



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:59 pm BST

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

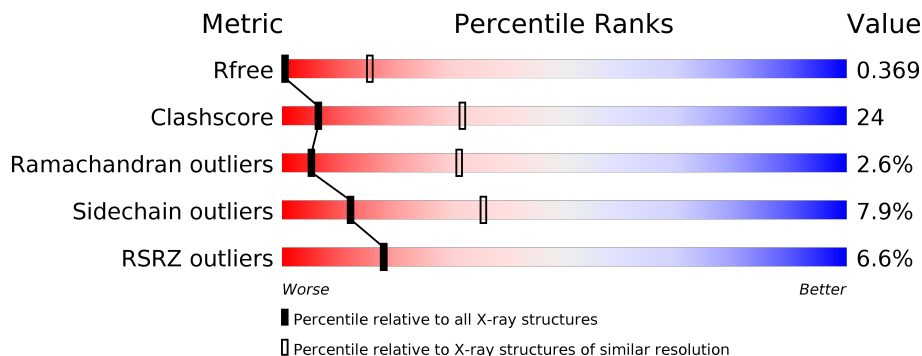
1 Overall quality at a glance i

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.






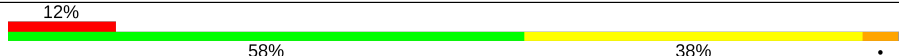
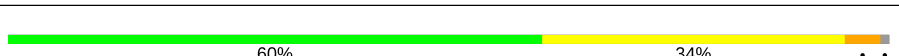
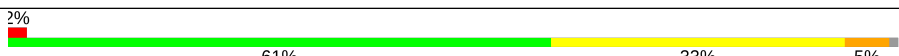
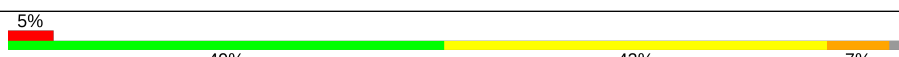
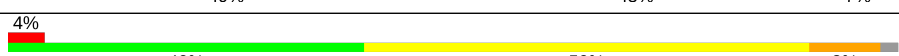

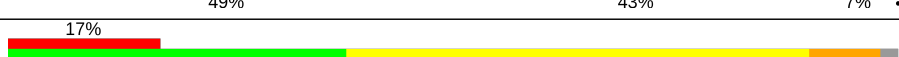

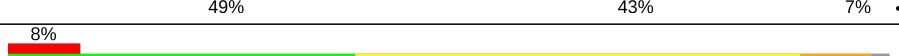
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	243	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	D	243	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	E	243	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 33%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	H	243	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	I	243	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 50%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>
1	M	243	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 52%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
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 [i](#)

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
			Total	C	N	O	S			
1	A	215	1600	1007	273	314	6	38	0	0
1	D	215	1600	1007	273	314	6	51	0	0
1	E	215	1600	1007	273	314	6	38	0	0
1	I	215	1600	1007	273	314	6	51	0	0
1	H	215	1600	1007	273	314	6	38	0	0
1	M	215	1600	1007	273	314	6	51	0	0

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

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

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

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

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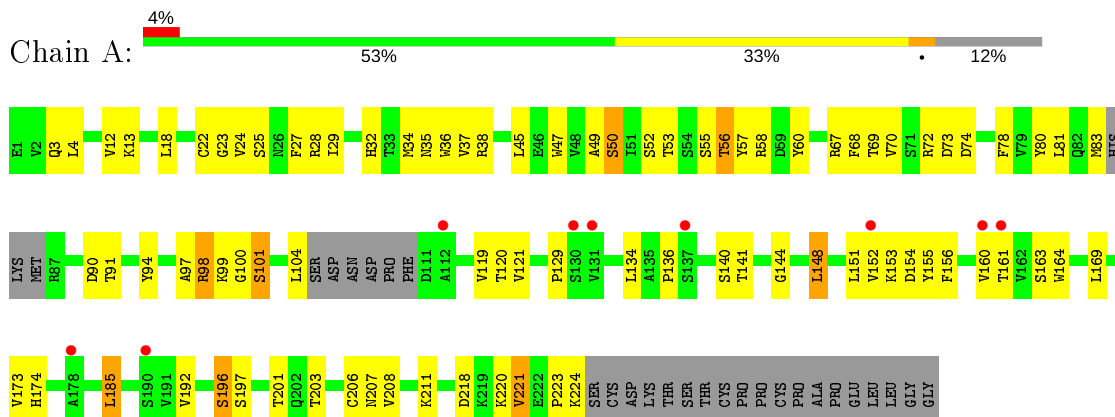
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Chain	Residue	Modelled	Actual	Comment	Reference
O	315	ASP	ASN	CONFLICT	UNP Q6PYX1
O	448	GLY	-	EXPRESSION TAG	UNP Q6PYX1
P	272	GLN	GLU	CONFLICT	UNP Q6PYX1
P	283	GLN	GLU	CONFLICT	UNP Q6PYX1
P	294	GLN	GLU	CONFLICT	UNP Q6PYX1
P	312	ASN	ASP	CONFLICT	UNP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

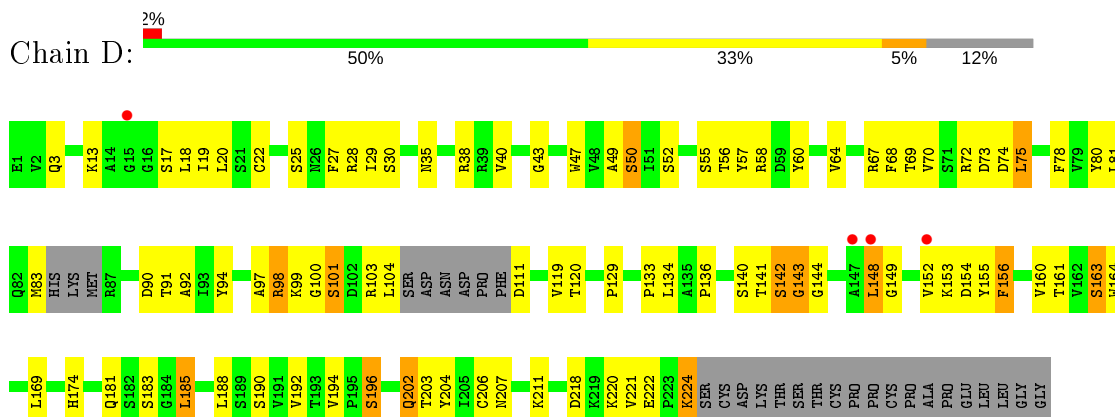
3 Residue-property plots [i](#)

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

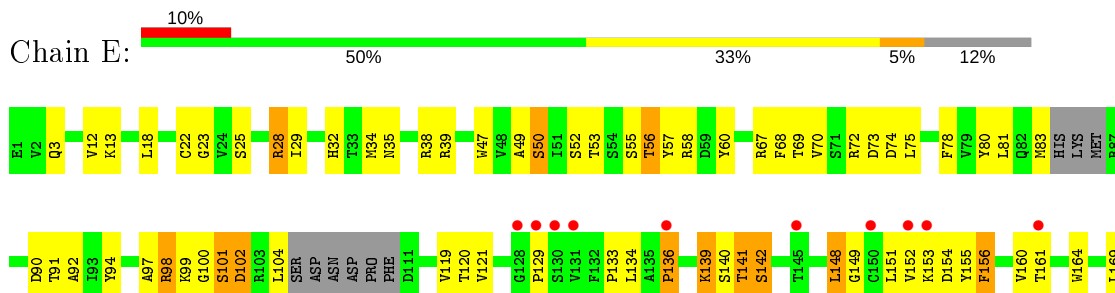
- Molecule 1: 2G12 IgG dimer heavy chain

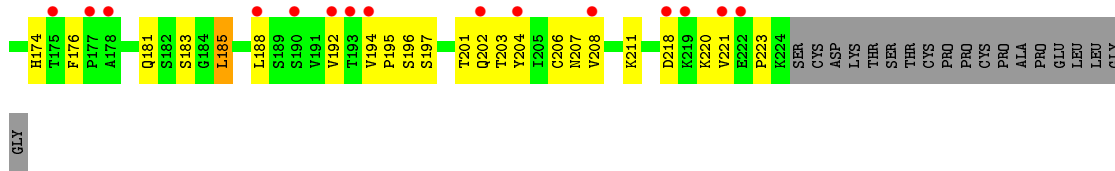


- Molecule 1: 2G12 IgG dimer heavy chain

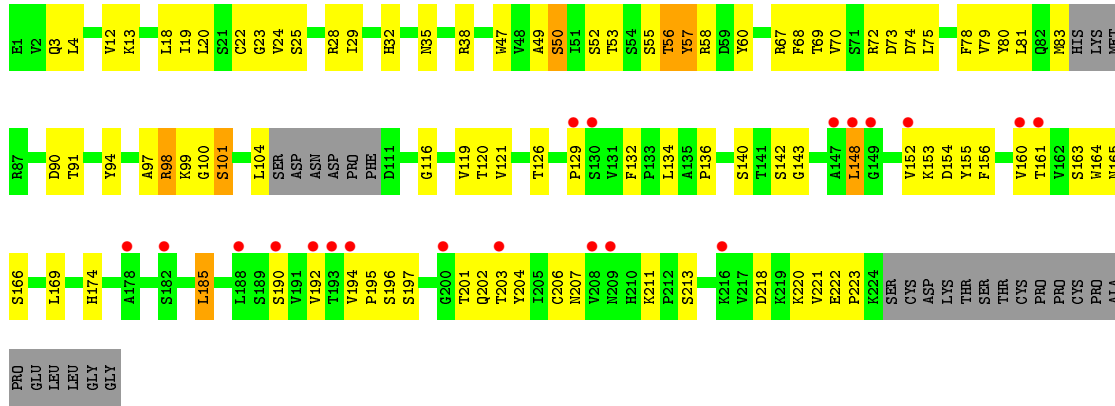


- Molecule 1: 2G12 IgG dimer heavy chain

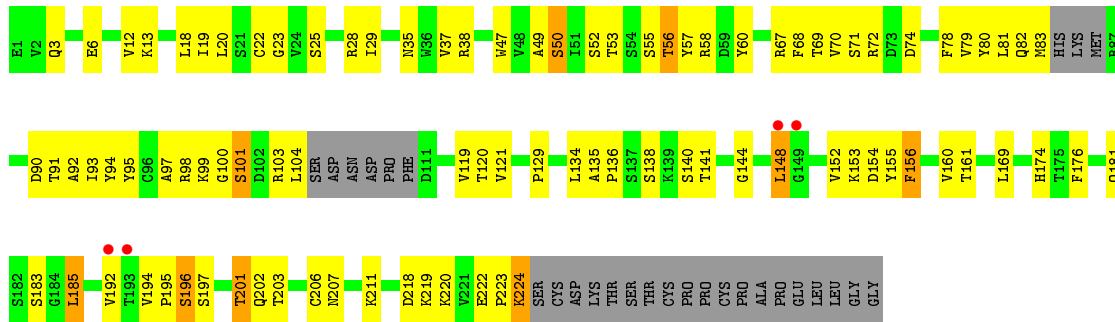




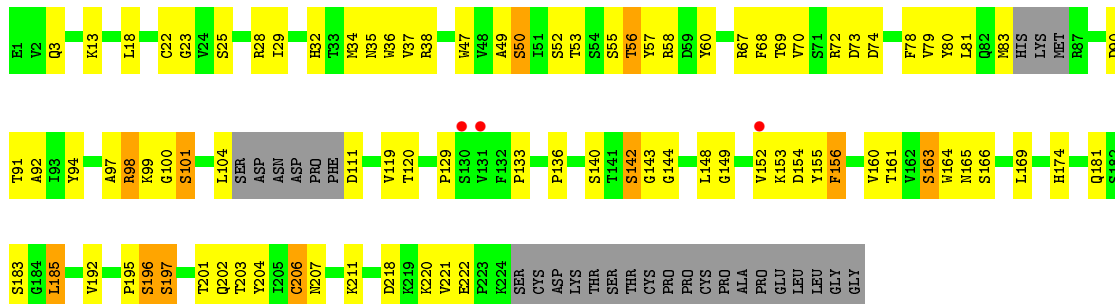
• Molecule 1: 2G12 IgG dimer heavy chain



• Molecule 1: 2G12 IgG dimer heavy chain

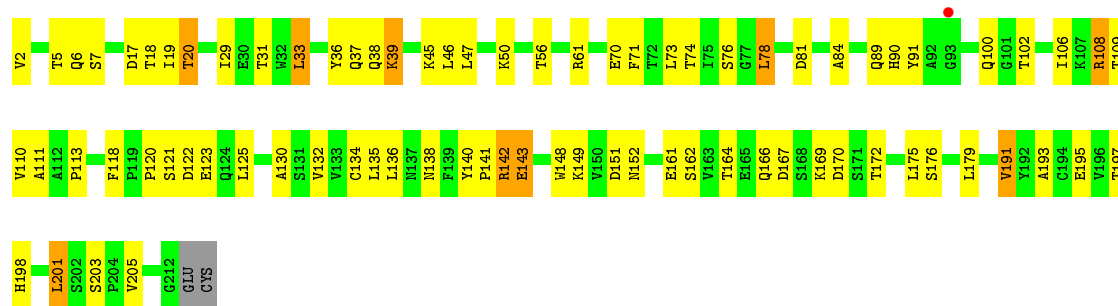


• Molecule 1: 2G12 IgG dimer heavy chain



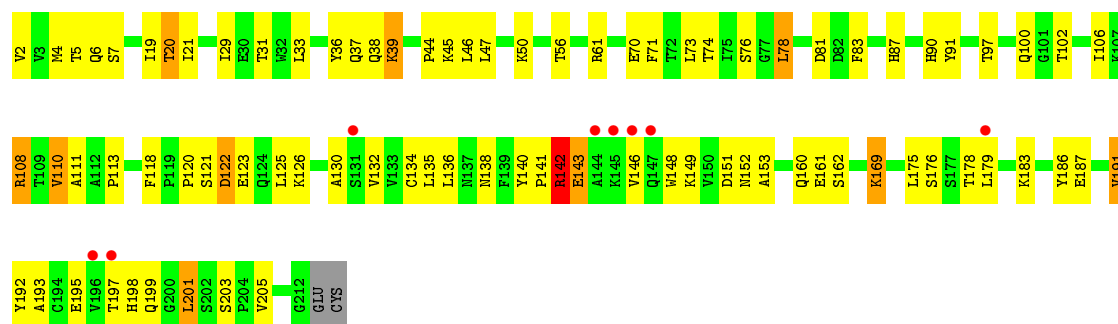
- Molecule 2: 2G12 IgG dimer light chain

Chain B: 



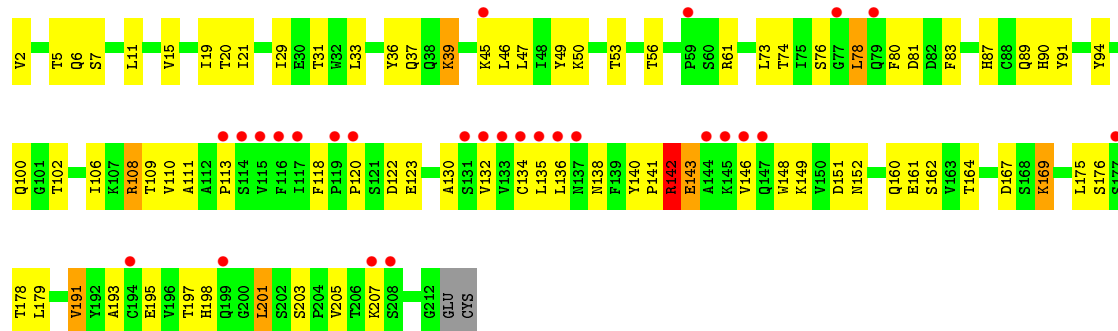
- Molecule 2: 2G12 IgG dimer light chain

Chain C: 



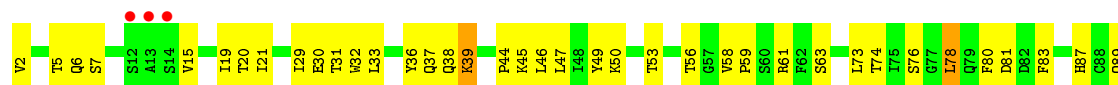
- Molecule 2: 2G12 IgG dimer light chain

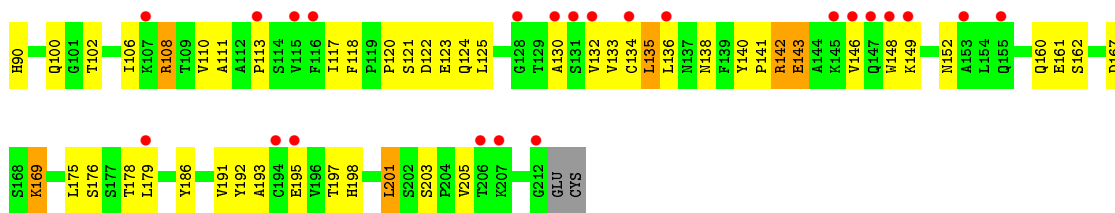
Chain F: 



- Molecule 2: 2G12 IgG dimer light chain

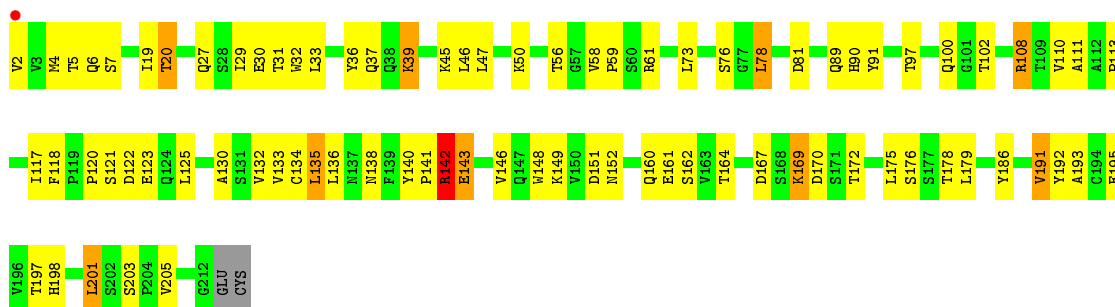
Chain G: 





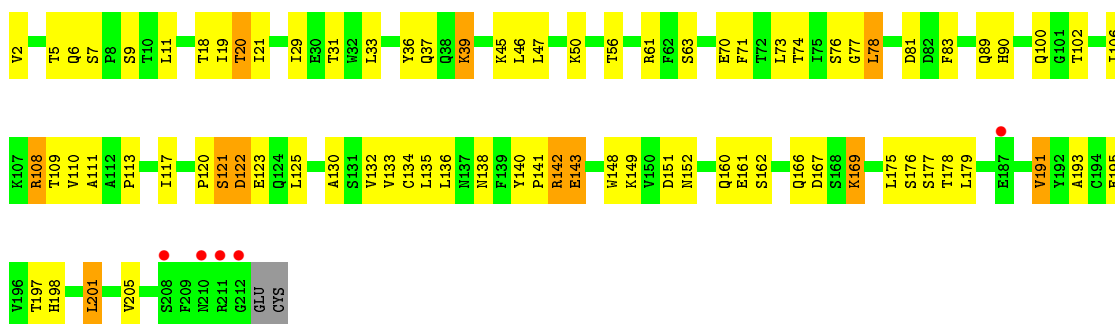
- Molecule 2: 2G12 IgG dimer light chain

Chain K: 60% 34%



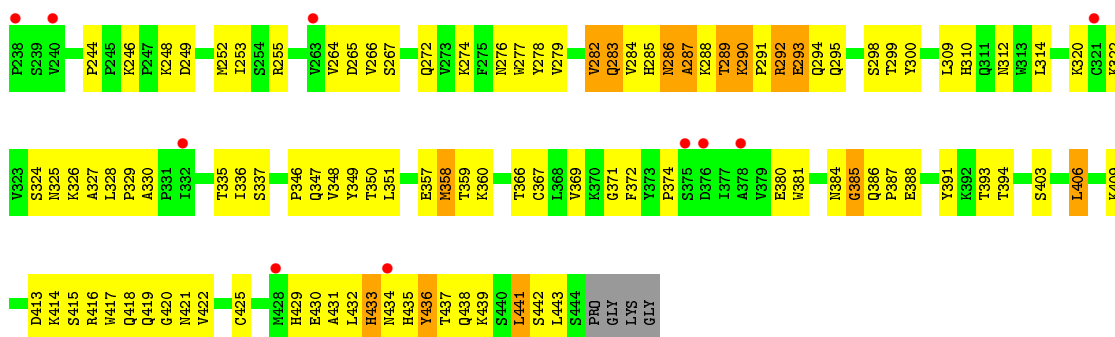
- Molecule 2: 2G12 IgG dimer light chain

