y	442	SER	2.3
3	O	441	LEU	2.3
1	E	74	ASP	2.3
3	J	265	ASP	2.3
2	K	119	PRO	2.3
2	F	212	GLY	2.3
1	E	33	THR	2.3
1	H	67	ARG	2.3
3	J	344	ARG	2.3
3	O	248	LYS	2.3
1	M	101	SER	2.3
2	B	35	TRP	2.3
2	C	181	LEU	2.3
2	K	26	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	443	LEU	2.3
1	I	195	PRO	2.3
2	F	90	HIS	2.3
3	O	315	ASP	2.3
2	F	117	ILE	2.3
1	E	1	GLU	2.3
2	B	100	GLN	2.3
3	N	386	GLN	2.3
3	X	388	GLU	2.3
3	O	388	GLU	2.3
2	G	108	ARG	2.3
3	J	292	ARG	2.3
2	B	56	THR	2.3
3	P	252	MET	2.3
2	C	148	TRP	2.3
2	C	174	SER	2.3
3	J	300	TYR	2.3
3	Y	424	SER	2.3
3	J	343	PRO	2.3
3	O	346	PRO	2.3
1	D	10	GLY	2.3
3	N	341	GLY	2.3
3	O	435	HIS	2.3
1	I	194	VAL	2.3
1	M	151	LEU	2.3
2	B	165	GLU	2.3
3	N	325	ASN	2.3
3	X	301	ARG	2.3
3	N	349	TYR	2.3
1	D	14	ALA	2.3
3	O	268	HIS	2.3
3	N	370	LYS	2.3
3	Y	317	LYS	2.3
1	I	11	LEU	2.3
2	C	142	ARG	2.3
2	F	155	GLN	2.3
1	I	33	THR	2.3
3	Y	411	THR	2.3
1	H	71	SER	2.3
2	F	171	SER	2.3
3	J	298	SER	2.3
3	O	253	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	159	PRO	2.3
2	K	99	GLY	2.3
2	L	59	PRO	2.3
2	L	204	PRO	2.3
3	O	329	PRO	2.3
2	B	188	LYS	2.3
3	Y	246	LYS	2.3
3	P	439	LYS	2.3
1	A	5	VAL	2.3
1	I	45	LEU	2.3
1	I	217	VAL	2.3
1	H	103	ARG	2.3
3	O	270	ASP	2.3
3	P	416	ARG	2.3
2	B	27	GLN	2.3
2	F	194	CYS	2.2
2	L	35	TRP	2.2
3	X	381	TRP	2.2
3	Y	243	PHE	2.2
3	P	393	THR	2.2
1	D	7	SER	2.2
1	M	100	GLY	2.2
3	X	246	LYS	2.2
3	O	395	PRO	2.2
1	E	31	ALA	2.2
1	E	112	ALA	2.2
2	G	191	VAL	2.2
2	L	133	VAL	2.2
2	L	199	GLN	2.2
3	J	258	GLU	2.2
2	L	173	TYR	2.2
1	E	96	CYS	2.2
1	I	65	LYS	2.2
3	Y	261	CYS	2.2
1	A	115	PRO	2.2
1	D	100	GLY	2.2
1	D	114	GLY	2.2
1	E	16	GLY	2.2
2	F	142	ARG	2.2
3	N	378	ALA	2.2
3	O	424	SER	2.2
1	H	46	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	185	ASP	2.2
3	O	336	ILE	2.2
3	Y	340	LYS	2.2
1	E	4	LEU	2.2
3	N	314	LEU	2.2
2	K	108	ARG	2.2
3	X	416	ARG	2.2
3	Y	344	ARG	2.2
2	L	60	SER	2.2
3	P	388	GLU	2.2
3	N	288	LYS	2.2
3	X	278	TYR	2.2
1	A	162	VAL	2.2
1	I	159	PRO	2.2
1	H	184	GLY	2.2
3	J	397	VAL	2.2
3	J	412	VAL	2.2
1	I	127	LYS	2.2
3	X	283	GLN	2.2
1	D	170	THR	2.2
2	L	180	THR	2.2
2	F	127	SER	2.2
3	P	375	SER	2.2
2	L	36	TYR	2.2
3	N	347	GLN	2.2
2	G	165	GLU	2.2
3	Y	258	GLU	2.2
3	P	259	VAL	2.2
1	A	102	ASP	2.2
3	O	292	ARG	2.2
1	D	149	GLY	2.2
3	N	441	LEU	2.2
3	Y	309	LEU	2.2
1	I	60	TYR	2.2
1	I	191	VAL	2.2
2	K	88	CYS	2.2
3	P	283	GLN	2.2
