



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 PM GMT

PDB ID : 4FHN
Title : Nup37-Nup120 full-length complex from Schizosaccharomyces pombe
Authors : Bilokapic, S.; Schwartz, T.U.
Deposited on : 2012-06-06
Resolution : 6.99 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

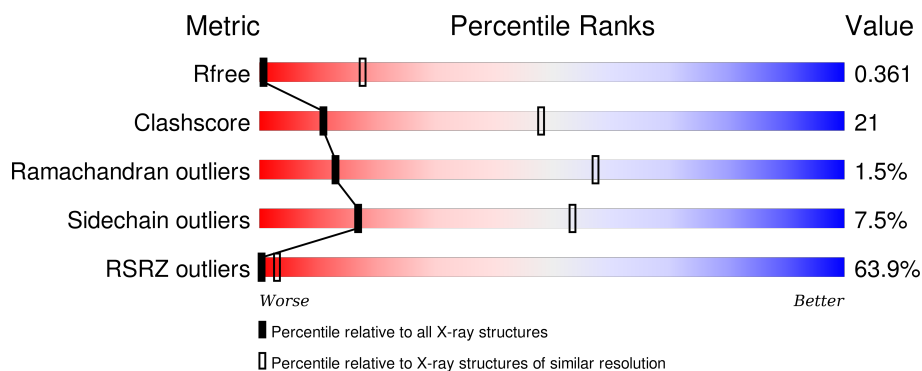
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.99 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}	91344	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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

Mol	Chain	Length	Quality of chain
1	A	394	<div> <div>70%</div> <div> <div>56%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	394	<div> <div>82%</div> <div> <div>56%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	1139	<div> <div>61%</div> <div> <div>45%</div> <div>40%</div> <div>5%</div> <div>10%</div> </div> </div>
2	D	1139	<div> <div>48%</div> <div> <div>45%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>
3	X	450	<div> <div>33%</div> <div> <div>59%</div> <div>38%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24772 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 NUCLEOPORIN NUP37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	0	0	0
			2638	1676	447	500	15			
1	C	344	Total	C	N	O	S	0	0	0
			2646	1680	449	502	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	PRO	-	EXPRESSION TAG	UNP O36030
A	-1	GLY	-	EXPRESSION TAG	UNP O36030
A	0	SER	-	EXPRESSION TAG	UNP O36030
C	-2	PRO	-	EXPRESSION TAG	UNP O36030
C	-1	GLY	-	EXPRESSION TAG	UNP O36030
C	0	SER	-	EXPRESSION TAG	UNP O36030

- Molecule 2 is a protein called Nucleoporin nup120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1022	Total	C	N	O	S	0	0	0
			8251	5335	1322	1563	31			
2	D	977	Total	C	N	O	S	0	0	0
			7871	5094	1258	1488	31			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	PRO	-	EXPRESSION TAG	UNP O43044
B	-1	GLY	-	EXPRESSION TAG	UNP O43044
B	0	SER	-	EXPRESSION TAG	UNP O43044
D	-2	PRO	-	EXPRESSION TAG	UNP O43044
D	-1	GLY	-	EXPRESSION TAG	UNP O43044
D	0	SER	-	EXPRESSION TAG	UNP O43044

- Molecule 3 is a protein called Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	442	Total	C	N	O	S	0	0	0
			3366	2119	594	632	21			

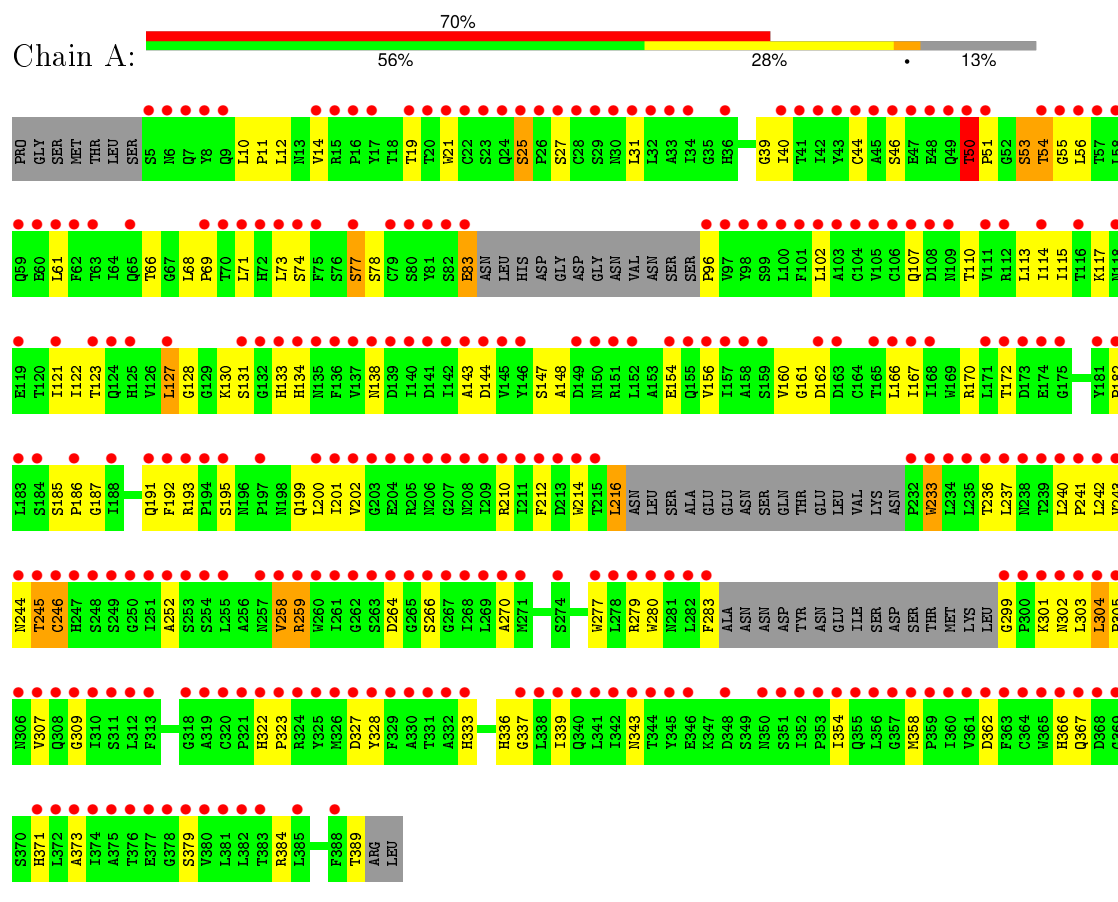
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
X	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
X	0	SER	-	EXPRESSION TAG	UNP Q8XDW9

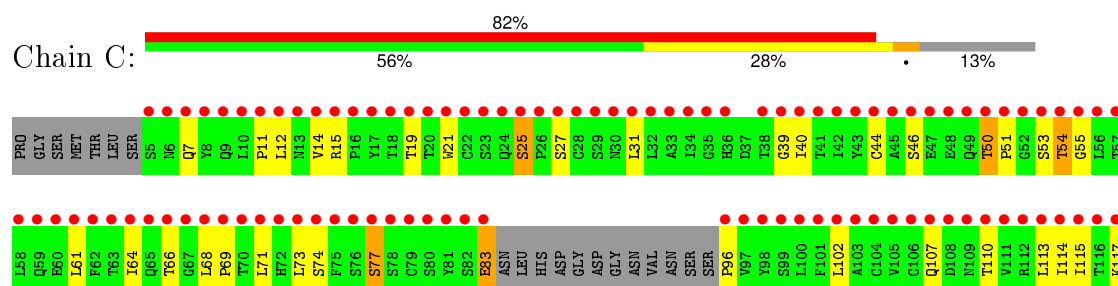
3 Residue-property plots

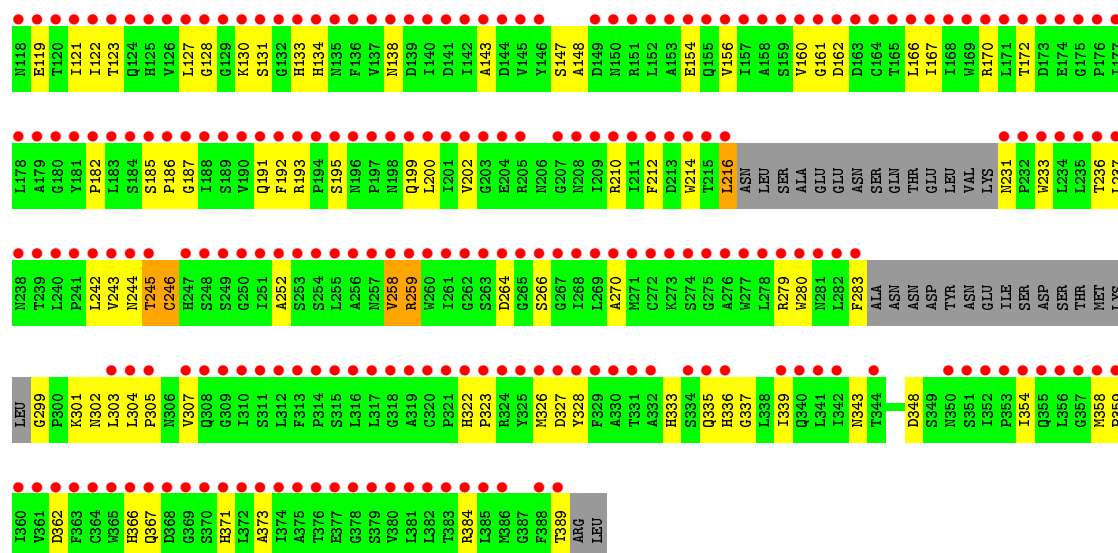
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

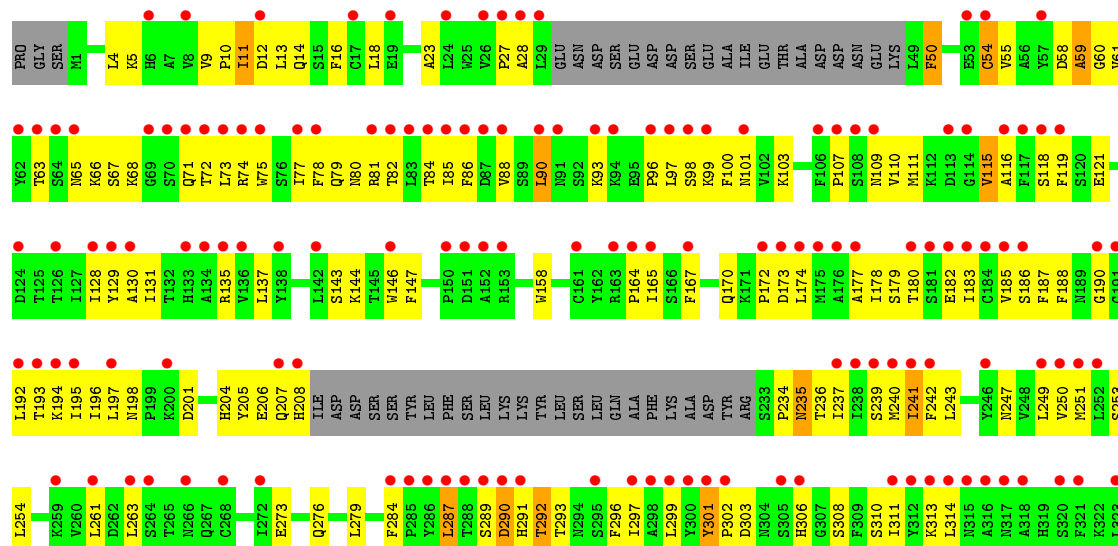
• Molecule 1: NUCLEOPORIN NUP37

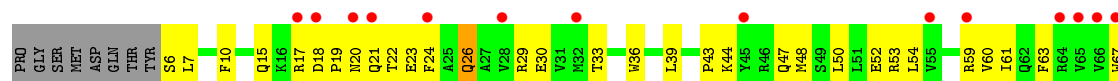


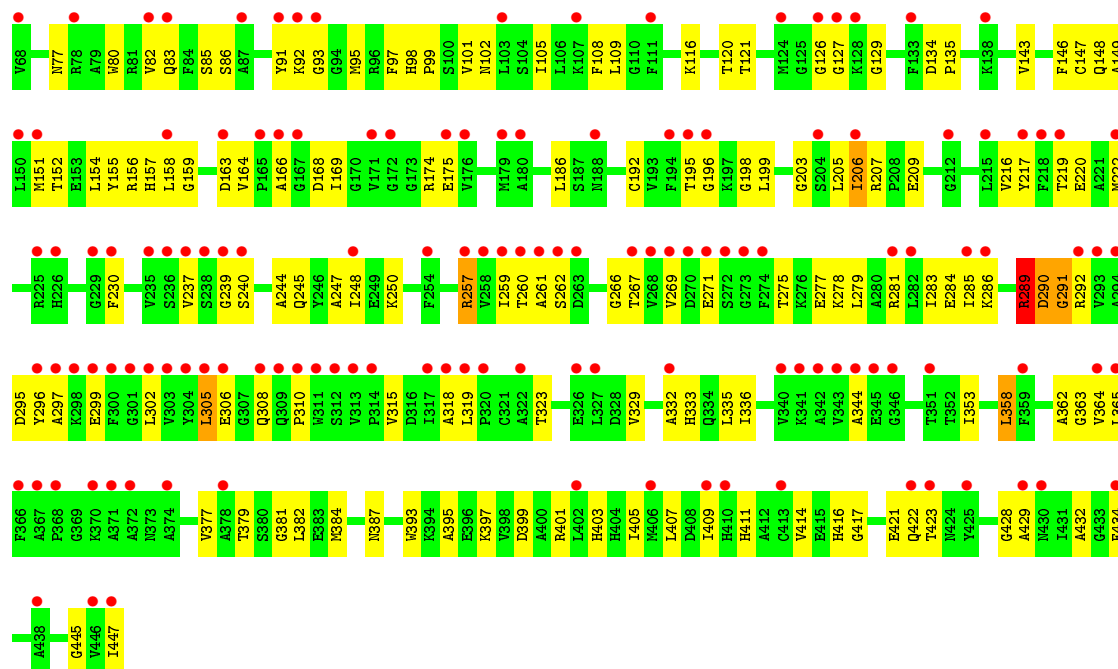
• Molecule 1: NUCLEOPORIN NUP37











4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	330.00 Å 330.00 Å 350.26 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.12 – 6.99 108.02 – 6.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (95.12-6.99) 99.5 (108.02-6.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.27	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 6.73 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.285 , 0.346 0.321 , 0.361	Depositor DCC
R_{free} test set	939 reflections (5.40%)	DCC
Wilson B-factor (Å ²)	456.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 693.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 18317 reflections	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	24772	wwPDB-VP
Average B, all atoms (Å ²)	672.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	0/2702	0.65	0/3689
1	C	0.29	0/2710	0.54	0/3701
2	B	0.37	0/8433	0.71	8/11445 (0.1%)
2	D	0.32	0/8039	0.57	1/10903 (0.0%)
3	X	0.41	0/3431	0.59	0/4630
All	All	0.35	0/25315	0.63	9/34368 (0.0%)

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	A	0	3
2	B	0	1
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	245	THR	N-CA-C	-7.16	91.68	111.00
2	B	72	THR	N-CA-C	6.09	127.44	111.00
2	B	916	LEU	CA-CB-CG	5.79	128.62	115.30
2	B	671	LEU	CA-CB-CG	5.70	128.41	115.30
2	B	73	LEU	CA-CB-CG	5.65	128.31	115.30
2	B	656	LEU	CA-CB-CG	5.49	127.93	115.30
2	B	942	LEU	CB-CG-CD1	-5.33	101.94	111.00
2	B	117	PHE	N-CA-C	5.03	124.59	111.00
2	D	656	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	233	TRP	Peptide
1	A	50	THR	Peptide
1	A	53	SER	Peptide
2	B	206	GLU	Peptide
2	D	206	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2638	0	2588	98	0
1	C	2646	0	2593	93	0
2	B	8251	0	8211	424	2
2	D	7871	0	7847	365	2
3	X	3366	0	3324	118	2
All	All	24772	0	24563	1038	4

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 21.