Chain L: 61% 33% 2% 5%

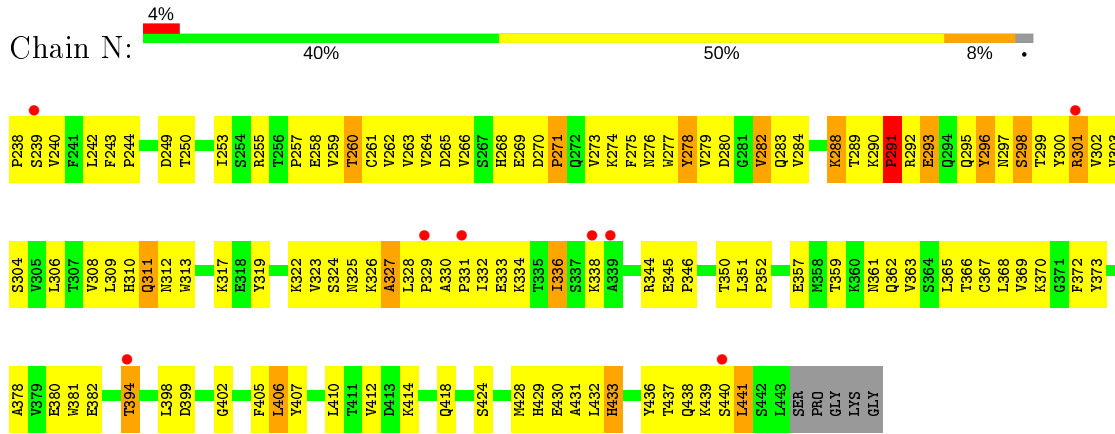


- Molecule 3: Hepatitis B virus receptor binding protein

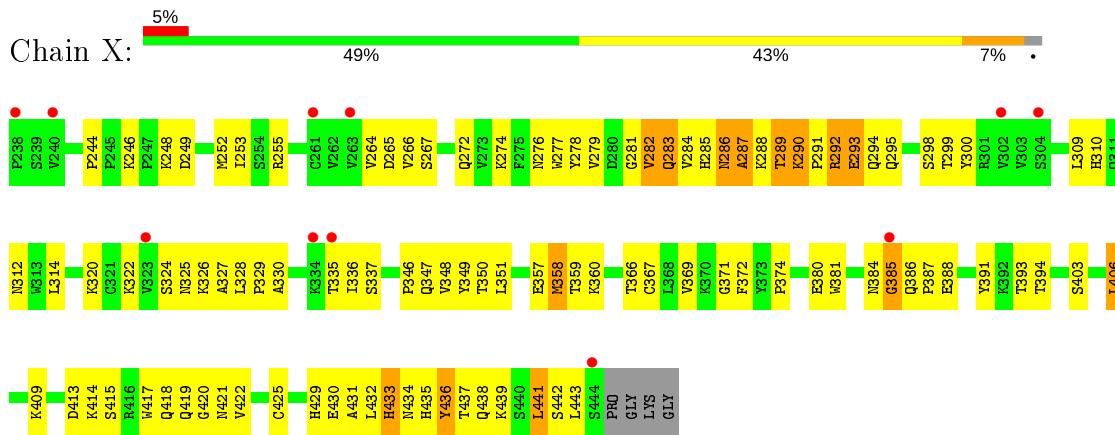
Chain J: 49% 43% 5% 7%



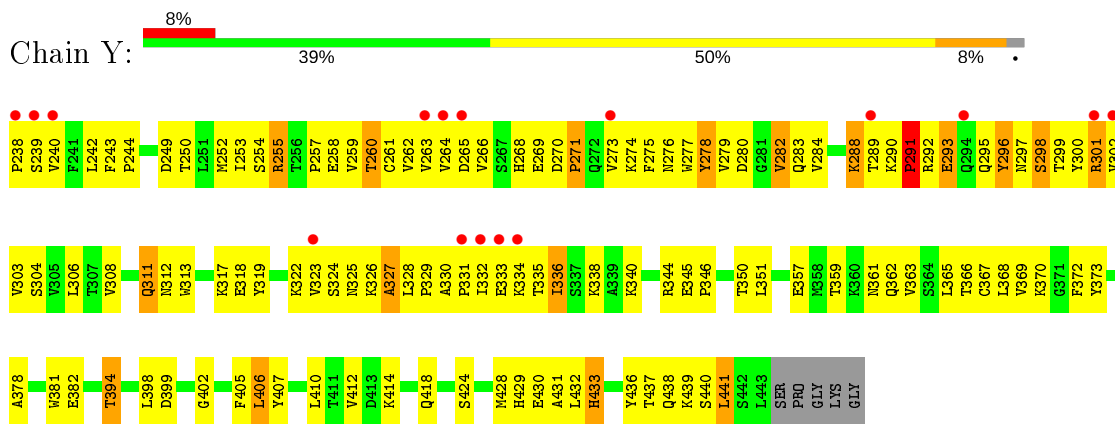
- Molecule 3: Hepatitis B virus receptor binding protein



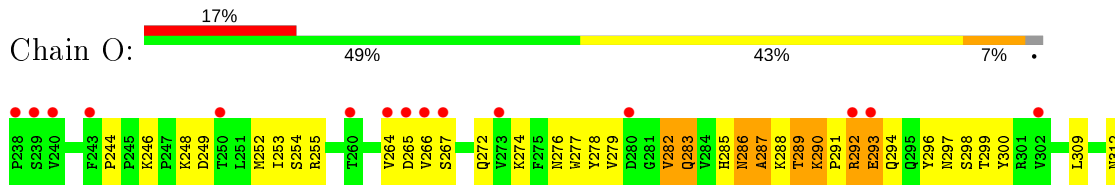
• Molecule 3: Hepatitis B virus receptor binding protein

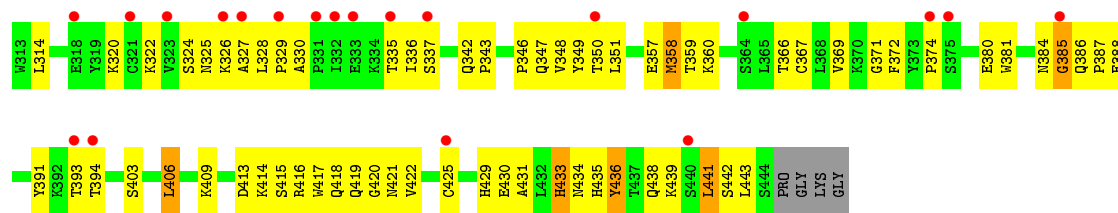


• Molecule 3: Hepatitis B virus receptor binding protein

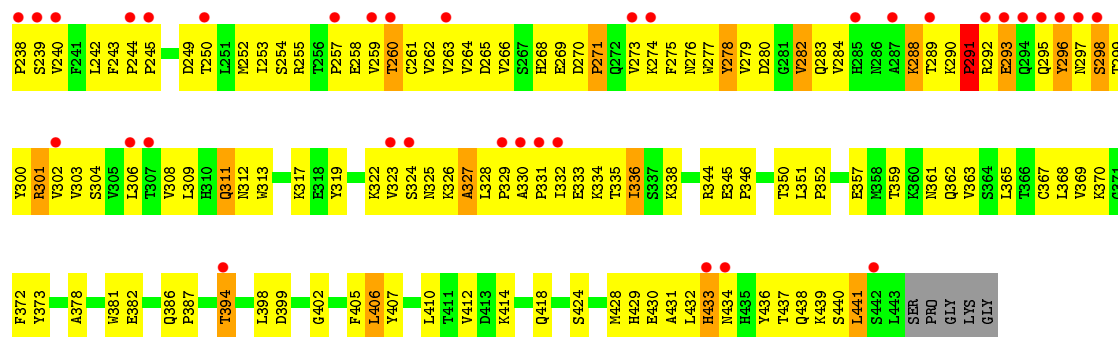


• Molecule 3: Hepatitis B virus receptor binding protein





● 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 – 7.43	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.75-8.00) 82.2 (39.75-7.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 7.33Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309, REFMAC	Depositor
R, R_{free}	0.359 , 0.369 0.359 , 0.369	Depositor DCC
R_{free} test set	1334 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	296.1	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 280.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.60	EDS
Total number of atoms	29250	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.69	1/1633 (0.1%)	0.95	4/2220 (0.2%)
1	D	0.63	0/1631	0.85	3/2214 (0.1%)
1	E	0.67	0/1633	0.93	4/2220 (0.2%)
1	H	0.63	0/1633	0.92	3/2220 (0.1%)
1	I	0.68	0/1631	0.83	3/2214 (0.1%)
1	M	0.68	2/1631 (0.1%)	0.85	3/2214 (0.1%)
2	B	0.63	0/1654	0.75	1/2246 (0.0%)
2	C	0.70	1/1654 (0.1%)	0.78	2/2246 (0.1%)
2	F	0.69	0/1654	0.77	2/2246 (0.1%)
2	G	0.69	1/1654 (0.1%)	0.77	1/2246 (0.0%)
2	K	0.63	0/1654	0.77	3/2246 (0.1%)
2	L	0.67	1/1654 (0.1%)	0.78	1/2246 (0.0%)
3	J	0.43	0/1706	0.68	0/2323
3	N	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	O	0.43	0/1706	0.68	0/2323
3	P	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
3	X	0.43	0/1706	0.68	0/2323
3	Y	0.48	1/1699 (0.1%)	0.67	2/2312 (0.1%)
All	All	0.60	9/29931 (0.0%)	0.78	36/40683 (0.1%)

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

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

All (9) bond length outliers are listed below:

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

All (36) bond angle outliers are listed below:

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

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

There are no chirality outliers.

All (6) planarity outliers are listed below:

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

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1600	0	1581	73	0
1	D	1600	0	1579	96	11
1	E	1600	0	1581	72	0
1	H	1600	0	1580	78	2
1	I	1600	0	1578	78	0
1	M	1600	0	1579	85	0
2	B	1618	0	1580	49	23
2	C	1618	0	1580	54	0
2	F	1618	0	1580	69	0
2	G	1618	0	1580	58	2
2	K	1618	0	1580	54	0
2	L	1618	0	1580	57	19
3	J	1660	0	1632	99	60
3	N	1654	0	1627	114	37
3	O	1660	0	1630	93	19

