



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 05:58 am BST

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

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

with specific help available everywhere you see the ⓘ symbol.

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

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

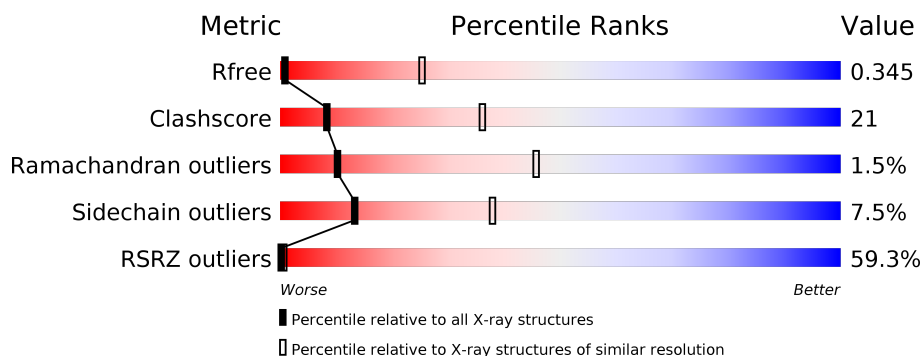
1 Overall quality at a glance ⓘ

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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)
RSRZ outliers	127900	1004 (9.50-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	394	<div> <div>68%</div> <div> <div>56%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>
1	C	394	<div> <div>80%</div> <div> <div>56%</div> <div>28%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	1139	<div> <div>57%</div> <div> <div>45%</div> <div>40%</div> <div>5%</div> <div>10%</div> </div> </div>
2	D	1139	<div> <div>44%</div> <div> <div>45%</div> <div>37%</div> <div>•</div> <div>14%</div> </div> </div>
3	X	450	<div> <div>27%</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			

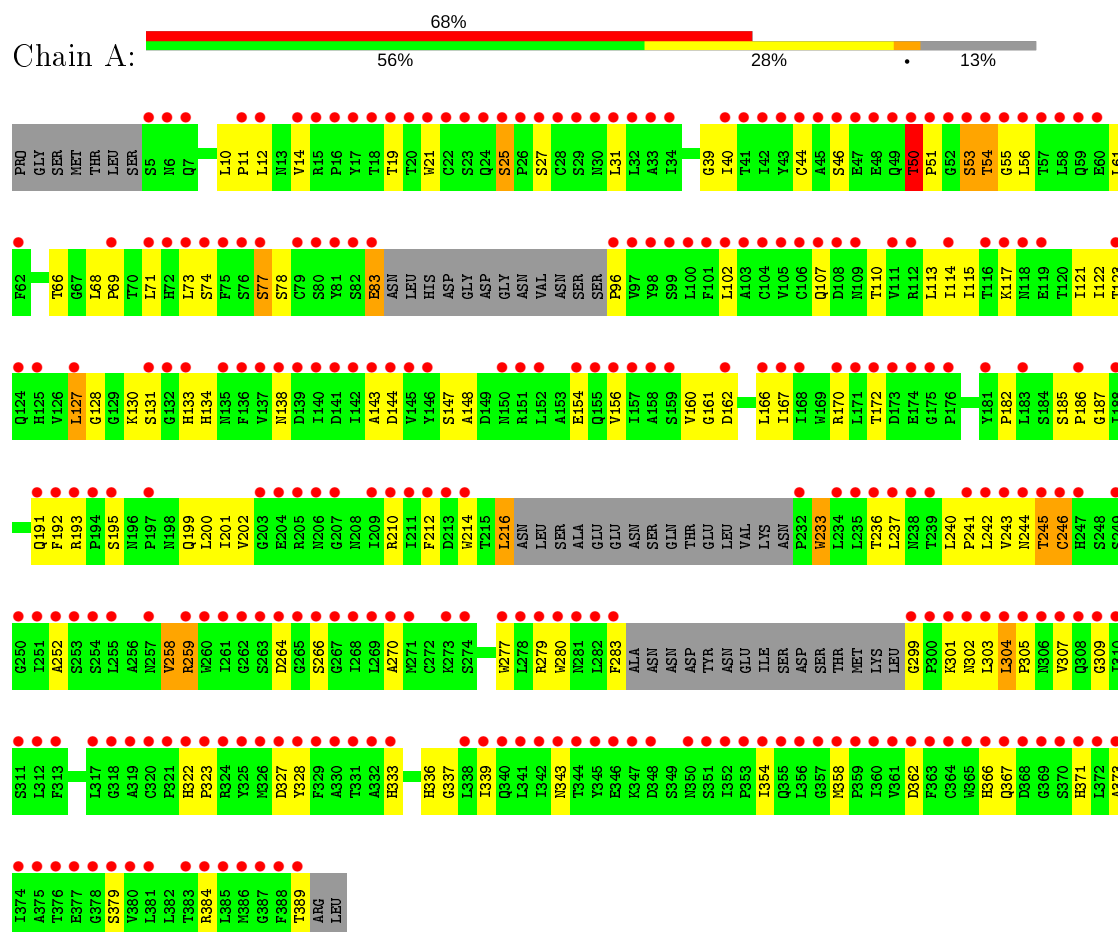
There are 3 discrepancies between the modelled and reference sequences:

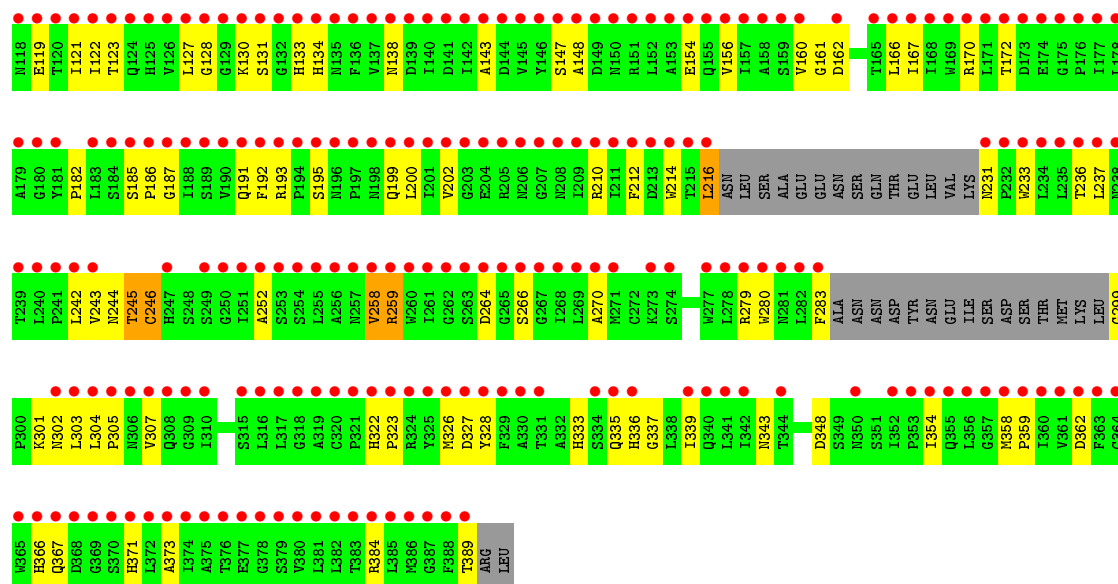
Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	PRO	-	EXPRESSION TAG	UNP Q8XDW9
X	-1	GLY	-	EXPRESSION TAG	UNP Q8XDW9
X	0	SER	-	EXPRESSION TAG	UNP Q8XDW9