All (1038) 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)
2:B:828:CYS:HA	2:B:831:LEU:HB2	1.40	1.01
2:B:174:LEU:HD11	2:B:240:MET:H	1.31	0.95
2:D:744:LYS:H	2:D:823:LYS:HD3	1.32	0.95
1:A:252:ALA:HB2	2:B:826:ASN:HD22	1.39	0.88
2:B:942:LEU:HD11	2:B:961:LEU:HG	1.56	0.86
2:D:174:LEU:HD11	2:D:240:MET:H	1.40	0.84
1:C:133:HIS:CD2	1:C:167:ILE:HD12	2.13	0.83
2:D:1015:SER:HB2	2:D:1018:CYS:HB2	1.62	0.82
2:D:93:LYS:H	2:D:96:PRO:HG3	1.45	0.82
2:B:1116:LEU:HB3	2:D:1067:LEU:HB3	1.60	0.81
2:B:93:LYS:H	2:B:96:PRO:HG3	1.46	0.81
3:X:60:VAL:HG22	3:X:82:VAL:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:ASP:HB2	2:B:1101:LYS:HE3	1.62	0.81
2:D:10:PRO:HG3	2:D:431:THR:HA	1.62	0.80
2:B:599:LEU:HD23	2:B:602:LEU:HD12	1.63	0.79
2:B:86:PHE:HB3	2:B:101:ASN:HD22	1.47	0.78
2:D:66:LYS:HG3	2:D:119:PHE:HB2	1.65	0.77
2:B:174:LEU:HB3	2:B:186:SER:HB3	1.65	0.77
2:D:86:PHE:HB3	2:D:101:ASN:HD22	1.48	0.77
2:B:10:PRO:HG3	2:B:431:THR:HA	1.64	0.77
3:X:59:ARG:NH1	3:X:83:GLN:OE1	2.17	0.77
2:B:66:LYS:HG3	2:B:119:PHE:HB2	1.66	0.76
2:D:174:LEU:HB3	2:D:186:SER:HB3	1.68	0.76
2:B:1124:THR:O	2:D:1027:ARG:NE	2.17	0.76
2:B:1116:LEU:HD13	2:D:1067:LEU:HD22	1.67	0.76
2:B:165:ILE:HD13	2:B:187:PHE:HE2	1.51	0.76
2:B:1027:ARG:NH2	2:D:1126:GLU:O	2.17	0.75
2:D:10:PRO:HB3	2:D:433:ILE:HD11	1.66	0.75
2:D:165:ILE:HD13	2:D:187:PHE:HE2	1.52	0.75
2:D:1102:LEU:HA	2:D:1105:LEU:HD12	1.67	0.75
2:D:740:LEU:HD13	2:D:827:ALA:HB1	1.69	0.74
2:D:1000:ASP:OD1	2:D:1028:TYR:OH	2.04	0.74
2:B:1126:GLU:O	2:D:1027:ARG:NH2	2.18	0.74
2:D:1026:TRP:CD1	2:D:1037:ALA:HB1	2.24	0.73
2:B:10:PRO:HB3	2:B:433:ILE:HD11	1.71	0.73
2:B:915:ALA:O	2:B:919:SER:OG	2.06	0.73
2:D:673:LEU:HD13	2:D:770:LEU:HD13	1.68	0.72
1:C:15:ARG:NH1	2:D:917:GLU:OE1	2.22	0.72
2:B:602:LEU:HD22	2:B:606:LEU:HD13	1.70	0.72
2:B:866:SER:OG	2:B:867:LEU:N	2.21	0.72
2:B:946:CYS:SG	2:B:974:PHE:HB3	2.29	0.71
3:X:60:VAL:HG13	3:X:82:VAL:HG22	1.70	0.71
2:B:839:PRO:HB2	2:B:869:LEU:HD11	1.71	0.71
2:B:942:LEU:HD22	2:B:958:LEU:HD23	1.73	0.71
1:A:193:ARG:NH1	1:A:199:GLN:OE1	2.21	0.70
1:A:154:GLU:HG2	1:A:172:THR:HG22	1.73	0.70
1:C:55:GLY:H	1:C:384:ARG:HH11	1.38	0.70
1:C:193:ARG:NH1	1:C:199:GLN:OE1	2.22	0.70
2:B:232:ARG:HG2	2:B:254:LEU:HD21	1.74	0.70
2:B:1067:LEU:HD22	2:D:1116:LEU:HD13	1.74	0.69
2:B:501:GLU:OE1	2:B:504:ARG:NH2	2.25	0.69
2:B:975:VAL:HA	2:B:978:LEU:HD12	1.74	0.69
2:B:412:ASN:ND2	2:B:594:GLU:OE2	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:GLY:HA2	2:B:236:THR:HA	1.74	0.69
2:B:247:ASN:HB3	2:B:263:LEU:HD12	1.75	0.69
2:D:1020:TYR:HA	2:D:1023:LEU:HD12	1.74	0.69
2:B:118:SER:HB3	2:B:129:TYR:HB2	1.73	0.69
2:B:1007:ALA:HA	2:B:1010:MET:HE2	1.74	0.69
2:D:708:TYR:HA	2:D:711:GLN:HG3	1.75	0.69
2:B:665:SER:HB3	2:B:777:ASN:HB3	1.75	0.69
1:A:303:LEU:HD21	2:B:479:GLN:HA	1.75	0.68
2:D:190:GLY:HA2	2:D:236:THR:HA	1.73	0.68
2:B:90:LEU:HA	2:B:669:PRO:HG3	1.74	0.68
2:B:174:LEU:HD11	2:B:240:MET:N	2.08	0.68
2:B:1022:ILE:HD13	2:B:1044:LEU:HD22	1.74	0.68
2:B:67:SER:HB2	2:B:73:LEU:HG	1.76	0.68
3:X:67:TRP:NE1	3:X:77:ASN:OD1	2.26	0.68
2:D:501:GLU:OE1	2:D:504:ARG:NH2	2.28	0.67
3:X:417:GLY:HA3	3:X:423:THR:HG23	1.76	0.67
2:B:116:ALA:O	2:B:130:ALA:HA	1.94	0.67
1:C:133:HIS:HD2	1:C:167:ILE:HD12	1.59	0.67
1:C:335:GLN:NE2	2:D:910:SER:OG	2.28	0.67
2:D:100:PHE:HE1	2:D:147:PHE:HA	1.59	0.67
2:B:100:PHE:HE1	2:B:147:PHE:HA	1.59	0.67
2:B:838:ASP:H	2:B:841:ALA:HB3	1.60	0.66
2:B:419:SER:HB2	2:B:471:LEU:HD21	1.76	0.66
2:B:192:LEU:HD11	2:B:251:MET:SD	2.35	0.66
1:C:339:ILE:HB	1:C:354:ILE:HB	1.77	0.66
2:D:192:LEU:HD11	2:D:251:MET:SD	2.34	0.66
2:D:174:LEU:HD11	2:D:240:MET:N	2.09	0.66
2:D:67:SER:HB2	2:D:73:LEU:HG	1.78	0.66
2:D:412:ASN:ND2	2:D:594:GLU:OE2	2.29	0.66
1:C:53:SER:OG	1:C:54:THR:N	2.27	0.66
1:A:53:SER:OG	1:A:54:THR:N	2.29	0.65
3:X:53:ARG:NH2	3:X:445:GLY:O	2.28	0.65
1:C:154:GLU:HG2	1:C:172:THR:HG22	1.76	0.65
1:A:301:LYS:HD3	2:B:479:GLN:HB3	1.77	0.65
2:D:236:THR:O	2:D:254:LEU:N	2.27	0.65
2:B:337:PRO:HG3	2:B:394:HIS:HE1	1.61	0.65
2:D:116:ALA:O	2:D:130:ALA:HA	1.95	0.65
2:B:239:SER:HB3	2:B:289:SER:HB2	1.79	0.65
1:A:339:ILE:HB	1:A:354:ILE:HB	1.79	0.65
1:A:117:LYS:HG2	1:A:122:ILE:HD13	1.78	0.65
2:D:72:THR:OG1	2:D:73:LEU:N	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:ILE:HA	2:B:253:SER:HA	1.78	0.65
1:A:110:THR:HG22	1:A:128:GLY:HA3	1.79	0.65
2:D:419:SER:HB2	2:D:471:LEU:HD21	1.78	0.65
2:D:971:LEU:HA	2:D:974:PHE:HD2	1.63	0.65
2:B:955:HIS:CE1	2:B:978:LEU:HD13	2.32	0.64
2:B:236:THR:O	2:B:254:LEU:N	2.29	0.64
2:B:953:ALA:C	2:B:955:HIS:H	2.00	0.64
2:B:364:ILE:HG23	2:B:522:ILE:HD12	1.79	0.64
2:B:72:THR:OG1	2:B:73:LEU:N	2.30	0.64
2:B:310:SER:OG	2:B:311:ILE:N	2.29	0.64
1:C:359:PRO:HD3	2:D:912:TYR:CZ	2.32	0.64
2:B:164:PRO:HB3	2:B:204:HIS:CD2	2.33	0.64
2:D:435:SER:HB2	2:D:512:LEU:HB3	1.78	0.64
3:X:149:ALA:O	3:X:152:THR:OG1	2.11	0.64
3:X:17:ARG:NH2	3:X:52:GLU:OE2	2.31	0.64
3:X:333:HIS:HA	3:X:336:ILE:HD12	1.80	0.63
2:D:337:PRO:HG3	2:D:394:HIS:HE1	1.62	0.63
2:D:249:LEU:HD23	2:D:261:LEU:HD23	1.81	0.63
2:D:237:ILE:HA	2:D:253:SER:HA	1.81	0.63
1:C:117:LYS:HG2	1:C:122:ILE:HD13	1.80	0.63
2:D:311:ILE:HB	2:D:332:ILE:HG13	1.81	0.63
2:D:639:LEU:HA	2:D:642:LEU:HD22	1.79	0.63
2:B:1003:LEU:HD12	2:B:1028:TYR:CG	2.34	0.63
1:A:200:LEU:HD11	1:A:212:PHE:HD2	1.63	0.63
2:D:79:GLN:HB3	2:D:82:THR:HB	1.80	0.63
3:X:291:GLY:O	3:X:292:ARG:NH1	2.31	0.62
2:D:975:VAL:HA	2:D:978:LEU:HD12	1.81	0.62
2:B:718:ASP:O	2:B:721:PHE:HB3	2.00	0.62
2:D:247:ASN:HB3	2:D:263:LEU:HD12	1.81	0.62
2:D:454:LYS:HD2	2:D:457:LYS:HD2	1.81	0.62
2:B:602:LEU:HB3	2:B:606:LEU:HD22	1.81	0.62
1:A:371:HIS:CE1	1:A:384:ARG:HD2	2.35	0.62
2:B:1043:LYS:HA	2:B:1046:ARG:HD2	1.80	0.62
2:D:118:SER:HB3	2:D:129:TYR:HB2	1.80	0.62
2:B:763:LEU:HD22	2:B:771:GLN:HG2	1.82	0.62
2:D:12:ASP:HB2	2:D:433:ILE:HG23	1.82	0.62
1:C:110:THR:HG22	1:C:128:GLY:HA3	1.81	0.62
2:B:74:ARG:HH22	2:B:144:LYS:HG2	1.63	0.62
2:B:1082:TRP:CZ3	2:B:1100:GLN:HA	2.34	0.62
2:D:945:ALA:O	2:D:949:GLY:N	2.28	0.62
2:D:90:LEU:HA	2:D:669:PRO:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1080:ASP:HB2	2:B:1101:LYS:CE	2.30	0.61
1:A:55:GLY:H	1:A:384:ARG:HH11	1.46	0.61
2:B:926:LYS:HZ1	2:B:930:ASP:H	1.48	0.61
2:D:310:SER:OG	2:D:311:ILE:N	2.31	0.61
2:D:349:PHE:HA	2:D:522:ILE:HD11	1.82	0.61
2:B:772:PHE:HD1	2:B:815:LEU:HD21	1.64	0.61
2:B:249:LEU:HD23	2:B:261:LEU:HD23	1.80	0.61
2:B:435:SER:HB2	2:B:512:LEU:HB3	1.82	0.61
2:B:958:LEU:HB3	2:B:971:LEU:HD13	1.82	0.61
2:D:619:TYR:CD2	2:D:700:SER:HA	2.36	0.61
1:C:371:HIS:CE1	1:C:384:ARG:HD2	2.35	0.61
2:D:364:ILE:HG23	2:D:522:ILE:HD12	1.83	0.61
1:C:7:GLN:OE1	2:D:950:LYS:NZ	2.34	0.61
2:D:239:SER:HB3	2:D:289:SER:HB2	1.83	0.61
2:D:767:ASN:HB3	2:D:770:LEU:HD11	1.82	0.60
2:B:695:PHE:CZ	2:B:724:LEU:HB3	2.36	0.60
2:D:310:SER:HA	2:D:332:ILE:H	1.65	0.60
2:B:79:GLN:HB3	2:B:82:THR:HB	1.83	0.60
2:B:543:ARG:HB3	2:B:679:ARG:HH12	1.66	0.60
1:A:130:LYS:HD3	2:B:609:TYR:HE1	1.66	0.60
2:B:68:LYS:HG3	2:B:121:GLU:HG2	1.81	0.60
2:B:1103:LEU:HD22	3:X:271:GLU:HB2	1.83	0.60
2:B:1026:TRP:HD1	2:B:1037:ALA:HB1	1.67	0.60
2:B:603:VAL:HG13	2:B:729:ARG:HD2	1.84	0.59
2:B:1113:HIS:HA	2:B:1116:LEU:HG	1.84	0.59
2:B:310:SER:HA	2:B:332:ILE:H	1.66	0.59
1:C:301:LYS:HD3	2:D:479:GLN:HB3	1.84	0.59
2:B:1058:GLU:HA	2:B:1061:PHE:HD2	1.67	0.59
2:D:913:ILE:HA	2:D:916:LEU:HB2	1.82	0.59
2:B:587:MET:HG2	2:B:591:THR:HG21	1.85	0.59
2:B:311:ILE:HB	2:B:332:ILE:HG13	1.83	0.59
2:D:976:ASN:OD1	2:D:1006:LYS:NZ	2.29	0.59
1:A:160:VAL:HB	1:A:187:GLY:HA3	1.83	0.59
3:X:168:ASP:OD1	3:X:169:ILE:N	2.33	0.59
2:B:668:SER:HB2	2:B:672:PHE:HD2	1.67	0.59
1:A:210:ARG:HH12	2:B:417:ASP:H	1.51	0.59
2:B:293:THR:HG23	2:B:353:SER:H	1.68	0.59
2:B:906:LEU:HD22	2:B:914:ASP:HB2	1.83	0.59
3:X:15:GLN:HG2	3:X:19:PRO:HA	1.83	0.59
2:B:835:LEU:HD21	2:B:841:ALA:HB1	1.83	0.59
2:D:1059:ARG:O	2:D:1063:ILE:HG13	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:VAL:HG22	2:D:78:PHE:HB3	1.83	0.59
3:X:98:HIS:HB3	3:X:101:VAL:HG23	1.85	0.59
3:X:216:VAL:HG21	3:X:250:LYS:HB3	1.84	0.59
2:D:1112:TYR:CE2	2:D:1116:LEU:HD11	2.38	0.59
2:D:693:GLU:HB3	2:D:697:PHE:CZ	2.38	0.59
2:D:587:MET:HG2	2:D:591:THR:HG21	1.85	0.59
2:D:798:LEU:HD23	2:D:801:ILE:HD12	1.83	0.59
2:B:838:ASP:O	2:B:842:VAL:N	2.36	0.59
2:B:164:PRO:HG2	2:B:195:ILE:HD13	1.83	0.59
2:B:1082:TRP:HZ2	3:X:305:LEU:HD22	1.68	0.58
2:B:349:PHE:HA	2:B:522:ILE:HD11	1.84	0.58
2:D:247:ASN:HB3	2:D:263:LEU:HB2	1.85	0.58
1:C:304:LEU:HD22	1:C:305:PRO:HD2	1.85	0.58
2:D:74:ARG:HH22	2:D:144:LYS:HG2	1.67	0.58
1:C:200:LEU:HD11	1:C:212:PHE:HD2	1.67	0.58
2:D:776:LEU:HD13	2:D:797:SER:HA	1.85	0.58
2:B:453:ASN:O	2:B:457:LYS:HG3	2.03	0.58
2:B:71:GLN:HB3	2:B:93:LYS:HE2	1.85	0.58
2:D:835:LEU:HD21	2:D:841:ALA:HB1	1.85	0.58
2:D:830:GLN:HG3	2:D:831:LEU:HD23	1.85	0.58
2:D:1112:TYR:CE1	2:D:1116:LEU:HD21	2.38	0.58
2:B:628:ASP:HB3	2:B:631:TYR:HD2	1.67	0.58
2:D:71:GLN:HB3	2:D:93:LYS:HE2	1.86	0.58
2:B:482:PRO:HA	2:B:489:TYR:HA	1.85	0.58
1:A:44:CYS:HB2	1:A:61:LEU:HD11	1.85	0.58
2:B:548:ILE:HD13	2:B:687:LYS:HD2	1.86	0.58
2:B:1103:LEU:HD13	3:X:271:GLU:H	1.68	0.58
2:B:812:VAL:HG21	2:B:835:LEU:HB2	1.86	0.58
2:B:668:SER:HB2	2:B:672:PHE:CD2	2.38	0.58
2:B:693:GLU:HB3	2:B:697:PHE:CZ	2.39	0.58
2:D:842:VAL:HG11	2:D:865:THR:HG21	1.85	0.58
2:B:985:ASN:O	2:B:989:ASN:ND2	2.37	0.58
2:B:989:ASN:O	2:B:993:PRO:HD3	2.04	0.58
3:X:18:ASP:HB3	3:X:21:GLN:HB2	1.85	0.58
2:B:708:TYR:HA	2:B:711:GLN:HG3	1.84	0.58
2:D:599:LEU:HD23	2:D:602:LEU:HD12	1.86	0.58
2:D:164:PRO:HB3	2:D:204:HIS:CD2	2.39	0.58
2:D:650:ASP:OD1	2:D:651:SER:N	2.37	0.57
2:D:734:LEU:HA	2:D:737:ASN:HB2	1.86	0.57
2:B:167:PHE:HD2	2:B:172:PRO:HD3	1.69	0.57
1:A:384:ARG:HH21	1:A:389:THR:HG21	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:535:TYR:HB2	2:D:538:LYS:O	2.05	0.57
1:C:44:CYS:HB2	1:C:61:LEU:HD11	1.86	0.57
1:C:160:VAL:HB	1:C:187:GLY:HA3	1.85	0.57
2:B:61:VAL:HG22	2:B:78:PHE:HB3	1.87	0.57
2:D:68:LYS:HG3	2:D:121:GLU:HG2	1.85	0.57
3:X:259:ILE:HG13	3:X:260:THR:HG23	1.86	0.57
2:D:314:LEU:HG	2:D:327:ILE:HG12	1.87	0.57
2:D:741:LEU:HA	2:D:768:THR:HB	1.86	0.57
1:A:304:LEU:HD22	1:A:305:PRO:HD2	1.85	0.57
2:D:313:LYS:HB3	2:D:329:LYS:HD3	1.86	0.57
2:B:337:PRO:HG3	2:B:394:HIS:CE1	2.40	0.57
2:D:847:LEU:HD23	2:D:850:LEU:HD12	1.86	0.57
2:B:445:ASN:HB2	2:B:448:SER:HB2	1.87	0.57
1:C:166:LEU:HD22	1:C:202:VAL:HG21	1.86	0.57
1:A:182:PRO:O	2:B:413:MET:HB2	2.04	0.57
2:D:453:ASN:O	2:D:457:LYS:HG3	2.04	0.57
2:D:482:PRO:HA	2:D:489:TYR:HA	1.86	0.57
2:B:65:ASN:HD21	2:B:73:LEU:HD21	1.70	0.57
2:D:639:LEU:HD13	2:D:701:LEU:HB3	1.87	0.57
1:A:166:LEU:HD22	1:A:202:VAL:HG21	1.87	0.57
2:D:996:ARG:HH11	2:D:1031:GLN:HG3	1.70	0.56
2:B:917:GLU:O	2:B:920:LEU:HB2	2.04	0.56
2:D:674:CYS:SG	2:D:767:ASN:ND2	2.77	0.56
2:B:1026:TRP:CD1	2:B:1037:ALA:HB1	2.40	0.56
2:B:935:ILE:HG23	2:B:967:LYS:HZ3	1.70	0.56
2:D:862:PHE:CZ	2:D:902:LEU:HD21	2.40	0.56
2:D:1026:TRP:HE1	2:D:1072:THR:HG22	1.71	0.56
3:X:219:THR:HB	3:X:230:PHE:CZ	2.41	0.56
1:A:333:HIS:HD2	1:A:336:HIS:H	1.52	0.56
3:X:54:LEU:HD22	3:X:434:PHE:HE1	1.71	0.56
2:D:619:TYR:HD2	2:D:700:SER:HA	1.68	0.56
2:D:1080:ASP:N	2:D:1101:LYS:HG2	2.21	0.56
2:B:770:LEU:O	2:B:773:PHE:N	2.39	0.56
2:B:956:VAL:O	2:B:960:VAL:HG23	2.04	0.56
2:D:912:TYR:CE2	2:D:947:ALA:HB1	2.41	0.56
1:A:21:TRP:CZ3	1:A:366:HIS:HD2	2.24	0.56
2:D:63:THR:HG1	2:D:521:SER:HG	1.54	0.56
2:B:237:ILE:HD13	2:B:251:MET:SD	2.46	0.55
1:C:242:LEU:HD13	1:C:305:PRO:HG3	1.87	0.55
1:A:242:LEU:HD13	1:A:305:PRO:HG3	1.88	0.55
2:D:549:GLU:O	2:D:553:GLU:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1121:VAL:HA	2:D:1124:THR:HG22	1.88	0.55
2:B:734:LEU:HA	2:B:737:ASN:HB2	1.87	0.55
3:X:159:GLY:O	3:X:163:ASP:N	2.38	0.55
3:X:209:GLU:N	3:X:209:GLU:OE1	2.38	0.55
1:C:71:LEU:HD11	2:D:860:ARG:CZ	2.36	0.55
2:B:118:SER:OG	2:B:177:ALA:HB2	2.06	0.55
2:D:337:PRO:HG3	2:D:394:HIS:CE1	2.41	0.55
2:B:549:GLU:O	2:B:553:GLU:HG2	2.05	0.55
2:B:12:ASP:H	2:B:433:ILE:HG13	1.71	0.55
3:X:379:THR:HA	3:X:382:LEU:HG	1.88	0.55
3:X:289:ARG:HH11	3:X:289:ARG:HG2	1.71	0.55
2:B:535:TYR:HB2	2:B:538:LYS:O	2.07	0.55
2:B:54:CYS:SG	2:B:55:VAL:N	2.79	0.55
1:C:107:GLN:HA	2:D:860:ARG:CZ	2.36	0.55
2:D:810:ASP:O	2:D:813:THR:OG1	2.21	0.55
3:X:148:GLN:O	3:X:152:THR:HG23	2.06	0.55
2:B:433:ILE:HG22	2:B:434:GLU:HG3	1.89	0.55
1:C:335:GLN:HE22	2:D:910:SER:C	2.10	0.55
2:D:982:GLY:HA3	2:D:987:LEU:HD11	1.89	0.55
2:D:177:ALA:HA	2:D:183:ILE:HG13	1.87	0.55
2:B:984:ILE:HG13	2:B:1024:PHE:CE2	2.41	0.55
2:B:194:LYS:HB3	2:B:205:TYR:HB2	1.89	0.55
2:B:12:ASP:HB2	2:B:433:ILE:HG23	1.88	0.54
2:B:247:ASN:HB3	2:B:263:LEU:HB2	1.89	0.54
2:B:450:VAL:O	2:B:454:LYS:N	2.38	0.54
1:C:21:TRP:CZ3	1:C:366:HIS:HD2	2.26	0.54
2:B:651:SER:O	2:B:655:ARG:HG3	2.07	0.54
1:C:384:ARG:HE	1:C:389:THR:HG21	1.71	0.54
2:B:177:ALA:HA	2:B:183:ILE:HG13	1.89	0.54
2:D:729:ARG:HH12	2:D:812:VAL:HG11	1.72	0.54
3:X:260:THR:HG22	3:X:269:VAL:HG22	1.88	0.54
1:C:384:ARG:HH21	1:C:389:THR:HG21	1.72	0.54
2:B:669:PRO:HD2	2:B:672:PHE:CD2	2.43	0.54
2:B:313:LYS:HD2	2:B:351:LEU:HD21	1.88	0.54
3:X:120:THR:O	3:X:121:THR:OG1	2.21	0.54
2:D:350:GLN:HG2	2:D:524:PHE:HB2	1.89	0.54
2:D:54:CYS:SG	2:D:55:VAL:N	2.80	0.54
2:D:1003:LEU:HD12	2:D:1028:TYR:CZ	2.43	0.54
1:C:55:GLY:H	1:C:384:ARG:NH1	2.06	0.54
3:X:219:THR:HB	3:X:230:PHE:CE2	2.42	0.54
2:D:738:SER:OG	2:D:738:SER:O	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:86:SER:HB3	3:X:91:TYR:CZ	2.42	0.54
2:B:79:GLN:HG3	2:B:80:ASN:N	2.23	0.54
2:B:548:ILE:HD11	2:B:687:LYS:HZ2	1.73	0.54
2:D:579:LEU:O	2:D:583:LEU:HG	2.08	0.54
2:B:241:ILE:HG22	2:B:250:VAL:HB	1.89	0.54
2:B:165:ILE:HD13	2:B:187:PHE:CE2	2.38	0.54
2:D:933:LEU:O	2:D:937:ILE:HG13	2.07	0.54
2:B:314:LEU:HG	2:B:327:ILE:HG12	1.89	0.54
2:D:695:PHE:CE1	2:D:724:LEU:HB3	2.42	0.54
1:A:107:GLN:HA	2:B:860:ARG:NH2	2.22	0.54
2:D:167:PHE:HD2	2:D:172:PRO:HD3	1.72	0.53
2:B:332:ILE:HG12	2:B:388:PHE:CE2	2.43	0.53
2:B:689:GLN:O	2:B:693:GLU:HG3	2.08	0.53
2:D:4:LEU:HG	2:D:393:SER:OG	2.08	0.53
3:X:6:SER:HB3	3:X:36:TRP:HE1	1.72	0.53
2:B:972:LEU:HD11	2:B:1005:ARG:HH11	1.73	0.53
2:D:306:HIS:ND1	2:D:308:SER:HB3	2.23	0.53
1:C:83:GLU:HA	1:C:96:PRO:HA	1.89	0.53
2:D:799:SER:O	2:D:803:ILE:HG12	2.08	0.53
2:D:65:ASN:HD21	2:D:73:LEU:HD21	1.73	0.53
3:X:275:THR:H	3:X:278:LYS:HB2	1.74	0.53
2:D:1080:ASP:H	2:D:1101:LYS:HG2	1.73	0.53
3:X:411:HIS:O	3:X:414:VAL:HG22	2.09	0.53
2:B:1083:ILE:HD13	2:B:1100:GLN:N	2.24	0.53
3:X:278:LYS:HB3	3:X:296:TYR:OH	2.08	0.53
3:X:267:THR:O	3:X:305:LEU:HG	2.08	0.53
2:B:840:ILE:HG23	2:B:875:GLN:HE21	1.72	0.53
2:D:815:LEU:HD22	2:D:819:LEU:HD11	1.91	0.53
2:B:185:VAL:HB	2:B:193:THR:HG22	1.91	0.53
2:D:12:ASP:H	2:D:433:ILE:HG13	1.73	0.53
1:A:11:PRO:HB2	1:A:14:VAL:HG23	1.90	0.53
2:B:842:VAL:HG11	2:B:865:THR:OG1	2.08	0.53
2:D:293:THR:HG23	2:D:353:SER:H	1.73	0.53
2:D:1109:VAL:O	2:D:1112:TYR:HB3	2.09	0.52
2:B:972:LEU:HD21	2:B:1005:ARG:HD3	1.91	0.52
2:D:460:ALA:O	2:D:462:THR:N	2.41	0.52
2:D:164:PRO:HG2	2:D:195:ILE:HD13	1.90	0.52
1:C:279:ARG:HB3	1:C:307:VAL:HG12	1.92	0.52
2:B:13:LEU:HA	2:B:16:PHE:HD2	1.75	0.52
3:X:175:GLU:H	3:X:175:GLU:CD	2.13	0.52
2:D:1066:TYR:CE1	2:D:1108:ILE:HB	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:771:GLN:HB3	2:B:819:LEU:HD22	1.91	0.52
1:A:237:LEU:HD13	1:A:280:TRP:CE2	2.44	0.52
3:X:23:GLU:N	3:X:23:GLU:OE1	2.43	0.52