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

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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:289:THR:HG22	3:N:290:LYS:H	1.48	0.78
3:X:314:LEU:HD22	3:X:430:GLU:HG3	1.62	0.78
3:P:263:VAL:O	3:P:301:ARG:HA	1.84	0.78
1:E:39:ARG:HD2	2:G:38:GLN:HE22	1.47	0.78
3:J:291:PRO:C	3:J:292:ARG:HD2	2.03	0.78
3:Y:263:VAL:O	3:Y:301:ARG:HA	1.84	0.78
3:Y:433:HIS:C	3:Y:433:HIS:N	2.37	0.78
1:D:75:LEU:HD22	1:I:57:TYR:CE1	2.19	0.77
3:N:433:HIS:C	3:N:433:HIS:CB	2.53	0.77
3:O:292:ARG:O	3:O:293:GLU:HB3	1.84	0.77
3:P:429:HIS:HD2	3:P:431:ALA:H	1.31	0.77
1:H:101:SER:HB2	1:H:104:LEU:H	1.47	0.77
1:I:207:ASN:ND2	1:I:218:ASP:OD2	2.19	0.76
3:J:292:ARG:O	3:J:293:GLU:HB3	1.85	0.76
3:P:433:HIS:CB	3:P:433:HIS:C	2.53	0.76
3:X:292:ARG:O	3:X:293:GLU:HB3	1.85	0.76
3:N:263:VAL:O	3:N:301:ARG:HA	1.84	0.76
3:P:429:HIS:CD2	3:P:431:ALA:H	2.03	0.76
3:N:429:HIS:CD2	3:N:431:ALA:H	2.03	0.76
3:Y:429:HIS:CD2	3:Y:431:ALA:H	2.03	0.76
3:Y:433:HIS:CB	3:Y:433:HIS:C	2.53	0.76
1:D:90:ASP:O	1:D:94:TYR:OH	2.03	0.76
3:O:272:GLN:NE2	3:O:326:LYS:HD2	2.01	0.75
3:Y:266:VAL:HB	3:Y:300:TYR:CB	2.15	0.75
3:N:266:VAL:HB	3:N:300:TYR:CB	2.15	0.75
1:D:75:LEU:HD13	1:I:57:TYR:CE1	2.22	0.75
3:P:266:VAL:HB	3:P:300:TYR:CB	2.15	0.75
3:J:272:GLN:NE2	3:J:326:LYS:HD2	2.01	0.75
1:M:91:THR:HG23	1:M:120:THR:HA	1.68	0.75
1:D:91:THR:HG23	1:D:120:THR:HA	1.68	0.75
1:H:3:GLN:HB2	1:H:25:SER:HB2	1.66	0.75
2:F:207:LYS:HZ3	1:M:201:THR:HB	1.46	0.75
3:X:429:HIS:CD2	3:X:431:ALA:H	2.05	0.75
1:D:75:LEU:HD22	1:I:57:TYR:CE2	2.20	0.74
3:J:429:HIS:CD2	3:J:431:ALA:H	2.05	0.74
3:N:328:LEU:HD12	3:N:329:PRO:HD2	1.69	0.74
1:H:207:ASN:ND2	1:H:218:ASP:OD2	2.20	0.74
3:P:365:LEU:HD12	3:P:410:LEU:HD23	1.69	0.74
1:H:224:LYS:HD2	1:H:224:LYS:N	2.03	0.74
3:N:365:LEU:HD12	3:N:410:LEU:HD23	1.69	0.74
3:O:429:HIS:CD2	3:O:431:ALA:H	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:272:GLN:NE2	3:X:326:LYS:HD2	2.01	0.74
1:I:152:VAL:HG11	1:I:160:VAL:HG11	1.69	0.73
3:Y:365:LEU:HD12	3:Y:410:LEU:HD23	1.69	0.73
3:J:295:GLN:OE1	1:M:195:PRO:HB3	1.89	0.73
1:A:197:SER:HB2	3:X:295:GLN:HE22	1.53	0.72
1:M:153:LYS:HG2	1:M:154:ASP:CG	2.10	0.72
1:A:153:LYS:HG2	1:A:154:ASP:CG	2.09	0.72
2:B:142:ARG:HG2	2:B:142:ARG:HH11	1.54	0.72
1:E:101:SER:HB2	1:E:104:LEU:H	1.54	0.72
1:H:18:LEU:HB3	1:H:83:MET:HE3	1.70	0.72
3:Y:328:LEU:HD12	3:Y:329:PRO:HD2	1.69	0.72
3:J:290:LYS:HZ2	2:L:109:THR:HG21	1.54	0.72
1:D:220:LYS:HE2	1:D:222:GLU:CD	2.10	0.72
3:P:328:LEU:HD12	3:P:329:PRO:HD2	1.69	0.72
3:J:295:GLN:NE2	1:M:197:SER:OG	2.23	0.72
1:A:197:SER:HB3	3:X:295:GLN:NE2	2.04	0.71
2:L:39:LYS:NZ	2:L:81:ASP:O	2.22	0.71
3:N:288:LYS:H	3:N:288:LYS:HD3	1.54	0.71
1:H:91:THR:HG23	1:H:120:THR:HA	1.71	0.71
2:L:142:ARG:HH11	2:L:142:ARG:HG2	1.56	0.71
1:D:153:LYS:HG2	1:D:154:ASP:CG	2.10	0.71
3:Y:288:LYS:HD3	3:Y:288:LYS:H	1.54	0.71
1:D:18:LEU:HB3	1:D:83:MET:HE3	1.73	0.71
3:P:288:LYS:HD3	3:P:288:LYS:H	1.54	0.71
1:H:153:LYS:HG2	1:H:154:ASP:CG	2.11	0.71
1:I:90:ASP:O	1:I:94:TYR:OH	2.05	0.70
2:G:142:ARG:HG2	2:G:142:ARG:HH11	1.55	0.70
2:G:143:GLU:OE2	2:G:143:GLU:N	2.24	0.70
2:G:39:LYS:NZ	2:G:81:ASP:O	2.20	0.70
3:J:290:LYS:HZ2	2:L:109:THR:CG2	2.05	0.70
3:J:290:LYS:NZ	2:L:109:THR:CG2	2.53	0.70
1:E:153:LYS:HG2	1:E:154:ASP:CG	2.13	0.70
1:M:207:ASN:ND2	1:M:218:ASP:OD2	2.25	0.69
3:X:422:VAL:HG22	3:X:442:SER:OG	1.92	0.69
3:J:252:MET:HB2	3:J:255:ARG:HG3	1.75	0.69
1:A:197:SER:HB3	3:X:295:GLN:HE22	1.56	0.69
1:I:204:TYR:O	1:I:221:VAL:N	2.26	0.69
2:C:136:LEU:HD13	2:C:175:LEU:HD22	1.75	0.69
1:A:101:SER:HB2	1:A:104:LEU:H	1.57	0.68
2:L:143:GLU:N	2:L:143:GLU:OE2	2.26	0.68
3:O:422:VAL:HG22	3:O:442:SER:OG	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:422:VAL:HG22	3:J:442:SER:OG	1.92	0.68
3:X:252:MET:HB2	3:X:255:ARG:HG3	1.75	0.68
1:A:90:ASP:O	1:A:94:TYR:OH	2.06	0.68
2:C:143:GLU:N	2:C:143:GLU:OE2	2.27	0.68
1:E:152:VAL:HG11	1:E:160:VAL:HG11	1.76	0.68
1:M:152:VAL:HG11	1:M:160:VAL:HG11	1.75	0.68
3:X:325:ASN:HD21	3:X:327:ALA:HB3	1.58	0.68
1:D:152:VAL:HG11	1:D:160:VAL:HG11	1.75	0.68
3:P:270:ASP:N	3:P:271:PRO:HD3	2.09	0.68
1:I:153:LYS:HG2	1:I:154:ASP:CG	2.15	0.67
3:O:252:MET:HB2	3:O:255:ARG:HG3	1.75	0.67
3:J:325:ASN:HD21	3:J:327:ALA:HB3	1.58	0.67
1:I:91:THR:HG23	1:I:120:THR:HA	1.76	0.67
3:N:270:ASP:N	3:N:271:PRO:HD3	2.09	0.67
3:O:418:GLN:HA	3:O:443:LEU:CD2	2.24	0.67
3:X:418:GLN:HA	3:X:443:LEU:CD2	2.24	0.67
1:E:136:PRO:HD3	1:E:148:LEU:HB3	1.77	0.67
3:O:325:ASN:HD21	3:O:327:ALA:HB3	1.58	0.67
2:F:142:ARG:HH11	2:F:142:ARG:HG2	1.60	0.67
2:C:39:LYS:NZ	2:C:81:ASP:O	2.21	0.67
3:J:429:HIS:HD2	3:J:431:ALA:H	1.42	0.67
3:J:418:GLN:HA	3:J:443:LEU:CD2	2.24	0.67
1:A:152:VAL:HG11	1:A:160:VAL:HG11	1.75	0.67
1:A:203:THR:HB	1:A:220:LYS:HE3	1.77	0.67
1:D:207:ASN:ND2	1:D:218:ASP:OD2	2.29	0.66
1:D:75:LEU:HD13	1:I:57:TYR:HE1	1.58	0.66
3:Y:270:ASP:N	3:Y:271:PRO:HD3	2.09	0.66
3:X:350:THR:HB	3:X:441:LEU:HG	1.77	0.66
3:O:325:ASN:ND2	3:O:327:ALA:HB3	2.10	0.66
3:O:350:THR:HB	3:O:441:LEU:HG	1.77	0.66
1:A:174:HIS:HE1	2:B:167:ASP:HB2	1.61	0.66
1:I:201:THR:OG1	1:I:202:GLN:N	2.28	0.66
3:J:325:ASN:ND2	3:J:327:ALA:HB3	2.10	0.66
3:J:350:THR:HB	3:J:441:LEU:HG	1.77	0.66
2:K:142:ARG:HH11	2:K:142:ARG:HG2	1.59	0.66
1:D:202:GLN:O	1:D:203:THR:HA	1.96	0.66
1:H:152:VAL:HG11	1:H:160:VAL:HG11	1.77	0.66
3:X:325:ASN:ND2	3:X:327:ALA:HB3	2.11	0.66
3:O:429:HIS:HD2	3:O:431:ALA:H	1.42	0.65
1:M:201:THR:HG1	1:M:202:GLN:N	1.94	0.65
3:P:290:LYS:HE3	3:P:292:ARG:HH22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:GLU:OE2	2:F:143:GLU:N	2.30	0.65
2:F:149:LYS:NZ	2:F:195:GLU:OE1	2.27	0.65
1:D:154:ASP:HB3	1:D:185:LEU:HD23	1.79	0.65
1:A:136:PRO:HD3	1:A:148:LEU:HB3	1.79	0.64
2:B:143:GLU:N	2:B:143:GLU:OE2	2.29	0.64
3:J:279:VAL:O	3:J:282:VAL:HG13	1.97	0.64
3:O:328:LEU:HG	3:O:330:ALA:O	1.98	0.64
3:X:429:HIS:HD2	3:X:431:ALA:H	1.43	0.64
2:B:29:ILE:HG21	2:B:90:HIS:HD2	1.62	0.64
2:F:37:GLN:O	2:F:45:LYS:N	2.30	0.64
3:Y:332:ILE:HG22	3:Y:333:GLU:N	2.13	0.64
2:C:149:LYS:NZ	2:C:195:GLU:OE1	2.26	0.64
3:P:330:ALA:HB1	3:P:331:PRO:HD2	1.80	0.64
3:O:279:VAL:O	3:O:282:VAL:HG13	1.97	0.64
3:X:328:LEU:HG	3:X:330:ALA:O	1.98	0.64
3:Y:290:LYS:HE3	3:Y:292:ARG:HH22	1.61	0.64
2:G:149:LYS:NZ	2:G:195:GLU:OE1	2.26	0.64
3:X:288:LYS:HD2	3:X:288:LYS:H	1.63	0.64
3:J:288:LYS:H	3:J:288:LYS:HD2	1.63	0.63
3:O:288:LYS:HD2	3:O:288:LYS:H	1.63	0.63
1:E:174:HIS:HE1	2:F:167:ASP:HB2	1.62	0.63
1:I:101:SER:HB2	1:I:104:LEU:H	1.63	0.63
2:K:143:GLU:OE2	2:K:143:GLU:N	2.31	0.63
3:N:290:LYS:HE3	3:N:292:ARG:HH22	1.61	0.63
3:N:332:ILE:HG22	3:N:333:GLU:N	2.13	0.63
3:P:332:ILE:HG22	3:P:333:GLU:N	2.13	0.63
3:J:290:LYS:HZ3	2:L:109:THR:HG21	1.61	0.63
3:J:328:LEU:HG	3:J:330:ALA:O	1.98	0.63
1:M:164:TRP:C	1:M:166:SER:H	2.02	0.63
1:M:204:TYR:O	1:M:221:VAL:N	2.32	0.63
3:N:330:ALA:HB1	3:N:331:PRO:HD2	1.79	0.63
1:A:154:ASP:HB3	1:A:185:LEU:HD23	1.80	0.63
1:E:201:THR:OG1	1:E:202:GLN:N	2.31	0.63
2:C:120:PRO:HG3	2:C:130:ALA:HB1	1.81	0.63
1:E:18:LEU:HB3	1:E:83:MET:HE3	1.79	0.63
3:J:290:LYS:NZ	2:L:109:THR:OG1	2.32	0.63
1:I:148:LEU:HB2	1:I:221:VAL:HG11	1.80	0.63
3:X:279:VAL:O	3:X:282:VAL:HG13	1.97	0.63
1:A:34:MET:SD	1:A:98:ARG:HB2	2.39	0.62
3:Y:330:ALA:HB1	3:Y:331:PRO:HD2	1.79	0.62
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:174:HIS:HE1	2:K:167:ASP:HB2	1.63	0.62
2:C:61:ARG:HB2	2:C:76:SER:O	1.99	0.62
2:C:142:ARG:HH11	2:C:142:ARG:HG2	1.63	0.62
1:D:75:LEU:CD2	1:I:57:TYR:CE1	2.82	0.62
1:E:203:THR:HB	1:E:220:LYS:HE3	1.81	0.62
1:H:154:ASP:HB3	1:H:185:LEU:HD23	1.82	0.62
3:O:384:ASN:O	3:O:386:GLN:N	2.31	0.62
2:K:136:LEU:HD13	2:K:175:LEU:HD22	1.82	0.62
2:C:29:ILE:HG21	2:C:90:HIS:HD2	1.64	0.62
2:G:136:LEU:HD13	2:G:175:LEU:HD22	1.80	0.62
1:I:18:LEU:HB3	1:I:83:MET:HE3	1.81	0.62
1:H:203:THR:HB	1:H:220:LYS:HE3	1.81	0.61
2:K:61:ARG:HB2	2:K:76:SER:O	2.00	0.61
2:G:37:GLN:O	2:G:45:LYS:N	2.29	0.61
2:G:29:ILE:HG21	2:G:90:HIS:HD2	1.64	0.61
1:M:163:SER:O	1:M:207:ASN:N	2.32	0.61
2:F:151:ASP:HA	2:F:191:VAL:HG12	1.81	0.61
1:M:99:LYS:HG2	1:M:100:GLY:N	2.14	0.61
2:C:37:GLN:O	2:C:45:LYS:N	2.31	0.61
2:B:149:LYS:NZ	2:B:195:GLU:OE1	2.32	0.61
3:P:394:THR:HG23	3:P:407:TYR:O	2.01	0.61
2:G:36:TYR:HB2	2:G:87:HIS:HB2	1.81	0.61
3:J:384:ASN:O	3:J:386:GLN:N	2.31	0.61
1:A:91:THR:HG23	1:A:120:THR:HA	1.83	0.60
2:F:136:LEU:HD13	2:F:175:LEU:HD22	1.82	0.60
2:G:120:PRO:HG3	2:G:130:ALA:HB1	1.83	0.60
1:A:99:LYS:HG2	1:A:100:GLY:N	2.16	0.60
3:N:406:LEU:HD12	3:N:406:LEU:C	2.22	0.60
1:D:99:LYS:HG2	1:D:100:GLY:N	2.16	0.60
1:D:203:THR:HB	1:D:220:LYS:HE3	1.83	0.60
3:X:417:TRP:CH2	3:X:441:LEU:HD22	2.37	0.60
3:J:417:TRP:CH2	3:J:441:LEU:HD22	2.37	0.60
3:J:421:ASN:N	3:J:421:ASN:HD22	2.00	0.60
1:M:18:LEU:HB3	1:M:83:MET:HE3	1.83	0.60
2:B:37:GLN:O	2:B:45:LYS:N	2.29	0.60
2:K:6:GLN:NE2	2:K:102:THR:OG1	2.35	0.60
3:P:406:LEU:HD12	3:P:406:LEU:C	2.22	0.60
3:X:384:ASN:O	3:X:386:GLN:N	2.31	0.60
3:Y:394:THR:HG23	3:Y:407:TYR:O	2.01	0.60
2:F:29:ILE:HG21	2:F:90:HIS:HD2	1.66	0.59
1:I:154:ASP:HB3	1:I:185:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:325:ASN:HD22	3:N:326:LYS:H	1.51	0.59
3:P:274:LYS:HE2	3:P:276:ASN:HD21	1.67	0.59
2:K:149:LYS:NZ	2:K:195:GLU:OE1	2.36	0.59
3:O:417:TRP:CH2	3:O:441:LEU:HD22	2.37	0.59
3:Y:406:LEU:C	3:Y:406:LEU:HD12	2.22	0.59
1:M:101:SER:HB2	1:M:104:LEU:H	1.66	0.59
3:N:257:PRO:HB2	3:N:308:VAL:HB	1.84	0.59
1:A:197:SER:CB	3:X:295:GLN:NE2	2.62	0.59
1:A:129:PRO:HB3	1:A:155:TYR:HB3	1.83	0.59
1:I:60:TYR:OH	1:I:69:THR:HA	2.03	0.59
1:H:99:LYS:HG2	1:H:100:GLY:N	2.17	0.59
2:L:120:PRO:HG3	2:L:130:ALA:HB1	1.85	0.59
3:N:274:LYS:HE2	3:N:276:ASN:HD21	1.67	0.59
3:P:257:PRO:HB2	3:P:308:VAL:HB	1.84	0.59
1:D:72:ARG:NE	1:D:74:ASP:OD1	2.30	0.59
1:H:72:ARG:NE	1:H:74:ASP:OD1	2.31	0.59
3:Y:325:ASN:HD22	3:Y:326:LYS:H	1.51	0.59
1:E:154:ASP:HB3	1:E:185:LEU:HD23	1.84	0.59
1:D:148:LEU:HD13	1:D:221:VAL:HB	1.85	0.59
2:K:37:GLN:O	2:K:45:LYS:N	2.33	0.59
2:L:29:ILE:HG21	2:L:90:HIS:HD2	1.67	0.59
3:N:394:THR:HG23	3:N:407:TYR:O	2.01	0.59
3:O:421:ASN:N	3:O:421:ASN:HD22	2.00	0.59
3:O:417:TRP:HH2	3:O:441:LEU:HD22	1.67	0.59
3:P:269:GLU:HG2	3:P:269:GLU:O	2.03	0.59
1:A:18:LEU:HB3	1:A:83:MET:HE3	1.83	0.59
3:P:296:TYR:CE1	3:P:301:ARG:HD3	2.38	0.59
1:D:75:LEU:CD2	1:I:57:TYR:CZ	2.69	0.58
3:J:417:TRP:HH2	3:J:441:LEU:HD22	1.67	0.58
3:P:279:VAL:O	3:P:279:VAL:HG23	2.03	0.58
3:X:433:HIS:ND1	3:X:434:ASN:OD1	2.36	0.58
1:M:133:PRO:HB3	1:M:221:VAL:HG22	1.85	0.58
3:N:269:GLU:O	3:N:269:GLU:HG2	2.03	0.58
3:O:276:ASN:HB2	3:O:322:LYS:HB3	1.86	0.58
3:Y:265:ASP:HA	3:Y:299:THR:HB	1.85	0.58
1:H:222:GLU:HB2	1:H:223:PRO:HD2	1.84	0.58
3:N:279:VAL:HG23	3:N:279:VAL:O	2.03	0.58
3:P:265:ASP:HA	3:P:299:THR:HB	1.86	0.58
3:X:421:ASN:N	3:X:421:ASN:HD22	2.00	0.58
3:Y:269:GLU:O	3:Y:269:GLU:HG2	2.03	0.58
2:G:201:LEU:HG	2:G:205:VAL:HG23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:415:SER:O	3:X:419:GLN:HG3	2.04	0.58
3:Y:274:LYS:HE2	3:Y:276:ASN:HD21	1.67	0.58
3:Y:296:TYR:CE1	3:Y:301:ARG:HD3	2.38	0.58
2:B:136:LEU:HD13	2:B:175:LEU:HD22	1.83	0.58
3:J:286:ASN:O	3:J:287:ALA:HB2	2.03	0.58
3:Y:424:SER:OG	3:Y:438:GLN:HG2	2.04	0.58
2:F:201:LEU:HG	2:F:205:VAL:HG23	1.86	0.58
1:H:169:LEU:HD21	1:H:192:VAL:HG21	1.85	0.58
1:H:201:THR:OG1	1:H:202:GLN:N	2.33	0.58
3:N:288:LYS:HE2	3:N:306:LEU:HD11	1.86	0.58
3:X:417:TRP:HH2	3:X:441:LEU:HD22	1.67	0.58
1:E:91:THR:HG23	1:E:120:THR:HA	1.85	0.58
1:H:129:PRO:HB3	1:H:155:TYR:HB3	1.84	0.58
1:I:99:LYS:HG2	1:I:100:GLY:N	2.18	0.58
1:M:164:TRP:O	1:M:166:SER:N	2.37	0.58
3:N:266:VAL:CB	3:N:300:TYR:HB2	2.28	0.58
3:O:286:ASN:O	3:O:287:ALA:HB2	2.03	0.58
3:N:424:SER:OG	3:N:438:GLN:HG2	2.04	0.58
2:B:39:LYS:NZ	2:B:81:ASP:O	2.27	0.58
2:C:201:LEU:HG	2:C:205:VAL:HG23	1.85	0.58
3:J:415:SER:O	3:J:419:GLN:HG3	2.04	0.58
3:P:288:LYS:HE2	3:P:306:LEU:HD11	1.86	0.58
3:Y:257:PRO:HB2	3:Y:308:VAL:HB	1.85	0.57
3:Y:288:LYS:HE2	3:Y:306:LEU:HD11	1.86	0.57
2:C:19:ILE:HG12	2:C:78:LEU:HD11	1.86	0.57
2:G:118:PHE:CD2	1:I:134:LEU:HD13	2.39	0.57
1:I:203:THR:HB	1:I:220:LYS:HE3	1.85	0.57
1:M:73:ASP:N	1:M:78:PHE:O	2.37	0.57
3:N:296:TYR:CE1	3:N:301:ARG:HD3	2.38	0.57
3:P:325:ASN:HD22	3:P:326:LYS:H	1.51	0.57
2: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:N:265:ASP:HA	3:N:299:THR:HB	1.85	0.57
3:O:415:SER:O	3:O:419:GLN:HG3	2.04	0.57
3:X:286:ASN:O	3:X:287:ALA:HB2	2.03	0.57
2:L:149:LYS:NZ	2:L:195:GLU:OE1	2.33	0.57
3:O:433:HIS:ND1	3:O:434:ASN:OD1	2.35	0.57
1:D:35:ASN:O	1:D:97:ALA:N	2.37	0.57
3:Y:279:VAL:HG23	3:Y:279:VAL:O	2.03	0.57
1:D:52:SER:O	1:D:72:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:LEU:CD1	1:I:57:TYR:CE1	2.86	0.57
3:J:433:HIS:ND1	3:J:434:ASN:OD1	2.36	0.57
3:X:320:LYS:HG3	3:X:335:THR:HG22	1.87	0.57
2:K:29:ILE:HG21	2:K:90:HIS:HD2	1.69	0.57
3:O:320:LYS:HG3	3:O:335:THR:HG22	1.87	0.57
3:P:311:GLN:CD	3:P:311:GLN:H	2.08	0.57
3:P:424:SER:OG	3:P:438:GLN:HG2	2.04	0.57
3:N:328:LEU:HG	3:N:330:ALA:O	2.05	0.57
3:J:276:ASN:HB2	3:J:322:LYS:HB3	1.86	0.56
3:J:320:LYS:HG3	3:J:335:THR:HG22	1.87	0.56
3:P:439:LYS:HE3	3:P:440:SER:O	2.05	0.56
1:D:144:GLY:O	1:D:196:SER:HB2	2.05	0.56
1:D:103:ARG:O	2:F:50:LYS:CE	2.53	0.56
1:A:153:LYS:HG2	1:A:154:ASP:OD2	2.06	0.56
2:G:6:GLN:NE2	2:G:102:THR:OG1	2.39	0.56
2:K:148:TRP:CE3	2:K:179:LEU:HD22	2.40	0.56
2:K:201:LEU:HG	2:K:205:VAL:HG23	1.87	0.56
2:K:37:GLN:HB2	2:K:47:LEU:HD11	1.87	0.56
3:X:276:ASN:HB2	3:X:322:LYS:HB3	1.86	0.56
2:C:6:GLN:NE2	2:C:102:THR:OG1	2.38	0.56
1:A:60:TYR:OH	1:A:69:THR:HA	2.04	0.56
2:G:19:ILE:HG12	2:G:78:LEU:HD11	1.88	0.56
1:H:136:PRO:HD3	1:H:148:LEU:HB3	1.87	0.56
3:N:311:GLN:CD	3:N:311:GLN:H	2.08	0.56
3:Y:325:ASN:ND2	3:Y:326:LYS:H	2.04	0.56
1:E:52:SER:O	1:E:72:ARG:NH1	2.37	0.56
3:N:301:ARG:HE	3:N:303:VAL:CG2	2.18	0.56
3:N:270:ASP:OD2	3:N:327:ALA:HB2	2.06	0.56
3:N:439:LYS:HE3	3:N:440:SER:O	2.05	0.56
3:P:270:ASP:OD2	3:P:327:ALA:HB2	2.06	0.56
3:P:328:LEU:HG	3:P:330:ALA:O	2.05	0.56
3:X:288:LYS:O	3:X:289:THR:O	2.24	0.56
3:Y:301:ARG:HE	3:Y:303:VAL:CG2	2.18	0.56
2:B:6:GLN:NE2	2:B:102:THR:OG1	2.38	0.56
3:Y:328:LEU:HG	3:Y:330:ALA:O	2.05	0.56
1:H:35:ASN:OD1	1:H:50:SER:HB2	2.06	0.56
3:O:328:LEU:HD12	3:O:329:PRO:HD2	1.88	0.56
3:Y:311:GLN:H	3:Y:311:GLN:CD	2.08	0.56
1:A:104:LEU:HD12	1:E:28:ARG:CG	2.20	0.56
1:D:129:PRO:HB3	1:D:155:TYR:HB3	1.87	0.56
2:F:120:PRO:HG3	2:F:130:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:288:LYS:O	3:J:289:THR:O	2.24	0.56
2:K:160:GLN:O	2:K:178:THR:N	2.36	0.56
3:N:325:ASN:ND2	3:N:326:LYS:H	2.04	0.56
1:D:38:ARG:HB3	1:D:94:TYR:CE2	2.41	0.55
1:H:58:ARG:NH1	1:H:70:VAL:O	2.39	0.55
2:L:160:GLN:O	2:L:178:THR:N	2.38	0.55
3:J:289:THR:O	3:J:290:LYS:HB2	2.07	0.55
3:O:288:LYS:O	3:O:289:THR:O	2.24	0.55
3:O:289:THR:O	3:O:290:LYS:HB2	2.07	0.55
3:P:301:ARG:HE	3:P:303:VAL:CG2	2.18	0.55
1:A:70:VAL:HA	1:A:80:TYR:O	2.06	0.55
1:D:164:TRP:HZ2	1:D:190:SER:O	1.90	0.55
1:D:169:LEU:HD21	1:D:192:VAL:HG21	1.88	0.55
1:D:60:TYR:OH	1:D:69:THR:HA	2.06	0.55
2:F:142:ARG:HG2	2:F:142:ARG:NH1	2.22	0.55
3:J:328:LEU:HD12	3:J:329:PRO:HD2	1.88	0.55
3:Y:266:VAL:CB	3:Y:300:TYR:HB2	2.28	0.55
3:P:325:ASN:ND2	3:P:326:LYS:H	2.04	0.55
2:B:19:ILE:HG12	2:B:78:LEU:HD11	1.88	0.55
2:C:37:GLN:HB2	2:C:47:LEU:HD11	1.89	0.55
1:D:101:SER:H	1:D:104:LEU:HD23	1.71	0.55
2:F:39:LYS:NZ	2:F:81:ASP:O	2.30	0.55
1:H:70:VAL:HA	1:H:80:TYR:O	2.06	0.55
2:K:39:LYS:NZ	2:K:81:ASP:O	2.30	0.55
1:M:60:TYR:OH	1:M:69:THR:HA	2.06	0.55
1:M:34:MET:SD	1:M:98:ARG:HB2	2.46	0.55
1:I:29:ILE:O	1:I:72:ARG:NH2	2.39	0.55
3:Y:439:LYS:HE3	3:Y:440:SER:O	2.05	0.55
1:A:47:TRP:NE1	1:A:49:ALA:O	2.40	0.55
1:E:35:ASN:OD1	1:E:50:SER:HB2	2.07	0.55
2:L:167:ASP:HB2	1:M:174:HIS:HE1	1.71	0.55
3:X:289:THR:O	3:X:290:LYS:HB2	2.07	0.55
3:Y:270:ASP:OD2	3:Y:327:ALA:HB2	2.06	0.55
1:H:94:TYR:CE1	1:H:119:VAL:HB	2.42	0.55
1:M:94:TYR:CE1	1:M:119:VAL:HB	2.42	0.55
3:O:414:LYS:HE2	3:O:418:GLN:NE2	2.22	0.55
1:D:133:PRO:HG2	1:D:224:LYS:HZ1	1.72	0.55
2:F:2:VAL:HG11	2:F:90:HIS:CD2	2.42	0.55
2:K:142:ARG:NH1	2:K:142:ARG:HG2	2.22	0.55
3:P:238:PRO:CG	3:P:328:LEU:HD13	2.37	0.55
3:P:275:PHE:HE1	3:P:302:VAL:HG12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HG	2:C:87:HIS:CE1	2.43	0.54
2:F:37:GLN:HB2	2:F:47:LEU:HD11	1.89	0.54
2:L:37:GLN:O	2:L:45:LYS:N	2.37	0.54
1:M:70:VAL:HA	1:M:80:TYR:O	2.06	0.54
3:X:328:LEU:HD12	3:X:329:PRO:HD2	1.88	0.54
1:M:68:PHE:CD1	1:M:83:MET:HA	2.42	0.54
3:X:414:LYS:HE2	3:X:418:GLN:NE2	2.22	0.54
3:N:240:VAL:O	3:N:334:LYS:HE3	2.08	0.54
3:O:282:VAL:O	3:O:283:GLN:CB	2.52	0.54
3:Y:240:VAL:O	3:Y:334:LYS:HE3	2.08	0.54
3:Y:238:PRO:CG	3:Y:328:LEU:HD13	2.37	0.54
2:B:91:TYR:HD1	1:D:99:LYS:NZ	2.04	0.54
1:H:135:ALA:HB3	1:H:224:LYS:HD3	1.89	0.54
2:K:162:SER:HB3	2:K:176:SER:OG	2.07	0.54
3:P:240:VAL:O	3:P:334:LYS:HE3	2.08	0.54
3:J:414:LYS:O	3:J:418:GLN:HG3	2.08	0.54
3:J:414:LYS:HE2	3:J:418:GLN:NE2	2.22	0.54
2:L:31:THR:OG1	2:L:50:LYS:HE2	2.07	0.54
3:N: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
3:N:238:PRO:CG	3:N:328:LEU:HD13	2.37	0.54
3:O:414:LYS:O	3:O:418:GLN:HG3	2.08	0.54
1:D:103:ARG:O	2:F:50:LYS:CD	2.56	0.54
2:K:120:PRO:HG3	2:K:130:ALA:HB1	1.89	0.54
2:L:6:GLN:NE2	2:L:102:THR:OG1	2.40	0.54
3:O:285:HIS:O	3:O:286:ASN:HB2	2.08	0.54
3:O:418:GLN:HA	3:O:443:LEU:HD22	1.90	0.54
1:E:60:TYR:OH	1:E:69:THR:HA	2.08	0.54
1:E:99:LYS:HG2	1:E:100:GLY:N	2.23	0.54
3:P:351:LEU:C	3:P:441:LEU:HD11	2.28	0.54
3:X:418:GLN:HA	3:X:443:LEU:HD22	1.90	0.54
3:Y:289:THR:HG22	3:Y:290:LYS:N	2.22	0.54
1:I:169:LEU:HD21	1:I:192:VAL:HG21	1.90	0.54
2:L:162:SER:HB3	2:L:176:SER:OG	2.07	0.54
3:Y:275:PHE:HE1	3:Y:302:VAL:HG12	1.72	0.54
1:E:70:VAL:HA	1:E:80:TYR:O	2.07	0.53
1:H:153:LYS:HG2	1:H:154:ASP:OD2	2.08	0.53
1:H:69:THR:C	1:H:81:LEU:HD12	2.28	0.53
1:I:22:CYS:O	1:I:78:PHE:HA	2.08	0.53
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.90	0.53
1:M:47:TRP:NE1	1:M:49:ALA:O	2.41	0.53