3 Residue-property plots

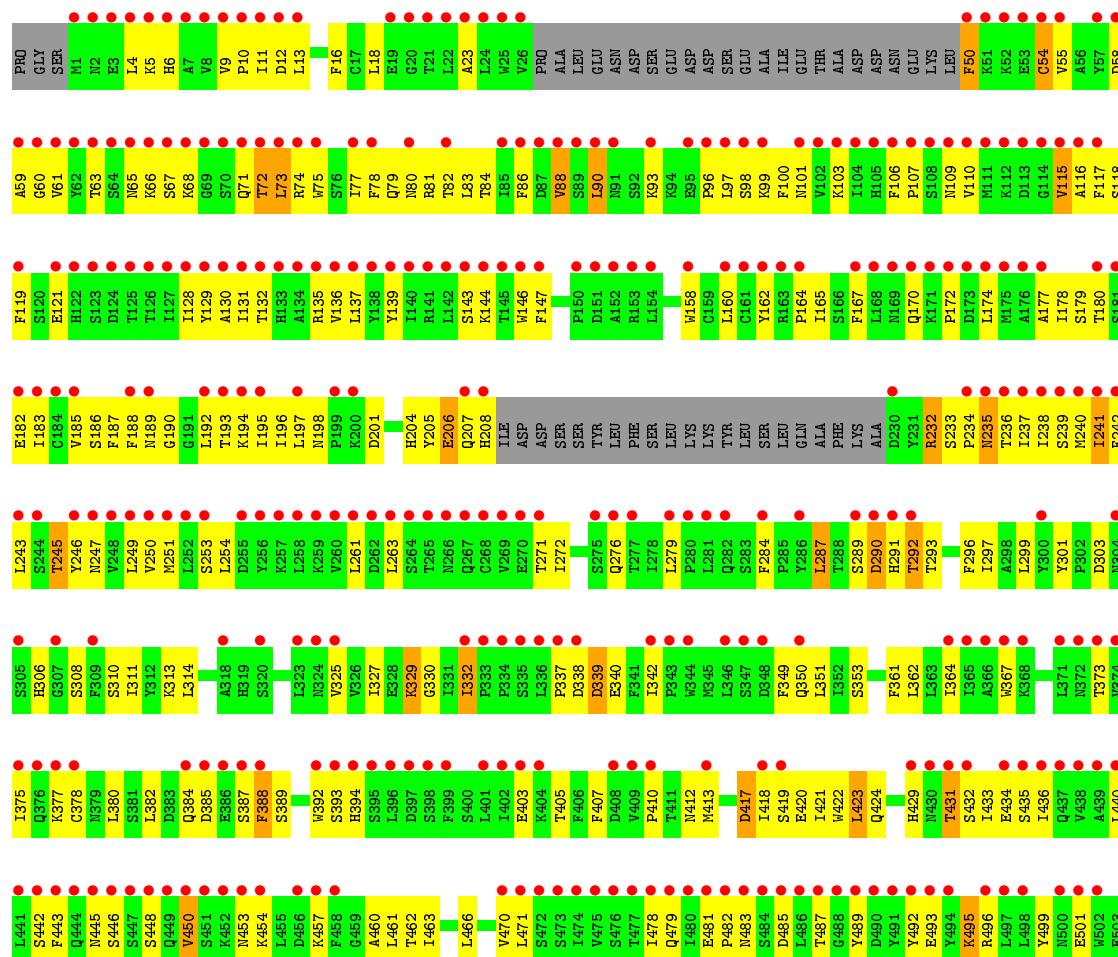
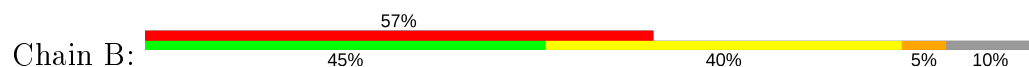
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