2:B:847:LEU:O	2:B:851:LYS:HG2	2.10	0.52
1:A:138:ASN:HD22	1:A:161:GLY:HA2	1.74	0.52
2:B:1067:LEU:O	2:B:1071:ASN:ND2	2.40	0.52
3:X:143:VAL:HG21	3:X:174:ARG:NH2	2.24	0.52
2:D:912:TYR:CZ	2:D:947:ALA:HB1	2.44	0.52
2:D:332:ILE:HG12	2:D:388:PHE:CE2	2.44	0.52
2:B:462:THR:O	2:B:466:LEU:HG	2.09	0.52
2:D:165:ILE:HD13	2:D:187:PHE:CE2	2.39	0.52
2:B:590:SER:O	2:B:594:GLU:HG2	2.10	0.52
1:C:237:LEU:HD13	1:C:280:TRP:CE2	2.45	0.52
2:B:454:LYS:HD2	2:B:457:LYS:HD2	1.92	0.52
2:B:63:THR:HG1	2:B:521:SER:HG	1.56	0.52
2:D:81:ARG:H	2:D:109:ASN:HB3	1.75	0.52
2:B:306:HIS:ND1	2:B:308:SER:HB3	2.25	0.52
2:B:1102:LEU:HA	2:B:1105:LEU:HD12	1.91	0.52
2:D:632:ILE:O	2:D:636:ILE:HG12	2.09	0.52
2:D:635:LEU:O	2:D:639:LEU:HG	2.09	0.52
2:B:81:ARG:H	2:B:109:ASN:HB3	1.74	0.52
2:D:1029:LYS:HB2	2:D:1037:ALA:HB2	1.92	0.52
2:D:237:ILE:HD13	2:D:251:MET:SD	2.49	0.52
2:B:953:ALA:O	2:B:955:HIS:N	2.43	0.52
2:B:926:LYS:NZ	2:B:930:ASP:H	2.08	0.52
1:C:333:HIS:HD2	1:C:336:HIS:H	1.55	0.52
3:X:399:ASP:O	3:X:403:HIS:HB2	2.09	0.52
1:A:83:GLU:HA	1:A:96:PRO:HA	1.92	0.52
2:B:955:HIS:O	2:B:958:LEU:HB2	2.10	0.52
2:B:4:LEU:HG	2:B:393:SER:OG	2.10	0.52
2:D:118:SER:OG	2:D:177:ALA:HB2	2.11	0.51
2:D:478:ILE:HD11	2:D:501:GLU:HG2	1.91	0.51
1:A:143:ALA:CB	1:A:192:PHE:HD2	2.23	0.51
3:X:196:GLY:O	3:X:207:ARG:NH2	2.43	0.51
2:D:1060:THR:O	2:D:1063:ILE:HB	2.10	0.51
2:B:164:PRO:HB3	2:B:204:HIS:NE2	2.26	0.51
2:D:816:VAL:HG11	2:D:832:ILE:HD13	1.92	0.51
2:B:650:ASP:OD1	2:B:651:SER:N	2.44	0.51
2:D:485:ASP:OD1	2:D:485:ASP:N	2.43	0.51
2:D:194:LYS:HB3	2:D:205:TYR:HB2	1.91	0.51
3:X:319:LEU:HD22	3:X:344:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:971:LEU:HD12	2:B:1002:LEU:HD11	1.91	0.51
2:B:1081:THR:H	2:B:1101:LYS:HZ2	1.57	0.51
2:B:478:ILE:HD11	2:B:501:GLU:HG2	1.92	0.51
1:A:130:LYS:O	1:A:134:HIS:NE2	2.41	0.51
2:B:767:ASN:HB3	2:B:770:LEU:HD11	1.92	0.51
2:B:377:LYS:HG2	2:B:393:SER:HB3	1.92	0.51
2:D:663:ASN:OD1	2:D:796:SER:OG	2.22	0.51
1:A:264:ASP:OD1	1:A:264:ASP:N	2.40	0.51
2:D:13:LEU:HA	2:D:16:PHE:HD2	1.76	0.51
1:A:337:GLY:HA3	1:A:358:MET:O	2.11	0.51
3:X:147:CYS:O	3:X:151:MET:HG2	2.11	0.51
1:C:264:ASP:OD1	1:C:264:ASP:N	2.42	0.51
2:D:1060:THR:HA	2:D:1063:ILE:HD12	1.93	0.51
2:D:100:PHE:CE1	2:D:147:PHE:HA	2.44	0.51
2:D:690:VAL:O	2:D:693:GLU:HB2	2.10	0.51
2:B:965:PRO:HG3	2:B:967:LYS:NZ	2.25	0.51
1:C:279:ARG:NH1	1:C:327:ASP:OD1	2.38	0.51
1:A:240:LEU:HB3	1:A:241:PRO:HD3	1.92	0.51
2:B:1113:HIS:O	2:B:1117:LYS:HG3	2.10	0.51
2:B:1112:TYR:OH	2:D:1112:TYR:OH	2.22	0.51
1:A:55:GLY:H	1:A:384:ARG:NH1	2.09	0.51
2:D:313:LYS:HD2	2:D:351:LEU:HD21	1.93	0.51
2:D:998:ASP:O	2:D:1002:LEU:HG	2.11	0.51
2:D:65:ASN:HB2	2:D:75:TRP:CD1	2.46	0.51
1:C:7:GLN:NE2	2:D:983:LYS:HD2	2.26	0.51
2:D:828:CYS:HA	2:D:831:LEU:HB2	1.92	0.51
2:B:524:PHE:CE1	2:B:531:THR:HA	2.45	0.51
1:A:212:PHE:HE1	1:A:233:TRP:CE3	2.29	0.51
2:B:969:SER:O	2:B:972:LEU:HB2	2.11	0.51
2:D:462:THR:O	2:D:466:LEU:HG	2.11	0.51
1:A:102:LEU:O	1:A:113:LEU:HD12	2.10	0.50
2:B:923:ASP:OD1	2:B:941:THR:OG1	2.18	0.50
2:B:695:PHE:CE1	2:B:724:LEU:HB3	2.45	0.50
3:X:54:LEU:HD22	3:X:434:PHE:CE1	2.46	0.50
2:D:492:TYR:OH	2:D:496:ARG:NH2	2.45	0.50
1:C:162:ASP:HA	1:C:186:PRO:HB3	1.93	0.50
3:X:416:HIS:CE1	3:X:432:ALA:HA	2.46	0.50
2:B:939:HIS:O	2:B:942:LEU:HB2	2.12	0.50
2:B:953:ALA:C	2:B:955:HIS:N	2.64	0.50
2:B:237:ILE:HG21	2:B:251:MET:SD	2.51	0.50
1:A:130:LYS:HD3	2:B:609:TYR:CE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:990:TYR:O	2:B:994:THR:HG23	2.12	0.50
2:D:815:LEU:O	2:D:819:LEU:HG	2.11	0.50
2:B:63:THR:OG1	2:B:521:SER:OG	2.29	0.50
1:A:258:VAL:HG13	1:A:270:ALA:HB2	1.93	0.50
1:A:114:ILE:HG23	1:A:121:ILE:HG23	1.93	0.50
1:A:133:HIS:CD2	1:A:167:ILE:HD12	2.46	0.50
2:D:642:LEU:HB3	2:D:645:PRO:HD3	1.92	0.50
2:D:812:VAL:HG21	2:D:835:LEU:HB2	1.93	0.50
1:C:40:ILE:HG23	1:C:73:LEU:HD11	1.93	0.50
2:B:546:TYR:HE1	2:B:791:HIS:CE1	2.29	0.50
2:D:723:SER:O	2:D:726:GLU:HB3	2.11	0.50
2:B:859:VAL:HG12	2:B:863:LYS:HE3	1.93	0.50
2:B:1060:THR:O	2:B:1063:ILE:HB	2.11	0.50
2:B:937:ILE:O	2:B:941:THR:OG1	2.29	0.50
2:D:636:ILE:HA	2:D:639:LEU:HD12	1.92	0.50
2:B:350:GLN:HG2	2:B:524:PHE:HB2	1.94	0.50
2:D:422:TRP:CZ2	2:D:499:TYR:HA	2.46	0.50
2:B:1112:TYR:HH	2:D:1112:TYR:HH	1.51	0.50
1:A:384:ARG:HE	1:A:389:THR:CG2	2.24	0.50
2:D:985:ASN:HA	2:D:988:LEU:HD12	1.93	0.50
2:B:170:GLN:OE1	2:B:208:HIS:NE2	2.44	0.50
2:D:676:SER:HB2	2:D:773:PHE:CE1	2.47	0.50
1:C:258:VAL:HG13	1:C:270:ALA:HB2	1.93	0.50
2:B:943:LYS:HG3	2:B:974:PHE:CZ	2.47	0.50
2:D:977:GLN:O	2:D:981:GLN:HG3	2.11	0.50
1:C:283:PHE:HB2	1:C:299:GLY:N	2.27	0.50
1:C:252:ALA:HB2	2:D:826:ASN:HD22	1.77	0.49
2:B:332:ILE:HG12	2:B:388:PHE:HE2	1.76	0.49
2:B:313:LYS:HB3	2:B:329:LYS:HD3	1.94	0.49
2:B:131:ILE:HG12	2:B:137:LEU:HD23	1.93	0.49
2:B:881:GLU:CB	2:B:901:HIS:HE1	2.25	0.49
2:D:742:LEU:HD22	2:D:826:ASN:HD21	1.77	0.49
2:D:767:ASN:OD1	2:D:768:THR:N	2.44	0.49
2:D:1119:VAL:O	2:D:1123:VAL:HG23	2.13	0.49
2:D:1047:TYR:O	2:D:1050:THR:OG1	2.31	0.49
2:D:1073:LEU:HD11	2:D:1105:LEU:HD13	1.94	0.49
2:B:86:PHE:HB3	2:B:101:ASN:ND2	2.21	0.49
2:B:873:THR:HG22	2:B:883:GLN:HE22	1.77	0.49
3:X:381:GLY:O	3:X:384:MET:HB2	2.11	0.49
1:C:231:ASN:ND2	2:D:491:TYR:OH	2.45	0.49
2:B:50:PHE:CZ	2:B:442:SER:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:92:LYS:HD2	3:X:164:VAL:O	2.12	0.49
1:A:192:PHE:HE1	1:A:200:LEU:HD22	1.77	0.49
3:X:95:MET:HA	3:X:129:GLY:O	2.13	0.49
3:X:83:GLN:HB3	3:X:91:TYR:CZ	2.48	0.49
2:B:1042:GLU:O	2:B:1045:SER:OG	2.24	0.49
2:D:546:TYR:HE1	2:D:791:HIS:NE2	2.10	0.49
2:B:129:TYR:OH	2:B:180:THR:O	2.31	0.49
2:D:9:VAL:HB	2:D:539:VAL:HG23	1.95	0.49
1:A:283:PHE:HB2	1:A:299:GLY:N	2.27	0.49
3:X:363:GLY:O	3:X:422:GLN:NE2	2.35	0.49
2:B:919:SER:HB2	2:B:941:THR:HG23	1.93	0.49
2:D:629:PRO:HA	2:D:632:ILE:HD12	1.95	0.49
1:A:280:TRP:CD1	1:A:305:PRO:HA	2.48	0.49
1:C:130:LYS:HE2	2:D:608:SER:HB3	1.95	0.49
2:D:1063:ILE:HG12	2:D:1112:TYR:HE1	1.78	0.49
2:B:172:PRO:HA	2:B:187:PHE:HD1	1.78	0.49
2:D:332:ILE:HG12	2:D:388:PHE:HE2	1.77	0.49
3:X:289:ARG:NH1	3:X:289:ARG:HG2	2.24	0.49
2:B:178:ILE:HD11	2:B:182:GLU:HB2	1.95	0.49
2:B:115:VAL:O	2:B:116:ALA:HB3	2.12	0.49
2:D:982:GLY:O	2:D:984:ILE:N	2.46	0.49
2:D:939:HIS:O	2:D:942:LEU:HB2	2.12	0.49
2:B:905:LYS:O	2:B:909:GLU:HG3	2.12	0.49
2:B:1063:ILE:HG12	2:B:1112:TYR:HE1	1.78	0.48
2:D:524:PHE:CE1	2:D:531:THR:HA	2.47	0.48
2:B:422:TRP:CZ2	2:B:499:TYR:HA	2.48	0.48
1:A:162:ASP:HA	1:A:186:PRO:HB3	1.94	0.48
2:B:1120:ALA:HA	2:B:1123:VAL:HG23	1.94	0.48
2:B:188:PHE:O	2:B:236:THR:OG1	2.25	0.48
2:B:9:VAL:HB	2:B:539:VAL:HG23	1.94	0.48
2:D:590:SER:O	2:D:594:GLU:HG2	2.12	0.48
2:B:817:GLU:HA	2:B:844:LEU:HD11	1.95	0.48
2:B:884:GLU:O	2:B:888:LYS:HG3	2.13	0.48
1:C:12:LEU:HD22	2:D:951:PHE:HB3	1.96	0.48
2:B:492:TYR:OH	2:B:496:ARG:NH2	2.46	0.48
2:D:86:PHE:HB3	2:D:101:ASN:ND2	2.22	0.48
2:B:1062:ILE:HA	2:B:1065:HIS:CD2	2.48	0.48
1:C:170:ARG:HD3	1:C:214:TRP:CZ3	2.48	0.48
3:X:222:MET:SD	3:X:365:LEU:HB3	2.53	0.48
2:D:170:GLN:OE1	2:D:208:HIS:NE2	2.46	0.48
2:B:733:PHE:CZ	2:B:812:VAL:HG23	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:945:ALA:HB1	2:D:954:ALA:CB	2.43	0.48
2:B:959:MET:SD	2:B:994:THR:HB	2.54	0.48
1:A:71:LEU:HD11	2:B:860:ARG:NH2	2.29	0.48
3:X:332:ALA:HA	3:X:335:LEU:HD12	1.94	0.48
2:D:284:PHE:CD2	2:D:287:LEU:HD13	2.48	0.48
2:B:460:ALA:O	2:B:462:THR:N	2.42	0.48
2:D:492:TYR:O	2:D:495:LYS:HB3	2.14	0.48
2:B:824:GLN:HG2	2:B:827:ALA:HB3	1.95	0.48
2:D:185:VAL:HB	2:D:193:THR:HG22	1.94	0.48
2:B:1105:LEU:HA	2:B:1108:ILE:HG12	1.94	0.48
2:D:768:THR:O	2:D:770:LEU:N	2.47	0.48
2:B:1045:SER:HA	2:B:1048:ILE:HD12	1.96	0.48
2:B:65:ASN:HB2	2:B:75:TRP:CD1	2.49	0.48
1:C:192:PHE:HE1	1:C:200:LEU:HD22	1.78	0.48
2:B:60:GLY:HA2	2:B:78:PHE:O	2.13	0.48
2:B:840:ILE:HG23	2:B:875:GLN:NE2	2.29	0.48
2:B:879:LEU:HA	2:B:879:LEU:HD23	1.68	0.48
3:X:43:PRO:O	3:X:47:GLN:NE2	2.38	0.48
2:B:913:ILE:O	2:B:916:LEU:HB2	2.13	0.48
2:B:600:ARG:HG3	2:B:834:TRP:NE1	2.28	0.48
2:D:433:ILE:HG22	2:D:434:GLU:HG3	1.96	0.48
2:D:742:LEU:HB2	2:D:824:GLN:HG3	1.96	0.48
2:B:1010:MET:O	2:B:1013:VAL:HG12	2.13	0.48
1:C:182:PRO:HB3	2:D:597:TYR:CZ	2.49	0.48
1:C:233:TRP:HD1	2:D:413:MET:SD	2.37	0.48
3:X:405:ILE:O	3:X:409:ILE:HG13	2.14	0.48
2:D:703:THR:HG23	2:D:704:SER:H	1.79	0.48
2:D:1066:TYR:CD2	2:D:1112:TYR:HB2	2.48	0.48
3:X:166:ALA:HB2	3:X:195:THR:OG1	2.12	0.48
1:C:130:LYS:O	1:C:134:HIS:NE2	2.40	0.48
2:D:60:GLY:HA2	2:D:78:PHE:O	2.13	0.48
1:A:280:TRP:CE2	1:A:305:PRO:HB3	2.49	0.48
2:D:1040:ILE:HG22	2:D:1044:LEU:HD11	1.94	0.48
2:B:241:ILE:CG2	2:B:250:VAL:HB	2.44	0.48
2:B:492:TYR:O	2:B:495:LYS:HB3	2.14	0.48
3:X:29:ARG:O	3:X:33:THR:OG1	2.18	0.48
2:B:98:SER:O	2:B:99:LYS:HD3	2.13	0.48
1:C:138:ASN:HD22	1:C:161:GLY:HA2	1.79	0.48
2:D:814:GLU:O	2:D:817:GLU:HB3	2.14	0.48
2:D:290:ASP:OD1	2:D:290:ASP:N	2.47	0.48
2:D:975:VAL:HA	2:D:978:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:763:LEU:HD21	2:B:774:SER:OG	2.14	0.47
3:X:306:GLU:O	3:X:308:GLN:HG3	2.14	0.47
2:D:673:LEU:HB2	2:D:770:LEU:HD22	1.95	0.47
3:X:333:HIS:CE1	3:X:358:LEU:HD11	2.49	0.47
2:D:353:SER:HB2	2:D:361:PHE:CD2	2.49	0.47
2:B:485:ASP:N	2:B:485:ASP:OD1	2.42	0.47
2:B:1015:SER:HB3	2:B:1018:CYS:HB2	1.95	0.47
3:X:237:VAL:H	3:X:260:THR:HG1	1.55	0.47
2:D:906:LEU:HD22	2:D:914:ASP:HB2	1.95	0.47
1:A:40:ILE:HG23	1:A:73:LEU:HD11	1.96	0.47
2:B:816:VAL:O	2:B:820:PHE:HB3	2.14	0.47
2:B:958:LEU:HD13	2:B:975:VAL:HG22	1.96	0.47
2:B:1067:LEU:HD13	2:D:1116:LEU:HD22	1.95	0.47
2:B:419:SER:O	2:B:423:LEU:HD12	2.14	0.47
1:C:337:GLY:HA3	1:C:358:MET:O	2.13	0.47
2:B:207:GLN:HG3	2:B:207:GLN:O	2.14	0.47
2:B:1109:VAL:O	2:B:1112:TYR:HB3	2.14	0.47
2:D:1063:ILE:HG12	2:D:1112:TYR:CE1	2.50	0.47
2:D:419:SER:O	2:D:423:LEU:HD12	2.14	0.47
2:D:968:LYS:HA	2:D:971:LEU:HD12	1.96	0.47
2:D:636:ILE:HD13	2:D:639:LEU:HD12	1.95	0.47
2:B:293:THR:CG2	2:B:353:SER:H	2.27	0.47
1:C:156:VAL:HG21	1:C:214:TRP:CH2	2.50	0.47
2:B:548:ILE:CD1	2:B:687:LYS:HD2	2.44	0.47
2:D:935:ILE:CG2	2:D:967:LYS:HZ3	2.28	0.47
1:A:39:GLY:HA2	1:A:66:THR:OG1	2.15	0.47
2:B:1101:LYS:O	2:B:1105:LEU:HG	2.14	0.47
2:D:826:ASN:N	2:D:826:ASN:OD1	2.43	0.47
2:D:13:LEU:HB3	2:D:674:CYS:SG	2.54	0.47
2:D:182:GLU:HG2	2:D:196:ILE:HG13	1.96	0.47
2:D:129:TYR:OH	2:D:180:THR:O	2.32	0.47
1:A:210:ARG:HH12	2:B:417:ASP:N	2.12	0.47
2:B:945:ALA:HB1	2:B:954:ALA:HB1	1.96	0.47
2:D:859:VAL:HG13	2:D:918:PHE:HZ	1.79	0.47
2:B:632:ILE:O	2:B:636:ILE:HG12	2.14	0.47
2:B:284:PHE:HD2	2:B:287:LEU:HD13	1.80	0.47
2:D:339:ASP:O	2:D:342:ILE:HB	2.13	0.47
2:D:241:ILE:HG22	2:D:250:VAL:HB	1.95	0.47
1:A:252:ALA:HB2	2:B:826:ASN:ND2	2.18	0.47
2:D:196:ILE:HD13	2:D:205:TYR:HE2	1.80	0.47
1:A:182:PRO:HB3	2:B:597:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:673:LEU:O	2:B:677:VAL:HG23	2.15	0.47
1:A:244:ASN:HB3	1:A:246:CYS:SG	2.55	0.47
1:A:279:ARG:HB3	1:A:307:VAL:HG12	1.96	0.47
2:D:405:THR:HB	2:D:589:PHE:CZ	2.50	0.47
2:D:955:HIS:HA	2:D:958:LEU:HB2	1.97	0.47
2:B:965:PRO:HG2	2:B:967:LYS:HG3	1.95	0.47
2:D:293:THR:CG2	2:D:353:SER:H	2.28	0.47
2:D:81:ARG:H	2:D:109:ASN:CB	2.28	0.47
1:A:195:SER:HB2	1:A:264:ASP:HA	1.96	0.47
2:B:131:ILE:HG12	2:B:137:LEU:CD2	2.45	0.47
2:B:705:GLN:O	2:B:709:GLU:HG3	2.15	0.47
2:B:339:ASP:O	2:B:342:ILE:HB	2.15	0.47
3:X:199:LEU:HD23	3:X:203:GLY:O	2.15	0.47
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.78	0.47
2:B:978:LEU:O	2:B:981:GLN:HB3	2.15	0.47
2:D:314:LEU:HD21	2:D:325:VAL:HG13	1.97	0.47
3:X:318:ALA:O	3:X:319:LEU:HD23	2.15	0.47
2:D:18:LEU:HD13	2:D:101:ASN:HB2	1.97	0.46
2:D:638:THR:O	2:D:642:LEU:HD13	2.15	0.46
2:B:652:LEU:HD23	2:B:655:ARG:NE	2.30	0.46
2:B:466:LEU:O	2:B:470:VAL:HG23	2.14	0.46
2:B:284:PHE:CD2	2:B:287:LEU:HD13	2.50	0.46
1:C:114:ILE:HG23	1:C:121:ILE:HG23	1.97	0.46
2:D:237:ILE:HG21	2:D:251:MET:SD	2.55	0.46
2:D:584:HIS:HB3	2:D:693:GLU:HG2	1.96	0.46
1:A:143:ALA:HB2	1:A:192:PHE:HD2	1.80	0.46
2:B:521:SER:O	2:B:534:ASN:HB2	2.15	0.46
2:B:828:CYS:O	2:B:832:ILE:HB	2.15	0.46
2:B:926:LYS:HZ2	2:B:933:LEU:HD23	1.79	0.46
2:B:718:ASP:O	2:B:722:LEU:HG	2.15	0.46
1:C:147:SER:OG	1:C:148:ALA:N	2.48	0.46
3:X:393:TRP:CG	3:X:397:LYS:HD3	2.50	0.46
2:B:1063:ILE:O	2:B:1067:LEU:HG	2.14	0.46
2:D:1062:ILE:HG22	2:D:1066:TYR:CE2	2.50	0.46
2:B:1101:LYS:O	2:B:1104:THR:HG23	2.16	0.46
2:B:178:ILE:HG21	2:B:263:LEU:HD21	1.97	0.46
2:B:815:LEU:HD22	2:B:819:LEU:HD11	1.97	0.46
2:D:289:SER:O	2:D:299:LEU:HB2	2.14	0.46
1:C:192:PHE:CE1	1:C:200:LEU:HD22	2.50	0.46
2:B:995:LEU:O	2:B:999:VAL:HG23	2.15	0.46
2:B:629:PRO:HA	2:B:632:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:139:TYR:HB3	2:B:160:LEU:O	2.16	0.46
2:B:672:PHE:HE1	2:B:790:LEU:HD23	1.81	0.46
2:B:984:ILE:HG21	2:B:1024:PHE:CG	2.51	0.46
1:A:147:SER:OG	1:A:148:ALA:N	2.48	0.46
1:A:191:GLN:OE1	1:A:259:ARG:HD2	2.16	0.46
2:D:172:PRO:HA	2:D:187:PHE:HD1	1.80	0.46
1:C:143:ALA:CB	1:C:192:PHE:HD2	2.29	0.46
2:D:241:ILE:CG2	2:D:250:VAL:HB	2.46	0.46
1:C:191:GLN:OE1	1:C:259:ARG:HD2	2.16	0.46
2:B:243:LEU:HD21	2:B:292:THR:HG21	1.97	0.46
2:B:826:ASN:O	2:B:829:MET:HB2	2.16	0.46
1:A:12:LEU:HD13	2:B:951:PHE:HD1	1.81	0.46
2:B:1116:LEU:HD22	2:D:1067:LEU:HD13	1.97	0.46
2:B:18:LEU:HD13	2:B:101:ASN:HB2	1.98	0.46
2:B:1017:PRO:HA	2:B:1020:TYR:HD2	1.81	0.46
1:A:170:ARG:HD3	1:A:214:TRP:CZ3	2.51	0.46
2:D:742:LEU:HD12	2:D:827:ALA:HB2	1.98	0.46
1:C:384:ARG:HE	1:C:389:THR:CG2	2.29	0.46
2:B:353:SER:HB2	2:B:361:PHE:CD2	2.51	0.46
1:A:283:PHE:C	2:B:487:THR:HB	2.35	0.46
2:B:690:VAL:O	2:B:693:GLU:HB2	2.16	0.46
1:C:130:LYS:HD3	2:D:609:TYR:CE1	2.51	0.46
2:D:340:GLU:HB3	2:D:342:ILE:HD13	1.98	0.46
1:C:11:PRO:HB2	1:C:14:VAL:HG23	1.98	0.46
2:D:1112:TYR:O	2:D:1116:LEU:HG	2.15	0.46
2:B:162:TYR:HE2	2:B:204:HIS:CE1	2.34	0.46
2:D:697:PHE:O	2:D:701:LEU:HG	2.16	0.46
2:D:450:VAL:O	2:D:454:LYS:N	2.37	0.46
2:D:948:ALA:O	2:D:950:LYS:HG2	2.16	0.46
1:A:134:HIS:HB3	2:B:605:ASP:OD1	2.16	0.46
2:D:828:CYS:O	2:D:832:ILE:HB	2.16	0.46
2:B:875:GLN:HB2	2:B:879:LEU:HG	1.98	0.46
2:D:466:LEU:O	2:D:470:VAL:HG23	2.15	0.46
2:D:1019:TRP:CZ2	2:D:1048:ILE:HD11	2.51	0.46
2:B:198:ASN:HB3	2:B:201:ASP:HB3	1.96	0.46
2:D:1025:SER:O	2:D:1029:LYS:HG2	2.15	0.46
2:D:708:TYR:OH	2:D:713:LYS:HD2	2.15	0.46
2:D:512:LEU:HA	2:D:512:LEU:HD22	1.86	0.46
2:D:178:ILE:HG21	2:D:263:LEU:HD21	1.97	0.46
2:D:671:LEU:HD12	2:D:672:PHE:H	1.81	0.46
2:D:50:PHE:CZ	2:D:442:SER:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1034:ARG:HH21	2:D:1076:LEU:HD22	1.81	0.46
2:B:832:ILE:HG13	2:B:835:LEU:HD22	1.97	0.45
3:X:333:HIS:NE2	3:X:358:LEU:HD11	2.30	0.45
2:D:639:LEU:HD22	2:D:701:LEU:HD13	1.98	0.45
2:D:695:PHE:CZ	2:D:724:LEU:HB3	2.51	0.45
2:D:198:ASN:HB3	2:D:201:ASP:HB3	1.97	0.45
1:C:322:HIS:HA	1:C:323:PRO:HD3	1.84	0.45
2:D:919:SER:HB2	2:D:941:THR:OG1	2.16	0.45
2:D:329:LYS:HB3	2:D:329:LYS:HZ2	1.82	0.45
2:D:284:PHE:HD2	2:D:287:LEU:HD13	1.81	0.45
1:A:78:SER:OG	1:A:144:ASP:OD2	2.27	0.45
1:C:243:VAL:O	1:C:245:THR:OG1	2.33	0.45
2:D:1104:THR:O	2:D:1108:ILE:HG23	2.17	0.45
2:B:815:LEU:O	2:B:819:LEU:HG	2.16	0.45
2:B:543:ARG:CB	2:B:679:ARG:HH12	2.30	0.45
2:B:680:VAL:HG11	2:B:773:PHE:HZ	1.81	0.45
2:B:5:LYS:HE2	2:B:549:GLU:HG3	1.97	0.45
1:A:156:VAL:HG21	1:A:214:TRP:CH2	2.51	0.45
1:C:102:LEU:O	1:C:113:LEU:HD12	2.16	0.45
3:X:85:SER:O	3:X:126:GLY:N	2.48	0.45
2:B:729:ARG:HH12	2:B:812:VAL:HG11	1.81	0.45
2:B:812:VAL:CG2	2:B:835:LEU:HB2	2.47	0.45