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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
2:B:142:ARG:HG2	2:B:142:ARG:NH1	2.18	0.53
3:N:351:LEU:C	3:N:441:LEU:HD11	2.28	0.53
3:X:285:HIS:O	3:X:286:ASN:HB2	2.08	0.53
3:Y:262:VAL:HG13	3:Y:303:VAL:HG22	1.90	0.53
3:Y:351:LEU:C	3:Y:441:LEU:HD11	2.28	0.53
1:D:35:ASN:OD1	1:D:50:SER:HB2	2.08	0.53
1:H:101:SER:H	1:H:104:LEU:CD2	2.21	0.53
3:P:322:LYS:HE3	3:P:333:GLU:OE2	2.08	0.53
3:P:266:VAL:CB	3:P:300:TYR:HB2	2.28	0.53
1:D:70:VAL:HA	1:D:80:TYR:O	2.09	0.53
3:J:285:HIS:O	3:J:286:ASN:HB2	2.08	0.53
2:L:142:ARG:CG	2:L:142:ARG:HH11	2.21	0.53
3:N:289:THR:HG22	3:N:290:LYS:N	2.21	0.53
3:Y:322:LYS:HE3	3:Y:333:GLU:OE2	2.08	0.53
1:A:37:VAL:HG22	1:A:47:TRP:HA	1.90	0.53
1:M:220:LYS:C	1:M:221:VAL:HA	2.29	0.53
3:X:351:LEU:HB2	3:X:366:THR:HB	1.90	0.53
1:I:72:ARG:NE	1:I:74:ASP:OD1	2.34	0.53
2:F:160:GLN:O	2:F:178:THR:N	2.41	0.53
2:G:149:LYS:HB2	2:G:193:ALA:HB3	1.91	0.53
1:I:101:SER:OG	1:I:104:LEU:HA	2.09	0.53
3:N:322:LYS:HE3	3:N:333:GLU:OE2	2.08	0.53
1:A:22:CYS:O	1:A:78:PHE:HA	2.09	0.53
2:B:151:ASP:HA	2:B:191:VAL:HG12	1.90	0.53
3:O:351:LEU:HB2	3:O:366:THR:HB	1.90	0.53
2:F:140:TYR:CD2	2:F:141:PRO:HA	2.44	0.52
2:G:37:GLN:HB2	2:G:47:LEU:HD11	1.91	0.52
1:H:38:ARG:HB3	1:H:94:TYR:CE2	2.44	0.52
3:Y:297:ASN:O	3:Y:298:SER:HB3	2.09	0.52
2:B:201:LEU:HG	2:B:205:VAL:HG23	1.90	0.52
1:D:94:TYR:CE1	1:D:119:VAL:HB	2.44	0.52
3:J:418:GLN:HA	3:J:443:LEU:HD22	1.90	0.52
1:E:101:SER:H	1:E:104:LEU:HD23	1.75	0.52
1:H:29:ILE:O	1:H:72:ARG:NH2	2.43	0.52
1:M:35:ASN:O	1:M:97:ALA:N	2.42	0.52
3:P:262:VAL:HG13	3:P:303:VAL:HG22	1.90	0.52
3:J:384:ASN:OD1	3:J:385:GLY:N	2.41	0.52
3:N:312:ASN:ND2	3:N:317:LYS:HD2	2.24	0.52
1:A:164:TRP:CH2	1:A:221:VAL:HG21	2.45	0.52
1:A:73:ASP:N	1:A:78:PHE:O	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:SER:HB2	1:D:104:LEU:H	1.75	0.52
2:L:142:ARG:NH1	2:L:142:ARG:HG2	2.19	0.52
2:G:160:GLN:O	2:G:178:THR:N	2.40	0.52
3:X:283:GLN:C	3:X:285:HIS:N	2.62	0.52
1:A:52:SER:O	1:A:72:ARG:NH1	2.42	0.52
1:I:35:ASN:OD1	1:I:50:SER:HB2	2.10	0.52
3:Y:312:ASN:ND2	3:Y:317:LYS:HD2	2.24	0.52
1:A:134:LEU:HD13	2:B:118:PHE:CD2	2.45	0.52
2:C:138:ASN:OD1	1:D:174:HIS:NE2	2.43	0.52
1:E:47:TRP:NE1	1:E:49:ALA:O	2.43	0.52
2:F:148:TRP:CE3	2:F:179:LEU:HD22	2.44	0.52
2:F:149:LYS:HB2	2:F:193:ALA:HB3	1.91	0.52
2:G:148:TRP:CE3	2:G:179:LEU:HD22	2.45	0.52
1:M:129:PRO:HB3	1:M:155:TYR:HB3	1.90	0.52
1:M:203:THR:HG21	1:M:220:LYS:HZ1	1.75	0.52
1:M:35:ASN:OD1	1:M:50:SER:HB2	2.09	0.52
3:N:296:TYR:HE1	3:N:301:ARG:HD3	1.74	0.52
2:B:142:ARG:HH11	2:B:142:ARG:CG	2.21	0.52
2:C:186:TYR:HA	2:C:192:TYR:OH	2.10	0.52
2:G:21:ILE:HG12	2:G:102:THR:HG21	1.91	0.52
3:J:436:TYR:CD1	3:J:436:TYR:C	2.84	0.52
2:K:151:ASP:HA	2:K:191:VAL:HG12	1.91	0.52
3:X:384:ASN:OD1	3:X:385:GLY:N	2.41	0.52
1:D:153:LYS:HG2	1:D:154:ASP:OD1	2.10	0.52
3:J:351:LEU:HB2	3:J:366:THR:HB	1.90	0.52
3:J:393:THR:HG22	3:J:394:THR:O	2.10	0.51
3:P:312:ASN:ND2	3:P:317:LYS:HD2	2.24	0.51
3:X:393:THR:HG22	3:X:394:THR:O	2.10	0.51
3:Y:296:TYR:HE1	3:Y:301:ARG:HD3	1.74	0.51
1:A:169:LEU:HD21	1:A:192:VAL:HG21	1.91	0.51
1:D: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:D:69:THR:C	1:D:81:LEU:HD12	2.31	0.51
1:E:134:LEU:HD13	2:F:118:PHE:CD2	2.46	0.51
2:G:61:ARG:HB2	2:G:76:SER:O	2.10	0.51
1:I:101:SER:H	1:I:104:LEU:HD23	1.76	0.51
1:M:53:THR:O	1:M:56:THR:OG1	2.28	0.51
3:N:325:ASN:ND2	3:N:326:LYS:N	2.59	0.51
3:P:325:ASN:ND2	3:P:326:LYS:N	2.59	0.51
2:C:140:TYR:CD2	2:C:141:PRO:HA	2.45	0.51
1:D:58:ARG:NH1	1:D:70:VAL:O	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:TRP:CZ2	1:E:192:VAL:HG12	2.46	0.51
1:D:74:ASP:HB3	2:F:94:TYR:HE1	1.74	0.51
2:G:31:THR:OG1	2:G:50:LYS:HE2	2.10	0.51
1:H:35:ASN:O	1:H:97:ALA:N	2.41	0.51
2:L:5:THR:HG23	2:L:100:GLN:HE22	1.75	0.51
3:X:429:HIS:O	3:X:435:HIS:HA	2.11	0.51
2:G:167:ASP:HB2	1:I:174:HIS:HE1	1.75	0.51
1:I:94:TYR:CE1	1:I:119:VAL:HB	2.46	0.51
1:M:52:SER:O	1:M:72:ARG:NH1	2.43	0.51
3:P:291:PRO:CB	3:P:304:SER:HA	2.37	0.51
3:Y:291:PRO:CB	3:Y:304:SER:HA	2.37	0.51
1:A:35:ASN:O	1:A:97:ALA:N	2.44	0.51
1:D:202:GLN:HB2	1:D:204:TYR:CZ	2.45	0.51
3:P:297:ASN:O	3:P:298:SER:HB3	2.09	0.51
3:X:350:THR:HB	3:X:441:LEU:CG	2.40	0.51
3:X:436:TYR:CD1	3:X:436:TYR:C	2.84	0.51
3:Y:291:PRO:HB3	3:Y:304:SER:CA	2.37	0.51
3:Y:325:ASN:ND2	3:Y:326:LYS:N	2.59	0.51
1:E:129:PRO:HB3	1:E:155:TYR:HB3	1.93	0.51
1:E:72:ARG:NE	1:E:74:ASP:OD1	2.33	0.51
1:D:29:ILE:O	1:D:72:ARG:NH2	2.44	0.51
2:G:113:PRO:HD3	2:G:198:HIS:CG	2.46	0.51
3:J:429:HIS:O	3:J:435:HIS:HA	2.11	0.51
3:O:393:THR:HG22	3:O:394:THR:O	2.10	0.51
3:O:429:HIS:O	3:O:435:HIS:HA	2.11	0.51
3:P:249:ASP:O	3:P:257:PRO:HG3	2.11	0.51
2:C:140:TYR:CG	2:C:141:PRO:HA	2.45	0.51
1:I:68:PHE:CD1	1:I:83:MET:HA	2.46	0.51
3:J:418:GLN:C	3:J:420:GLY:H	2.15	0.51
2:L:73:LEU:HD12	2:L:74:THR:H	1.76	0.51
2:L:19:ILE:HG12	2:L:78:LEU:HD11	1.91	0.51
3:O:350:THR:HB	3:O:441:LEU:CG	2.40	0.51
3:X:418:GLN:C	3:X:420:GLY:H	2.15	0.51
2:G:113:PRO:HD2	2:G:201:LEU:HD22	1.93	0.51
1:I:70:VAL:HA	1:I:80:TYR:O	2.10	0.51
1:H:134:LEU:HD13	2:K:118:PHE:CD2	2.46	0.51
3:O:384:ASN:OD1	3:O:385:GLY:N	2.41	0.51
3:Y:378:ALA:HB3	3:Y:428:MET:HB2	1.92	0.51
2:G:142:ARG:NH1	2:G:142:ARG:HG2	2.20	0.50
1:M:144:GLY:O	1:M:196:SER:HB2	2.10	0.50
3:O:443:LEU:HG	3:O:443:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:261:CYS:HB2	3:Y:277:TRP:CZ2	2.47	0.50
1:A:35:ASN:OD1	1:A:50:SER:HB2	2.11	0.50
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.92	0.50
1:E:94:TYR:CE1	1:E:119:VAL:HB	2.46	0.50
1:M:23:GLY:HA2	1:M:78:PHE:CD2	2.46	0.50
3:X:360:LYS:O	3:X:414:LYS:HD2	2.11	0.50
1:H:68:PHE:CD1	1:H:83:MET:HA	2.47	0.50
3:N:249:ASP:O	3:N:257:PRO:HG3	2.11	0.50
3:N:297:ASN:O	3:N:298:SER:HB3	2.09	0.50
3:N:291:PRO:CB	3:N:304:SER:HA	2.37	0.50
2:F:36:TYR:HE2	2:F:89:GLN:HB3	1.76	0.50
2:G:36:TYR:CE1	2:G:46:LEU:HD13	2.46	0.50
3:X:294:GLN:O	3:X:300:TYR:CD1	2.65	0.50
3:Y:249:ASP:C	3:Y:257:PRO:HG3	2.32	0.50
1:D:38:ARG:HD3	1:D:94:TYR:CE2	2.46	0.50
1:I:220:LYS:HE2	1:I:222:GLU:HG3	1.93	0.50
1:M:153:LYS:HG2	1:M:154:ASP:OD1	2.11	0.50
1:M:195:PRO:C	1:M:197:SER:H	2.14	0.50
3:O:418:GLN:C	3:O:420:GLY:H	2.15	0.50
2:C:148:TRP:CE3	2:C:179:LEU:HD22	2.46	0.50
1:E:169:LEU:HD21	1:E:192:VAL:HG21	1.93	0.50
1:I:52:SER:O	1:I:72:ARG:NH1	2.44	0.50
2:L:148:TRP:CE3	2:L:179:LEU:HD22	2.47	0.50
1:M:169:LEU:HD21	1:M:192:VAL:HG21	1.94	0.50
1:M:133:PRO:HB2	1:M:221:VAL:HG13	1.92	0.50
3:N:432:LEU:CD1	3:N:437:THR:HG22	2.42	0.50
3:O:360:LYS:O	3:O:414:LYS:HD2	2.11	0.50
3:P:249:ASP:C	3:P:257:PRO:HG3	2.32	0.50
3:P:278:TYR:CD1	3:P:278:TYR:N	2.79	0.50
2:F:21:ILE:HG12	2:F:102:THR:HG21	1.92	0.50
3:J:283:GLN:C	3:J:285:HIS:N	2.63	0.50
3:N:291:PRO:HB3	3:N:304:SER:CA	2.37	0.50
3:O:294:GLN:O	3:O:300:TYR:CD1	2.65	0.50
1:A:67:ARG:C	1:A:68:PHE:HD1	2.15	0.50
3:N:261:CYS:HB2	3:N:277:TRP:CZ2	2.47	0.50
3:N:378:ALA:HB3	3:N:428:MET:HB2	1.92	0.50
3:P:332:ILE:CG2	3:P:333:GLU:N	2.74	0.50
3:P:406:LEU:HD12	3:P:406:LEU:O	2.12	0.50
3:P:432:LEU:CD1	3:P:437:THR:HG22	2.42	0.50
3:Y:249:ASP:O	3:Y:257:PRO:HG3	2.10	0.50
3:Y:292:ARG:O	3:Y:293:GLU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ASP:N	1:D:78:PHE:O	2.44	0.50
1:E:34:MET:SD	1:E:98:ARG:HB2	2.52	0.50
2:F:140:TYR:CG	2:F:141:PRO:HA	2.47	0.50
3:J:380:GLU:O	3:J:425:CYS:HA	2.12	0.50
2:L:121:SER:O	2:L:125:LEU:HB2	2.11	0.50
3:O:436:TYR:C	3:O:436:TYR:CD1	2.84	0.50
3:P:250:THR:HG22	3:P:257:PRO:HB3	1.94	0.50
3:P:289:THR:HG22	3:P:290:LYS:N	2.21	0.50
1:H:38:ARG:NH1	1:H:90:ASP:HA	2.27	0.49
3:J:360:LYS:O	3:J:414:LYS:HD2	2.11	0.49
1:M:58:ARG:NH1	1:M:70:VAL:O	2.44	0.49
3:N:250:THR:HG22	3:N:257:PRO:HB3	1.94	0.49
3:N:278:TYR:N	3:N:278:TYR:CD1	2.79	0.49
3:N:332:ILE:CG2	3:N:333:GLU:N	2.74	0.49
3:P:291:PRO:HB3	3:P:304:SER:CA	2.37	0.49
3:Y:406:LEU:HD12	3:Y:406:LEU:O	2.12	0.49
3:X:409:LYS:HB2	3:Y:407:TYR:OH	2.12	0.49
1:D:92:ALA:N	1:D:119:VAL:O	2.44	0.49
3:J:443:LEU:HG	3:J:443:LEU:O	2.11	0.49
3:O:380:GLU:O	3:O:425:CYS:HA	2.12	0.49
3:P:378:ALA:HB3	3:P:428:MET:HB2	1.92	0.49
1:E:67:ARG:C	1:E:68:PHE:HD1	2.15	0.49
1:H:92:ALA:HB3	1:H:94:TYR:CE1	2.47	0.49
3:J:294:GLN:O	3:J:300:TYR:CD1	2.65	0.49
3:J:357:GLU:C	3:J:359:THR:H	2.15	0.49
3:O:292:ARG:O	3:O:293:GLU:CB	2.58	0.49
3:O:357:GLU:C	3:O:359:THR:H	2.15	0.49
3:Y:278:TYR:N	3:Y:278:TYR:CD1	2.79	0.49
3:Y:350:THR:HB	3:Y:441:LEU:HG	1.95	0.49
1:I:129:PRO:HB3	1:I:155:TYR:HB3	1.93	0.49
1:I:47:TRP:NE1	1:I:49:ALA:O	2.45	0.49
3:P:296:TYR:HE1	3:P:301:ARG:HD3	1.74	0.49
3:X:278:TYR:HB2	3:X:320:LYS:HB3	1.95	0.49
3:Y:332:ILE:CG2	3:Y:333:GLU:N	2.74	0.49
2:F:19:ILE:HG12	2:F:78:LEU:HD11	1.93	0.49
1:I:12:VAL:O	1:I:121:VAL:HA	2.13	0.49
1:M:164:TRP:CE2	1:M:206:CYS:HB2	2.47	0.49
3:N:292:ARG:O	3:N:293:GLU:HB3	2.12	0.49
3:O:246:LYS:HB2	3:O:249:ASP:OD2	2.12	0.49
3:X:357:GLU:C	3:X:359:THR:H	2.15	0.49
3:X:443:LEU:HG	3:X:443:LEU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:THR:HG23	2:B:100:GLN:HE22	1.77	0.49
1:E:58:ARG:NH1	1:E:70:VAL:O	2.44	0.49
3:J:278:TYR:HB2	3:J:320:LYS:HB3	1.94	0.49
2:K:19:ILE:HG12	2:K:78:LEU:HD11	1.94	0.49
3:X:246:LYS:HB2	3:X:249:ASP:OD2	2.12	0.49
2:G:138:ASN:OD1	1:I:174:HIS:NE2	2.45	0.49
2:G:142:ARG:CG	2:G:142:ARG:HH11	2.22	0.49
2:G:5:THR:HG23	2:G:100:GLN:HE22	1.77	0.49
1:H:38:ARG:HD3	1:H:94:TYR:CE2	2.48	0.49
2:K:117:ILE:HG13	2:K:133:VAL:O	2.12	0.49
3:P:398:LEU:HD11	3:P:402:GLY:HA2	1.95	0.49
3:P:369:VAL:O	3:P:405:PHE:HA	2.12	0.49
3:X:380:GLU:O	3:X:425:CYS:HA	2.12	0.49
3:Y:369:VAL:O	3:Y:405:PHE:HA	2.13	0.49
3:Y:432:LEU:CD1	3:Y:437:THR:HG22	2.42	0.49
2:G:83:PHE:CE1	2:G:106:ILE:HG12	2.48	0.49
1:H:38:ARG:HB3	1:H:94:TYR:CD2	2.48	0.49
3:N:249:ASP:C	3:N:257:PRO:HG3	2.32	0.49
3:N:406:LEU:HD12	3:N:406:LEU:O	2.12	0.49
3:O:283:GLN:CD	3:O:287:ALA:HB2	2.33	0.49
1:E:23:GLY:HA2	1:E:78:PHE:CD2	2.48	0.49
1:I:101:SER:H	1:I:104:LEU:CD2	2.26	0.49
1:I:23:GLY:HA2	1:I:78:PHE:CD2	2.48	0.49
3:J:409:LYS:HB2	3:N:407:TYR:OH	2.12	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
3:Y:250:THR:HG22	3:Y:257:PRO:HB3	1.94	0.49
1:A:53:THR:O	1:A:56:THR:OG1	2.31	0.49
1:H:60:TYR:OH	1:H:69:THR:HA	2.13	0.49
3:J:283:GLN:CD	3:J:287:ALA:HB2	2.34	0.49
3:O:388:GLU:OE2	3:O:416:ARG:NH2	2.42	0.49
3:P:261:CYS:HB2	3:P:277:TRP:CZ2	2.47	0.49
3:X:283:GLN:CD	3:X:287:ALA:HB2	2.34	0.49
3:Y:398:LEU:HD11	3:Y:402:GLY:HA2	1.95	0.49
1:E:153:LYS:HG2	1:E:154:ASP:OD2	2.13	0.48
1:E:73:ASP:N	1:E:78:PHE:O	2.42	0.48
1:H:176:PHE:CD1	2:K:176:SER:HB3	2.48	0.48
1:H:69:THR:O	1:H:81:LEU:HD12	2.13	0.48
3:N:311:GLN:N	3:N:311:GLN:NE2	2.53	0.48
3:N:398:LEU:HD11	3:N:402:GLY:HA2	1.95	0.48
3:O:248:LYS:O	3:O:255:ARG:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:31:THR:O	2:G:50:LYS:HA	2.13	0.48
1:H:202:GLN:O	1:H:203:THR:HA	2.12	0.48
2:L:201:LEU:HG	2:L:205:VAL:HG23	1.95	0.48
3:X:248:LYS:O	3:X:255:ARG:HD3	2.13	0.48
1:A:38:ARG:HB3	1:A:94:TYR:CE2	2.48	0.48
3:J:350:THR:HB	3:J:441:LEU:CG	2.40	0.48
2:L:140:TYR:CG	2:L:141:PRO:HA	2.48	0.48
1:M:22:CYS:O	1:M:78:PHE:HA	2.12	0.48
3:X:277:TRP:O	3:X:283:GLN:HB3	2.13	0.48
1:A:197:SER:HB3	3:X:295:GLN:CD	2.34	0.48
1:A:69:THR:C	1:A:81:LEU:HD12	2.33	0.48
2:C:149:LYS:HB2	2:C:193:ALA:HB3	1.94	0.48
1:E:68:PHE:CD1	1:E:83:MET:HA	2.48	0.48
1:H:47:TRP:NE1	1:H:49:ALA:O	2.46	0.48
1:I:67:ARG:C	1:I:68:PHE:HD1	2.17	0.48
3:P:292:ARG:O	3:P:293:GLU:HB3	2.12	0.48
3:X: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
2:G:2:VAL:HG11	2:G:90:HIS:CD2	2.48	0.48
1:I:35:ASN:O	1:I:97:ALA:N	2.45	0.48
1:M:29:ILE:O	1:M:72:ARG:NH2	2.46	0.48
1:A:32:HIS:ND1	1:A:98:ARG:HG3	2.29	0.48
2:B:20:THR:HG22	2:B:73:LEU:O	2.13	0.48
3:J:277:TRP:O	3:J:283:GLN:HB3	2.13	0.48
2:L:61:ARG:HB2	2:L:76:SER:O	2.14	0.48
3:N:350:THR:HB	3:N:441:LEU:HG	1.95	0.48
3:O:266:VAL:O	3:O:300:TYR:HB2	2.13	0.48
2:F:108:ARG:NH1	2:F:111:ALA:HB2	2.28	0.48
1:I:153:LYS:HG2	1:I:154:ASP:OD2	2.13	0.48
3:J:248:LYS:O	3:J:255:ARG:HD3	2.13	0.48
1:M:72:ARG:NE	1:M:74:ASP:OD1	2.36	0.48
2:K:91:TYR:CD1	1:M:99:LYS:NZ	2.81	0.48
3:N:369:VAL:O	3:N:405:PHE:HA	2.12	0.48
3:O:278:TYR:HB2	3:O:320:LYS:HB3	1.95	0.48
3:P:244:PRO:HB3	3:P:336:ILE:HD11	1.95	0.48
3:P:259:VAL:HG23	3:P:308:VAL:CG2	2.43	0.48
3:P:350:THR:HB	3:P:441:LEU:HG	1.95	0.48
2:B:140:TYR:CG	2:B:141:PRO:HA	2.49	0.48
2:G:149:LYS:HZ1	2:G:195:GLU:CD	2.13	0.48
2:G:162:SER:HB3	2:G:176:SER:OG	2.13	0.48
2:G:169:LYS:HB3	2:G:169:LYS:NZ	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:101:SER:N	1:I:104:LEU:HD23	2.29	0.48
2:G:118:PHE:CG	1:I:134:LEU:HB3	2.49	0.48
3:J:246:LYS:HB2	3:J:249:ASP:OD2	2.12	0.48
1:M:92:ALA:N	1:M:119:VAL:O	2.46	0.48
3:X:358:MET:O	3:X:414:LYS:HE3	2.14	0.48
3:O:277:TRP:O	3:O:283:GLN:HB3	2.13	0.48
3:X:371:GLY:HA2	3:X:403:SER:OG	2.14	0.48
2:C:142:ARG:HG2	2:C:142:ARG:NH1	2.28	0.48
3:J:388:GLU:OE1	3:J:388:GLU:HA	2.14	0.48
2:L:21:ILE:HG12	2:L:102:THR:HG21	1.95	0.48
1:M:149:GLY:O	1:M:221:VAL:HG21	2.14	0.48
3:O:283:GLN:C	3:O:285:HIS:N	2.63	0.48
3:P:312:ASN:HB3	3:P:319:TYR:OH	2.14	0.48
3:X:388:GLU:OE1	3:X:388:GLU:HA	2.14	0.48
3:Y:311:GLN:NE2	3:Y:311:GLN:N	2.53	0.48
3:Y:244:PRO:HB3	3:Y:336:ILE:HD11	1.95	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
1:H:69:THR:O	1:H:81:LEU:HA	2.13	0.47
3:J:371:GLY:HA2	3:J:403:SER:OG	2.14	0.47
3:J:358:MET:O	3:J:414:LYS:HE3	2.14	0.47
3:J:414:LYS:HG2	3:J:418:GLN:NE2	2.29	0.47
3:N:259:VAL:HG23	3:N:308:VAL:CG2	2.43	0.47
3:O:358:MET:O	3:O:414:LYS:HE3	2.14	0.47
3:X:414:LYS:HG2	3:X:418:GLN:NE2	2.29	0.47
2:C:169:LYS:NZ	2:C:169:LYS:HB3	2.29	0.47
3:J:292:ARG:O	3:J:293:GLU:CB	2.58	0.47
2:L:140:TYR:CD2	2:L:141:PRO:HA	2.49	0.47
3:N:312:ASN:HB3	3:N:319:TYR:OH	2.14	0.47
3:O:414:LYS:HG2	3:O:418:GLN:NE2	2.29	0.47
3:Y:312:ASN:HB3	3:Y:319:TYR:OH	2.14	0.47
3:J:266:VAL:O	3:J:300:TYR:HB2	2.13	0.47
3:J:388:GLU:OE2	3:J:416:ARG:NH2	2.42	0.47
2:L:169:LYS:NZ	2:L:169:LYS:HB3	2.29	0.47
2:L:151:ASP:HA	2:L:191:VAL:HG12	1.95	0.47
1:A:23:GLY:HA2	1:A:78:PHE:CD2	2.50	0.47
1:D:67:ARG:C	1:D:68:PHE:HD1	2.18	0.47
1:E:102:ASP:N	1:E:102:ASP:OD1	2.47	0.47
2:F:142:ARG:CG	2:F:142:ARG:HH11	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:SER:O	1:H:72:ARG:NH1	2.47	0.47
3:N:279:VAL:O	3:N:282:VAL:HG22	2.15	0.47
3:X:282:VAL:O	3:X:283:GLN:CB	2.52	0.47
3:X:288:LYS:H	3:X:288:LYS:CD	2.27	0.47
3:Y:259:VAL:HG23	3:Y:308:VAL:CG2	2.43	0.47
2:C:113:PRO:HD3	2:C:198:HIS:CG	2.50	0.47
1:D:98:ARG:NH2	1:D:111:ASP:OD2	2.35	0.47
1:H:153:LYS:HG2	1:H:154:ASP:OD1	2.14	0.47
1:M:101:SER:OG	1:M:104:LEU:HA	2.14	0.47
1:M:203:THR:HG21	1:M:220:LYS:NZ	2.30	0.47
3:P:275:PHE:HZ	3:P:302:VAL:O	1.98	0.47
2:B:29:ILE:HG21	2:B:90:HIS:CD2	2.47	0.47
2:B:61:ARG:HB2	2:B:76:SER:O	2.15	0.47
2:C:162:SER:HB3	2:C:176:SER:OG	2.15	0.47
2:F:6:GLN:NE2	2:F:102:THR:OG1	2.48	0.47
2:K:113:PRO:HD3	2:K:198:HIS:CG	2.49	0.47
2:K:121:SER:O	2:K:125:LEU:HB2	2.14	0.47
1:H:174:HIS:HB3	2:K:164:THR:HG21	1.97	0.47
1:M:153:LYS:HG2	1:M:154:ASP:OD2	2.14	0.47
3:P:432:LEU:HD22	3:P:437:THR:HB	1.97	0.47
3:X:438:GLN:O	3:X:439:LYS:HD3	2.15	0.47
2:F:11:LEU:HD22	2:F:19:ILE:HD12	1.97	0.47
1:H:67:ARG:C	1:H:68:PHE:HD1	2.18	0.47
1:I:68:PHE:HB3	1:I:81:LEU:HD11	1.95	0.47
3:J:288:LYS:H	3:J:288:LYS:CD	2.27	0.47
1:H:134:LEU:HB3	2:K:118:PHE:CG	2.49	0.47
2:K:4:MET:HG2	2:K:97:THR:HG23	1.95	0.47
3:N:244:PRO:HB3	3:N:336:ILE:HD11	1.95	0.47
3:N:322:LYS:HG3	3:N:333:GLU:HG2	1.97	0.47
3:P:308:VAL:HG11	3:P:313:TRP:HB2	1.97	0.47
2:C:31:THR:O	2:C:50:LYS:HA	2.14	0.47
2:F:167:ASP:OD2	2:F:169:LYS:HG3	2.15	0.47
2:L:20:THR:HG22	2:L:73:LEU:O	2.14	0.47
1:M:203:THR:HB	1:M:220:LYS:HE3	1.96	0.47
3:Y:322:LYS:HG3	3:Y:333:GLU:HG2	1.97	0.47
2:C:118:PHE:CD2	1:D:134:LEU:HD13	2.50	0.47
1:I:126:THR:HB	1:I:213:SER:HB3	1.97	0.47
1:I:53:THR:O	1:I:56:THR:OG1	2.32	0.47
3:O:289:THR:CG2	3:O:290:LYS:N	2.78	0.47
3:Y:275:PHE:HZ	3:Y:302:VAL:O	1.97	0.47
1:A:99:LYS:NZ	2:C:91:TYR:CD1	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:68:PHE:O	1:H:69:THR:OG1	2.31	0.47
3:J:438:GLN:O	3:J:439:LYS:HD3	2.15	0.47
1:M:164:TRP:C	1:M:166:SER:N	2.67	0.47
3:N:432:LEU:HD22	3:N:437:THR:HB	1.97	0.47
3:P:368:LEU:HD12	3:P:369:VAL:H	1.79	0.47
3:Y:279:VAL:O	3:Y:282:VAL:HG22	2.15	0.47
1:H:19:ILE:C	1:H:20:LEU:HD23	2.36	0.46
2:K:108:ARG:NH1	2:K:111:ALA:HB2	2.30	0.46
2:L:31:THR:O	2:L:50:LYS:HA	2.15	0.46
1:M:92:ALA:HB3	1:M:94:TYR:CE1	2.50	0.46
3:O:438:GLN:O	3:O:439:LYS:HD3	2.15	0.46
3:P:279:VAL:O	3:P:282:VAL:HG22	2.15	0.46
3:P:322:LYS:HG3	3:P:333:GLU:HG2	1.97	0.46
3:Y:308:VAL:HG11	3:Y:313:TRP:HB2	1.97	0.46
2:B:36:TYR:CE1	2:B:46:LEU:HD13	2.51	0.46
2:C:5:THR:HG23	2:C:100:GLN:HE22	1.80	0.46
2:K:36:TYR:HE2	2:K:89:GLN:HB3	1.81	0.46
1:M:101:SER:H	1:M:104:LEU:CD2	2.28	0.46
3:N:278:TYR:CE2	3:N:284:VAL:HG22	2.50	0.46
3:O:371:GLY:HA2	3:O:403:SER:OG	2.14	0.46
3:P:261:CYS:HB2	3:P:277:TRP:CH2	2.50	0.46
3:Y:300:TYR:HB3	3:Y:301:ARG:H	1.37	0.46
1:A:68:PHE:CD1	1:A:83:MET:HA	2.51	0.46
2:B:148:TRP:CE3	2:B:179:LEU:HD22	2.51	0.46
1:D:69:THR:O	1:D:81:LEU:HD12	2.15	0.46
2:G:146:VAL:HB	2:G:161:GLU:OE2	2.15	0.46
1:H:101:SER:OG	1:H:104:LEU:HA	2.15	0.46
1:I:220:LYS:HE2	1:I:222:GLU:CG	2.46	0.46
3:J:421:ASN:N	3:J:421:ASN:ND2	2.64	0.46
3:N:308:VAL:HG11	3:N:313:TRP:HB2	1.97	0.46
3:O:388:GLU:OE1	3:O:388:GLU:HA	2.14	0.46
3:O:421:ASN:N	3:O:421:ASN:ND2	2.64	0.46
2:B:201:LEU:HB3	2:B:203:SER:O	2.16	0.46
2:F:83:PHE:CE1	2:F:106:ILE:HG12	2.51	0.46
3:X:289:THR:CG2	3:X:290:LYS:N	2.78	0.46
3:X:421:ASN:N	3:X:421:ASN:ND2	2.64	0.46
3:Y:361:ASN:ND2	3:Y:362:GLN:HG3	2.31	0.46
2:B:140:TYR:CD2	2:B:141:PRO:HA	2.50	0.46
2:B:149:LYS:HB2	2:B:193:ALA:HB3	1.96	0.46
2:B:31:THR:O	2:B:50:LYS:HA	2.15	0.46
1:D:154:ASP:HA	1:D:185:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:ILE:O	1:E:72:ARG:NH2	2.48	0.46
2:G:36:TYR:HE2	2:G:89:GLN:HB3	1.81	0.46
1:H:103:ARG:O	1:H:104:LEU:HB2	2.15	0.46
1:I:52:SER:OG	1:I:56:THR:N	2.49	0.46
3:N:432:LEU:HD11	3:N:437:THR:HG22	1.98	0.46
3:P:278:TYR:CE2	3:P:284:VAL:HG22	2.50	0.46
3:P:300:TYR:O	3:P:301:ARG:HB2	2.16	0.46
3:X:286:ASN:O	3:X:287:ALA:CB	2.63	0.46
2:B:113:PRO:HD3	2:B:198:HIS:CG	2.50	0.46
2:B:162:SER:HB3	2:B:176:SER:OG	2.16	0.46
2:K:140:TYR:CG	2:K:141:PRO:HA	2.50	0.46
2:L:2:VAL:HG11	2:L:90:HIS:CD2	2.51	0.46
3:N:361:ASN:ND2	3:N:362:GLN:HG3	2.31	0.46
3:Y:261:CYS:HB2	3:Y:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD11	3:Y:437:THR:HG22	1.98	0.46
1:H:144:GLY:O	1:H:196:SER:HB2	2.15	0.46
1:M:22:CYS:N	1:M:79:VAL:O	2.48	0.46
3:O:265:ASP:HA	3:O:299:THR:HB	1.98	0.46
3:Y:278:TYR:CE2	3:Y:284:VAL:HG22	2.50	0.46
1:H:92:ALA:N	1:H:119:VAL:O	2.47	0.46
3:N:275:PHE:HZ	3:N:302:VAL:O	1.98	0.46
3:N:368:LEU:HD12	3:N:369:VAL:H	1.79	0.46
3:O:288:LYS:CD	3:O:288:LYS:H	2.27	0.46
1:E:153:LYS:HG2	1:E:154:ASP:OD1	2.15	0.46
3:J:265:ASP:HA	3:J:299:THR:HB	1.98	0.46
3:J:289:THR:CG2	3:J:290:LYS:N	2.78	0.46
3:N:261:CYS:HB2	3:N:277:TRP:CH2	2.50	0.46
3:Y:432:LEU:HD22	3:Y:437:THR:HB	1.97	0.46
1:H:22:CYS:O	1:H:78:PHE:HA	2.15	0.46
3:J:266:VAL:HB	3:J:300:TYR:HB2	1.98	0.46
2:K:146:VAL:HB	2:K:161:GLU:OE2	2.16	0.46
3:P:344:ARG:O	3:P:372:PHE:HA	2.16	0.46
3:P:432:LEU:HD11	3:P:437:THR:HG22	1.98	0.46
2:C:36:TYR:CE1	2:C:46:LEU:HD13	2.50	0.45
2:F:113:PRO:HD2	2:F:201:LEU:HD22	1.98	0.45
1:I:69:THR:C	1:I:81:LEU:HD12	2.36	0.45
2:L:106:ILE:O	2:L:166:GLN:NE2	2.46	0.45
3:N:300:TYR:O	3:N:301:ARG:CB	2.64	0.45
3:N:344:ARG:O	3:N:372:PHE:HA	2.16	0.45
3:P:439:LYS:HD2	3:P:439:LYS:HA	1.81	0.45
3:Y:368:LEU:HD12	3:Y:369:VAL:H	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:HIS:HB3	2:B:164:THR:HG21	1.98	0.45
2:C:121:SER:O	2:C:125:LEU:HB2	2.16	0.45
1:M:69:THR:C	1:M:81:LEU:HD12	2.36	0.45
1:A:94:TYR:CE1	1:A:119:VAL:HB	2.51	0.45
1:H:135:ALA:CB	1:H:224:LYS:HD3	2.47	0.45
2:L:83:PHE:CE1	2:L:106:ILE:HG12	2.52	0.45
3:N:242:LEU:HD13	3:N:336:ILE:HG22	1.98	0.45
3:P:433:HIS:CA	3:P:434:ASN:N	2.69	0.45
1:A:101:SER:H	1:A:104:LEU:HD23	1.82	0.45
2:G:124:GLN:NE2	1:I:132:PHE:CE2	2.85	0.45
2:K:142:ARG:HH11	2:K:142:ARG:CG	2.25	0.45
1:M:32:HIS:ND1	1:M:98:ARG:HG3	2.31	0.45
3:P:300:TYR:O	3:P:301:ARG:CB	2.65	0.45
3:P:311:GLN:N	3:P:311:GLN:NE2	2.53	0.45
3:P:361:ASN:ND2	3:P:362:GLN:HG3	2.31	0.45
3:Y:300:TYR:O	3:Y:301:ARG:HB2	2.16	0.45
1:A:29:ILE:O	1:A:72:ARG:NH2	2.49	0.45
1:E:69:THR:C	1:E:81:LEU:HD12	2.37	0.45
2:F:162:SER:HB3	2:F:176:SER:OG	2.16	0.45
2:F:5:THR:HG23	2:F:100:GLN:HE22	1.81	0.45
1:H:53:THR:O	1:H:56:THR:OG1	2.34	0.45
3:J:278:TYR:N	3:J:278:TYR:CD1	2.85	0.45
3:N:269:GLU:C	3:N:271:PRO:HD3	2.36	0.45
3:O:286:ASN:O	3:O:287:ALA:CB	2.63	0.45
3:X:265:ASP:HA	3:X:299:THR:HB	1.98	0.45
3:Y:279:VAL:O	3:Y:280:ASP:HB2	2.16	0.45
3:Y:242:LEU:HD13	3:Y:336:ILE:HG22	1.98	0.45
1:A:72:ARG:NE	1:A:74:ASP:OD1	2.38	0.45
2:C:146:VAL:HB	2:C:161:GLU:OE2	2.17	0.45
1:D:22:CYS:O	1:D:78:PHE:HA	2.16	0.45
1:E:32:HIS:ND1	1:E:98:ARG:HG3	2.31	0.45
3:J:244:PRO:HB3	3:J:336:ILE:HD13	1.99	0.45
3:O:342:GLN:HA	3:O:343:PRO:HD3	1.83	0.45
3:Y:290:LYS:HE3	3:Y:292:ARG:HH12	1.82	0.45
1:A:164:TRP:CZ3	1:A:221:VAL:HG21	2.52	0.45
1:D:101:SER:N	1:D:104:LEU:HD23	2.31	0.45
2:F:36:TYR:CE1	2:F:46:LEU:HD13	2.52	0.45
2:K:31:THR:O	2:K:50:LYS:HA	2.16	0.45
1:M:101:SER:N	1:M:104:LEU:HD23	2.31	0.45
3:N:265:ASP:HA	3:N:299:THR:CB	2.47	0.45
3:N:279:VAL:O	3:N:280:ASP:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:326:LYS:C	3:N:328:LEU:H	2.20	0.45
3:P:406:LEU:CD1	3:P:406:LEU:C	2.85	0.45
3:Y:344:ARG:O	3:Y:372:PHE:HA	2.16	0.45
2:B:31:THR:OG1	2:B:50:LYS:HE2	2.15	0.45
2:C:113:PRO:HD2	2:C:201:LEU:HD22	1.99	0.45
1:D:101:SER:H	1:D:104:LEU:CD2	2.29	0.45
1:E:101:SER:N	1:E:104:LEU:HD23	2.32	0.45
1:E:101:SER:OG	1:E:104:LEU:HA	2.17	0.45
1:E:195:PRO:C	1:E:197:SER:H	2.20	0.45
2:G:108:ARG:NH1	2:G:111:ALA:HB2	2.32	0.45
1:I:164:TRP:HZ2	1:I:190:SER:O	1.99	0.45
2:K:140:TYR:CD2	2:K:141:PRO:HA	2.52	0.45
3:P:269:GLU:C	3:P:271:PRO:HD3	2.36	0.45
3:Y:406:LEU:C	3:Y:406:LEU:CD1	2.84	0.45
1:E:101:SER:H	1:E:104:LEU:CD2	2.29	0.45
2:F:113:PRO:HD3	2:F:198:HIS:CG	2.52	0.45
2:F:31:THR:OG1	2:F:50:LYS:HE2	2.15	0.45
3:N:300:TYR:O	3:N:301:ARG:HB2	2.16	0.45
3:P:279:VAL:O	3:P:280:ASP:HB2	2.17	0.45
3:Y:265:ASP:HA	3:Y:299:THR:CB	2.47	0.45
3:Y:300:TYR:O	3:Y:301:ARG:CB	2.65	0.45
3:Y:301:ARG:HG2	3:Y:303:VAL:HG23	1.99	0.45
3:Y:323:VAL:HG12	3:Y:324:SER:N	2.32	0.45
1:A:101:SER:H	1:A:104:LEU:CD2	2.30	0.45
1:E:133:PRO:HB3	1:E:221:VAL:HG22	1.99	0.45
1:E:3:GLN:HB2	1:E:25:SER:CB	2.41	0.45
2:F:31:THR:O	2:F:50:LYS:HA	2.16	0.45
3:N:323:VAL:HG12	3:N:324:SER:N	2.32	0.45
3:N:406:LEU:CD1	3:N:406:LEU:C	2.85	0.45
3:P:290:LYS:HE3	3:P:292:ARG:HH12	1.82	0.45
3:X:266:VAL:HB	3:X:300:TYR:HB2	1.98	0.45
1:D:91:THR:HG23	1:D:120:THR:HG22	1.99	0.44
1:E:38:ARG:HB3	1:E:94:TYR:CE2	2.52	0.44
1:H:37:VAL:HG22	1:H:47:TRP:HA	1.98	0.44
3:J:286:ASN:O	3:J:287:ALA:CB	2.63	0.44
3:N:238:PRO:CB	3:N:328:LEU:HD13	2.47	0.44
3:O:346:PRO:CB	3:O:372:PHE:HB3	2.39	0.44
3:O:374:PRO:O	3:O:429:HIS:HE1	2.00	0.44
3:Y:345:GLU:HA	3:Y:431:ALA:HB3	1.99	0.44
1:E:148:LEU:HD12	1:E:164:TRP:CH2	2.53	0.44
2:F:61:ARG:HB2	2:F:76:SER:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:VAL:HG22	1:H:194:VAL:HG13	2.00	0.44
2:K:149:LYS:HB2	2:K:193:ALA:HB3	1.99	0.44
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.32	0.44
3:P:238:PRO:CB	3:P:328:LEU:HD13	2.47	0.44
3:X:244:PRO:HB3	3:X:336:ILE:HD13	1.99	0.44
1:A:12:VAL:O	1:A:121:VAL:HA	2.17	0.44
3:J:347:GLN:NE2	3:J:349:TYR:OH	2.51	0.44
3:P: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
3:X:291:PRO:O	3:X:292:ARG:HD2	2.17	0.44
3:Y:238:PRO:CB	3:Y:328:LEU:HD13	2.47	0.44
1:D:64:VAL:HB	1:D:68:PHE:CD2	2.53	0.44
3:J:278:TYR:HA	3:J:282:VAL:O	2.18	0.44
2:K:27:GLN:O	2:K:29:ILE:HG23	2.17	0.44
3:P:345:GLU:HA	3:P:431:ALA:HB3	1.99	0.44
3:X:287:ALA:O	3:X:288:LYS:C	2.56	0.44
1:A:153:LYS:HG2	1:A:154:ASP:OD1	2.16	0.44
2:C:2:VAL:HG11	2:C:90:HIS:CD2	2.53	0.44
1:D:192:VAL:HG22	1:D:194:VAL:HG13	1.99	0.44
2:F:36:TYR:HB2	2:F:87:HIS:HB2	1.99	0.44
2:G:124:GLN:HB2	1:I:132:PHE:CD1	2.52	0.44
1:I:58:ARG:NH1	1:I:70:VAL:O	2.49	0.44
3:J:309:LEU:O	3:J:312:ASN:N	2.51	0.44
3:N:345:GLU:HA	3:N:431:ALA:HB3	1.98	0.44
3:O:266:VAL:HB	3:O:300:TYR:HB2	1.98	0.44
3:O:347:GLN:NE2	3:O:349:TYR:OH	2.51	0.44
3:X:309:LEU:O	3:X:312:ASN:N	2.51	0.44
3:Y:269:GLU:C	3:Y:271:PRO:HD3	2.36	0.44
1:H:18:LEU:CB	1:H:83:MET:HE3	2.43	0.44
3:J:264:VAL:O	3:J:265:ASP:HB2	2.18	0.44
3:J:287:ALA:O	3:J:288:LYS:C	2.56	0.44
3:J:346:PRO:CB	3:J:372:PHE:HB3	2.39	0.44
3:J:248:LYS:NZ	3:J:380:GLU:OE2	2.47	0.44
2:K:30:GLU:HB2	2:K:32:TRP:CD1	2.53	0.44
3:P:326:LYS:C	3:P:328:LEU:H	2.20	0.44
3:P:363:VAL:HG22	3:P:412:VAL:O	2.18	0.44
3:X:278:TYR:HA	3:X:282:VAL:O	2.18	0.44
3:Y:239:SER:HB3	3:Y:264:VAL:CG2	2.47	0.44
1:A:69:THR:O	1:A:81:LEU:HD12	2.18	0.44
1:D:188:LEU:O	1:D:188:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:149:LYS:HZ1	2:F:195:GLU:CD	2.18	0.44
1:E:174:HIS:HB3	2:F:164:THR:HG21	1.99	0.44
1:H:92:ALA:HB3	1:H:94:TYR:CZ	2.53	0.44
3:N:290:LYS:HE3	3:N:292:ARG:HH12	1.82	0.44
3:O:291:PRO:O	3:O:292:ARG:HD2	2.18	0.44
3:P:278:TYR:HE2	3:P:284:VAL:HG22	1.83	0.44
3:P:323:VAL:HG12	3:P:324:SER:N	2.32	0.44
3:X:278:TYR:N	3:X:278:TYR:CD1	2.85	0.44
3:Y:363:VAL:HG22	3:Y:412:VAL:O	2.18	0.44
1:E:12:VAL:O	1:E:121:VAL:HA	2.18	0.44
1:E:194:VAL:HG21	1:E:204:TYR:CZ	2.53	0.44
3:N:301:ARG:HG2	3:N:303:VAL:HG23	1.99	0.44
3:Y:278:TYR:HE2	3:Y:284:VAL:HG22	1.83	0.44
3:Y:439:LYS:HA	3:Y:439:LYS:HD2	1.82	0.44
2:B:108:ARG:NH1	2:B:111:ALA:HB2	2.33	0.44
1:H:23:GLY:HA2	1:H:78:PHE:CD2	2.52	0.44
2:L:117:ILE:HG13	2:L:133:VAL:O	2.17	0.44
1:M:185:LEU:HA	1:M:185:LEU:HD12	1.78	0.44
3:O:309:LEU:O	3:O:312:ASN:N	2.51	0.44
1:A:38:ARG:HD3	1:A:94:TYR:CE2	2.53	0.43
1:E:35:ASN:O	1:E:97:ALA:N	2.48	0.43
1:H:22:CYS:N	1:H:79:VAL:O	2.51	0.43
3:N:278:TYR:HE2	3:N:284:VAL:HG22	1.83	0.43
3:N:363:VAL:HG22	3:N:412:VAL:O	2.18	0.43
3:O:296:TYR:HB3	3:O:297:ASN:H	1.56	0.43
3:O:244:PRO:HB3	3:O:336:ILE:HD13	1.99	0.43
2:L:70:GLU:HG3	2:L:71:PHE:N	2.32	0.43
1:M:68:PHE:HB3	1:M:81:LEU:HD11	2.00	0.43
3:O:278:TYR:CD1	3:O:278:TYR:N	2.85	0.43
3:P:242:LEU:HA	3:P:242:LEU:HD23	1.86	0.43
1:A:69:THR:O	1:A:81:LEU:HA	2.18	0.43
1:E:136:PRO:HG2	1:E:223:PRO:HG3	1.99	0.43
1:I:22:CYS:N	1:I:79:VAL:O	2.47	0.43
2:K:170:ASP:OD1	2:K:172:THR:OG1	2.19	0.43
2:K:186:TYR:HA	2:K:192:TYR:OH	2.18	0.43
3:O:278:TYR:HA	3:O:282:VAL:O	2.18	0.43
3:X:347:GLN:NE2	3:X:349:TYR:OH	2.50	0.43
3:Y:326:LYS:C	3:Y:328:LEU:H	2.20	0.43
2:C:136:LEU:HB2	2:C:175:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:22:CYS:O	1:E:78:PHE:HA	2.18	0.43
1:E:68:PHE:HB3	1:E:81:LEU:HD11	2.00	0.43
2:F:207:LYS:HZ3	1:M:201:THR:CB	2.17	0.43
2:G:121:SER:O	2:G:125:LEU:HB2	2.19	0.43
2:L:113:PRO:HD3	2:L:198:HIS:CG	2.52	0.43
1:M:98:ARG:NH2	1:M:111:ASP:OD2	2.37	0.43
3:O:264:VAL:O	3:O:265:ASP:HB2	2.18	0.43
3:X:374:PRO:O	3:X:429:HIS:HE1	2.00	0.43
1:H:101:SER:H	1:H:104:LEU:HD22	1.83	0.43
1:I:60:TYR:CE2	1:I:69:THR:HA	2.54	0.43
2:K:20:THR:HG22	2:K:73:LEU:O	2.19	0.43
3:N:239:SER:HB3	3:N:264:VAL:CG2	2.47	0.43
3:N:351:LEU:HA	3:N:352:PRO:HD3	1.91	0.43
3:P:258:GLU:HA	3:P:308:VAL:HG23	1.99	0.43
3:P:338:LYS:NZ	3:P:430:GLU:OE2	2.52	0.43
3:X:348:VAL:O	3:X:439:LYS:HG3	2.19	0.43
3:Y:338:LYS:NZ	3:Y:430:GLU:OE2	2.52	0.43
1:A:154:ASP:HA	1:A:185:LEU:HB3	2.01	0.43
2:B:36:TYR:HE2	2:B:89:GLN:HB3	1.83	0.43
1:D:156:PHE:HB3	1:D:185:LEU:HD12	2.00	0.43
1:E:181:GLN:C	1:E:183:SER:H	2.21	0.43
2:K:2:VAL:HG11	2:K:90:HIS:CD2	2.53	0.43
2:K:31:THR:OG1	2:K:50:LYS:HE2	2.18	0.43
2:L:63:SER:O	2:L:74:THR:N	2.52	0.43
3:P:325:ASN:HD22	3:P:326:LYS:N	2.15	0.43
3:P:414:LYS:O	3:P:418:GLN:HG3	2.19	0.43
3:Y:252:MET:SD	3:Y:428:MET:HE3	2.58	0.43
2:B:121:SER:O	2:B:125:LEU:HB2	2.18	0.43
2:C:83:PHE:CE1	2:C:106:ILE:HG12	2.53	0.43
2:G:161:GLU:HA	2:G:176:SER:O	2.18	0.43
1:I:194:VAL:HG21	1:I:204:TYR:CZ	2.54	0.43
3:J:374:PRO:O	3:J:429:HIS:HE1	2.00	0.43
3:N:414:LYS:O	3:N:418:GLN:HG3	2.19	0.43
1:A:27:PHE:CE1	1:A:29:ILE:HG22	2.53	0.43
1:A:3:GLN:HB2	1:A:25:SER:CB	2.41	0.43
2:C:20:THR:HG22	2:C:73:LEU:O	2.18	0.43
1:I:163:SER:O	1:I:164:TRP:CD1	2.71	0.43
1:I:222:GLU:HA	1:I:223:PRO:HD3	1.86	0.43
3:J:348:VAL:O	3:J:439:LYS:HG3	2.19	0.43
1:M:38:ARG:HB3	1:M:94:TYR:CE2	2.54	0.43
1:M:67:ARG:C	1:M:68:PHE:HD1	2.22	0.43