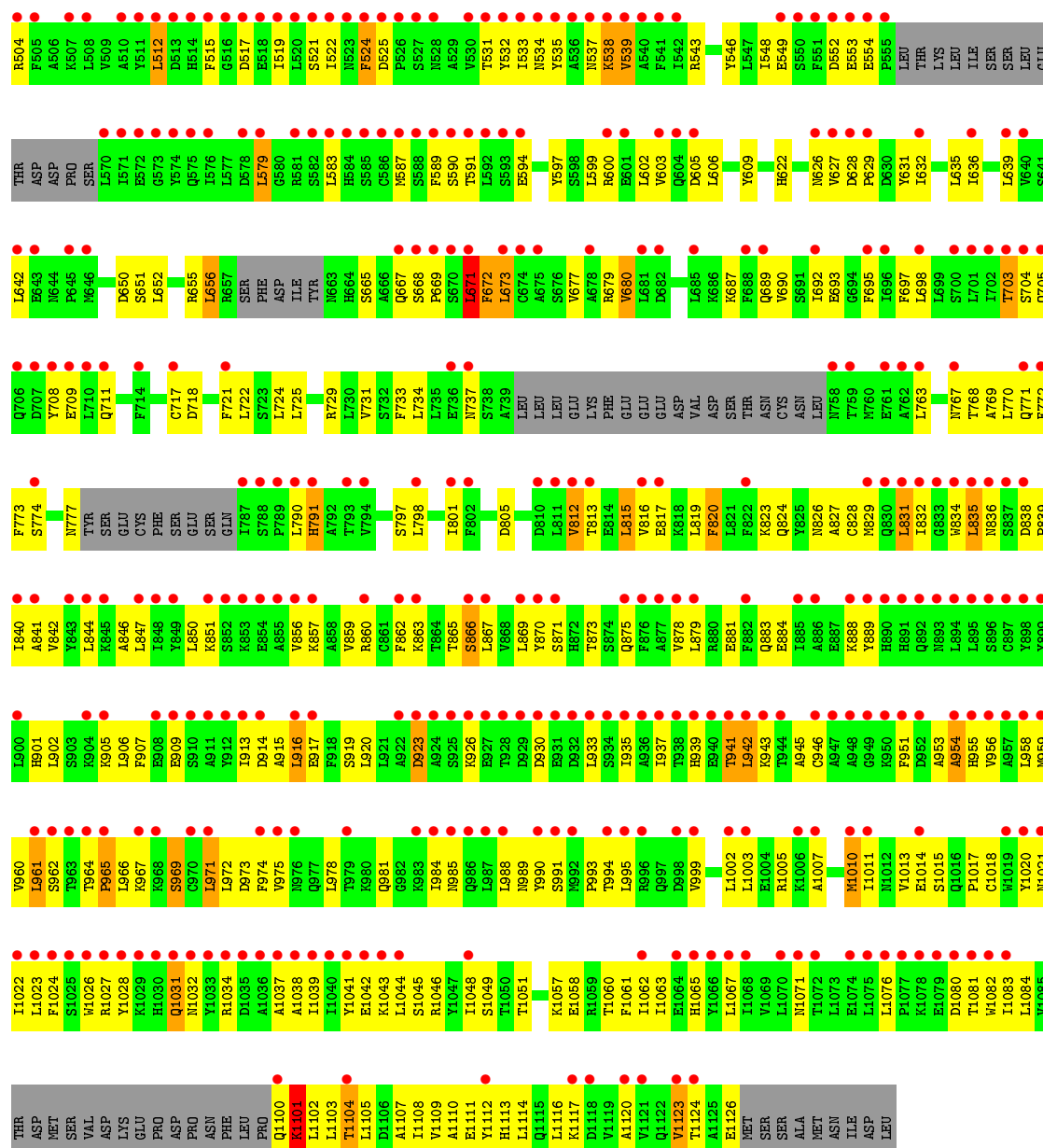
• Molecule 1: NUCLEOPORIN NUP37

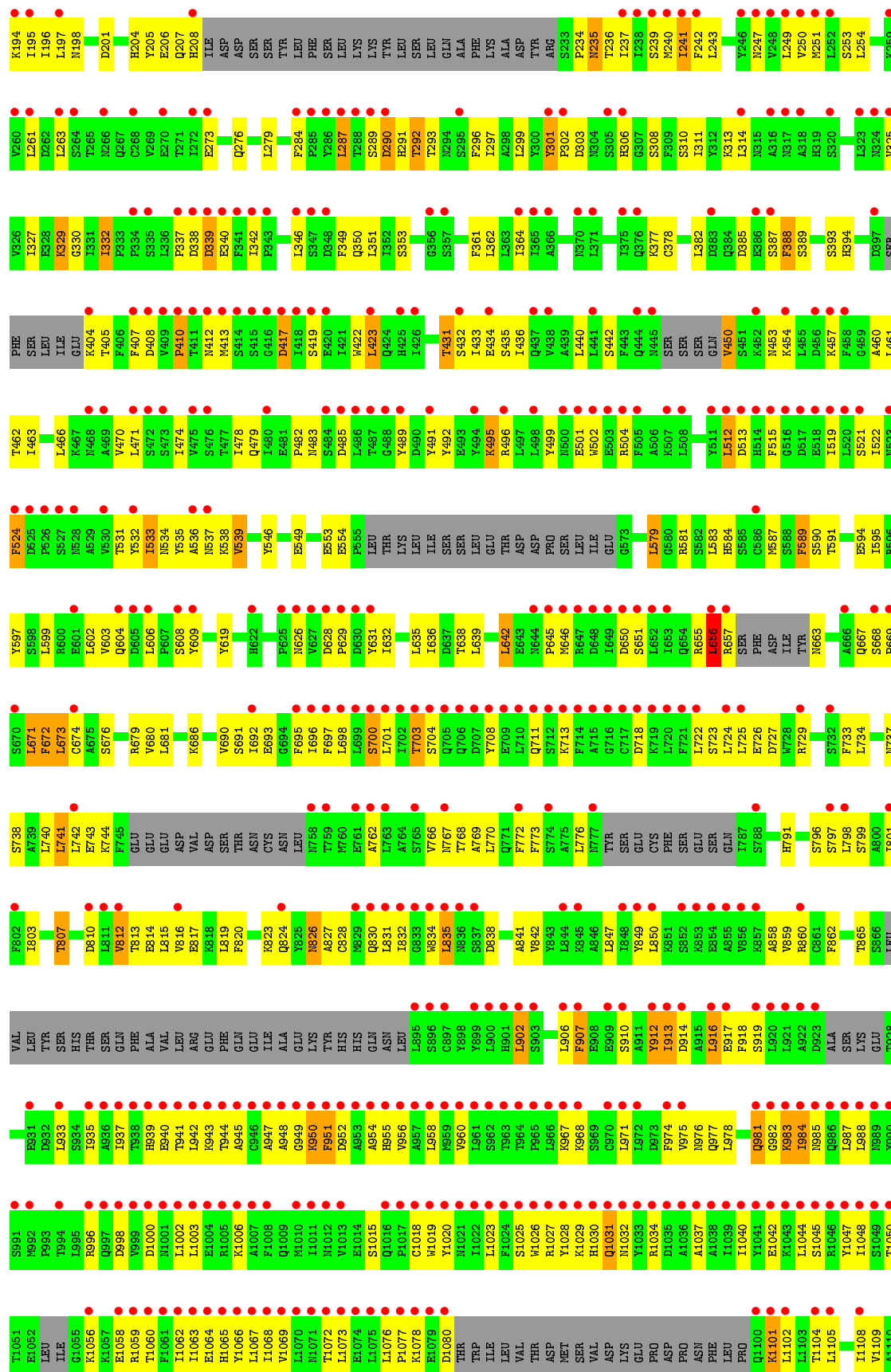


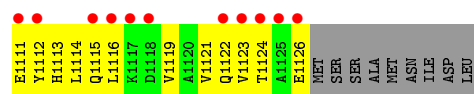


• Molecule 2: Nucleoporin nup120

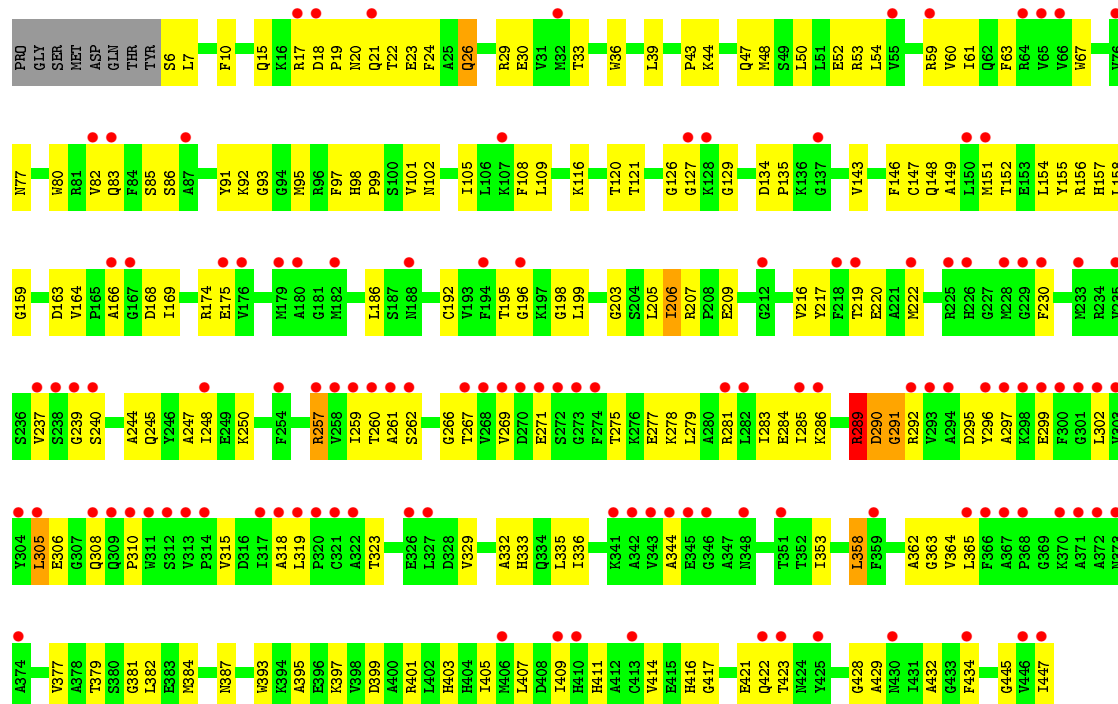








• Molecule 3: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α , β , γ	330.00Å 330.00Å 350.26Å 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 6.73Å)	Xtriage
Refinement program	PHENIX 1.7.3 _928	Depositor
R, R_{free}	0.285 , 0.346 0.280 , 0.345	Depositor DCC
R_{free} test set	939 reflections (5.13%)	wwPDB-VP
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 , 684.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.33	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
2:B:1080:ASP:HB2	2:B:1101:LYS:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:60:VAL:HG22	3:X:82:VAL:HG13	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:10:PRO:HG3	2:B:431:THR:HA	1.64	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
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:B:1124:THR:O	2:D:1027:ARG:NE	2.17	0.76
2:D:174:LEU:HB3	2:D:186:SER:HB3	1.68	0.76
2:B:165:ILE:HD13	2:B:187:PHE:HE2	1.51	0.76