3:X:83:GLN:HB3	3:X:91:TYR:CE1	2.51	0.45
2:D:768:THR:C	2:D:770:LEU:H	2.19	0.45
2:B:1028:TYR:O	2:B:1031:GLN:HB3	2.15	0.45
2:D:377:LYS:HG2	2:D:393:SER:HB3	1.97	0.45
2:D:803:ILE:HG21	2:D:807:THR:HG23	1.99	0.45
3:X:281:ARG:O	3:X:284:GLU:HB2	2.16	0.45
3:X:353:ILE:HD12	3:X:353:ILE:H	1.82	0.45
2:B:1044:LEU:O	2:B:1048:ILE:HG13	2.17	0.45
1:A:11:PRO:HB2	1:A:14:VAL:CG2	2.47	0.45
2:B:81:ARG:H	2:B:109:ASN:CB	2.29	0.45
2:B:97:LEU:O	2:B:99:LYS:HG2	2.17	0.45
2:D:1105:LEU:O	2:D:1108:ILE:HG12	2.17	0.45
2:D:639:LEU:O	2:D:642:LEU:HB2	2.17	0.45
3:X:239:GLY:N	3:X:262:SER:OG	2.37	0.45
1:A:277:TRP:CZ2	1:A:309:GLY:HA3	2.51	0.45
1:C:343:ASN:H	1:C:348:ASP:HB2	1.82	0.45
2:B:1010:MET:SD	2:B:1021:ASN:HB3	2.57	0.45
1:C:160:VAL:HG11	1:C:202:VAL:HG13	1.99	0.45
1:C:130:LYS:HD3	2:D:609:TYR:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:279:LEU:O	3:X:283:ILE:HG13	2.17	0.45
2:D:276:GLN:HB3	2:D:279:LEU:HD23	1.99	0.45
2:D:131:ILE:HG12	2:D:137:LEU:HD23	1.98	0.45
2:B:81:ARG:HA	2:B:109:ASN:HA	1.98	0.45
2:D:668:SER:HB2	2:D:672:PHE:HD2	1.82	0.45
1:A:243:VAL:O	1:A:245:THR:OG1	2.35	0.45
2:D:158:TRP:H	2:D:158:TRP:HE3	1.64	0.45
2:B:417:ASP:HB2	2:B:418:ILE:H	1.52	0.45
1:A:107:GLN:HE22	2:B:860:ARG:HG2	1.80	0.45
2:B:870:TYR:O	2:B:871:SER:OG	2.33	0.45
2:B:916:LEU:CD2	2:B:945:ALA:HA	2.47	0.45
2:D:1019:TRP:CH2	2:D:1048:ILE:HD11	2.51	0.45
2:B:955:HIS:HA	2:B:958:LEU:HD12	1.99	0.45
1:C:51:PRO:C	1:C:53:SER:H	2.18	0.45
2:D:1058:GLU:O	2:D:1062:ILE:HG13	2.17	0.44
2:B:75:TRP:CE3	2:B:539:VAL:HG13	2.51	0.44
2:B:1103:LEU:CD1	3:X:271:GLU:H	2.29	0.44
2:D:587:MET:SD	2:D:696:ILE:HD13	2.57	0.44
1:C:107:GLN:HA	2:D:860:ARG:NH2	2.32	0.44
2:B:881:GLU:HB3	2:B:901:HIS:HE1	1.82	0.44
3:X:206:ILE:HD11	3:X:395:ALA:HB1	1.99	0.44
2:D:12:ASP:HB2	2:D:433:ILE:CG2	2.45	0.44
1:A:53:SER:O	1:A:384:ARG:HD3	2.17	0.44
2:D:595:ILE:HD13	2:D:696:ILE:HD11	1.98	0.44
1:C:212:PHE:HE1	1:C:233:TRP:CE3	2.34	0.44
1:A:21:TRP:CZ2	1:A:373:ALA:HB2	2.52	0.44
2:B:340:GLU:HB3	2:B:342:ILE:HD13	2.00	0.44
2:D:474:ILE:HG12	2:D:502:TRP:CZ2	2.52	0.44
2:D:28:ALA:HB1	2:D:107:PRO:HB3	1.98	0.44
2:D:436:ILE:O	2:D:440:LEU:HG	2.18	0.44
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.81	0.44
2:B:1023:LEU:O	2:B:1026:TRP:HB3	2.18	0.44
2:D:602:LEU:HD22	2:D:606:LEU:HD13	1.99	0.44
2:D:907:PHE:HE2	2:D:943:LYS:HD3	1.83	0.44
2:B:382:LEU:HD21	2:B:389:SER:H	1.82	0.44
2:B:1082:TRP:CH2	2:B:1100:GLN:HG3	2.52	0.44
1:C:195:SER:HB2	1:C:264:ASP:HA	1.99	0.44
2:D:23:ALA:HA	2:D:103:LYS:O	2.18	0.44
2:B:579:LEU:O	2:B:583:LEU:HG	2.17	0.44
2:D:196:ILE:HD13	2:D:205:TYR:CE2	2.52	0.44
2:D:77:ILE:HB	2:D:84:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:940:GLU:O	2:D:944:THR:HG23	2.17	0.44
2:D:97:LEU:HD21	2:D:762:ALA:N	2.33	0.44
2:B:1060:THR:HG22	2:B:1063:ILE:HD12	2.00	0.44
1:A:210:ARG:NH1	2:B:417:ASP:OD1	2.50	0.44
1:C:280:TRP:CE2	1:C:305:PRO:HB3	2.53	0.44
2:D:838:ASP:O	2:D:842:VAL:N	2.43	0.44
2:D:533:ILE:HD12	2:D:535:TYR:HE1	1.83	0.44
1:C:236:THR:HG21	2:D:417:ASP:OD1	2.18	0.44
2:B:622:HIS:O	2:B:627:VAL:HG21	2.16	0.44
2:B:600:ARG:HG3	2:B:834:TRP:HE1	1.82	0.44
1:A:302:ASN:O	1:A:303:LEU:HD23	2.17	0.44
1:A:51:PRO:C	1:A:53:SER:H	2.18	0.44
2:B:1058:GLU:O	2:B:1062:ILE:HG13	2.17	0.44
2:B:77:ILE:HB	2:B:84:THR:OG1	2.18	0.44
2:D:382:LEU:HD21	2:D:389:SER:H	1.83	0.44
2:B:436:ILE:O	2:B:440:LEU:HG	2.17	0.44
2:B:1039:ILE:HG23	2:B:1083:ILE:HG13	2.00	0.44
2:D:1115:GLN:O	2:D:1119:VAL:HG23	2.17	0.44
2:B:844:LEU:HA	2:B:844:LEU:HD23	1.63	0.44
3:X:261:ALA:O	3:X:267:THR:HG23	2.18	0.44
2:B:1013:VAL:HG13	2:B:1015:SER:H	1.83	0.44
1:C:280:TRP:CD1	1:C:305:PRO:HA	2.53	0.44
3:X:205:LEU:C	3:X:207:ARG:H	2.21	0.44
2:D:914:ASP:O	2:D:918:PHE:HD1	2.01	0.44
2:D:243:LEU:HD21	2:D:292:THR:HG21	2.00	0.44
3:X:245:GLN:O	3:X:248:ILE:HB	2.17	0.44
2:B:385:ASP:HB3	2:B:387:SER:HB3	2.00	0.44
2:D:207:GLN:O	2:D:207:GLN:HG3	2.18	0.44
2:B:88:VAL:HB	2:B:671:LEU:HD23	1.99	0.44
2:B:66:LYS:CG	2:B:119:PHE:HB2	2.43	0.43
2:D:249:LEU:HB2	2:D:261:LEU:HB3	2.00	0.43
2:B:543:ARG:HB3	2:B:679:ARG:HH22	1.82	0.43
3:X:379:THR:HA	3:X:382:LEU:CG	2.48	0.43
3:X:289:ARG:HH11	3:X:289:ARG:CG	2.30	0.43
3:X:36:TRP:HA	3:X:39:LEU:HD12	2.00	0.43
2:B:871:SER:H	2:B:883:GLN:HG2	1.83	0.43
2:B:798:LEU:HA	2:B:801:ILE:HD12	2.00	0.43
2:B:703:THR:HG23	2:B:704:SER:H	1.83	0.43
1:C:25:SER:HB2	1:C:77:SER:HA	2.00	0.43
2:B:4:LEU:HD23	2:B:4:LEU:HA	1.86	0.43
3:X:151:MET:SD	3:X:154:LEU:HD23	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:61:ILE:HG22	3:X:63:PHE:HD1	1.81	0.43
1:C:252:ALA:HB2	2:D:826:ASN:HB3	2.00	0.43
1:A:192:PHE:CE1	1:A:200:LEU:HD22	2.52	0.43
1:A:279:ARG:NH1	1:A:327:ASP:OD1	2.43	0.43
2:D:417:ASP:OD1	2:D:417:ASP:N	2.50	0.43
2:D:301:TYR:HA	2:D:302:PRO:HD3	1.88	0.43
2:B:955:HIS:HE1	2:B:978:LEU:HD13	1.81	0.43
2:B:933:LEU:O	2:B:937:ILE:HG13	2.17	0.43
2:D:651:SER:O	2:D:655:ARG:HG3	2.18	0.43
1:A:138:ASN:OD1	2:B:857:LYS:NZ	2.49	0.43
2:B:463:ILE:HA	2:B:466:LEU:HG	1.98	0.43
2:B:945:ALA:HB1	2:B:954:ALA:CB	2.48	0.43
2:D:131:ILE:HG12	2:D:137:LEU:CD2	2.47	0.43
3:X:266:GLY:HA3	3:X:305:LEU:O	2.19	0.43
2:B:889:TYR:CG	2:B:933:LEU:HD13	2.53	0.43
2:B:178:ILE:HG13	2:B:179:SER:N	2.33	0.43
2:D:362:LEU:HD12	2:D:378:CYS:O	2.18	0.43
2:D:1030:HIS:HA	2:D:1034:ARG:CG	2.48	0.43
1:A:10:LEU:HG	1:A:379:SER:HA	2.01	0.43
2:B:279:LEU:HD21	2:B:303:ASP:HA	2.00	0.43
1:A:115:ILE:HB	1:A:123:THR:HB	2.01	0.43
2:B:158:TRP:HE3	2:B:158:TRP:H	1.64	0.43
2:B:290:ASP:OD1	2:B:290:ASP:N	2.51	0.43
2:D:978:LEU:O	2:D:982:GLY:N	2.50	0.43
2:B:768:THR:C	2:B:770:LEU:H	2.21	0.43
2:D:1111:GLU:HA	2:D:1114:LEU:HD12	1.99	0.43
1:A:25:SER:HB2	1:A:77:SER:HA	2.01	0.43
2:D:173:ASP:HB2	2:D:188:PHE:CE1	2.53	0.43
2:D:812:VAL:CG2	2:D:835:LEU:HB2	2.48	0.43
2:B:988:LEU:O	2:B:991:SER:OG	2.26	0.43
2:B:445:ASN:OD1	2:B:446:SER:N	2.51	0.43
1:C:69:PRO:HD2	1:C:107:GLN:HB2	2.01	0.43
1:C:39:GLY:HA2	1:C:66:THR:OG1	2.19	0.43
3:X:277:GLU:H	3:X:277:GLU:CD	2.21	0.43
3:X:109:LEU:HA	3:X:109:LEU:HD23	1.88	0.43
1:A:322:HIS:HA	1:A:323:PRO:HD3	1.84	0.43
2:B:991:SER:O	2:B:994:THR:OG1	2.37	0.43
2:D:329:LYS:HB3	2:D:329:LYS:NZ	2.33	0.43
2:D:287:LEU:HD12	2:D:346:LEU:O	2.19	0.43
2:D:198:ASN:HB3	2:D:201:ASP:CB	2.49	0.43
2:D:733:PHE:HA	2:D:834:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:TRP:CE3	2:D:539:VAL:HG13	2.53	0.43
2:B:417:ASP:OD1	2:B:417:ASP:N	2.52	0.43
2:D:1076:LEU:HA	2:D:1077:PRO:HD3	1.84	0.43
2:B:245:THR:HG23	2:B:246:TYR:HD1	1.84	0.43
3:X:157:HIS:O	3:X:158:LEU:HD23	2.18	0.43
2:D:1073:LEU:HD21	2:D:1105:LEU:HD13	2.00	0.43
2:B:12:ASP:HB2	2:B:433:ILE:CG2	2.48	0.43
2:D:407:PHE:CG	2:D:422:TRP:CH2	3.07	0.43
3:X:116:LYS:HD3	3:X:377:VAL:HG21	2.00	0.43
2:B:23:ALA:HA	2:B:103:LYS:O	2.18	0.43
2:B:182:GLU:HG2	2:B:196:ILE:HG13	2.00	0.42
2:B:289:SER:O	2:B:299:LEU:HB2	2.18	0.42
3:X:198:GLY:O	3:X:203:GLY:N	2.52	0.42
1:C:115:ILE:HB	1:C:123:THR:HB	2.00	0.42
1:A:19:THR:HG22	1:A:362:ASP:HB3	2.01	0.42
2:D:11:ILE:HA	2:D:14:GLN:CD	2.40	0.42
2:D:767:ASN:HB3	2:D:770:LEU:HD21	2.01	0.42
2:B:238:ILE:HG23	2:B:239:SER:H	1.84	0.42
2:B:242:PHE:HD1	2:B:249:LEU:HD13	1.84	0.42
1:A:69:PRO:HD2	1:A:107:GLN:HB2	2.00	0.42
2:B:380:LEU:HD23	2:B:389:SER:O	2.19	0.42
3:X:61:ILE:O	3:X:80:TRP:HA	2.19	0.42
1:A:328:TYR:CE1	1:A:343:ASN:HB2	2.54	0.42
2:B:635:LEU:O	2:B:639:LEU:HG	2.19	0.42
2:B:1038:ALA:O	2:B:1041:TYR:HB2	2.18	0.42
2:B:923:ASP:OD1	2:B:937:ILE:HG22	2.20	0.42
2:B:196:ILE:HD13	2:B:205:TYR:CE2	2.54	0.42
2:B:471:LEU:HA	2:B:471:LEU:HD23	1.78	0.42
2:D:75:TRP:O	2:D:85:ILE:HG13	2.20	0.42
2:D:79:GLN:HG3	2:D:80:ASN:N	2.35	0.42
2:D:603:VAL:HG13	2:D:729:ARG:HD2	2.01	0.42
2:D:340:GLU:HG3	2:D:340:GLU:O	2.20	0.42
1:C:302:ASN:O	1:C:303:LEU:HD23	2.20	0.42
1:C:19:THR:HG22	1:C:362:ASP:HB3	2.01	0.42
2:D:235:ASN:O	2:D:235:ASN:ND2	2.47	0.42
3:X:237:VAL:N	3:X:260:THR:OG1	2.32	0.42
3:X:44:LYS:HA	3:X:47:GLN:HG2	2.00	0.42
2:D:98:SER:O	2:D:99:LYS:HD3	2.19	0.42
2:B:729:ARG:NH1	2:B:836:ASN:HB2	2.34	0.42
2:B:994:THR:OG1	2:B:999:VAL:HG22	2.20	0.42
1:A:182:PRO:HB3	2:B:597:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:429:ALA:O	3:X:432:ALA:N	2.52	0.42
2:B:276:GLN:HB3	2:B:279:LEU:HD23	2.00	0.42
2:D:59:ALA:O	2:D:536:ALA:HB1	2.20	0.42
3:X:93:GLY:HA3	3:X:127:GLY:O	2.18	0.42
2:B:1014:GLU:HG3	2:B:1014:GLU:O	2.18	0.42
2:B:421:ILE:H	2:B:421:ILE:HG13	1.67	0.42
2:B:1113:HIS:HA	2:B:1116:LEU:CD1	2.50	0.42
2:D:1068:ILE:O	2:D:1072:THR:HG23	2.19	0.42
2:B:162:TYR:HE2	2:B:204:HIS:HE1	1.66	0.42
2:D:81:ARG:HA	2:D:109:ASN:HA	2.01	0.42
2:B:797:SER:OG	2:B:798:LEU:N	2.52	0.42
2:B:1100:GLN:O	2:B:1101:LYS:NZ	2.50	0.42
2:B:432:SER:O	2:B:433:ILE:HD13	2.20	0.42
2:D:178:ILE:HD11	2:D:182:GLU:HB2	2.01	0.42
1:A:299:GLY:N	2:B:489:TYR:HH	2.18	0.42
1:C:21:TRP:CZ2	1:C:373:ALA:HB2	2.54	0.42
2:B:823:LYS:HB3	2:B:824:GLN:H	1.62	0.42
3:X:217:TYR:O	3:X:220:GLU:HB3	2.19	0.42
3:X:134:ASP:HA	3:X:135:PRO:HD3	1.88	0.42
2:D:1069:VAL:O	2:D:1073:LEU:HG	2.19	0.42
2:B:926:LYS:HZ3	2:B:930:ASP:HB2	1.85	0.42
2:B:233:SER:O	2:B:235:ASN:N	2.51	0.42
2:D:956:VAL:O	2:D:960:VAL:HG23	2.19	0.42
2:D:143:SER:O	2:D:146:TRP:HB3	2.20	0.42
2:B:6:HIS:CE1	2:B:375:ILE:HD12	2.55	0.42
2:B:698:LEU:HD23	2:B:698:LEU:HA	1.91	0.42
2:D:423:LEU:HD11	2:D:471:LEU:HG	2.01	0.42
2:B:731:VAL:O	2:B:734:LEU:HB2	2.19	0.42
2:D:681:LEU:HD12	2:D:738:SER:OG	2.20	0.42
2:B:1017:PRO:HA	2:B:1020:TYR:CD2	2.55	0.42
2:B:198:ASN:HB3	2:B:201:ASP:CB	2.50	0.42
3:X:281:ARG:NE	3:X:299:GLU:OE2	2.53	0.42
2:D:1056:LYS:HE2	2:D:1122:GLN:OE1	2.19	0.42
2:B:271:THR:C	2:B:272:ILE:HD12	2.40	0.42
2:D:1066:TYR:CE2	2:D:1112:TYR:HB2	2.54	0.42
2:D:1105:LEU:O	2:D:1109:VAL:HG23	2.20	0.42
3:X:292:ARG:HB2	3:X:295:ASP:CG	2.40	0.42
2:B:984:ILE:HG21	2:B:1024:PHE:CD1	2.55	0.42
1:C:328:TYR:CE1	1:C:343:ASN:HB2	2.55	0.42
2:D:279:LEU:HD11	2:D:303:ASP:H	1.83	0.42
2:B:798:LEU:HD23	2:B:801:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:192:CYS:HB2	3:X:387:ASN:OD1	2.20	0.42
3:X:297:ALA:HA	3:X:302:LEU:HB2	2.02	0.42
2:D:1062:ILE:HA	2:D:1065:HIS:ND1	2.35	0.41
2:D:432:SER:O	2:D:433:ILE:HD13	2.20	0.41
2:B:100:PHE:CE1	2:B:147:PHE:HA	2.45	0.41
1:C:237:LEU:HD13	1:C:280:TRP:CD2	2.55	0.41
2:B:768:THR:OG1	2:B:769:ALA:N	2.53	0.41
2:D:521:SER:O	2:D:534:ASN:HB2	2.20	0.41
1:A:107:GLN:HA	2:B:860:ARG:CZ	2.50	0.41
2:B:420:GLU:O	2:B:424:GLN:HG3	2.20	0.41
2:B:367:TRP:O	2:B:373:THR:HG23	2.20	0.41
2:B:1112:TYR:O	2:B:1116:LEU:HG	2.20	0.41
3:X:50:LEU:O	3:X:53:ARG:HB2	2.19	0.41
2:D:581:ARG:HG3	2:D:693:GLU:OE2	2.19	0.41
1:C:143:ALA:HB3	1:C:192:PHE:HD2	1.85	0.41
2:B:990:TYR:O	2:B:993:PRO:HD2	2.20	0.41
3:X:21:GLN:HB3	3:X:24:PHE:HB3	2.01	0.41
3:X:20:ASN:O	3:X:22:THR:N	2.50	0.41
2:B:106:PHE:HB3	2:B:107:PRO:HD2	2.02	0.41
3:X:97:PHE:CE2	3:X:146:PHE:HE2	2.38	0.41
1:C:326:MET:HB3	1:C:326:MET:HE2	1.89	0.41
2:B:1111:GLU:HA	2:B:1114:LEU:HD12	2.02	0.41
2:B:1107:ALA:O	2:B:1110:ALA:HB3	2.20	0.41
2:B:961:LEU:HA	2:B:961:LEU:HD22	1.85	0.41
2:B:1112:TYR:CZ	2:B:1116:LEU:HD21	2.56	0.41
2:D:1064:GLU:HA	2:D:1067:LEU:HG	2.01	0.41
2:B:1100:GLN:HB3	2:B:1104:THR:CG2	2.50	0.41
2:B:1082:TRP:CZ2	3:X:305:LEU:HD22	2.50	0.41
1:C:53:SER:O	1:C:384:ARG:HD3	2.19	0.41
1:A:160:VAL:HG11	1:A:202:VAL:HG13	2.01	0.41
3:X:260:THR:HG21	3:X:310:PRO:HB3	2.02	0.41
2:B:1081:THR:O	2:B:1101:LYS:NZ	2.54	0.41
2:B:73:LEU:HD11	2:B:525:ASP:OD2	2.21	0.41
1:C:170:ARG:HD3	1:C:214:TRP:HZ3	1.85	0.41
2:D:656:LEU:HD13	2:D:657:ARG:HG2	2.02	0.41
3:X:362:ALA:HB3	3:X:364:VAL:HG23	2.03	0.41
2:D:1042:GLU:O	2:D:1045:SER:OG	2.21	0.41
2:B:481:GLU:HB3	2:B:493:GLU:OE1	2.20	0.41
2:B:196:ILE:HD13	2:B:205:TYR:HE2	1.84	0.41
2:D:602:LEU:HD22	2:D:606:LEU:HD22	2.03	0.41
2:D:5:LYS:HE2	2:D:549:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:LYS:NZ	2:B:329:LYS:HB3	2.35	0.41
2:D:772:PHE:HD1	2:D:815:LEU:HD21	1.86	0.41
2:B:847:LEU:O	2:B:850:LEU:HB2	2.20	0.41
2:B:951:PHE:CE2	2:B:953:ALA:HB2	2.56	0.41
2:D:385:ASP:HB3	2:D:387:SER:HB3	2.03	0.41
2:B:143:SER:O	2:B:146:TRP:HB3	2.20	0.41
3:X:286:LYS:HD2	3:X:286:LYS:HA	1.72	0.41
2:B:1063:ILE:HG12	2:B:1112:TYR:CE1	2.56	0.41
2:B:423:LEU:HD11	2:B:471:LEU:HG	2.02	0.41
1:A:236:THR:HG21	2:B:417:ASP:OD1	2.20	0.41
2:B:708:TYR:HA	2:B:711:GLN:CG	2.50	0.41
2:D:549:GLU:OE1	2:D:686:LYS:NZ	2.30	0.41
3:X:379:THR:O	3:X:382:LEU:HB2	2.21	0.41
1:A:191:GLN:O	1:A:201:ILE:HG22	2.21	0.41
1:C:210:ARG:HH12	2:D:417:ASP:H	1.68	0.41
2:B:279:LEU:HD11	2:B:303:ASP:H	1.84	0.41
1:C:64:ILE:HG12	1:C:119:GLU:HA	2.02	0.41
1:C:244:ASN:HB3	1:C:246:CYS:SG	2.61	0.41
2:B:378:CYS:HB2	2:B:392:TRP:CZ3	2.55	0.41
2:B:405:THR:HB	2:B:589:PHE:CZ	2.55	0.41
2:D:242:PHE:HD1	2:D:249:LEU:HD13	1.85	0.41
3:X:98:HIS:CG	3:X:99:PRO:HD2	2.55	0.41
3:X:216:VAL:O	3:X:230:PHE:HE2	2.03	0.41
2:D:4:LEU:HA	2:D:4:LEU:HD23	1.91	0.41
2:B:407:PHE:CG	2:B:422:TRP:CH2	3.09	0.41
1:A:170:ARG:HD3	1:A:214:TRP:HZ3	1.85	0.41
2:B:132:THR:OG1	2:B:136:VAL:HG22	2.21	0.41
2:B:1080:ASP:OD1	2:B:1082:TRP:NE1	2.49	0.41
2:D:115:VAL:O	2:D:116:ALA:HB3	2.21	0.41
2:D:471:LEU:HA	2:D:471:LEU:HD23	1.75	0.41
2:D:847:LEU:HD23	2:D:847:LEU:HA	1.89	0.41
2:D:815:LEU:HA	2:D:815:LEU:HD23	1.83	0.41
3:X:92:LYS:HZ1	3:X:166:ALA:HB2	1.86	0.41
2:D:718:ASP:O	2:D:722:LEU:HG	2.21	0.41
1:A:384:ARG:HE	1:A:389:THR:HG21	1.86	0.41
2:B:314:LEU:HD21	2:B:325:VAL:HG13	2.01	0.41
3:X:199:LEU:HD23	3:X:203:GLY:C	2.41	0.41
2:D:84:THR:HG22	2:D:103:LYS:HG3	2.02	0.41
2:B:83:LEU:HG	2:B:84:THR:N	2.36	0.41
3:X:245:GLN:HG3	3:X:245:GLN:H	1.62	0.41
2:B:846:ALA:HB1	2:B:862:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:408:ASP:O	2:D:410:PRO:HD3	2.21	0.41
2:D:628:ASP:HB3	2:D:631:TYR:HD2	1.86	0.41
2:B:1112:TYR:CE2	2:B:1116:LEU:HD11	2.57	0.40
1:A:51:PRO:O	1:A:53:SER:N	2.45	0.40
1:A:143:ALA:HB3	1:A:192:PHE:CD2	2.57	0.40
1:C:182:PRO:O	2:D:413:MET:HB2	2.22	0.40
2:B:875:GLN:OE1	2:B:879:LEU:HG	2.21	0.40
2:D:243:LEU:HD23	2:D:243:LEU:HA	1.89	0.40
3:X:244:ALA:O	3:X:247:ALA:HB3	2.21	0.40
2:B:1112:TYR:CE1	2:B:1116:LEU:HD21	2.56	0.40
2:D:165:ILE:HG21	2:D:187:PHE:HZ	1.85	0.40
3:X:333:HIS:O	3:X:336:ILE:HB	2.20	0.40
2:D:724:LEU:O	2:D:727:ASP:HB2	2.21	0.40
3:X:416:HIS:HB2	3:X:428:GLY:HA2	2.02	0.40
2:B:362:LEU:HD12	2:B:378:CYS:O	2.21	0.40
2:D:849:TYR:HB3	2:D:858:ALA:HB2	2.03	0.40
2:D:1066:TYR:HE1	2:D:1108:ILE:HB	1.86	0.40
2:D:1113:HIS:HA	2:D:1116:LEU:HG	2.02	0.40
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.97	0.40
1:C:200:LEU:HD23	1:C:214:TRP:CD1	2.57	0.40
1:C:182:PRO:HB3	2:D:597:TYR:CE2	2.57	0.40
2:B:193:THR:HA	2:B:206:GLU:HA	2.04	0.40
2:B:913:ILE:HG13	2:B:916:LEU:HD12	2.03	0.40
2:B:733:PHE:HA	2:B:834:TRP:CZ3	2.56	0.40
2:B:962:SER:HB3	2:B:971:LEU:HD11	2.03	0.40
2:B:926:LYS:NZ	2:B:933:LEU:HD23	2.35	0.40
2:D:178:ILE:HG13	2:D:179:SER:N	2.36	0.40
2:B:548:ILE:O	2:B:552:ASP:HB2	2.21	0.40
2:B:995:LEU:HA	2:B:995:LEU:HD23	1.87	0.40
2:D:362:LEU:HD11	2:D:377:LYS:HB2	2.03	0.40
2:D:463:ILE:HA	2:D:466:LEU:HG	2.04	0.40
3:X:26:GLN:O	3:X:30:GLU:HG3	2.20	0.40
1:A:127:LEU:HA	1:A:127:LEU:HD23	1.94	0.40
3:X:257:ARG:HG3	3:X:257:ARG:O	2.20	0.40
3:X:7:LEU:O	3:X:10:PHE:HB3	2.22	0.40
2:B:1105:LEU:O	2:B:1108:ILE:HG12	2.22	0.40
1:A:56:LEU:HB2	1:A:371:HIS:NE2	2.37	0.40
1:A:212:PHE:CE1	1:A:233:TRP:CE3	3.08	0.40
2:B:767:ASN:HB3	2:B:770:LEU:HD21	2.03	0.40
2:B:673:LEU:HD13	2:B:770:LEU:HD13	2.04	0.40
3:X:289:ARG:HB3	3:X:290:ASP:H	1.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:102:ASN:OD1	3:X:105:ILE:N	2.30	0.40