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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:201:LEU:HB3	2:G:203:SER:O	2.19	0.43
2:G:49:TYR:CE2	2:G:53:THR:HB	2.54	0.43
1:H:60:TYR:CE2	1:H:69:THR:HA	2.53	0.43
2:L:149:LYS:HB2	2:L:193:ALA:HB3	2.00	0.43
3:N:238:PRO:HB2	3:N:328:LEU:HD13	2.01	0.43
3:X:346:PRO:CB	3:X:372:PHE:HB3	2.39	0.43
1:A:144:GLY:O	1:A:196:SER:HB2	2.19	0.43
2:B:70:GLU:HG3	2:B:71:PHE:N	2.33	0.43
2:C:108:ARG:NH1	2:C:111:ALA:HB2	2.34	0.43
2:C:186:TYR:HA	2:C:192:TYR:HH	1.83	0.43
1:D:18:LEU:CB	1:D:83:MET:HE3	2.47	0.43
1:D:103:ARG:N	2:F:50:LYS:NZ	2.60	0.43
2:L:161:GLU:HA	2:L:176:SER:O	2.18	0.43
3:O:287:ALA:O	3:O:288:LYS:C	2.56	0.43
3:P:386:GLN:HA	3:P:387:PRO:HD3	1.76	0.43
3:X:264:VAL:O	3:X:265:ASP:HB2	2.18	0.43
3:Y:291:PRO:O	3:Y:292:ARG:HB3	2.19	0.43
3:Y:258:GLU:HA	3:Y:308:VAL:HG23	1.99	0.43
1:D:194:VAL:HG21	1:D:204:TYR:CZ	2.54	0.42
1:D:19:ILE:C	1:D:20:LEU:HD23	2.39	0.42
2:K:161:GLU:HA	2:K:176:SER:O	2.19	0.42
2:L:167:ASP:CB	1:M:174:HIS:HE1	2.32	0.42
3:N:338:LYS:NZ	3:N:430:GLU:OE2	2.52	0.42
3:P:266:VAL:HB	3:P:300:TYR:CD2	2.54	0.42
3:P:301:ARG:HG2	3:P:303:VAL:HG23	1.99	0.42
2:B:161:GLU:HA	2:B:176:SER:O	2.19	0.42
1:D:149:GLY:O	1:D:221:VAL:HG11	2.18	0.42
2:F:161:GLU:HA	2:F:176:SER:O	2.19	0.42
2:F:201:LEU:HB3	2:F:203:SER:O	2.19	0.42
3:N:266:VAL:HB	3:N:300:TYR:CD2	2.54	0.42
3:P:368:LEU:HD12	3:P:369:VAL:N	2.34	0.42
2:B:38:GLN:O	2:B:84:ALA:HB1	2.20	0.42
2:G:29:ILE:HG21	2:G:90:HIS:CD2	2.50	0.42
1:H:156:PHE:CD1	1:H:156:PHE:C	2.92	0.42
3:J:384:ASN:CG	3:J:385:GLY:H	2.22	0.42
2:L:36:TYR:HE2	2:L:89:GLN:HB3	1.85	0.42
1:M:37:VAL:HG22	1:M:47:TRP:HA	2.01	0.42
1:M:69:THR:O	1:M:81:LEU:HD12	2.20	0.42
3:O:274:LYS:HE2	3:O:324:SER:HB2	2.02	0.42