2:B:1116:LEU:HD13	2:D:1067:LEU:HD22	1.67	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:412:ASN:ND2	2:B:594:GLU:OE2	2.25	0.69
2:B:975:VAL:HA	2:B:978:LEU:HD12	1.74	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:B:118:SER:HB3	2:B:129:TYR:HB2	1.73	0.69
2:D:1020:TYR:HA	2:D:1023:LEU:HD12	1.74	0.69
2:B:1007:ALA:HA	2:B:1010:MET:HE2	1.74	0.69
2:B:665:SER:HB3	2:B:777:ASN:HB3	1.75	0.69
2:D:708:TYR:HA	2:D:711:GLN:HG3	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
2:B:116:ALA:O	2:B:130:ALA:HA	1.94	0.67
3:X:417:GLY:HA3	3:X:423:THR:HG23	1.76	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:419:SER:HB2	2:B:471:LEU:HD21	1.76	0.66
2:B:838:ASP:H	2:B:841:ALA:HB3	1.60	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
1:C:154:GLU:HG2	1:C:172:THR:HG22	1.76	0.65
3:X:53:ARG:NH2	3:X:445:GLY:O	2.28	0.65
1:A:301:LYS:HD3	2:B:479:GLN:HB3	1.77	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:D:236:THR:O	2:D:254:LEU:N	2.27	0.65
1:A:117:LYS:HG2	1:A:122:ILE:HD13	1.78	0.65
1:A:339:ILE:HB	1:A:354:ILE:HB	1.79	0.65
2:B:239:SER:HB3	2:B:289:SER:HB2	1.79	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)
1:A:110:THR:HG22	1:A:128:GLY:HA3	1.79	0.65