All (4) 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)
2:B:189:ASN:O	2:D:404:LYS:NZ[8_555]	2.07	0.13
3:X:156:ARG:NH1	3:X:186:LEU:O[12_544]	2.13	0.07
3:X:155:TYR:OH	3:X:186:LEU:O[12_544]	2.16	0.04
2:B:384:GLN:NE2	2:D:273:GLU:OE1[6_554]	2.17	0.03

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	335/394 (85%)	315 (94%)	19 (6%)	1 (0%)	46	83
1	C	336/394 (85%)	319 (95%)	16 (5%)	1 (0%)	46	83
2	B	1006/1139 (88%)	869 (86%)	117 (12%)	20 (2%)	9	51
2	D	951/1139 (84%)	821 (86%)	108 (11%)	22 (2%)	8	48
3	X	440/450 (98%)	420 (96%)	17 (4%)	3 (1%)	26	71
All	All	3068/3516 (87%)	2744 (89%)	277 (9%)	47 (2%)	13	57

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	965	PRO
2	D	951	PHE
3	X	206	ILE
3	X	289	ARG
1	A	50	THR

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Mol	Chain	Res	Type
2	B	115	VAL
2	B	410	PRO
2	B	856	VAL
2	B	1101	LYS
1	C	50	THR
2	D	27	PRO
2	D	115	VAL
2	D	626	ASN
2	D	952	ASP
3	X	291	GLY
2	B	59	ALA
2	B	234	PRO
2	B	287	LEU
2	B	403	GLU
2	B	495	LYS
2	B	626	ASN
2	D	59	ALA
2	D	287	LEU
2	D	410	PRO
2	D	461	LEU
2	D	495	LYS
2	D	698	LEU
2	D	950	LYS
2	D	983	LYS
2	B	110	VAL
2	B	135	ARG
2	B	815	LEU
2	B	954	ALA
2	B	1051	THR
2	D	234	PRO
2	D	769	ALA
2	D	1032	ASN
2	B	1032	ASN
2	D	110	VAL
2	D	135	ARG
2	D	1078	LYS
2	B	461	LEU
2	B	517	ASP
2	D	111	MET
2	D	984	ILE
2	B	330	GLY
2	D	330	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/345 (87%)	278 (93%)	21 (7%)	19	56
1	C	300/345 (87%)	280 (93%)	20 (7%)	20	57
2	B	940/1050 (90%)	859 (91%)	81 (9%)	13	47
2	D	897/1050 (85%)	828 (92%)	69 (8%)	16	52
3	X	347/354 (98%)	330 (95%)	17 (5%)	31	66
All	All	2783/3144 (88%)	2575 (92%)	208 (8%)	17	53

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	27	SER
1	A	31	LEU
1	A	46	SER
1	A	50	THR
1	A	54	THR
1	A	68	LEU
1	A	74	SER
1	A	77	SER
1	A	83	GLU
1	A	127	LEU
1	A	131	SER
1	A	185	SER
1	A	216	LEU
1	A	245	THR
1	A	246	CYS
1	A	258	VAL
1	A	259	ARG
1	A	266	SER
1	A	304	LEU
1	A	367	GLN
2	B	11	ILE
2	B	50	PHE

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Mol	Chain	Res	Type
2	B	54	CYS
2	B	58	ASP
2	B	88	VAL
2	B	90	LEU
2	B	128	ILE
2	B	197	LEU
2	B	232	ARG
2	B	235	ASN
2	B	241	ILE
2	B	290	ASP
2	B	291	HIS
2	B	292	THR
2	B	296	PHE
2	B	297	ILE
2	B	301	TYR
2	B	329	LYS
2	B	332	ILE
2	B	338	ASP
2	B	339	ASP
2	B	388	PHE
2	B	417	ASP
2	B	423	LEU
2	B	429	HIS
2	B	431	THR
2	B	443	PHE
2	B	450	VAL
2	B	483	ASN
2	B	512	LEU
2	B	515	PHE
2	B	519	ILE
2	B	524	PHE
2	B	532	TYR
2	B	533	ILE
2	B	537	ASN
2	B	538	LYS
2	B	539	VAL
2	B	554	GLU
2	B	579	LEU
2	B	642	LEU
2	B	656	LEU
2	B	667	GLN
2	B	671	LEU

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Mol	Chain	Res	Type
2	B	672	PHE
2	B	673	LEU
2	B	680	VAL
2	B	692	ILE
2	B	703	THR
2	B	717	CYS
2	B	725	LEU
2	B	791	HIS
2	B	805	ASP
2	B	812	VAL
2	B	813	THR
2	B	820	PHE
2	B	831	LEU
2	B	835	LEU
2	B	866	SER
2	B	878	VAL
2	B	902	LEU
2	B	907	PHE
2	B	923	ASP
2	B	941	THR
2	B	961	LEU
2	B	964	THR
2	B	966	LEU
2	B	969	SER
2	B	971	LEU
2	B	973	ASP
2	B	1010	MET
2	B	1011	ILE
2	B	1031	GLN
2	B	1034	ARG
2	B	1049	SER
2	B	1057	LYS
2	B	1076	LEU
2	B	1084	LEU
2	B	1101	LYS
2	B	1104	THR
2	B	1123	VAL
1	C	25	SER
1	C	27	SER
1	C	31	LEU
1	C	46	SER
1	C	50	THR

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Mol	Chain	Res	Type
1	C	54	THR
1	C	68	LEU
1	C	74	SER
1	C	77	SER
1	C	83	GLU
1	C	127	LEU
1	C	131	SER
1	C	185	SER
1	C	216	LEU
1	C	245	THR
1	C	246	CYS
1	C	258	VAL
1	C	259	ARG
1	C	266	SER
1	C	367	GLN
2	D	11	ILE
2	D	50	PHE
2	D	54	CYS
2	D	58	ASP
2	D	88	VAL
2	D	90	LEU
2	D	128	ILE
2	D	197	LEU
2	D	235	ASN
2	D	241	ILE
2	D	290	ASP
2	D	291	HIS
2	D	292	THR
2	D	296	PHE
2	D	297	ILE
2	D	301	TYR
2	D	329	LYS
2	D	332	ILE
2	D	338	ASP
2	D	339	ASP
2	D	388	PHE
2	D	417	ASP
2	D	423	LEU
2	D	431	THR
2	D	450	VAL
2	D	483	ASN
2	D	512	LEU

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Mol	Chain	Res	Type
2	D	513	ASP
2	D	515	PHE
2	D	519	ILE
2	D	524	PHE
2	D	532	TYR
2	D	533	ILE
2	D	537	ASN
2	D	539	VAL
2	D	554	GLU
2	D	579	LEU
2	D	589	PHE
2	D	604	GLN
2	D	642	LEU
2	D	646	MET
2	D	656	LEU
2	D	667	GLN
2	D	671	LEU
2	D	672	PHE
2	D	673	LEU
2	D	679	ARG
2	D	680	VAL
2	D	691	SER
2	D	692	ILE
2	D	700	SER
2	D	703	THR
2	D	725	LEU
2	D	741	LEU
2	D	743	GLU
2	D	766	VAL
2	D	807	THR
2	D	812	VAL
2	D	820	PHE
2	D	826	ASN
2	D	835	LEU
2	D	902	LEU
2	D	907	PHE
2	D	912	TYR
2	D	913	ILE
2	D	916	LEU
2	D	981	GLN
2	D	1031	GLN
2	D	1101	LYS

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Mol	Chain	Res	Type
3	X	26	GLN
3	X	48	MET
3	X	108	PHE
3	X	240	SER
3	X	257	ARG
3	X	285	ILE
3	X	289	ARG
3	X	290	ASP
3	X	305	LEU
3	X	315	VAL
3	X	323	THR
3	X	329	VAL
3	X	358	LEU
3	X	401	ARG
3	X	407	LEU
3	X	421	GLU
3	X	447	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	204	HIS
2	B	394	HIS
2	B	528	ASN
2	B	791	HIS
2	B	901	HIS
2	B	955	HIS
2	B	989	ASN
2	B	1100	GLN
1	C	231	ASN
1	C	335	GLN
2	D	101	ASN
2	D	204	HIS
2	D	394	HIS
2	D	528	ASN
2	D	758	ASN
3	X	117	ASN

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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	343/394 (87%)	3.98	276 (80%) 0 2	358, 705, 903, 929	0
1	C	344/394 (87%)	7.82	324 (94%) 0 1	5, 817, 978, 997	0
2	B	1022/1139 (89%)	3.28	698 (68%) 0 3	273, 650, 901, 955	0
2	D	977/1139 (85%)	3.11	551 (56%) 0 3	298, 714, 927, 984	0
3	X	442/450 (98%)	1.76	149 (33%) 0 4	219, 451, 760, 881	0
All	All	3128/3516 (88%)	3.59	1998 (63%) 0 3	5, 667, 929, 997	0