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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
3:Y:266:VAL:HB	3:Y:300:TYR:CD2	2.54	0.42
1:A:58:ARG:NH1	1:A:70:VAL:O	2.52	0.42
1:I:164:TRP:O	1:I:166:SER:N	2.53	0.42
2:K:91:TYR:HD1	1:M:99:LYS:HZ3	1.66	0.42
3:Y:296:TYR:OH	3:Y:301:ARG:NH1	2.46	0.42
1:A:101:SER:N	1:A:104:LEU:HD23	2.34	0.42
1:D:153:LYS:NZ	1:D:181:GLN:OE1	2.23	0.42
2:F:29:ILE:HG21	2:F:90:HIS:CD2	2.52	0.42
1:H:68:PHE:HB3	1:H:81:LEU:HD11	2.01	0.42
3:J:291:PRO:O	3:J:292:ARG:HD2	2.17	0.42
3:N:258:GLU:HA	3:N:308:VAL:HG23	1.99	0.42
3:O:336:ILE:HG12	3:O:337:SER:N	2.35	0.42
3:X:336:ILE:HG12	3:X:337:SER:N	2.35	0.42
3:Y:357:GLU:C	3:Y:359:THR:H	2.23	0.42
3:Y:368:LEU:HD12	3:Y:369:VAL:N	2.34	0.42
3:Y:414:LYS:O	3:Y:418:GLN:HG3	2.18	0.42
1:A:185:LEU:HA	1:A:185:LEU:HD12	1.78	0.42
1:A:38:ARG:NH1	1:A:90:ASP:HA	2.34	0.42
2:C:160:GLN:O	2:C:178:THR:N	2.44	0.42
1:D:185:LEU:HA	1:D:185:LEU:HD12	1.76	0.42
1:D:74:ASP:HB3	2:F:94:TYR:CE1	2.54	0.42
1:E:38:ARG:HD3	1:E:94:TYR:CE2	2.55	0.42
2:G:63:SER:O	2:G:74:THR:N	2.50	0.42
2:F:91:TYR:HD1	1:I:99:LYS:NZ	2.17	0.42
3:N:368:LEU:HD12	3:N:369:VAL:N	2.34	0.42
3:O:369:VAL:HB	3:O:406:LEU:HD12	2.02	0.42
3:P:296:TYR:OH	3:P:301:ARG:NH1	2.46	0.42
3:X:283:GLN:C	3:X:285:HIS:H	2.23	0.42
1:A:197:SER:HB3	3:X:295:GLN:OE1	2.20	0.42
3:X:384:ASN:CG	3:X:385:GLY:H	2.22	0.42
2:C:21:ILE:HG12	2:C:102:THR:HG21	2.02	0.42
1:E:152:VAL:HG22	1:E:208:VAL:HG21	2.01	0.42
1:I:153:LYS:HG2	1:I:154:ASP:OD1	2.20	0.42
3:J:391:TYR:CD2	3:J:391:TYR:C	2.93	0.42
1:E:149:GLY:HA2	1:E:164:TRP:CH2	2.55	0.42
1:E:53:THR:O	1:E:56:THR:OG1	2.38	0.42
1:E:60:TYR:CE2	1:E:69:THR:HA	2.54	0.42
1:H:38:ARG:HA	1:H:93:ILE:O	2.19	0.42
3:J:336:ILE:HG12	3:J:337:SER:N	2.35	0.42