1	D	87	ARG	2.2
3	N	301	ARG	2.2
1	M	135	ALA	2.1
2	G	59	PRO	2.1
3	X	330	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	N	372	PHE	2.1
3	J	389	ASN	2.1
3	X	288	LYS	2.1
3	Y	306	LEU	2.1
3	J	393	THR	2.1
1	A	174	HIS	2.1
3	N	310	HIS	2.1
1	M	160	VAL	2.1
3	J	444	SER	2.1
3	X	259	VAL	2.1
1	I	168	ALA	2.1
3	J	313	TRP	2.1
3	O	261	CYS	2.1
1	M	212	PRO	2.1
1	A	148	LEU	2.1
1	A	220	LYS	2.1
1	I	219	LYS	2.1
1	I	220	LYS	2.1
1	H	20	LEU	2.1
1	M	205	ILE	2.1
2	F	136	LEU	2.1
3	N	361	ASN	2.1
2	G	87	HIS	2.1
2	K	64	GLY	2.1
1	I	115	PRO	2.1
2	K	45	LYS	2.1
3	N	387	PRO	2.1
1	E	150	CYS	2.1
1	M	2	VAL	2.1
3	J	379	VAL	2.1
1	A	33	THR	2.1
1	D	172	GLY	2.1
2	K	147	GLN	2.1
1	D	127	LYS	2.1
2	B	30	GLU	2.1
2	L	161	GLU	2.1
3	P	287	ALA	2.1
1	D	212	PRO	2.1
3	X	439	LYS	2.1
3	O	288	LYS	2.1
3	P	423	PHE	2.1
2	B	170	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
3	J	413	ASP	2.1
1	H	192	VAL	2.1
3	J	305	VAL	2.1
3	Y	266	VAL	2.1
1	A	103	ARG	2.1
3	J	276	ASN	2.1
3	X	421	ASN	2.1
2	C	31	THR	2.1
1	D	71	SER	2.1
1	D	122	SER	2.1
1	I	147	ALA	2.1
2	C	9	SER	2.1
2	F	67	SER	2.1
2	L	67	SER	2.1
2	L	123	GLU	2.1
2	L	175	LEU	2.1
3	J	388	GLU	2.1
3	P	254	SER	2.1
1	D	223	PRO	2.1
1	I	218	ASP	2.1
3	X	261	CYS	2.1
3	Y	301	ARG	2.1
2	C	91	TYR	2.1
1	A	8	GLY	2.1
1	I	203	THR	2.1
1	M	220	LYS	2.1
2	F	39	LYS	2.1
3	J	338	LYS	2.1
3	P	275	PHE	2.1
1	A	223	PRO	2.1
3	X	267	SER	2.1
3	Y	396	PRO	2.1
3	O	403	SER	2.1
1	H	72	ARG	2.1
1	H	74	ASP	2.1
3	X	265	ASP	2.1
2	F	149	LYS	2.1
3	J	278	TYR	2.1
3	O	368	LEU	2.1
2	L	153	ALA	2.1
1	M	120	THR	2.1
3	J	342	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
3	Y	272	GLN	2.1
2	C	161	GLU	2.1
2	G	131	SER	2.1
1	D	191	VAL	2.1
3	N	240	VAL	2.1
3	N	369	VAL	2.1
1	E	100	GLY	2.0
2	B	106	ILE	2.0
3	O	321	CYS	2.0
1	D	35	ASN	2.0
2	B	172	THR	2.0
2	G	204	PRO	2.0
3	O	384	ASN	2.0
1	A	196	SER	2.0
1	I	101	SER	2.0
2	F	191	VAL	2.0
3	J	239	SER	2.0
3	X	400	SER	2.0
3	Y	275	PHE	2.0
1	E	144	GLY	2.0
2	B	96	ALA	2.0
2	F	57	GLY	2.0
2	K	128	GLY	2.0
1	E	79	VAL	2.0
1	I	192	VAL	2.0
3	Y	416	ARG	2.0
1	E	50	SER	2.0
2	F	7	SER	2.0
2	K	60	SER	2.0
3	O	365	LEU	2.0
2	K	51	ALA	2.0
1	I	164	TRP	2.0
3	P	284	VAL	2.0
1	A	161	THR	2.0
2	C	73	LEU	2.0
2	G	56	THR	2.0
3	O	355	ARG	2.0
2	G	126	LYS	2.0
3	Y	360	LYS	2.0
2	K	76	SER	2.0
3	X	337	SER	2.0
1	A	176	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.