All (1998) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	ILE	34.1
1	C	102	LEU	26.4
1	C	33	ALA	25.0
1	C	320	CYS	23.4
1	C	321	PRO	22.7
1	C	167	ILE	22.7
2	D	715	ALA	22.5
1	C	20	THR	22.4
2	D	716	GLY	21.8
2	D	704	SER	21.1
2	D	706	GLN	20.8
1	C	45	ALA	20.2
1	C	32	LEU	19.8
1	C	113	LEU	18.5
1	C	43	TYR	18.2
2	D	288	THR	18.2
1	C	159	SER	18.1
1	C	364	CYS	18.0
2	B	487	THR	18.0
1	C	77	SER	18.0

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Mol	Chain	Res	Type	RSRZ
1	C	62	PHE	17.8
1	C	79	CYS	17.2
2	D	705	GLN	17.2
1	C	24	GLN	17.0
1	C	21	TRP	17.0
1	C	46	SER	16.8
1	C	44	CYS	16.7
1	C	60	GLU	16.6
2	B	928	THR	16.4
2	D	717	CYS	16.3
1	C	64	ILE	16.2
1	C	40	ILE	16.2
1	C	50	THR	16.0
1	C	143	ALA	15.9
2	D	700	SER	15.8
1	C	34	ILE	15.8
1	C	76	SER	15.5
1	C	100	LEU	15.4
1	C	30	ASN	15.4
1	C	57	THR	15.3
1	C	65	GLN	15.2
1	C	363	PHE	15.1
1	C	56	LEU	15.1
1	C	155	GLN	15.1
2	D	718	ASP	15.1
1	C	61	LEU	15.0
1	C	19	THR	15.0
1	C	74	SER	14.7
1	C	66	THR	14.7
1	C	382	LEU	14.4
1	C	7	GLN	14.3
1	C	75	PHE	14.2
1	C	83	GLU	14.2
2	D	1038	ALA	14.2
1	C	124	GLN	14.1
1	C	41	THR	14.1
1	C	98	TYR	14.0
1	C	373	ALA	13.9
1	C	101	PHE	13.9
1	C	47	GLU	13.8
1	C	5	SER	13.7
1	C	42	ILE	13.4

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Mol	Chain	Res	Type	RSRZ
1	C	96	PRO	13.4
1	C	51	PRO	13.4
1	C	48	GLU	13.4
1	C	330	ALA	13.2
1	C	78	SER	13.2
1	C	166	LEU	13.2
2	D	1080	ASP	13.0
2	B	87	ASP	12.9
1	C	59	GLN	12.9
1	C	58	LEU	12.9
1	C	144	ASP	12.9
1	C	63	THR	12.8
2	B	172	PRO	12.7
2	D	949	GLY	12.7
1	C	171	LEU	12.7
1	C	180	GLY	12.7
2	D	703	THR	12.6
1	C	25	SER	12.5
1	C	6	ASN	12.5
2	D	702	ILE	12.5
1	C	125	HIS	12.5
2	D	709	GLU	12.3
1	C	168	ILE	12.3
2	D	707	ASP	12.3
1	C	179	ALA	12.2
1	C	261	ILE	12.2
1	C	53	SER	12.1
1	C	259	ARG	12.1
2	D	107	PRO	12.1
1	C	118	ASN	12.1
1	C	358	MET	12.0
1	C	31	LEU	12.0
1	C	103	ALA	12.0
2	B	180	THR	11.9
2	D	487	THR	11.9
2	D	712	SER	11.8
1	A	299	GLY	11.8
2	B	930	ASP	11.8
2	D	698	LEU	11.5
1	C	52	GLY	11.5
1	C	319	ALA	11.5
1	C	158	ALA	11.5

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Mol	Chain	Res	Type	RSRZ
2	D	1039	ILE	11.4
1	C	359	PRO	11.4
2	B	537	ASN	11.4
2	B	335	SER	11.3
1	C	80	SER	11.2
2	B	208	HIS	11.2
2	D	711	GLN	11.2
2	D	646	MET	11.1
1	C	115	ILE	11.1
2	D	1041	TYR	11.0
1	C	374	ILE	11.0
2	D	701	LEU	10.9
1	C	55	GLY	10.9
2	D	947	ALA	10.9
1	C	202	VAL	10.9
1	C	54	THR	10.9
1	C	262	GLY	10.8
2	D	1040	ILE	10.8
2	D	713	LYS	10.8
2	B	536	ALA	10.8
2	D	1037	ALA	10.7
1	C	383	THR	10.7
1	C	212	PHE	10.7
2	B	670	SER	10.7
1	C	269	LEU	10.7
2	D	240	MET	10.7
1	A	30	ASN	10.7
1	C	377	GLU	10.7
1	C	157	ILE	10.6
2	B	552	ASP	10.6
2	D	946	CYS	10.6
1	C	49	GLN	10.5
2	D	708	TYR	10.4
1	A	261	ILE	10.4
2	D	410	PRO	10.4
1	C	381	LEU	10.4
1	C	141	ASP	10.3
1	C	322	HIS	10.3
2	D	714	PHE	10.3
1	C	142	ILE	10.2
1	C	81	TYR	10.1
2	B	926	LYS	10.1

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Mol	Chain	Res	Type	RSRZ
1	C	156	VAL	10.1
1	C	123	THR	10.0
1	C	181	TYR	10.0
1	C	365	TRP	10.0
2	D	1042	GLU	10.0
1	C	170	ARG	9.9
1	C	362	ASP	9.8
2	B	488	GLY	9.8
1	C	264	ASP	9.8
2	B	893	ASN	9.7
2	B	8	VAL	9.7
1	C	249	SER	9.7
1	C	372	LEU	9.7
1	A	253	SER	9.7
2	D	239	SER	9.7
2	D	1026	TRP	9.7
2	D	1076	LEU	9.6
1	A	43	TYR	9.6
1	C	97	VAL	9.5
1	C	23	SER	9.5
1	A	98	TYR	9.4
1	A	82	SER	9.4
2	D	696	ILE	9.4
1	C	361	VAL	9.4
1	C	112	ARG	9.4
2	D	1074	GLU	9.4
2	D	986	GLN	9.4
1	C	67	GLY	9.4
2	D	1044	LEU	9.4
1	C	239	THR	9.4
2	B	6	HIS	9.3
2	B	59	ALA	9.3
2	B	50	PHE	9.3
1	C	357	GLY	9.3
2	B	7	ALA	9.3
1	C	172	THR	9.2
2	D	710	LEU	9.2
1	C	22	CYS	9.2
2	D	193	THR	9.2
2	B	520	LEU	9.2
1	C	213	ASP	9.1
2	D	186	SER	9.1

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Mol	Chain	Res	Type	RSRZ
2	B	97	LEU	9.1
1	A	262	GLY	9.1
1	C	329	PHE	9.1
1	C	82	SER	9.1
2	D	1075	LEU	9.1
1	C	119	GLU	9.0
1	C	263	SER	9.0
2	D	948	ALA	8.9
2	D	1035	ASP	8.9
1	A	81	TYR	8.9
2	B	113	ASP	8.9
2	D	945	ALA	8.9
1	C	104	CYS	8.9
1	C	209	ILE	8.9
2	D	991	SER	8.9
1	C	270	ALA	8.9
1	C	376	THR	8.8
1	A	23	SER	8.8
1	C	197	PRO	8.8
2	D	983	LYS	8.8
2	B	929	ASP	8.8
2	D	605	ASP	8.8
1	C	250	GLY	8.8
1	C	360	ILE	8.8
2	D	1019	TRP	8.7
2	D	1071	ASN	8.7
2	D	912	TYR	8.7
1	A	96	PRO	8.7
2	D	29	LEU	8.7
1	A	118	ASN	8.7
2	B	170	GLN	8.7
2	B	554	GLU	8.7
1	A	173	ASP	8.6
2	B	448	SER	8.6
2	B	991	SER	8.6
2	D	1003	LEU	8.6
2	D	1022	ILE	8.6
2	B	517	ASP	8.5
1	C	99	SER	8.5
2	D	289	SER	8.5
2	D	1073	LEU	8.5
2	D	417	ASP	8.5

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Mol	Chain	Res	Type	RSRZ
1	C	214	TRP	8.5
2	D	1072	THR	8.5
2	D	955	HIS	8.5
2	D	921	LEU	8.4
2	B	477	THR	8.4
3	X	310	PRO	8.4
1	C	194	PRO	8.4
1	C	195	SER	8.4
2	B	282	GLN	8.3
2	B	705	GLN	8.3
1	A	329	PHE	8.3
1	A	34	ILE	8.3
2	B	519	ILE	8.2
2	D	942	LEU	8.2
1	C	8	TYR	8.1
1	C	317	LEU	8.1
2	D	28	ALA	8.1
1	C	371	HIS	8.0
2	D	1043	LYS	8.0
3	X	293	VAL	8.0
1	C	253	SER	8.0
1	C	29	SER	7.9
1	A	83	GLU	7.9
1	A	326	MET	7.9
1	C	9	GLN	7.9
2	D	958	LEU	7.9
1	A	141	ASP	7.9
1	C	116	THR	7.9
1	C	375	ALA	7.9
2	B	173	ASP	7.9
2	D	408	ASP	7.8
1	A	24	GLN	7.8
1	A	281	ASN	7.8
2	D	833	GLY	7.8
2	B	706	GLN	7.8
1	A	358	MET	7.8
2	B	449	GLN	7.8
1	C	366	HIS	7.8
1	C	154	GLU	7.7
2	B	867	LEU	7.7
2	B	238	ILE	7.7
2	B	516	GLY	7.7

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Mol	Chain	Res	Type	RSRZ
2	B	72	THR	7.7
1	C	28	CYS	7.7
2	D	645	PRO	7.7
1	C	380	VAL	7.7
2	B	889	TYR	7.7
2	D	174	LEU	7.7
2	B	540	ALA	7.6
2	D	1021	ASN	7.6
1	C	215	THR	7.6
1	C	117	LYS	7.6
2	B	553	GLU	7.6
2	B	61	VAL	7.6
2	D	287	LEU	7.6
1	A	357	GLY	7.6
2	D	185	VAL	7.6
2	D	1064	GLU	7.6
2	B	374	VAL	7.6
1	C	211	ILE	7.6
2	B	518	GLU	7.6
1	A	45	ALA	7.5
1	C	16	PRO	7.5
3	X	268	VAL	7.5
1	C	15	ARG	7.5
2	D	176	ALA	7.5
1	A	356	LEU	7.5
3	X	344	ALA	7.5
1	A	340	GLN	7.5
2	D	1067	LEU	7.5
2	B	668	SER	7.4
2	D	476	SER	7.4
1	C	126	VAL	7.4
2	D	347	SER	7.4
1	C	252	ALA	7.4
1	A	29	SER	7.4
2	D	1031	GLN	7.4
2	B	834	TRP	7.4
1	A	33	ALA	7.4
2	B	169	ASN	7.4
2	D	1020	TYR	7.4
1	A	239	THR	7.4
1	C	323	PRO	7.4
1	A	97	VAL	7.3

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Mol	Chain	Res	Type	RSRZ
2	B	395	SER	7.3
2	B	515	PHE	7.3
1	C	165	THR	7.3
2	B	375	ILE	7.3
2	D	184	CYS	7.3
2	D	1025	SER	7.3
1	C	200	LEU	7.3
1	A	107	GLN	7.3
2	B	266	ASN	7.3
2	D	1028	TYR	7.3
1	C	169	TRP	7.2
2	B	539	VAL	7.2
2	B	700	SER	7.2
1	A	322	HIS	7.2
1	C	201	ILE	7.2
2	B	142	LEU	7.2
1	A	74	SER	7.2
1	A	344	THR	7.2
2	D	721	PHE	7.2
1	C	11	PRO	7.2
2	D	950	LYS	7.2
2	B	927	GLU	7.2
1	A	150	ASN	7.2
1	C	238	ASN	7.2
2	B	450	VAL	7.1
1	A	279	ARG	7.1
2	B	347	SER	7.1
2	B	473	SER	7.1
2	B	74	ARG	7.1
1	C	107	GLN	7.1
1	A	31	LEU	7.1
2	B	86	PHE	7.1
2	D	192	LEU	7.1
2	D	845	LYS	7.1
1	C	10	LEU	7.1
2	B	440	LEU	7.1
2	B	444	GLN	7.1
1	A	327	ASP	7.1
2	D	922	ALA	7.1
2	B	950	LYS	7.0
3	X	303	VAL	7.0
1	A	60	GLU	7.0

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Mol	Chain	Res	Type	RSRZ
2	B	535	TYR	7.0
2	D	627	VAL	7.0
2	B	955	HIS	7.0
1	C	331	THR	7.0
2	B	138	TYR	7.0
1	C	210	ARG	7.0
1	A	328	TYR	7.0
1	A	32	LEU	7.0
1	A	269	LEU	6.9
3	X	302	LEU	6.9
2	D	988	LEU	6.9
2	D	27	PRO	6.9
2	D	488	GLY	6.9
2	B	397	ASP	6.9
1	C	27	SER	6.9
2	B	88	VAL	6.9
1	C	173	ASP	6.9
2	B	26	VAL	6.9
3	X	260	THR	6.9
2	B	71	GLN	6.8
2	D	1069	VAL	6.8
1	A	341	LEU	6.8
1	A	374	ILE	6.8
2	B	866	SER	6.8
2	D	191	GLY	6.8
1	A	325	TYR	6.8
1	C	111	VAL	6.8
1	C	177	ILE	6.8
2	B	996	ARG	6.8
1	C	378	GLY	6.8
2	B	126	THR	6.8
1	A	205	ARG	6.8
1	C	231	ASN	6.8
2	B	1019	TRP	6.8
1	C	260	TRP	6.8
2	B	886	ALA	6.8
1	A	342	ILE	6.8
2	D	1023	LEU	6.8
2	B	175	MET	6.7
2	B	183	ILE	6.7
2	B	447	SER	6.7
2	D	1079	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	58	LEU	6.7
1	C	237	LEU	6.7
1	A	300	PRO	6.7
2	B	882	PHE	6.7
1	C	267	GLY	6.7
2	B	93	LYS	6.7
1	C	309	GLY	6.7
2	D	1000	ASP	6.7
2	D	668	SER	6.6
2	B	195	ILE	6.6
1	C	316	LEU	6.6
2	D	134	ALA	6.6
2	B	242	PHE	6.6
1	A	152	LEU	6.6
1	C	216	LEU	6.6
2	B	135	ARG	6.6
2	B	587	MET	6.6
1	C	73	LEU	6.6
2	D	695	PHE	6.5
2	B	171	LYS	6.5
2	B	555	PRO	6.5
2	B	63	THR	6.5
2	B	386	GLU	6.5
2	D	1070	LEU	6.5
2	B	376	GLN	6.5
1	C	384	ARG	6.5
1	C	356	LEU	6.5
2	D	1036	ALA	6.5
1	C	203	GLY	6.5
2	D	647	ARG	6.5
1	C	268	ILE	6.5
2	B	60	GLY	6.5
2	B	833	GLY	6.5
2	B	457	LYS	6.5
1	A	234	LEU	6.5
2	D	1007	ALA	6.4
1	C	234	LEU	6.4
2	B	114	GLY	6.4
2	B	439	ALA	6.4
2	B	485	ASP	6.4
2	B	410	PRO	6.4
1	C	145	VAL	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	41	THR	6.3
2	D	1045	SER	6.3
1	A	266	SER	6.3
2	D	97	LEU	6.3
2	D	286	TYR	6.3
2	D	943	LYS	6.3
2	D	954	ALA	6.3
2	B	998	ASP	6.3
2	D	719	LYS	6.3
2	B	451	SER	6.3
1	C	325	TYR	6.3
2	D	386	GLU	6.3
1	A	366	HIS	6.2
2	D	990	TYR	6.2
1	A	365	TRP	6.2
2	B	933	LEU	6.2
1	C	134	HIS	6.2
2	B	189	ASN	6.2
2	B	107	PRO	6.2
2	D	944	THR	6.2
1	A	104	CYS	6.2
2	B	486	LEU	6.2
2	B	669	PRO	6.2
1	A	144	ASP	6.2
2	B	789	PRO	6.2
2	B	438	VAL	6.2
2	D	832	ILE	6.2
1	A	308	GLN	6.2
2	B	241	ILE	6.2
2	D	172	PRO	6.1
2	D	699	LEU	6.1
1	C	341	LEU	6.1
2	B	109	ASN	6.1
2	B	584	HIS	6.1
2	D	1100	GLN	6.1
2	B	443	PHE	6.1
2	D	1046	ARG	6.1
2	B	774	SER	6.1
2	D	939	HIS	6.1
2	B	454	LYS	6.1
2	D	485	ASP	6.1
2	B	673	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
2	D	1004	GLU	6.1
3	X	261	ALA	6.0
1	C	71	LEU	6.0
1	A	283	PHE	6.0
1	A	211	ILE	6.0
2	D	992	MET	6.0
2	D	195	ILE	6.0
1	A	302	ASN	6.0
2	B	1026	TRP	6.0
2	D	486	LEU	6.0
1	A	268	ILE	6.0
2	B	3	GLU	6.0
2	B	181	SER	6.0
2	B	504	ARG	6.0
3	X	367	ALA	6.0
1	C	205	ARG	5.9
2	D	175	MET	5.9
2	B	207	GLN	5.9
2	B	163	ARG	5.9
2	B	532	TYR	5.9
1	A	307	VAL	5.9
1	A	174	GLU	5.9
1	A	100	LEU	5.9
1	C	127	LEU	5.9
2	D	628	ASP	5.9
2	D	1047	TYR	5.9
1	C	175	GLY	5.9
2	B	5	LYS	5.9
2	D	1024	PHE	5.9
1	C	340	GLN	5.9
2	D	899	TYR	5.9
2	B	194	LYS	5.9
2	B	453	ASN	5.8
2	D	1068	ILE	5.9
2	B	501	GLU	5.8
2	B	836	ASN	5.8
2	D	251	MET	5.8
2	B	161	CYS	5.8
2	B	1024	PHE	5.8
2	B	176	ALA	5.8
2	B	62	TYR	5.8
3	X	274	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
2	B	432	SER	5.8
1	A	143	ALA	5.8
2	B	489	TYR	5.8
2	B	514	HIS	5.8
2	B	1002	LEU	5.8
2	B	167	PHE	5.8
2	D	173	ASP	5.8
2	D	418	ILE	5.8
2	D	340	GLU	5.8
2	D	856	VAL	5.8
2	B	112	LYS	5.8
2	D	957	ALA	5.8
1	C	191	GLN	5.8
2	B	999	VAL	5.8
1	A	375	ALA	5.8
2	D	914	ASP	5.8
3	X	226	HIS	5.7
2	B	570	LEU	5.7
1	A	267	GLY	5.7
1	A	166	LEU	5.7
1	C	232	PRO	5.7
2	B	923	ASP	5.7
2	D	759	THR	5.7
2	D	626	ASN	5.7
2	B	551	PHE	5.7
2	D	419	SER	5.7
1	A	263	SER	5.7
1	C	176	PRO	5.7
2	B	1071	ASN	5.7
2	D	648	ASP	5.7
2	B	193	THR	5.7
1	C	39	GLY	5.7
2	B	108	SER	5.7
1	C	308	GLN	5.7
2	B	367	TRP	5.7
1	C	350	ASN	5.7
2	B	704	SER	5.7
1	C	251	ILE	5.7
1	A	278	LEU	5.6
2	B	164	PRO	5.6
2	B	279	LEU	5.6
1	C	277	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
2	B	90	LEU	5.6
1	A	145	VAL	5.6
1	A	339	ILE	5.6
3	X	343	VAL	5.6
2	D	763	LEU	5.6
1	A	353	PRO	5.6
2	D	609	TYR	5.6
2	D	1048	ILE	5.6
2	D	208	HIS	5.6
2	B	1082	TRP	5.6
2	D	669	PRO	5.6
2	B	252	LEU	5.6
1	A	42	ILE	5.6
1	C	233	TRP	5.6
1	A	277	TRP	5.6
2	D	896	SER	5.6
2	B	54	CYS	5.6
2	B	549	GLU	5.6
2	D	938	THR	5.6
1	A	319	ALA	5.6
2	B	870	TYR	5.6
1	C	354	ILE	5.6
2	D	1006	LYS	5.6
1	A	352	ILE	5.6
2	B	125	THR	5.5
2	B	474	ILE	5.5
2	B	1080	ASP	5.5
2	D	504	ARG	5.5
1	C	120	THR	5.5
1	C	326	MET	5.5
1	A	249	SER	5.5
1	C	379	SER	5.5
2	B	484	SER	5.5
2	B	925	SER	5.5
3	X	294	ALA	5.5
2	B	344	TRP	5.5
2	B	1031	GLN	5.5
1	C	178	LEU	5.5
2	D	917	GLU	5.5
2	B	96	PRO	5.5
1	C	122	ILE	5.5
2	B	240	MET	5.5