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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
1:M:38:ARG:HD3	1:M:94:TYR:CE2	2.55	0.42
3:N:357:GLU:C	3:N:359:THR:H	2.23	0.42
3:P:238:PRO:HB2	3:P:328:LEU:HD13	2.01	0.42
3:Y:238:PRO:HB2	3:Y:328:LEU:HD13	2.01	0.42
1:D:220:LYS:HE2	1:D:222:GLU:OE1	2.19	0.42
1:H:101:SER:N	1:H:104:LEU:HD22	2.35	0.42
1:I:32:HIS:ND1	1:I:98:ARG:HG3	2.35	0.42
3:X:369:VAL:HB	3:X:406:LEU:HD12	2.02	0.42
3:Y:328:LEU:HD12	3:Y:329:PRO:CD	2.47	0.42
1:A:38:ARG:HB3	1:A:94:TYR:CD2	2.55	0.42
1:H:6:GLU:OE1	1:H:95:TYR:HA	2.20	0.42
1:I:195:PRO:C	1:I:197:SER:H	2.23	0.42
3:J:274:LYS:HE2	3:J:324:SER:HB2	2.01	0.42
3:J:367:CYS:HB2	3:J:381:TRP:CH2	2.55	0.42
2:K:58:VAL:HA	2:K:59:PRO:HD3	1.91	0.42
2:L:29:ILE:HG21	2:L:90:HIS:CD2	2.53	0.42
3:N:350:THR:HB	3:N:441:LEU:CD1	2.50	0.42
3:X:391:TYR:C	3:X:391:TYR:CD2	2.92	0.42
2:C:4:MET:SD	2:C:90:HIS:HB2	2.59	0.41
1:D:40:VAL:O	1:D:43:GLY:N	2.45	0.41
2:L:138:ASN:OD1	1:M:174:HIS:NE2	2.52	0.41
2:L:161:GLU:HG2	2:L:177:SER:HB2	2.02	0.41
3:O:367:CYS:HB2	3:O:381:TRP:CH2	2.55	0.41
3:Y:276:ASN:HB3	3:Y:278:TYR:CE1	2.56	0.41
2:C:183:LYS:HE2	2:C:187:GLU:OE1	2.20	0.41
1:D:163:SER:OG	1:D:207:ASN:HB2	2.20	0.41
1:D:181:GLN:C	1:D:183:SER:H	2.23	0.41
1:D:47:TRP:NE1	1:D:49:ALA:O	2.53	0.41
1:E:38:ARG:NH1	1:E:90:ASP:HA	2.35	0.41
2:F:49:TYR:CE2	2:F:53:THR:HB	2.55	0.41
2:G:58:VAL:HA	2:G:59:PRO:HD3	1.97	0.41
2:G:133:VAL:HG21	1:I:134:LEU:HD21	2.01	0.41
3:J:282:VAL:O	3:J:283:GLN:CB	2.52	0.41
3:N:268:HIS:O	3:N:271:PRO:CG	2.68	0.41
3:P:296:TYR:HB3	3:P:297:ASN:H	1.34	0.41
3:P:350:THR:HB	3:P:441:LEU:CD1	2.50	0.41
3:X:314:LEU:HD23	3:X:314:LEU:HA	1.87	0.41
3:Y:268:HIS:O	3:Y:271:PRO:CG	2.68	0.41
1:A:173:VAL:HG22	1:A:192:VAL:HB	2.01	0.41
1:A:99:LYS:HZ3	2:C:91:TYR:HD1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:PHE:CE1	2:K:176:SER:HB3	2.55	0.41
3:J:328:LEU:HD12	3:J:329:PRO:CD	2.50	0.41
2:L:11:LEU:HD22	2:L:19:ILE:HD12	2.02	0.41
1:M:23:GLY:HA2	1:M:78:PHE:CE2	2.54	0.41
1:M:38:ARG:HB3	1:M:94:TYR:CD2	2.55	0.41
3:N:291:PRO:O	3:N:292:ARG:HB3	2.19	0.41
3:O:391:TYR:C	3:O:391:TYR:CD2	2.92	0.41
3:P:276:ASN:HB3	3:P:278:TYR:CE1	2.55	0.41
1:D:30:SER:HB3	1:D:74:ASP:HB3	2.01	0.41
1:E:188:LEU:HD12	1:E:188:LEU:O	2.20	0.41
1:I:4:LEU:HG	1:I:24:VAL:HG12	2.02	0.41
2:K:36:TYR:CE1	2:K:46:LEU:HD13	2.55	0.41
3:O:328:LEU:HD12	3:O:329:PRO:CD	2.50	0.41
2:B:113:PRO:HD2	2:B:201:LEU:HD22	2.03	0.41
2:B:138:ASN:C	2:B:172:THR:HB	2.41	0.41
2:G:38:GLN:HA	2:G:44:PRO:HA	2.02	0.41
2:G:73:LEU:HD12	2:G:74:THR:H	1.84	0.41
1:H:68:PHE:HA	1:H:82:GLN:O	2.20	0.41
3:O:386:GLN:HA	3:O:387:PRO:HD3	1.88	0.41
3:P:268:HIS:O	3:P:271:PRO:CG	2.68	0.41
3:X:386:GLN:HG3	3:X:387:PRO:HD2	2.02	0.41
3:Y:350:THR:HB	3:Y:441:LEU:CD1	2.50	0.41
1:A:160:VAL:HG13	1:A:208:VAL:HG13	2.02	0.41
2:C:110:VAL:HG13	2:C:199:GLN:HG2	2.02	0.41
2:G:167:ASP:CG	1:I:174:HIS:HE1	2.23	0.41
1:H:219:LYS:HE2	1:H:219:LYS:HB2	1.91	0.41
1:M:181:GLN:C	1:M:183:SER:H	2.24	0.41
3:N:367:CYS:HB2	3:N:381:TRP:CZ2	2.56	0.41
3:O:283:GLN:C	3:O:285:HIS:H	2.23	0.41
3:O:384:ASN:CG	3:O:385:GLY:H	2.22	0.41
3:X:367:CYS:HB2	3:X:381:TRP:CH2	2.55	0.41
2:B:106:ILE:O	2:B:166:GLN:NE2	2.48	0.41
2:C:38:GLN:HA	2:C:44:PRO:HA	2.03	0.41
2:G:15:VAL:HG21	2:G:80:PHE:CZ	2.56	0.41
2:L:5:THR:CG2	2:L:100:GLN:HE22	2.33	0.41
3:X:274:LYS:HE2	3:X:324:SER:HB2	2.02	0.41
3:Y:335:THR:O	3:Y:336:ILE:HB	2.21	0.41
2:B:2:VAL:HG11	2:B:90:HIS:CD2	2.56	0.41
2:C:151:ASP:HA	2:C:191:VAL:HG12	2.02	0.41
2:G:140:TYR:CG	2:G:141:PRO:HA	2.56	0.41
2:L:100:GLN:N	2:L:100:GLN:OE1	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:367:CYS:HB2	3:Y:381:TRP:CZ2	2.56	0.41
2:C:149:LYS:HA	2:C:153:ALA:O	2.21	0.41
1:E:34:MET:O	1:E:50:SER:HA	2.21	0.41
2:G:30:GLU:HB2	2:G:32:TRP:CD1	2.56	0.41
1:H:160:VAL:HG12	1:H:160:VAL:O	2.20	0.41
1:H:195:PRO:C	1:H:197:SER:H	2.23	0.41
1:I:94:TYR:O	1:I:116:GLY:HA2	2.20	0.41
3:J:386:GLN:HG3	3:J:387:PRO:HD2	2.02	0.41
2:K:201:LEU:HB3	2:K:203:SER:O	2.20	0.41
2:L:167:ASP:CG	1:M:174:HIS:CE1	2.94	0.41
3:N:350:THR:HB	3:N:441:LEU:CG	2.51	0.41
3:O:252:MET:HB2	3:O:255:ARG:CG	2.49	0.41
3:O:386:GLN:HG3	3:O:387:PRO:HD2	2.02	0.41
3:P:273:VAL:HB	3:P:302:VAL:HG21	2.03	0.41
3:P:357:GLU:C	3:P:359:THR:H	2.23	0.41
3:P:350:THR:HB	3:P:441:LEU:CG	2.51	0.41
2:C:70:GLU:HG3	2:C:71:PHE:N	2.35	0.41
1:H:12:VAL:O	1:H:121:VAL:HA	2.20	0.41
2:K:4:MET:SD	2:K:90:HIS:HB2	2.61	0.41
1:M:34:MET:O	1:M:50:SER:HA	2.19	0.41
3:N:273:VAL:HB	3:N:302:VAL:HG21	2.03	0.41
3:X:386:GLN:HA	3:X:387:PRO:HD3	1.88	0.41
3:Y:351:LEU:HB2	3:Y:366:THR:HB	2.03	0.41
2:B:33:LEU:HA	2:B:89:GLN:O	2.21	0.41
1:D:17:SER:HA	1:D:83:MET:O	2.21	0.41
2:F:73:LEU:HD12	2:F:74:THR:H	1.85	0.41
2:G:186:TYR:HA	2:G:192:TYR:OH	2.20	0.41
1:I:73:ASP:N	1:I:78:PHE:O	2.50	0.41
3:J:283:GLN:C	3:J:285:HIS:H	2.23	0.41
2:L:122:ASP:HA	2:L:125:LEU:HB3	2.03	0.41
3:P:308:VAL:HG12	3:P:309:LEU:N	2.36	0.41
3:X:328:LEU:HD12	3:X:329:PRO:CD	2.50	0.41
3:Y:273:VAL:HB	3:Y:302:VAL:HG21	2.03	0.41
1:A:152:VAL:HG22	1:A:208:VAL:HG21	2.03	0.40
1:A:4:LEU:HG	1:A:24:VAL:HG12	2.02	0.40
2:C:122:ASP:O	2:C:126:LYS:HB2	2.20	0.40
1:D:164:TRP:HH2	1:D:221:VAL:HG21	1.85	0.40
1:D:27:PHE:CE1	1:D:29:ILE:HG22	2.57	0.40
1:M:38:ARG:NH1	1:M:90:ASP:HA	2.35	0.40
3:N:351:LEU:HB2	3:N:366:THR:HB	2.03	0.40
3:P:245:PRO:HB3	3:P:258:GLU:H	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:61:ARG:O	2:C:76:SER:N	2.36	0.40
2:C:73:LEU:HD12	2:C:74:THR:H	1.86	0.40
1:D:156:PHE:C	1:D:156:PHE:CD1	2.94	0.40
1:E:156:PHE:C	1:E:156:PHE:CD1	2.94	0.40
2:F:108:ARG:HD3	2:F:109:THR:N	2.35	0.40
1:E:176:PHE:CD2	2:F:164:THR:HG23	2.56	0.40
2:G:117:ILE:HG13	2:G:133:VAL:O	2.21	0.40
2:L:36:TYR:CE1	2:L:46:LEU:HD13	2.56	0.40
3:N:276:ASN:HB3	3:N:278:TYR:CE1	2.56	0.40
3:N:308:VAL:HG12	3:N:309:LEU:N	2.37	0.40
3:O:289:THR:HG22	3:O:290:LYS:N	2.36	0.40
3:X:289:THR:HG22	3:X:290:LYS:N	2.37	0.40
3:Y:242:LEU:HD23	3:Y:242:LEU:HA	1.85	0.40
2:B:108:ARG:HD3	2:B:109:THR:N	2.36	0.40
2:B:73:LEU:HD12	2:B:74:THR:H	1.86	0.40
2:C:149:LYS:HZ1	2:C:195:GLU:CD	2.18	0.40
3:J:328:LEU:HA	3:J:329:PRO:HD3	1.94	0.40
3:P:335:THR:O	3:P:336:ILE:HB	2.21	0.40
3:P:367:CYS:HB2	3:P:381:TRP:CZ2	2.56	0.40
3:P:350:THR:HB	3:P:441:LEU:HD12	2.03	0.40
2:B:91:TYR:CD1	1:D:99:LYS:NZ	2.86	0.40
1:E:101:SER:CB	1:E:104:LEU:H	2.29	0.40
1:E:181:GLN:C	1:E:183:SER:N	2.75	0.40
1:H:181:GLN:C	1:H:183:SER:H	2.24	0.40
1:H:58:ARG:NH1	1:H:71:SER:OG	2.52	0.40
1:M:69:THR:O	1:M:81:LEU:HA	2.20	0.40
3:X:432:LEU:HD22	3:X:437:THR:HB	2.04	0.40
2:B:170:ASP:OD1	2:B:172:THR:OG1	2.23	0.40
1:D:220:LYS:HE2	1:D:222:GLU:OE2	2.21	0.40
1:E:38:ARG:HB2	1:E:92:ALA:CB	2.52	0.40
2:F:15:VAL:HG21	2:F:80:PHE:CZ	2.56	0.40
2:G:167:ASP:CG	1:I:174:HIS:CE1	2.95	0.40
1:I:19:ILE:C	1:I:20:LEU:HD23	2.41	0.40
1:I:38:ARG:NH1	1:I:90:ASP:HA	2.37	0.40
3:J:432:LEU:HD22	3:J:437:THR:HB	2.04	0.40
2:K:29:ILE:HG21	2:K:90:HIS:CD2	2.54	0.40
2:K:5:THR:HG23	2:K:100:GLN:HE22	1.86	0.40
1:M:156:PHE:CD1	1:M:156:PHE:C	2.94	0.40
3:P:351:LEU:HA	3:P:352:PRO:HD3	1.91	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:252:MET:O	3:Y:253:ILE:CG1[12_555]	0.41	1.79
3:J:252:MET:O	3:X:253:ILE:CD1[12_545]	0.48	1.72
3:O:253:ILE:CA	3:O:253:ILE:CB[10_444]	0.59	1.61
3:J:253:ILE:CD1	3:X:252:MET:O[12_545]	0.66	1.54
3:Y:253:ILE:CA	3:Y:253:ILE:CA[12_555]	0.70	1.50
2:B:18:THR:CA	3:J:285:HIS:ND1[12_545]	0.71	1.49
2:B:18:THR:CA	3:J:285:HIS:CE1[12_545]	0.71	1.49
3:J:253:ILE:CG1	3:X:252:MET:C[12_545]	0.73	1.47
3:X:284:VAL:CG1	2:L:18:THR:CG2[12_545]	0.86	1.34
3:J:253:ILE:CG1	3:X:253:ILE:N[12_545]	0.87	1.33
3:Y:253:ILE:CA	3:Y:253:ILE:C[12_555]	0.87	1.33
3:O:253:ILE:CB	3:O:253:ILE:CB[10_444]	0.96	1.24
3:N:310:HIS:CD2	3:P:253:ILE:CD1[6_445]	1.05	1.15
3:N:380:GLU:OE1	3:P:433:HIS:NE2[6_445]	1.05	1.15
3:X:285:HIS:CG	2:L:18:THR:OG1[12_545]	1.10	1.10
3:J:253:ILE:CD1	3:X:252:MET:C[12_545]	1.17	1.03
3:Y:382:GLU:OE2	3:Y:433:HIS:CG[12_555]	1.19	1.01
3:Y:253:ILE:CG2	3:Y:255:ARG:N[12_555]	1.20	1.00
3:J:253:ILE:CB	3:X:253:ILE:N[12_545]	1.20	1.00
3:O:253:ILE:CD1	3:O:254:SER:N[10_444]	1.22	0.98
2:B:18:THR:C	3:J:285:HIS:ND1[12_545]	1.25	0.95
3:N:253:ILE:CG2	3:P:253:ILE:C[6_445]	1.25	0.95
2:B:18:THR:N	3:J:285:HIS:CG[12_545]	1.25	0.95
3:N:253:ILE:N	3:P:253:ILE:N[6_445]	1.28	0.92
3:N:380:GLU:OE1	3:P:433:HIS:CE1[6_445]	1.30	0.90
3:X:285:HIS:ND1	2:L:18:THR:OG1[12_545]	1.30	0.90
1:D:143:GLY:O	3:Y:280:ASP:CG[8_555]	1.31	0.89
2:B:18:THR:OG1	3:J:285:HIS:CD2[12_545]	1.32	0.88
3:Y:382:GLU:OE2	3:Y:433:HIS:CB[12_555]	1.32	0.88
2:B:18:THR:N	3:J:285:HIS:ND1[12_545]	1.33	0.87
3:N:253:ILE:CG2	3:P:253:ILE:CA[6_445]	1.34	0.86
3:N:433:HIS:CG	3:P:382:GLU:OE2[6_445]	1.35	0.85
3:X:283:GLN:N	2:L:18:THR:O[12_545]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD1[8_555]	1.35	0.85
1:D:143:GLY:O	3:Y:280:ASP:OD2[8_555]	1.35	0.85
1:D:143:GLY:C	3:Y:280:ASP:OD2[8_555]	1.35	0.85
3:J:253:ILE:N	3:X:253:ILE:CG1[12_545]	1.36	0.84
3:N:253:ILE:CB	3:P:253:ILE:CA[6_445]	1.37	0.83
3:Y:253:ILE:N	3:Y:253:ILE:N[12_555]	1.37	0.83
1:D:144:GLY:N	3:Y:280:ASP:OD2[8_555]	1.37	0.83
3:J:253:ILE:CA	3:X:253:ILE:CG1[12_545]	1.39	0.81
3:O:253:ILE:CA	3:O:253:ILE:CG2[10_444]	1.40	0.80

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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:N:253:ILE:CA	3:P:253:ILE:N[6_445]	1.41	0.79
3:J:252:MET:C	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CA	3:P:253:ILE:CA[6_445]	1.42	0.78
3:J:252:MET:O	3:X:253:ILE:CG1[12_545]	1.42	0.78
3:N:253:ILE:CG1	3:P:252:MET:C[6_445]	1.44	0.76
3:Y:253:ILE:CG2	3:Y:254:SER:C[12_555]	1.45	0.75
3:X:281:GLY:O	2:L:20:THR:OG1[12_545]	1.45	0.75
3:J:253:ILE:CA	3:X:253:ILE:CA[12_545]	1.46	0.74
3:J:310:HIS:NE2	3:X:253:ILE:CG2[12_545]	1.46	0.74
3:O:253:ILE:C	3:O:253:ILE:CG2[10_444]	1.47	0.73
1:D:144:GLY:CA	3:Y:280:ASP:OD2[8_555]	1.48	0.72
3:O:253:ILE:O	3:O:253:ILE:CG2[10_444]	1.48	0.72
3:Y:253:ILE:C	3:Y:253:ILE:CB[12_555]	1.48	0.72
3:Y:436:TYR:CD1	3:Y:436:TYR:CD1[12_555]	1.48	0.72
3:J:253:ILE:CB	3:X:253:ILE:CA[12_545]	1.49	0.71
3:J:253:ILE:CG1	3:X:252:MET:O[12_545]	1.50	0.70
3:N:310:HIS:CD2	3:P:253:ILE:CG1[6_445]	1.50	0.70
3:N:253:ILE:CB	3:P:253:ILE:N[6_445]	1.51	0.69
3:O:253:ILE:C	3:O:253:ILE:CG1[10_444]	1.51	0.69
2:B:18:THR:CA	3:J:285:HIS:NE2[12_545]	1.51	0.69
3:N:310:HIS:NE2	3:P:253:ILE:CD1[6_445]	1.51	0.69
3:O:253:ILE:CA	3:O:253:ILE:CG1[10_444]	1.54	0.66
3:J:253:ILE:CA	3:X:253:ILE:CB[12_545]	1.55	0.65
2:B:18:THR:CA	3:J:285:HIS:CG[12_545]	1.57	0.63
3:Y:252:MET:C	3:Y:253:ILE:CG1[12_555]	1.58	0.62
3:X:285:HIS:NE2	2:L:77:GLY:N[12_545]	1.58	0.62
3:Y:253:ILE:N	3:Y:254:SER:N[12_555]	1.60	0.60
3:Y:382:GLU:OE2	3:Y:433:HIS:CD2[12_555]	1.60	0.60
3:J:436:TYR:CD1	3:X:436:TYR:CE1[12_545]	1.61	0.59
1:D:142:SER:CB	3:Y:318:GLU:OE2[8_555]	1.62	0.58
3:N:436:TYR:CD1	3:P:436:TYR:CD1[6_445]	1.62	0.58
3:N:433:HIS:CD2	3:P:382:GLU:OE2[6_445]	1.65	0.55
3:N:253:ILE:C	3:P:253:ILE:CG2[6_445]	1.65	0.55
3:N:253:ILE:CG1	3:P:252:MET:O[6_445]	1.66	0.54
3:J:252:MET:C	3:X:253:ILE:CD1[12_545]	1.67	0.53
3:X:285:HIS:CB	2:L:18:THR:OG1[12_545]	1.67	0.53
3:J:310:HIS:CE1	3:X:253:ILE:CG2[12_545]	1.68	0.52
3:J:253:ILE:CB	3:X:252:MET:C[12_545]	1.69	0.51
2:B:18:THR:CB	3:J:285:HIS:CG[12_545]	1.69	0.51
2:B:18:THR:N	3:J:285:HIS:CD2[12_545]	1.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:380:GLU:OE1	3:X:433:HIS:NE2[12_545]	1.71	0.49
3:X:285:HIS:ND1	2:L:18:THR:CB[12_545]	1.71	0.49
3:Y:253:ILE:N	3:Y:253:ILE:CA[12_555]	1.71	0.49
3:N:253:ILE:CA	3:P:253:ILE:CB[6_445]	1.72	0.48
3:J:253:ILE:CA	3:X:253:ILE:N[12_545]	1.72	0.48
2:B:18:THR:C	3:J:285:HIS:CE1[12_545]	1.73	0.47
3:N:253:ILE:CA	3:P:253:ILE:CG2[6_445]	1.73	0.47
3:O:253:ILE:C	3:O:253:ILE:CB[10_444]	1.73	0.47
3:J:436:TYR:CD1	3:X:436:TYR:CD1[12_545]	1.74	0.46
3:O:253:ILE:C	3:O:253:ILE:CD1[10_444]	1.75	0.45
3:N:253:ILE:CG2	3:P:252:MET:O[6_445]	1.75	0.45
3:Y:252:MET:O	3:Y:253:ILE:CD1[12_555]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CB[10_444]	1.75	0.45
3:O:253:ILE:N	3:O:253:ILE:CG1[10_444]	1.75	0.45
3:N:253:ILE:O	3:P:253:ILE:CG2[6_445]	1.76	0.44
3:N:253:ILE:CD1	3:P:252:MET:O[6_445]	1.77	0.43
3:X:285:HIS:ND1	2:L:18:THR:CA[12_545]	1.77	0.43
3:X:284:VAL:CB	2:L:18:THR:CG2[12_545]	1.78	0.42
3:Y:253:ILE:CA	3:Y:254:SER:N[12_555]	1.78	0.42
3:X:281:GLY:O	2:L:20:THR:N[12_545]	1.78	0.42
2:B:18:THR:CB	3:J:285:HIS:ND1[12_545]	1.79	0.41
3:Y:252:MET:O	3:Y:253:ILE:CB[12_555]	1.79	0.41
1:D:143:GLY:C	3:Y:280:ASP:CG[8_555]	1.80	0.40
3:J:253:ILE:CG2	3:X:310:HIS:NE2[12_545]	1.80	0.40
2:B:18:THR:N	3:J:285:HIS:CE1[12_545]	1.81	0.39
3:J:253:ILE:C	3:X:253:ILE:CG1[12_545]	1.83	0.37
3:J:253:ILE:CG1	3:X:253:ILE:CA[12_545]	1.84	0.36
2:B:18:THR:O	3:J:285:HIS:ND1[12_545]	1.84	0.36
3:X:285:HIS:N	2:L:18:THR:CB[12_545]	1.84	0.36
2:B:18:THR:CB	3:J:285:HIS:CD2[12_545]	1.85	0.35
3:N:253:ILE:CB	3:P:252:MET:C[6_445]	1.85	0.35
3:N:253:ILE:CG2	3:P:253:ILE:N[6_445]	1.86	0.34
3:N:310:HIS:NE2	3:P:253:ILE:CB[6_445]	1.86	0.34
3:Y:253:ILE:N	3:Y:253:ILE:C[12_555]	1.87	0.33
3:N:433:HIS:CB	3:P:382:GLU:OE2[6_445]	1.87	0.33
2:B:18:THR:CA	3:J:285:HIS:CD2[12_545]	1.89	0.31
2:B:18:THR:CG2	3:J:284:VAL:CG1[12_545]	1.90	0.30
3:J:253:ILE:CG2	3:X:253:ILE:CA[12_545]	1.91	0.29
3:Y:253:ILE:C	3:Y:253:ILE:CG2[12_555]	1.91	0.29
3:Y:253:ILE:O	3:Y:253:ILE:CB[12_555]	1.92	0.28
3:Y:253:ILE:CA	3:Y:253:ILE:O[12_555]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:253:ILE:CG2	3:P:254:SER:N[6_445]	1.93	0.27
3:N:310:HIS:NE2	3:P:253:ILE:CG1[6_445]	1.93	0.27
3:J:253:ILE:N	3:X:253:ILE:N[12_545]	1.93	0.27
3:Y:436:TYR:CD1	3:Y:436:TYR:CE1[12_555]	1.93	0.27
1:D:143:GLY:C	3:Y:280:ASP:OD1[8_555]	1.95	0.25
3:X:283:GLN:CA	2:L:18:THR:O[12_545]	1.96	0.24
3:N:253:ILE:CD1	3:P:249:ASP:O[6_445]	1.96	0.24
3:O:253:ILE:N	3:O:253:ILE:CD1[10_444]	1.97	0.23
3:X:285:HIS:N	2:L:18:THR:OG1[12_545]	1.97	0.23
3:Y:253:ILE:CA	3:Y:253:ILE:CB[12_555]	1.97	0.23
2:B:18:THR:N	3:J:285:HIS:NE2[12_545]	1.98	0.22
1:D:141:THR:CG2	3:Y:340:LYS:NZ[8_555]	1.99	0.21
3:Y:253:ILE:O	3:Y:253:ILE:CG2[12_555]	2.00	0.20
2:B:18:THR:OG1	3:J:285:HIS:NE2[12_545]	2.00	0.20
3:J:252:MET:SD	3:X:434:ASN:ND2[12_545]	2.00	0.20
3:N:253:ILE:CG2	3:P:252:MET:C[6_445]	2.01	0.19
2:B:18:THR:CB	3:J:285:HIS:CE1[12_545]	2.01	0.19
3:N:253:ILE:CB	3:P:252:MET:O[6_445]	2.01	0.19
2:B:18:THR:OG1	3:J:285:HIS:CG[12_545]	2.03	0.17
3:O:253:ILE:CG2	3:O:253:ILE:CG2[10_444]	2.03	0.17
2:B:18:THR:CB	3:J:285:HIS:NE2[12_545]	2.04	0.16
3:N:253:ILE:CG1	3:P:253:ILE:N[6_445]	2.04	0.16
3:J:253:ILE:CD1	3:X:252:MET:CA[12_545]	2.04	0.16
3:O:252:MET:CE	3:O:434:ASN:ND2[10_444]	2.04	0.16
3:O:253:ILE:CB	3:O:253:ILE:CG2[10_444]	2.05	0.15
3:X:285:HIS:CE1	2:L:77:GLY:N[12_545]	2.06	0.14
3:J:436:TYR:CE1	3:X:436:TYR:CD1[12_545]	2.06	0.14
3:X:281:GLY:O	2:L:20:THR:CB[12_545]	2.06	0.14
3:X:285:HIS:CA	2:L:18:THR:OG1[12_545]	2.07	0.13
3:N:253:ILE:CG2	3:P:253:ILE:O[6_445]	2.07	0.13
3:J:253:ILE:N	3:X:253:ILE:CB[12_545]	2.08	0.12
1:D:142:SER:CA	3:Y:318:GLU:OE2[8_555]	2.08	0.12
3:J:310:HIS:CD2	3:X:253:ILE:CG2[12_545]	2.08	0.12
3:Y:249:ASP:O	3:Y:253:ILE:CD1[12_555]	2.09	0.11
3:X:285:HIS:NE2	2:L:76:SER:C[12_545]	2.09	0.11
3:N:382:GLU:OE2	3:P:433:HIS:CB[6_445]	2.10	0.10
2:B:17:ASP:O	3:J:285:HIS:NE2[12_545]	2.10	0.10
3:J:253:ILE:CG1	3:X:252:MET:CA[12_545]	2.10	0.10
3:J:436:TYR:CE1	3:X:436:TYR:CE1[12_545]	2.11	0.09
3:O:253:ILE:CB	3:O:253:ILE:CG1[10_444]	2.11	0.09
3:O:253:ILE:CA	3:O:253:ILE:CA[10_444]	2.11	0.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:253:ILE:CG2	3:X:310:HIS:CD2[12_545]	2.12	0.08
3:J:380:GLU:OE1	3:X:433:HIS:CE1[12_545]	2.12	0.08
3:N:380:GLU:CD	3:P:433:HIS:NE2[6_445]	2.14	0.06
2:G:50:LYS:NZ	1:H:103:ARG:C[8_445]	2.15	0.05
2:G:50:LYS:NZ	1:H:103:ARG:CA[8_445]	2.16	0.04
3:N:436:TYR:CE1	3:P:436:TYR:O[6_445]	2.17	0.03
3:Y:382:GLU:CD	3:Y:433:HIS:CD2[12_555]	2.17	0.03
3:J:253:ILE:CB	3:X:252:MET:O[12_545]	2.18	0.02
3:X:284:VAL:CA	2:L:18:THR:CG2[12_545]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/243 (85%)	184 (89%)	19 (9%)	4 (2%)	8	38
1	D	204/243 (84%)	185 (91%)	15 (7%)	4 (2%)	7	38
1	E	207/243 (85%)	186 (90%)	18 (9%)	3 (1%)	11	46
1	H	207/243 (85%)	187 (90%)	16 (8%)	4 (2%)	8	38
1	I	204/243 (84%)	182 (89%)	17 (8%)	5 (2%)	5	32
1	M	204/243 (84%)	186 (91%)	13 (6%)	5 (2%)	5	32
2	B	209/213 (98%)	187 (90%)	21 (10%)	1 (0%)	29	69
2	C	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	29	69
2	F	209/213 (98%)	184 (88%)	24 (12%)	1 (0%)	29	69
2	G	209/213 (98%)	186 (89%)	22 (10%)	1 (0%)	29	69
2	K	209/213 (98%)	185 (88%)	23 (11%)	1 (0%)	29	69
2	L	209/213 (98%)	186 (89%)	21 (10%)	2 (1%)	15	55
3	J	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	N	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	P	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20
3	X	205/211 (97%)	174 (85%)	20 (10%)	11 (5%)	2	19
3	Y	204/211 (97%)	177 (87%)	17 (8%)	10 (5%)	2	20
All	All	3714/4002 (93%)	3276 (88%)	343 (9%)	95 (3%)	5	31

All (95) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	A	141	THR
1	A	223	PRO
1	D	136	PRO
1	D	140	SER
1	D	142	SER
1	E	141	THR
1	I	136	PRO
1	I	140	SER
1	I	142	SER
3	J	283	GLN
3	J	287	ALA
3	J	289	THR
3	J	433	HIS
3	N	298	SER
3	N	301	ARG
3	X	283	GLN
3	X	287	ALA
3	X	289	THR
3	X	433	HIS
3	Y	298	SER
3	Y	301	ARG
1	H	138	SER
1	H	140	SER
1	H	141	THR
1	M	136	PRO
1	M	140	SER
1	M	142	SER
1	M	165	ASN
3	O	283	GLN
3	O	287	ALA
3	O	289	THR

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Mol	Chain	Res	Type
3	O	433	HIS
3	P	298	SER
3	P	301	ARG
1	E	142	SER
2	F	110	VAL
2	G	110	VAL
1	I	165	ASN
3	J	267	SER
3	J	298	SER
3	N	271	PRO
3	X	267	SER
3	X	298	SER
3	Y	271	PRO
1	H	201	THR
3	O	267	SER
3	O	298	SER
3	P	271	PRO
3	J	293	GLU
3	N	282	VAL
3	N	291	PRO
3	N	293	GLU
3	X	293	GLU
3	Y	282	VAL
3	Y	291	PRO
3	Y	293	GLU
2	K	110	VAL
3	O	293	GLU
3	P	282	VAL
3	P	291	PRO
3	P	293	GLU
2	B	110	VAL
2	C	110	VAL
3	J	286	ASN
3	J	358	MET
3	J	385	GLY
3	N	283	GLN
3	N	295	GLN
3	X	286	ASN
3	X	358	MET
3	X	385	GLY
3	Y	283	GLN
3	Y	295	GLN

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

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	180/205 (88%)	163 (91%)	17 (9%)	8	28
1	D	180/205 (88%)	162 (90%)	18 (10%)	7	26
1	E	180/205 (88%)	162 (90%)	18 (10%)	7	26
1	H	180/205 (88%)	165 (92%)	15 (8%)	11	34
1	I	180/205 (88%)	165 (92%)	15 (8%)	11	34
1	M	180/205 (88%)	163 (91%)	17 (9%)	8	28
2	B	182/184 (99%)	164 (90%)	18 (10%)	8	26
2	C	182/184 (99%)	165 (91%)	17 (9%)	9	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	182/184 (99%)	164 (90%)	18 (10%)	8	26
2	G	182/184 (99%)	164 (90%)	18 (10%)	8	26
2	K	182/184 (99%)	163 (90%)	19 (10%)	7	24
2	L	182/184 (99%)	164 (90%)	18 (10%)	8	26
3	J	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	N	192/196 (98%)	180 (94%)	12 (6%)	18	43
3	O	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	P	192/196 (98%)	180 (94%)	12 (6%)	18	43
3	X	193/196 (98%)	187 (97%)	6 (3%)	40	62
3	Y	192/196 (98%)	180 (94%)	12 (6%)	18	43
All	All	3327/3510 (95%)	3065 (92%)	262 (8%)	12	35

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

Mol	Chain	Res	Type
1	A	13	LYS
1	A	50	SER
1	A	55	SER
1	A	56	THR
1	A	57	TYR
1	A	98	ARG
1	A	101	SER
1	A	148	LEU
1	A	156	PHE
1	A	161	THR
1	A	163	SER
1	A	185	LEU
1	A	196	SER
1	A	206	CYS
1	A	211	LYS
1	A	221	VAL
1	A	224	LYS
2	B	7	SER
2	B	20	THR
2	B	33	LEU
2	B	39	LYS
2	B	56	THR
2	B	78	LEU

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Mol	Chain	Res	Type
2	B	108	ARG
2	B	122	ASP
2	B	123	GLU
2	B	132	VAL
2	B	134	CYS
2	B	142	ARG
2	B	143	GLU
2	B	152	ASN
2	B	169	LYS
2	B	191	VAL
2	B	197	THR
2	B	201	LEU
2	C	7	SER
2	C	20	THR
2	C	33	LEU
2	C	39	LYS
2	C	56	THR
2	C	78	LEU
2	C	108	ARG
2	C	122	ASP
2	C	123	GLU
2	C	132	VAL
2	C	134	CYS
2	C	142	ARG
2	C	152	ASN
2	C	169	LYS
2	C	191	VAL
2	C	197	THR
2	C	201	LEU
1	D	13	LYS
1	D	50	SER
1	D	55	SER
1	D	56	THR
1	D	57	TYR
1	D	75	LEU
1	D	98	ARG
1	D	101	SER
1	D	148	LEU
1	D	156	PHE
1	D	161	THR
1	D	163	SER
1	D	185	LEU

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Mol	Chain	Res	Type
1	D	196	SER
1	D	202	GLN
1	D	206	CYS
1	D	211	LYS
1	D	224	LYS
1	E	13	LYS
1	E	50	SER
1	E	55	SER
1	E	56	THR
1	E	57	TYR
1	E	75	LEU
1	E	98	ARG
1	E	101	SER
1	E	102	ASP
1	E	139	LYS
1	E	141	THR
1	E	148	LEU
1	E	156	PHE
1	E	161	THR
1	E	185	LEU
1	E	196	SER
1	E	206	CYS
1	E	211	LYS
2	F	7	SER
2	F	20	THR
2	F	33	LEU
2	F	39	LYS
2	F	56	THR
2	F	78	LEU
2	F	108	ARG
2	F	122	ASP
2	F	123	GLU
2	F	132	VAL
2	F	134	CYS
2	F	142	ARG
2	F	143	GLU
2	F	152	ASN
2	F	169	LYS
2	F	191	VAL
2	F	197	THR
2	F	201	LEU
2	G	7	SER

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Mol	Chain	Res	Type
2	G	20	THR
2	G	33	LEU
2	G	39	LYS
2	G	56	THR
2	G	78	LEU
2	G	108	ARG
2	G	122	ASP
2	G	123	GLU
2	G	132	VAL
2	G	134	CYS
2	G	135	LEU
2	G	142	ARG
2	G	152	ASN
2	G	169	LYS
2	G	191	VAL
2	G	197	THR
2	G	201	LEU
1	I	13	LYS
1	I	50	SER
1	I	55	SER
1	I	56	THR
1	I	57	TYR
1	I	75	LEU
1	I	98	ARG
1	I	101	SER
1	I	148	LEU
1	I	156	PHE
1	I	161	THR
1	I	185	LEU
1	I	196	SER
1	I	206	CYS
1	I	211	LYS
3	J	282	VAL
3	J	292	ARG
3	J	406	LEU
3	J	413	ASP
3	J	436	TYR
3	J	441	LEU
3	N	255	ARG
3	N	260	THR
3	N	278	TYR
3	N	288	LYS

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Mol	Chain	Res	Type
3	N	291	PRO
3	N	296	TYR
3	N	311	GLN
3	N	370	LYS
3	N	394	THR
3	N	399	ASP
3	N	406	LEU
3	N	441	LEU
3	X	282	VAL
3	X	292	ARG
3	X	406	LEU
3	X	413	ASP
3	X	436	TYR
3	X	441	LEU
3	Y	255	ARG
3	Y	260	THR
3	Y	278	TYR
3	Y	288	LYS
3	Y	291	PRO
3	Y	296	TYR
3	Y	311	GLN
3	Y	370	LYS
3	Y	394	THR
3	Y	399	ASP
3	Y	406	LEU
3	Y	441	LEU
1	H	13	LYS
1	H	50	SER
1	H	55	SER
1	H	56	THR
1	H	57	TYR
1	H	98	ARG
1	H	101	SER
1	H	148	LEU
1	H	156	PHE
1	H	161	THR
1	H	185	LEU
1	H	196	SER
1	H	206	CYS
1	H	211	LYS
1	H	224	LYS
2	K	7	SER

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Mol	Chain	Res	Type
2	K	20	THR
2	K	33	LEU
2	K	39	LYS
2	K	56	THR
2	K	78	LEU
2	K	108	ARG
2	K	122	ASP
2	K	123	GLU
2	K	132	VAL
2	K	134	CYS
2	K	135	LEU
2	K	142	ARG
2	K	143	GLU
2	K	152	ASN
2	K	169	LYS
2	K	191	VAL
2	K	197	THR
2	K	201	LEU
2	L	7	SER
2	L	9	SER
2	L	20	THR
2	L	33	LEU
2	L	39	LYS
2	L	56	THR
2	L	78	LEU
2	L	108	ARG
2	L	122	ASP
2	L	123	GLU
2	L	132	VAL
2	L	134	CYS
2	L	142	ARG
2	L	152	ASN
2	L	169	LYS
2	L	191	VAL
2	L	197	THR
2	L	201	LEU
1	M	13	LYS
1	M	50	SER
1	M	55	SER
1	M	56	THR
1	M	57	TYR
1	M	98	ARG

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

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

Mol	Chain	Res	Type
2	B	6	GLN
2	B	90	HIS
2	C	87	HIS
2	C	90	HIS
2	F	90	HIS
2	G	6	GLN
2	G	38	GLN
2	G	87	HIS
2	G	90	HIS

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Mol	Chain	Res	Type
3	J	272	GLN
3	J	283	GLN
3	J	311	GLN
3	J	325	ASN
3	J	347	GLN
3	J	361	ASN
3	J	390	ASN
3	J	418	GLN
3	J	419	GLN
3	J	421	ASN
3	J	429	HIS
3	N	272	GLN
3	N	276	ASN
3	N	283	GLN
3	N	286	ASN
3	N	311	GLN
3	N	312	ASN
3	N	325	ASN
3	N	342	GLN
3	N	361	ASN
3	N	389	ASN
3	N	390	ASN
3	N	419	GLN
3	N	429	HIS
3	N	434	ASN
3	N	438	GLN
3	X	272	GLN
3	X	283	GLN
3	X	311	GLN
3	X	325	ASN
3	X	347	GLN
3	X	361	ASN
3	X	390	ASN
3	X	418	GLN
3	X	419	GLN
3	X	421	ASN
3	X	429	HIS
3	Y	272	GLN
3	Y	276	ASN
3	Y	283	GLN
3	Y	286	ASN
3	Y	311	GLN

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

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

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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.32	9 (4%) 35 32	114, 118, 126, 134	0
1	D	207/243 (85%)	0.25	4 (1%) 66 59	113, 118, 125, 139	0
1	E	209/243 (86%)	0.77	25 (11%) 4 8	178, 182, 190, 198	0
1	H	209/243 (86%)	0.23	4 (1%) 66 59	96, 100, 107, 115	0
1	I	207/243 (85%)	0.61	20 (9%) 7 11	177, 182, 189, 203	0
1	M	207/243 (85%)	0.16	3 (1%) 75 66	94, 100, 107, 121	0
2	B	211/213 (99%)	0.10	1 (0%) 91 85	113, 118, 124, 139	0
2	C	211/213 (99%)	0.27	8 (3%) 40 36	113, 118, 123, 143	0
2	F	211/213 (99%)	0.89	27 (12%) 3 7	177, 182, 188, 203	0
2	G	211/213 (99%)	0.86	26 (12%) 4 8	177, 182, 187, 207	0
2	K	211/213 (99%)	0.27	1 (0%) 91 85	94, 100, 105, 120	0
2	L	211/213 (99%)	0.23	5 (2%) 59 52	94, 100, 105, 124	0
3	J	207/211 (98%)	0.58	10 (4%) 30 29	176, 176, 176, 176	0
3	N	206/211 (97%)	0.60	8 (3%) 39 35	179, 179, 179, 179	0
3	O	207/211 (98%)	0.99	35 (16%) 1 4	274, 274, 274, 274	0
3	P	206/211 (97%)	0.96	35 (16%) 1 4	277, 277, 277, 277	0
3	X	207/211 (98%)	0.52	11 (5%) 26 26	167, 167, 167, 167	0
3	Y	206/211 (97%)	0.55	16 (7%) 13 15	171, 171, 171, 171	0
All	All	3753/4002 (93%)	0.51	248 (6%) 18 18	94, 167, 277, 277	0

All (248) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	134	CYS	7.1
3	O	238	PRO	6.0
1	E	193	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	190	SER	5.2
1	I	152	VAL	5.1
3	Y	239	SER	4.8
2	G	147	GLN	4.6
2	G	134	CYS	4.5
1	E	130	SER	4.3
1	M	130	SER	4.3
3	P	273	VAL	4.2
2	C	145	LYS	4.1
3	O	265	ASP	4.0
3	Y	302	VAL	4.0
3	P	293	GLU	3.8
3	P	295	GLN	3.8
3	O	239	SER	3.8
1	I	129	PRO	3.7
3	P	302	VAL	3.7
2	F	132	VAL	3.7
1	E	152	VAL	3.6
1	D	152	VAL	3.6
2	C	197	THR	3.6
2	F	116	PHE	3.6
3	O	393	THR	3.5
1	I	182	SER	3.5
3	Y	333	GLU	3.5
3	Y	238	PRO	3.5
3	P	294	GLN	3.5
3	O	394	THR	3.4
3	X	302	VAL	3.4
1	E	131	VAL	3.4
3	P	292	ARG	3.4
1	E	222	GLU	3.4
2	F	114	SER	3.3
2	F	115	VAL	3.3
3	X	444	SER	3.3
3	O	440	SER	3.3
3	P	259	VAL	3.3
1	E	129	PRO	3.2
1	E	175	THR	3.2
2	F	147	GLN	3.2
3	O	332	ILE	3.2
1	I	130	SER	3.2
3	Y	240	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	131	VAL	3.2
3	P	274	LYS	3.1
2	G	212	GLY	3.1
1	I	161	THR	3.1
1	E	194	VAL	3.1
2	F	146	VAL	3.1
1	E	161	THR	3.1
3	N	394	THR	3.1
1	I	160	VAL	3.1
2	F	177	SER	3.0
3	Y	263	VAL	3.0
1	H	148	LEU	3.0
3	O	264	VAL	3.0
1	A	152	VAL	3.0
2	G	146	VAL	3.0
3	P	244	PRO	3.0
3	Y	264	VAL	3.0
2	C	147	GLN	3.0
2	G	116	PHE	3.0
2	F	135	LEU	3.0
1	I	147	ALA	3.0
2	G	107	LYS	2.9
2	F	131	SER	2.9
3	P	239	SER	2.9
2	F	120	PRO	2.9
2	G	145	LYS	2.9
1	H	192	VAL	2.9
2	F	45	LYS	2.9
3	P	434	ASN	2.9
1	I	149	GLY	2.8
1	A	160	VAL	2.8
3	O	266	VAL	2.8
1	I	200	GLY	2.8
2	L	187	GLU	2.8
2	C	131	SER	2.8
3	P	238	PRO	2.8
3	J	240	VAL	2.8
2	F	144	ALA	2.8
2	G	13	ALA	2.8
1	E	204	TYR	2.7
2	G	148	TRP	2.7
3	Y	289	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	P	240	VAL	2.7
3	P	323	VAL	2.7
3	X	263	VAL	2.7
2	C	144	ALA	2.7
3	Y	301	ARG	2.7
2	C	146	VAL	2.7
3	P	330	ALA	2.7
2	F	117	ILE	2.7
3	O	337	SER	2.7
3	P	332	ILE	2.7
3	O	326	LYS	2.7
2	G	155	GLN	2.7
2	C	179	LEU	2.7
2	G	195	GLU	2.7
3	P	433	HIS	2.6
3	J	376	ASP	2.6
1	I	203	THR	2.6
2	C	196	VAL	2.6
2	F	136	LEU	2.6
2	G	12	SER	2.6
1	A	137	SER	2.6
3	J	428	MET	2.6
1	I	208	VAL	2.6
2	G	194	CYS	2.6
2	G	14	SER	2.6
3	X	240	VAL	2.6
3	P	245	PRO	2.6
2	G	131	SER	2.6
3	O	350	THR	2.6
2	F	199	GLN	2.5
1	D	147	ALA	2.5
2	K	2	VAL	2.5
2	F	137	ASN	2.5
1	H	193	THR	2.5
1	I	192	VAL	2.5
3	O	273	VAL	2.5
3	P	297	ASN	2.5
2	F	77	GLY	2.5
2	L	212	GLY	2.5
3	P	442	SER	2.5
1	A	130	SER	2.5
1	E	128	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	219	LYS	2.5
2	F	145	LYS	2.5
3	P	296	TYR	2.5
2	F	79	GLN	2.5
1	E	178	ALA	2.5
1	I	188	LEU	2.5
2	F	207	LYS	2.4
3	N	338	LYS	2.4
3	P	298	SER	2.4
3	Y	332	ILE	2.4
1	E	136	PRO	2.4
2	F	194	CYS	2.4
1	E	218	ASP	2.4
3	J	378	ALA	2.4
3	O	333	GLU	2.4
2	G	128	GLY	2.4
1	D	148	LEU	2.4
3	X	304	SER	2.4
3	O	329	PRO	2.4
3	O	385	GLY	2.4
3	Y	273	VAL	2.4
3	X	385	GLY	2.3
3	O	260	THR	2.3
3	O	243	PHE	2.3
3	X	335	THR	2.3
1	I	209	ASN	2.3
2	G	130	ALA	2.3
3	P	331	PRO	2.3
3	O	331	PRO	2.3
1	A	161	THR	2.3
3	Y	334	LYS	2.3
3	O	323	VAL	2.3
3	N	329	PRO	2.3
3	O	375	SER	2.3
3	Y	265	ASP	2.3
1	E	221	VAL	2.3
3	J	238	PRO	2.3
2	G	206	THR	2.3
3	O	321	CYS	2.3
2	F	208	SER	2.3
2	G	132	VAL	2.3
3	X	323	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
3	O	364	SER	2.3
3	O	280	ASP	2.2
1	A	190	SER	2.2
1	E	150	CYS	2.2
2	F	133	VAL	2.2
3	N	331	PRO	2.2
3	P	257	PRO	2.2
1	A	112	ALA	2.2
3	J	321	CYS	2.2
2	B	93	GLY	2.2
2	F	59	PRO	2.2
1	A	178	ALA	2.2
1	D	15	GLY	2.2
3	P	263	VAL	2.2
3	P	260	THR	2.2
3	X	334	LYS	2.2
3	N	301	ARG	2.2
3	O	327	ALA	2.2
3	X	238	PRO	2.2
2	G	153	ALA	2.2
1	E	153	LYS	2.2
3	P	306	LEU	2.2
3	N	239	SER	2.2
2	G	115	VAL	2.1
3	N	440	SER	2.1
3	P	324	SER	2.1
2	G	113	PRO	2.1
3	J	434	ASN	2.1
3	P	250	THR	2.1
3	P	394	THR	2.1
1	I	148	LEU	2.1
3	O	292	ARG	2.1
1	E	208	VAL	2.1
3	Y	323	VAL	2.1
1	E	145	THR	2.1
3	X	261	CYS	2.1
1	I	178	ALA	2.1
1	I	216	LYS	2.1
3	O	335	THR	2.1
3	P	289	THR	2.1
1	M	152	VAL	2.1
2	F	113	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
3	Y	294	GLN	2.1
2	G	149	LYS	2.1
3	J	263	VAL	2.1
3	J	332	ILE	2.1
1	H	149	GLY	2.1
3	O	250	THR	2.1
3	O	240	VAL	2.1
3	P	329	PRO	2.1
3	P	307	THR	2.1
2	L	210	ASN	2.1
3	N	339	ALA	2.1
1	E	188	LEU	2.0
1	M	131	VAL	2.0
3	O	302	VAL	2.0
3	O	374	PRO	2.0
3	P	285	HIS	2.0
2	G	136	LEU	2.0
2	G	207	LYS	2.0
1	E	202	GLN	2.0
3	Y	331	PRO	2.0
3	P	287	ALA	2.0
1	E	192	VAL	2.0
3	O	425	CYS	2.0
1	I	194	VAL	2.0
3	O	267	SER	2.0
3	O	293	GLU	2.0
3	O	318	GLU	2.0
1	I	193	THR	2.0
3	J	375	SER	2.0
2	L	211	ARG	2.0
2	F	119	PRO	2.0
2	G	179	LEU	2.0
1	E	177	PRO	2.0
1	I	190	SER	2.0
2	L	208	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.