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Mol	Chain	Res	Type	RSRZ
2	D	87	ASP	5.5
1	A	28	CYS	5.5
2	B	137	LEU	5.5
2	D	1066	TYR	5.4
2	D	989	ASN	5.4
3	X	309	GLN	5.4
1	A	151	ARG	5.4
2	D	444	GLN	5.4
2	B	897	CYS	5.4
1	C	258	VAL	5.4
2	D	940	GLU	5.4
3	X	300	PHE	5.4
1	A	116	THR	5.4
2	B	994	THR	5.4
1	C	151	ARG	5.4
2	D	953	ALA	5.4
2	B	898	TYR	5.4
1	C	192	PHE	5.4
2	B	533	ILE	5.4
1	A	330	ALA	5.4
2	D	1034	ARG	5.4
1	C	140	ILE	5.4
2	D	356	GLY	5.4
1	A	280	TRP	5.4
2	B	184	CYS	5.4
3	X	262	SER	5.4
1	A	368	ASP	5.4
1	C	152	LEU	5.4
2	B	237	ILE	5.4
2	B	505	PHE	5.4
2	B	435	SER	5.3
1	A	72	HIS	5.3
2	B	239	SER	5.3
1	A	350	ASN	5.3
2	D	1063	ILE	5.3
1	A	15	ARG	5.3
1	C	105	VAL	5.3
2	B	1067	LEU	5.3
3	X	297	ALA	5.3
2	D	290	ASP	5.3
2	B	696	ILE	5.3
1	A	338	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	132	GLY	5.3
2	B	146	TRP	5.3
2	D	151	ASP	5.3
2	D	670	SER	5.3
1	A	183	LEU	5.3
2	B	408	ASP	5.3
1	A	56	LEU	5.3
1	C	18	THR	5.3
2	B	394	HIS	5.3
2	B	829	MET	5.3
1	C	198	ASN	5.3
1	C	133	HIS	5.3
1	C	26	PRO	5.3
2	B	436	ILE	5.3
2	D	108	SER	5.3
2	D	1011	ILE	5.3
1	A	259	ARG	5.3
2	D	897	CYS	5.3
1	C	17	TYR	5.3
2	D	902	LEU	5.3
1	A	321	PRO	5.2
1	A	21	TRP	5.2
3	X	296	TYR	5.2
3	X	425	TYR	5.2
2	B	482	PRO	5.2
1	A	112	ARG	5.2
3	X	269	VAL	5.2
1	C	13	ASN	5.2
2	B	626	ASN	5.2
1	A	331	THR	5.2
2	D	1032	ASN	5.2
2	B	133	HIS	5.2
2	B	862	PHE	5.2
1	A	377	GLU	5.2
2	B	909	GLU	5.2
1	C	121	ILE	5.2
1	A	264	ASP	5.2
2	B	1035	ASP	5.2
2	B	91	ASN	5.2
2	B	762	ALA	5.2
3	X	271	GLU	5.2
2	B	894	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	B	434	GLU	5.2
2	D	241	ILE	5.2
2	B	174	LEU	5.2
1	A	367	GLN	5.1
1	A	209	ILE	5.1
2	B	419	SER	5.1
2	D	404	LYS	5.1
3	X	366	PHE	5.1
2	D	1065	HIS	5.1
2	D	500	ASN	5.1
2	B	1022	ILE	5.1
3	X	238	SER	5.1
1	C	247	HIS	5.1
2	B	481	GLU	5.1
2	B	144	LYS	5.1
2	D	1030	HIS	5.1
2	D	1124	THR	5.1
1	C	131	SER	5.1
2	B	140	ILE	5.1
2	D	72	THR	5.1
2	B	758	ASN	5.1
2	B	912	TYR	5.1
2	D	348	ASP	5.1
1	C	310	ILE	5.1
1	A	388	PHE	5.0
2	B	130	ALA	5.0
2	D	342	ILE	5.0
1	C	128	GLY	5.0
2	B	913	ILE	5.0
2	B	334	PRO	5.0
2	D	300	TYR	5.0
1	A	351	SER	5.0
2	D	520	LEU	5.0
2	D	1002	LEU	5.0
1	C	265	GLY	5.0
1	C	196	ASN	5.0
2	B	1076	LEU	5.0
2	B	1034	ARG	5.0
2	B	932	ASP	5.0
2	D	26	VAL	5.0
2	D	507	LYS	5.0
1	A	146	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	277	THR	5.0
1	A	140	ILE	5.0
2	B	4	LEU	5.0
2	B	1003	LEU	5.0
2	D	1112	TYR	5.0
3	X	258	VAL	4.9
1	A	50	THR	4.9
2	B	538	LYS	4.9
1	A	362	ASP	4.9
1	C	385	LEU	4.9
1	A	57	THR	4.9
2	B	98	SER	4.9
2	B	446	SER	4.9
2	B	832	ILE	4.9
2	D	941	THR	4.9
1	C	186	PRO	4.9
2	B	152	ALA	4.9
3	X	365	LEU	4.9
1	C	353	PRO	4.9
2	B	701	LEU	4.9
2	B	89	SER	4.9
2	B	771	GLN	4.9
2	B	493	GLU	4.9
2	B	141	ARG	4.9
2	B	841	ALA	4.9
2	B	1066	TYR	4.9
1	C	12	LEU	4.9
2	B	111	MET	4.9
3	X	237	VAL	4.9
2	B	885	ILE	4.9
2	D	649	ILE	4.9
2	B	604	GLN	4.8
3	X	267	THR	4.8
1	A	102	LEU	4.8
2	B	892	GLN	4.8
2	D	604	GLN	4.8
2	B	922	ALA	4.8
2	B	280	PRO	4.8
1	A	142	ILE	4.8
1	C	328	TYR	4.8
1	A	25	SER	4.8
2	B	947	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	338	ASP	4.8
1	C	266	SER	4.8
3	X	371	ALA	4.8
2	B	23	ALA	4.8
2	B	1081	THR	4.8
1	A	282	LEU	4.8
2	D	1077	PRO	4.8
2	D	860	ARG	4.8
2	D	834	TRP	4.8
2	B	1100	GLN	4.8
1	A	106	CYS	4.8
1	A	354	ILE	4.8
1	C	342	ILE	4.8
2	B	946	CYS	4.8
2	B	502	TRP	4.8
2	B	1124	THR	4.8
2	B	387	SER	4.7
2	D	473	SER	4.7
2	D	913	ILE	4.7
1	C	278	LEU	4.7
2	D	855	ALA	4.7
2	D	985	ASN	4.7
2	B	472	SER	4.7
1	C	109	ASN	4.7
2	D	519	ILE	4.7
1	A	376	THR	4.7
2	D	194	LYS	4.7
1	A	369	GLY	4.7
2	B	19	GLU	4.7
2	B	286	TYR	4.7
1	A	254	SER	4.7
2	B	914	ASP	4.7
2	B	948	ALA	4.7
2	B	403	GLU	4.7
2	B	263	LEU	4.7
2	B	586	CYS	4.7
1	C	274	SER	4.7
2	B	150	PRO	4.7
2	D	472	SER	4.7
3	X	127	GLY	4.7
1	C	236	THR	4.7
2	B	674	CYS	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	505	PHE	4.7
2	B	675	ALA	4.6
2	B	507	LYS	4.6
2	B	1025	SER	4.6
2	D	503	GLU	4.6
1	A	260	TRP	4.6
2	B	1040	ILE	4.6
2	D	183	ILE	4.6
1	C	72	HIS	4.6
2	D	963	THR	4.6
2	B	275	SER	4.6
2	D	415	SER	4.6
2	D	916	LEU	4.6
1	A	103	ALA	4.6
2	D	697	PHE	4.6
2	B	110	VAL	4.6
2	B	629	PRO	4.6
2	B	1028	TYR	4.6
1	C	280	TRP	4.6
1	C	35	GLY	4.6
1	A	312	LEU	4.6
1	C	242	LEU	4.6
1	C	135	ASN	4.6
2	B	371	LEU	4.6
2	D	1033	TYR	4.6
2	B	525	ASP	4.6
2	B	251	MET	4.6
2	B	77	ILE	4.6
2	B	151	ASP	4.6
2	B	1021	ASN	4.6
2	B	99	LYS	4.6
2	B	835	LEU	4.6
1	A	246	CYS	4.5
2	B	988	LEU	4.5
2	D	1029	LYS	4.5
2	B	790	LEU	4.5
2	B	934	SER	4.5
2	B	1041	TYR	4.5
2	D	285	PRO	4.5
2	B	761	GLU	4.5
1	A	99	SER	4.5
2	D	829	MET	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	399	PHE	4.5
2	D	515	PHE	4.5
1	A	44	CYS	4.5
2	B	124	ASP	4.5
2	B	185	VAL	4.5
2	B	276	GLN	4.5
1	A	247	HIS	4.5
2	B	106	PHE	4.5
2	B	627	VAL	4.5
2	D	501	GLU	4.5
1	C	139	ASP	4.5
2	B	471	LEU	4.5
2	B	478	ILE	4.5
1	A	332	ALA	4.5
3	X	342	ALA	4.5
1	A	214	TRP	4.5
2	D	498	LEU	4.5
2	D	552	ASP	4.5
2	D	163	ARG	4.5
2	B	1075	LEU	4.5
3	X	368	PRO	4.5
1	C	130	LYS	4.5
2	B	585	SER	4.5
3	X	341	LYS	4.4
1	A	133	HIS	4.4
2	B	136	VAL	4.4
2	B	385	ASP	4.4
1	A	71	LEU	4.4
1	A	114	ILE	4.4
2	B	115	VAL	4.4
2	B	521	SER	4.4
1	A	137	VAL	4.4
1	A	310	ILE	4.4
2	D	762	ALA	4.4
1	A	14	VAL	4.4
1	A	26	PRO	4.4
2	D	854	GLU	4.4
2	D	346	LEU	4.4
2	D	1062	ILE	4.4
2	B	582	SER	4.4
1	A	309	GLY	4.4
1	C	137	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	363	PHE	4.4
2	B	788	SER	4.4
2	D	720	LEU	4.4
2	D	920	LEU	4.4
1	A	181	TYR	4.4
2	B	366	ALA	4.4
2	B	958	LEU	4.4
3	X	308	GLN	4.4
1	C	162	ASP	4.4
1	C	368	ASP	4.4
2	B	70	SER	4.4
2	B	541	PHE	4.4
2	B	843	TYR	4.4
2	B	445	ASN	4.3
1	A	62	PHE	4.3
2	D	918	PHE	4.3
2	B	53	GLU	4.3
2	B	373	THR	4.3
2	B	129	TYR	4.3
1	C	311	SER	4.3
2	B	528	ASN	4.3
1	A	131	SER	4.3
2	B	513	ASP	4.3
2	D	830	GLN	4.3
2	B	1062	ILE	4.3
2	D	411	THR	4.3
1	A	372	LEU	4.3
1	A	7	GLN	4.3
1	C	199	GLN	4.3
2	D	915	ALA	4.3
2	B	671	LEU	4.3
1	A	235	LEU	4.3
2	D	452	LYS	4.3
1	A	306	ASN	4.3
3	X	320	PRO	4.3
2	B	896	SER	4.3
1	A	159	SER	4.3
2	D	177	ALA	4.3
2	B	1023	LEU	4.3
2	D	118	SER	4.3
2	D	426	ILE	4.3
1	A	210	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	386	MET	4.2
1	A	343	ASN	4.2
2	B	763	LEU	4.2
2	B	603	VAL	4.2
2	B	75	TRP	4.2
1	A	301	LYS	4.2
2	B	348	ASP	4.2
2	B	418	ILE	4.2
2	B	1065	HIS	4.2
1	A	138	ASN	4.2
2	D	1027	ARG	4.2
2	D	606	LEU	4.2
1	C	174	GLU	4.2
2	B	1030	HIS	4.2
3	X	292	ARG	4.2
1	A	157	ILE	4.2
3	X	326	GLU	4.2
2	B	497	LEU	4.2
3	X	423	THR	4.2
1	A	73	LEU	4.2
1	A	158	ALA	4.2
2	B	441	LEU	4.2
2	B	1112	TYR	4.2
2	D	437	GLN	4.2
2	B	954	ALA	4.2
1	C	352	ILE	4.2
1	A	245	THR	4.2
2	B	143	SER	4.2
2	B	1044	LEU	4.2
1	C	38	THR	4.2
2	B	534	ASN	4.2
2	B	337	PRO	4.2
2	D	335	SER	4.2
2	B	572	GLU	4.2
1	C	318	GLY	4.2
2	B	628	ASP	4.2
2	D	936	ALA	4.2
1	C	129	GLY	4.1
2	D	180	THR	4.1
1	C	235	LEU	4.1
2	D	512	LEU	4.1
2	B	117	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	476	SER	4.1
2	D	923	ASP	4.1
2	D	365	ILE	4.1
2	D	972	LEU	4.1
1	C	70	THR	4.1
2	D	494	TYR	4.1
2	D	968	LYS	4.1
3	X	240	SER	4.1
2	B	899	TYR	4.1
2	B	944	THR	4.1
2	B	583	LEU	4.1
2	D	601	GLU	4.1
2	D	316	ALA	4.1
2	B	837	SER	4.1
2	B	639	LEU	4.1
2	B	949	GLY	4.1
2	D	71	GLN	4.1
2	D	484	SER	4.1
2	B	1120	ALA	4.1
2	B	437	GLN	4.1
2	D	608	SER	4.1
2	B	249	LEU	4.1
2	B	1007	ALA	4.1
3	X	225	ARG	4.1
2	D	129	TYR	4.1
2	B	479	GLN	4.0
2	B	812	VAL	4.0
1	A	381	LEU	4.0
2	B	431	THR	4.0
1	C	275	GLY	4.0
2	B	967	LYS	4.0
2	B	9	VAL	4.0
1	C	283	PHE	4.0
2	B	830	GLN	4.0
1	C	257	ASN	4.0
1	C	14	VAL	4.0
2	D	996	ARG	4.0
2	D	1126	GLU	4.0
2	B	963	THR	4.0
2	B	937	ILE	4.0
2	D	508	LEU	4.0
2	D	383	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	301	TYR	4.0
2	D	325	VAL	4.0
1	A	355	GLN	4.0
2	D	1012	ASN	4.0
2	B	119	PHE	4.0
1	C	106	CYS	4.0
2	B	116	ALA	4.0
3	X	313	VAL	4.0
1	C	208	ASN	4.0
2	B	590	SER	4.0
2	B	512	LEU	4.0
1	A	186	PRO	4.0
2	D	152	ALA	4.0
2	B	78	PHE	4.0
1	A	22	CYS	4.0
2	B	128	ILE	3.9
2	B	667	GLN	3.9
1	A	111	VAL	3.9
3	X	327	LEU	3.9
2	B	707	ASP	3.9
1	A	5	SER	3.9
1	A	379	SER	3.9
2	D	91	ASN	3.9
1	A	345	TYR	3.9
2	D	387	SER	3.9
2	B	895	LEU	3.9
2	D	376	GLN	3.9
2	B	522	ILE	3.9
1	C	110	THR	3.9
2	D	903	SER	3.9
2	D	135	ARG	3.9
2	B	365	ILE	3.9
2	B	692	ILE	3.9
2	B	1029	LYS	3.9
1	C	183	LEU	3.9
2	B	132	THR	3.9
2	B	396	LEU	3.9
2	B	500	ASN	3.9
2	D	313	LYS	3.9
2	B	58	ASP	3.9
2	B	103	LYS	3.9
2	D	951	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	441	LEU	3.9
2	B	122	HIS	3.9
1	A	212	PHE	3.9
1	C	339	ILE	3.9
2	B	759	THR	3.9
2	D	86	PHE	3.9
2	D	312	TYR	3.9
2	B	636	ILE	3.9
2	B	1038	ALA	3.9
1	A	313	PHE	3.9
2	B	134	ALA	3.9
1	A	324	ARG	3.9
2	B	121	GLU	3.9
2	B	1032	ASN	3.9
2	B	917	GLU	3.9
1	A	172	THR	3.9
2	D	438	VAL	3.9
2	B	1020	TYR	3.8
3	X	370	LYS	3.8
2	B	350	GLN	3.8
2	D	1078	LYS	3.8
3	X	304	TYR	3.8
2	D	901	HIS	3.8
2	B	1006	LYS	3.8
1	C	193	ARG	3.8
2	B	709	GLU	3.8
2	B	678	ALA	3.8
2	B	767	ASN	3.8
2	D	722	LEU	3.8
1	A	55	GLY	3.8
1	A	175	GLY	3.8
2	D	964	THR	3.8
3	X	311	TRP	3.8
2	B	372	ASN	3.8
1	A	305	PRO	3.8
2	B	1	MET	3.8
2	D	343	PRO	3.8
1	C	153	ALA	3.8
2	B	247	ASN	3.7
2	D	1018	CYS	3.7
2	D	106	PHE	3.7
3	X	18	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	494	TYR	3.7
2	D	93	LYS	3.7
2	D	457	LYS	3.7
3	X	259	ILE	3.7
1	A	255	LEU	3.7
1	A	270	ALA	3.7
2	B	527	SER	3.7
3	X	406	MET	3.7
2	B	1027	ARG	3.7
2	D	774	SER	3.7
2	D	987	LEU	3.7
2	B	581	ARG	3.7
1	C	146	TYR	3.7
2	D	54	CYS	3.7
1	C	248	SER	3.7
2	B	364	ILE	3.7
2	D	919	SER	3.7
2	D	416	GLY	3.7
2	D	263	LEU	3.7
2	D	725	LEU	3.7
2	B	1079	GLU	3.7
2	B	856	VAL	3.7
1	C	276	ALA	3.7
2	B	51	LYS	3.7
2	D	314	LEU	3.7
2	D	900	LEU	3.7
2	D	74	ARG	3.7
2	D	207	GLN	3.7
1	C	108	ASP	3.7
2	D	237	ILE	3.7
1	A	195	SER	3.7
2	D	984	ILE	3.7
3	X	346	GLY	3.7
2	B	940	GLU	3.7
1	A	380	VAL	3.7
2	B	192	LEU	3.7
2	D	657	ARG	3.7
2	B	542	ILE	3.7
1	A	132	GLY	3.6
2	B	943	LYS	3.6
3	X	318	ALA	3.6
2	D	88	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	306	HIS	3.6
2	D	1001	ASN	3.6
1	A	77	SER	3.6
1	A	371	HIS	3.6
2	B	962	SER	3.6
1	C	344	THR	3.6
2	B	703	THR	3.6
2	B	197	LEU	3.6
2	B	230	ASP	3.6
2	B	672	PHE	3.6
2	D	259	LYS	3.6
2	B	1121	VAL	3.6
2	B	442	SER	3.6
1	A	197	PRO	3.6
2	B	235	ASN	3.6
2	D	164	PRO	3.6
1	C	324	ARG	3.6
2	B	131	ILE	3.6
1	A	27	SER	3.6
1	A	194	PRO	3.6
2	B	304	ASN	3.6
1	C	315	SER	3.6
1	C	279	ARG	3.6
2	D	525	ASP	3.6
1	A	167	ILE	3.6
2	B	470	VAL	3.6
2	D	1049	SER	3.6
2	B	300	TYR	3.6
2	D	1010	MET	3.6
2	B	483	ASN	3.6
2	B	900	LEU	3.6
3	X	305	LEU	3.6
2	B	398	SER	3.6
1	A	124	GLN	3.6
2	D	6	HIS	3.6
2	B	860	ARG	3.6
2	D	375	ILE	3.6
2	B	200	LYS	3.6
2	B	377	LYS	3.6
2	B	145	THR	3.6
3	X	319	LEU	3.6
1	A	135	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	1039	ILE	3.6
3	X	196	GLY	3.6
2	B	1042	GLU	3.5
2	B	857	LYS	3.5
2	D	777	ASN	3.5
2	B	975	VAL	3.5
2	D	366	ALA	3.5
1	A	59	GLN	3.5
2	B	413	MET	3.5
2	D	692	ILE	3.5
2	D	895	LEU	3.5
2	D	511	TYR	3.5
2	D	999	VAL	3.5
2	B	508	LEU	3.5
2	B	939	HIS	3.5
2	B	1037	ALA	3.5
1	A	359	PRO	3.5
2	B	57	TYR	3.5
3	X	218	PHE	3.5
1	A	203	GLY	3.5
1	C	149	ASP	3.5
2	D	1102	LEU	3.5
1	A	265	GLY	3.5
2	D	516	GLY	3.5
2	B	101	ASN	3.5
1	A	360	ILE	3.5
2	D	674	CYS	3.5
1	A	311	SER	3.5
1	C	163	ASP	3.5
1	A	80	SER	3.5
2	D	765	SER	3.5
3	X	299	GLU	3.5
1	A	171	LEU	3.5
3	X	219	THR	3.5
1	C	334	SER	3.5
2	D	998	ASP	3.5
2	B	801	ILE	3.5
2	D	1111	GLU	3.5
2	D	252	LEU	3.4
2	B	409	VAL	3.4
2	D	502	TRP	3.4
2	D	906	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	801	ILE	3.4
2	B	336	LEU	3.4
2	B	24	LEU	3.4
2	B	831	LEU	3.4
2	D	853	LYS	3.4
2	D	629	PRO	3.4
2	B	936	ALA	3.4
1	A	75	PHE	3.4
2	B	765	SER	3.4
2	B	368	LYS	3.4
3	X	422	GLN	3.4
2	B	182	GLU	3.4
1	A	244	ASN	3.4
1	A	204	GLU	3.4
1	A	323	PRO	3.4
1	C	243	VAL	3.4
2	D	1108	ILE	3.4
2	B	878	VAL	3.4
3	X	257	ARG	3.4
2	B	942	LEU	3.4
2	D	413	MET	3.4
2	B	924	ALA	3.4
3	X	301	GLY	3.4
2	B	1118	ASP	3.4
2	D	849	TYR	3.4
2	B	492	TYR	3.4
3	X	239	GLY	3.4
2	D	952	ASP	3.4
1	A	40	ILE	3.4
2	B	918	PHE	3.4
2	D	305	SER	3.4
2	B	916	LEU	3.4
2	D	454	LYS	3.4
2	B	1068	ILE	3.4
2	D	98	SER	3.4
2	D	434	GLU	3.4
1	A	136	PHE	3.4
2	D	475	VAL	3.4
1	A	304	LEU	3.4
1	A	156	VAL	3.3
2	D	491	TYR	3.3
2	B	452	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	987	LEU	3.3
1	C	389	THR	3.3
2	D	997	GLN	3.3
2	B	496	ARG	3.3
2	B	902	LEU	3.3
2	B	177	ALA	3.3
2	D	357	SER	3.3
2	B	838	ASP	3.3
2	D	1050	THR	3.3
2	D	1117	LYS	3.3
2	D	302	PRO	3.3
2	B	261	LEU	3.3
2	D	57	TYR	3.3
2	D	407	PHE	3.3
2	B	578	ASP	3.3
1	A	16	PRO	3.3
1	C	187	GLY	3.3
2	B	811	LEU	3.3
1	A	348	ASP	3.3
2	B	139	TYR	3.3
2	D	138	TYR	3.3
1	C	184	SER	3.3
1	C	367	GLN	3.3
2	B	550	SER	3.3
2	B	1072	THR	3.3
1	C	254	SER	3.3
2	B	503	GLU	3.3
2	B	970	CYS	3.3
3	X	17	ARG	3.3
2	B	702	ILE	3.3
2	B	600	ARG	3.3
2	B	888	LYS	3.3
1	C	241	PRO	3.3
1	A	383	THR	3.3
2	B	816	VAL	3.3
3	X	222	MET	3.3
2	D	153	ARG	3.3
2	B	346	LEU	3.3
2	D	666	ALA	3.3
2	B	1117	LYS	3.3
1	C	138	ASN	3.3
1	C	150	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	80	ASN	3.3
1	C	281	ASN	3.2
2	D	1101	LYS	3.2
2	B	506	ALA	3.2
2	D	554	GLU	3.2
3	X	270	ASP	3.2
2	B	698	LEU	3.2
1	A	162	ASP	3.2
2	B	191	GLY	3.2
2	B	844	LEU	3.2
2	B	323	LEU	3.2
3	X	107	LYS	3.2
2	B	851	LYS	3.2
2	B	891	HIS	3.2
2	B	95	GLU	3.2
2	B	404	LYS	3.2
2	B	911	ALA	3.2
2	B	938	THR	3.2
2	D	344	TRP	3.2
2	D	742	LEU	3.2
2	B	243	LEU	3.2
2	D	971	LEU	3.2
2	B	737	ASN	3.2
2	B	840	ILE	3.2
2	B	875	GLN	3.2
1	A	168	ILE	3.2
2	B	632	ILE	3.2
2	D	496	ARG	3.2
2	B	292	THR	3.2
2	B	992	MET	3.2
2	B	165	ILE	3.2
2	B	972	LEU	3.2
1	C	335	GLN	3.2
2	B	695	PHE	3.2
2	B	123	SER	3.2
2	B	1113	HIS	3.2
1	A	119	GLU	3.2
3	X	194	PHE	3.2
2	D	1005	ARG	3.2
2	B	127	ILE	3.2
2	B	985	ASN	3.2
1	A	155	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	17	TYR	3.2
1	A	207	GLY	3.2
1	C	370	SER	3.2
2	B	301	TYR	3.2
2	B	772	PHE	3.2
2	D	423	LEU	3.2
1	C	273	LYS	3.2
2	D	836	ASN	3.2
1	C	190	VAL	3.1
2	B	1010	MET	3.1
2	B	591	THR	3.1
1	C	36	HIS	3.1
2	D	119	PHE	3.1
2	B	984	ILE	3.1
2	D	117	PHE	3.1
2	D	898	TYR	3.1
2	D	477	THR	3.1
1	A	139	ASP	3.1
2	B	901	HIS	3.1
2	B	990	TYR	3.1
1	C	207	GLY	3.1
2	B	979	THR	3.1
3	X	236	SER	3.1
2	D	90	LEU	3.1
2	D	336	LEU	3.1
3	X	21	GLN	3.1
2	D	1008	PHE	3.1
3	X	66	VAL	3.1
1	A	46	SER	3.1
1	A	242	LEU	3.1
1	A	346	GLU	3.1
2	D	469	ALA	3.1
2	B	511	TYR	3.1
2	B	689	GLN	3.1
2	B	961	LEU	3.1
1	C	204	GLU	3.1
2	B	919	SER	3.1
2	D	337	PRO	3.1
2	B	571	ILE	3.1
1	A	182	PRO	3.1
2	D	850	LEU	3.1
2	D	70	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	167	PHE	3.1
2	B	971	LEU	3.1
2	B	393	SER	3.1
1	C	68	LEU	3.1
2	D	126	THR	3.1
2	B	1115	GLN	3.1
2	D	113	ASP	3.1
2	D	644	ASN	3.1
2	D	364	ILE	3.1
2	D	1125	ALA	3.1
1	A	188	ILE	3.1
1	A	206	ASN	3.1
2	B	976	ASN	3.1
2	B	147	PHE	3.1
2	B	268	CYS	3.1
1	C	160	VAL	3.1
2	D	772	PHE	3.1
3	X	248	ILE	3.1
2	B	531	THR	3.1
1	C	189	SER	3.1
2	B	85	ILE	3.1
3	X	345	GLU	3.1
1	A	61	LEU	3.1
2	B	1116	LEU	3.1
2	B	968	LYS	3.1
2	B	849	TYR	3.1
2	D	1059	ARG	3.1
3	X	179	MET	3.1
2	D	114	GLY	3.0
2	D	133	HIS	3.0
2	D	650	ASP	3.0
2	D	53	GLU	3.0
1	A	373	ALA	3.0
2	D	935	ILE	3.0
1	C	312	LEU	3.0
2	B	974	PHE	3.0
3	X	166	ALA	3.0
2	D	339	ASP	3.0
1	A	191	GLN	3.0
2	D	909	GLU	3.0
1	C	69	PRO	3.0
2	B	682	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	773	PHE	3.0
2	D	1105	LEU	3.0
1	A	318	GLY	3.0
2	D	341	PHE	3.0
1	C	240	LEU	3.0
2	B	188	PHE	3.0
3	X	195	THR	3.0
1	A	20	THR	3.0
2	D	812	VAL	3.0
2	D	586	CYS	3.0
2	B	1104	THR	3.0
2	B	12	ASP	3.0
2	B	910	SER	3.0
2	D	527	SER	3.0
1	A	51	PRO	3.0
2	B	908	GLU	3.0
2	B	153	ARG	3.0
2	D	261	LEU	3.0
2	D	250	VAL	3.0
2	D	956	VAL	3.0
2	B	498	LEU	3.0
2	B	162	TYR	3.0
2	D	528	ASN	3.0
2	D	831	LEU	3.0
2	B	206	GLU	3.0
3	X	263	ASP	3.0
2	B	510	ALA	3.0
2	D	907	PHE	3.0
1	A	202	VAL	3.0
1	C	164	CYS	3.0
2	D	767	ASN	3.0
1	A	192	PHE	3.0
1	A	252	ALA	2.9
2	D	161	CYS	2.9
2	B	384	GLN	2.9
2	B	1083	ILE	2.9
2	B	1036	ALA	2.9
2	B	253	SER	2.9
2	B	297	ILE	2.9
2	D	824	GLN	2.9
2	B	509	VAL	2.9
2	D	967	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	182	PRO	2.9
2	B	69	GLY	2.9
2	B	1048	ILE	2.9
2	D	349	PHE	2.9
2	B	291	HIS	2.9
2	B	863	LYS	2.9
2	B	1123	VAL	2.9
2	B	303	ASP	2.9
1	C	185	SER	2.9
2	B	576	ILE	2.9
2	B	325	VAL	2.9
1	A	385	LEU	2.9
2	D	432	SER	2.9
2	D	1013	VAL	2.9
2	B	469	ALA	2.9
2	B	1070	LEU	2.9
2	D	8	VAL	2.9
1	A	243	VAL	2.9
2	B	688	PHE	2.9
1	A	63	THR	2.9
3	X	317	ILE	2.9
2	B	234	PRO	2.9
2	D	937	ILE	2.9
1	A	19	THR	2.9
2	B	640	VAL	2.9
2	B	1009	GLN	2.9
2	B	1033	TYR	2.9
2	D	12	ASP	2.9
2	D	852	SER	2.9
2	D	965	PRO	2.9
2	D	142	LEU	2.9
1	A	69	PRO	2.9
2	B	523	ASN	2.9
2	B	941	THR	2.9
1	C	136	PHE	2.9
2	B	246	TYR	2.9
1	A	271	MET	2.9
1	C	271	MET	2.9
1	C	332	ALA	2.9
1	A	108	ASP	2.9
1	A	163	ASP	2.9
2	B	845	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	VAL	2.9
2	B	2	ASN	2.9
1	C	188	ILE	2.9
1	C	244	ASN	2.9
2	D	816	VAL	2.9
3	X	235	VAL	2.9
1	A	79	CYS	2.9
2	D	837	SER	2.9
3	X	413	CYS	2.9
2	D	324	ASN	2.8
2	B	187	PHE	2.8
2	B	475	VAL	2.8
3	X	55	VAL	2.8
1	A	101	PHE	2.8
2	B	499	TYR	2.8
2	D	62	TYR	2.8
2	D	1116	LEU	2.8
2	B	324	ASN	2.8
2	D	414	SER	2.8
2	B	798	LEU	2.8
2	D	96	PRO	2.8
2	D	440	LEU	2.8
2	D	1104	THR	2.8
1	A	258	VAL	2.8
1	C	327	ASP	2.8
2	B	1011	ILE	2.8
2	B	1069	VAL	2.8
3	X	82	VAL	2.8
2	D	673	LEU	2.8
2	D	961	LEU	2.8
3	X	282	LEU	2.8
2	D	409	VAL	2.8
1	A	123	THR	2.8
2	B	721	PHE	2.8
3	X	32	MET	2.8
1	A	125	HIS	2.8
2	B	847	LEU	2.8
3	X	410	HIS	2.8
1	C	369	GLY	2.8
2	B	530	VAL	2.8
2	B	904	LYS	2.8
2	D	758	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	848	ILE	2.8
3	X	92	LYS	2.8
2	B	64	SER	2.8
2	B	278	ILE	2.8
2	B	458	PHE	2.8
2	B	877	ALA	2.8
2	D	65	ASN	2.8
2	D	445	ASN	2.8
2	B	82	THR	2.8
2	B	813	THR	2.8
1	A	208	ASN	2.8
2	D	181	SER	2.8
3	X	447	ILE	2.8
3	X	359	PHE	2.8
2	D	69	GLY	2.8
2	B	903	SER	2.8
2	B	995	LEU	2.8
2	B	951	PHE	2.7
2	B	848	ILE	2.7
2	D	165	ILE	2.7
2	B	22	LEU	2.7
2	B	320	SER	2.7
2	B	411	THR	2.7
3	X	351	THR	2.7
2	D	532	TYR	2.7
1	C	388	PHE	2.7
2	B	605	ASP	2.7
2	B	764	ALA	2.7
1	A	6	ASN	2.7
2	D	24	LEU	2.7
2	D	297	ILE	2.7
2	D	602	LEU	2.7
2	D	320	SER	2.7
1	A	320	CYS	2.7
2	B	456	ASP	2.7
2	B	1063	ILE	2.7
2	D	363	LEU	2.7
2	D	536	ALA	2.7
3	X	430	ASN	2.7
2	B	407	PHE	2.7
3	X	230	PHE	2.7
2	B	92	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	318	ALA	2.7
2	B	579	LEU	2.7
1	C	351	SER	2.7
2	B	160	LEU	2.7
1	A	236	THR	2.7
2	B	643	GLU	2.7
1	A	303	LEU	2.7
2	D	266	ASN	2.7
1	A	250	GLY	2.7
3	X	273	GLY	2.7
1	A	274	SER	2.7
2	D	974	PHE	2.7
1	A	237	LEU	2.7
3	X	64	ARG	2.7
2	D	537	ASN	2.7
1	A	49	GLN	2.7
2	B	524	PHE	2.7
3	X	180	ALA	2.7
2	B	905	LYS	2.7
2	D	1060	THR	2.7
3	X	175	GLU	2.7
2	D	600	ARG	2.7
1	A	333	HIS	2.7
3	X	167	GLY	2.7
2	B	102	VAL	2.7
2	D	405	THR	2.7
3	X	176	VAL	2.7
2	B	353	SER	2.6
2	B	601	GLU	2.6
2	B	890	HIS	2.6
2	B	256	TYR	2.6
2	D	299	LEU	2.6
2	D	811	LEU	2.6
2	D	672	PHE	2.6
2	B	352	ILE	2.6
2	D	1017	PRO	2.6
1	A	149	ASP	2.6
2	D	338	ASP	2.6
3	X	87	ALA	2.6
2	D	311	ILE	2.6
1	A	238	ASN	2.6
2	D	802	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	332	ILE	2.6
2	B	964	THR	2.6
3	X	286	LYS	2.6
2	B	65	ASN	2.6
1	A	165	THR	2.6
2	D	318	ALA	2.6
2	B	915	ALA	2.6
1	C	313	PHE	2.6
2	B	1014	GLU	2.6
2	D	905	LYS	2.6
2	B	646	MET	2.6
2	D	470	VAL	2.6
3	X	165	PRO	2.6
2	B	264	SER	2.6
3	X	409	ILE	2.6
2	B	794	VAL	2.6
2	D	99	LYS	2.6
2	D	835	LEU	2.6
2	D	497	LEU	2.6
2	D	603	VAL	2.6
2	B	190	GLY	2.6
2	B	906	LEU	2.6
2	B	965	PRO	2.6
2	D	150	PRO	2.6
2	B	1064	GLU	2.6
2	B	236	THR	2.6
2	D	911	ALA	2.5
2	D	471	LEU	2.5
2	B	281	LEU	2.5
3	X	124	MET	2.5
2	D	238	ILE	2.5
3	X	65	VAL	2.5
2	B	345	MET	2.5
2	B	259	LYS	2.5
2	D	317	ASN	2.5
2	B	158	TRP	2.5
1	C	307	VAL	2.5
2	B	417	ASP	2.5
2	D	412	ASN	2.5
2	D	468	ASN	2.5
3	X	285	ILE	2.5
2	B	526	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	1123	VAL	2.5
2	B	316	ALA	2.5
1	A	241	PRO	2.5
2	D	334	PRO	2.5
2	B	871	SER	2.5
1	C	304	LEU	2.5
2	B	311	ILE	2.5
2	D	77	ILE	2.5
2	B	105	HIS	2.5
2	D	456	ASP	2.5
1	A	70	THR	2.5
2	B	677	VAL	2.5
2	D	489	TYR	2.5
2	D	517	ASP	2.5
1	C	314	PRO	2.5
3	X	314	PRO	2.5
2	D	675	ALA	2.5
3	X	172	GLY	2.5
2	B	250	VAL	2.5
2	D	910	SER	2.5
3	X	312	SER	2.5
1	C	282	LEU	2.5
2	B	594	GLU	2.4
2	D	295	SER	2.4
2	D	761	GLU	2.4
2	B	52	LYS	2.4
2	B	168	LEU	2.4
2	B	986	GLN	2.4
2	D	370	ASN	2.4
2	D	397	ASP	2.4
3	X	434	PHE	2.4
1	A	36	HIS	2.4
2	B	73	LEU	2.4
2	D	128	ILE	2.4
2	D	327	ILE	2.4
3	X	138	LYS	2.4
2	B	791	HIS	2.4
2	B	309	PHE	2.4
2	D	667	GLN	2.4
3	X	281	ARG	2.4
2	B	855	ALA	2.4
2	D	130	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
3	X	24	PHE	2.4
2	D	420	GLU	2.4
3	X	150	LEU	2.4
1	A	109	ASN	2.4
2	D	771	GLN	2.4
2	D	1058	GLU	2.4
2	B	284	PHE	2.4
2	B	274	LEU	2.4
2	D	63	THR	2.4
3	X	402	LEU	2.4
3	X	298	LYS	2.4
2	B	817	GLU	2.4
2	B	869	LEU	2.4
2	D	625	PRO	2.4
2	B	793	THR	2.4
1	A	257	ASN	2.4
1	A	378	GLY	2.4
2	B	307	GLY	2.4
2	D	124	ASP	2.4
3	X	217	TYR	2.4
3	X	446	VAL	2.4
1	A	193	ARG	2.4
2	B	412	ASN	2.4
2	D	656	LEU	2.4
2	B	729	ARG	2.4
2	B	787	ILE	2.4
3	X	163	ASP	2.4
1	C	355	GLN	2.4
2	B	267	GLN	2.4
3	X	83	GLN	2.4
1	C	305	PRO	2.4
2	D	388	PHE	2.4
3	X	378	ALA	2.4
2	B	854	GLU	2.4
2	B	931	GLU	2.4
2	D	1122	GLN	2.4
2	B	305	SER	2.4
3	X	374	ALA	2.4
2	D	392	TRP	2.3
2	D	367	TRP	2.3
2	D	81	ARG	2.3
2	D	798	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	PRO	2.3
2	D	242	PHE	2.3
2	D	246	TYR	2.3
1	A	65	GLN	2.3
2	B	693	GLU	2.3
2	B	1045	SER	2.3
2	D	653	ILE	2.3
2	B	265	THR	2.3
2	D	1118	ASP	2.3
1	C	255	LEU	2.3
2	B	55	VAL	2.3
2	B	642	LEU	2.3
2	B	491	TYR	2.3
2	B	624	TYR	2.3
2	D	291	HIS	2.3
2	D	959	MET	2.3
2	B	802	PHE	2.3
2	D	729	ARG	2.3
2	B	679	ARG	2.3
2	B	466	LEU	2.3
2	D	75	TRP	2.3
3	X	28	VAL	2.3
1	C	272	CYS	2.3
1	A	213	ASP	2.3
2	D	962	SER	2.3
2	B	21	THR	2.3
1	A	251	ILE	2.3
2	B	104	ILE	2.3
2	D	518	GLU	2.3
2	D	200	LYS	2.3
2	D	1115	GLN	2.3
1	A	361	VAL	2.3
2	B	118	SER	2.3
2	B	714	PHE	2.3
2	B	810	ASP	2.3
2	B	11	ILE	2.3
3	X	340	VAL	2.3
3	X	212	GLY	2.3
2	B	685	LEU	2.3
3	X	128	LYS	2.3
2	B	676	SER	2.3
2	D	136	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	490	ASP	2.3
2	B	592	LEU	2.3
2	D	84	THR	2.3
2	D	378	CYS	2.3
2	D	390	CYS	2.3
2	B	935	ILE	2.3
3	X	322	ALA	2.3
3	X	68	VAL	2.3
2	B	717	CYS	2.2
2	D	321	PHE	2.2
2	D	499	TYR	2.2
3	X	372	ALA	2.2
2	D	994	THR	2.2
2	D	64	SER	2.2
2	D	350	GLN	2.2
2	D	1009	GLN	2.2
2	D	116	ALA	2.2
2	D	857	LYS	2.2
2	D	639	LEU	2.2
1	A	184	SER	2.2
2	B	426	ILE	2.2
1	C	245	THR	2.2
2	B	879	LEU	2.2
2	D	333	PRO	2.2
3	X	229	GLY	2.2
2	B	887	GLU	2.2
2	B	199	PRO	2.2
2	D	298	ALA	2.2
2	D	272	ILE	2.2
1	A	48	GLU	2.2
1	A	8	TYR	2.2
1	A	54	THR	2.2
2	D	826	ASN	2.2
2	B	257	LYS	2.2
2	B	876	PHE	2.2
1	A	47	GLU	2.2
1	C	303	LEU	2.2
2	D	83	LEU	2.2
2	D	109	ASN	2.2
3	X	103	LEU	2.2
3	X	254	PHE	2.2
2	B	625	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	83	LEU	2.2
2	D	264	SER	2.2
1	C	336	HIS	2.2
1	A	154	GLU	2.2
2	D	94	LYS	2.2
2	B	1000	ASP	2.2
3	X	188	ASN	2.2
1	A	382	LEU	2.2
2	B	290	ASP	2.2
2	B	545	PRO	2.2
2	B	822	PHE	2.2
2	D	671	LEU	2.2
2	D	101	ASN	2.2
2	B	392	TRP	2.2
2	D	640	VAL	2.2
2	D	863	LYS	2.2
1	A	215	THR	2.2
1	A	337	GLY	2.2
2	B	388	PHE	2.2
2	D	190	GLY	2.2
2	D	622	HIS	2.2
3	X	45	TYR	2.2
2	B	480	ILE	2.2
3	X	151	MET	2.2
3	X	306	GLU	2.2
2	B	248	VAL	2.2
2	D	975	VAL	2.2
2	B	271	THR	2.2
2	B	351	LEU	2.2
3	X	133	PHE	2.2
2	D	284	PHE	2.2
2	D	351	LEU	2.2
2	B	736	GLU	2.2
1	A	233	TRP	2.2
2	B	422	TRP	2.2
2	D	249	LEU	2.2
2	D	970	CYS	2.2
2	B	289	SER	2.2
2	D	960	VAL	2.1
2	B	852	SER	2.1
2	B	697	PHE	2.1
2	B	262	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	82	THR	2.1
3	X	429	ALA	2.1
2	D	458	PHE	2.1
2	D	474	ILE	2.1
2	D	724	LEU	2.1
1	A	9	GLN	2.1
1	A	127	LEU	2.1
2	B	258	LEU	2.1
2	D	323	LEU	2.1
2	D	844	LEU	2.1
2	D	933	LEU	2.1
1	A	364	CYS	2.1
2	B	81	ARG	2.1
2	D	514	HIS	2.1
2	B	1043	LYS	2.1
2	D	146	TRP	2.1
3	X	78	ARG	2.1
2	B	645	PRO	2.1
2	D	465	GLU	2.1
2	D	530	VAL	2.1
2	D	969	SER	2.1
1	A	134	HIS	2.1
2	B	1073	LEU	2.1
3	X	204	SER	2.1
2	B	25	TRP	2.1
2	B	631	TYR	2.1
2	B	708	TYR	2.1
2	D	509	VAL	2.1
2	B	907	PHE	2.1
2	B	10	PRO	2.1
2	B	983	LYS	2.1
2	B	548	ILE	2.1
2	D	315	ASN	2.1
2	D	632	ILE	2.1
3	X	126	GLY	2.1
1	A	248	SER	2.1
3	X	438	ALA	2.1
1	A	240	LEU	2.1
2	B	684	ILE	2.1
2	D	182	GLU	2.1
1	A	200	LEU	2.1
2	B	66	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1059	ARG	2.1
3	X	158	LEU	2.1
3	X	215	LEU	2.1
2	D	435	SER	2.1
2	B	363	LEU	2.1
1	C	161	GLY	2.1
3	X	272	SER	2.1
2	D	78	PHE	2.1
2	B	959	MET	2.1
2	D	19	GLU	2.1
2	B	17	CYS	2.1
2	D	268	CYS	2.1
2	B	699	LEU	2.1
2	B	378	CYS	2.1
1	A	121	ILE	2.1
1	C	256	ALA	2.1
2	B	302	PRO	2.1
2	B	13	LEU	2.1
2	D	521	SER	2.1
3	X	93	GLY	2.1
3	X	91	TYR	2.0
3	X	364	VAL	2.0
2	D	332	ILE	2.0
2	D	931	GLU	2.0
2	B	298	ALA	2.0
2	B	945	ALA	2.0
3	X	67	TRP	2.0
3	X	111	PHE	2.0
2	B	94	LYS	2.0
2	D	73	LEU	2.0
2	D	17	CYS	2.0
2	D	197	LEU	2.0
3	X	332	ALA	2.0
2	B	842	VAL	2.0
3	X	20	ASN	2.0
2	B	952	ASP	2.0
3	X	171	VAL	2.0
1	A	201	ILE	2.0
3	X	59	ARG	2.0
2	B	546	TYR	2.0
2	D	828	CYS	2.0
2	D	85	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	X	206	ILE	2.0
2	D	859	VAL	2.0
2	B	733	PHE	2.0
2	B	1074	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.