2:B:237:ILE:HA	2:B:253:SER:HA	1.78	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:236:THR:O	2:B:254:LEU:N	2.29	0.64
2:B:955:HIS:CE1	2:B:978:LEU:HD13	2.32	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
2:D:337:PRO:HG3	2:D:394:HIS:HE1	1.62	0.63
3:X:333:HIS:HA	3:X:336:ILE:HD12	1.80	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
2:B:1003:LEU:HD12	2:B:1028:TYR:CG	2.34	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
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
2:D:975:VAL:HA	2:D:978:LEU:HD12	1.81	0.62
3:X:291:GLY:O	3:X:292:ARG:NH1	2.31	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:B:763:LEU:HD22	2:B:771:GLN:HG2	1.82	0.62
2:D:118:SER:HB3	2:D:129:TYR:HB2	1.80	0.62
2:B:74:ARG:HH22	2:B:144:LYS:HG2	1.63	0.62
1:C:110:THR:HG22	1:C:128:GLY:HA3	1.81	0.62
2:D:12:ASP:HB2	2:D:433:ILE:HG23	1.82	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)
1:A:55:GLY:H	1:A:384:ARG:HH11	1.46	0.61
2:B:1080:ASP:HB2	2:B:1101:LYS:CE	2.30	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:B:695:PHE:CZ	2:B:724:LEU:HB3	2.36	0.60
2:D:767:ASN:HB3	2:D:770:LEU:HD11	1.82	0.60
2:D:310:SER:HA	2:D:332:ILE:H	1.65	0.60
1:A:130:LYS:HD3	2:B:609:TYR:HE1	1.66	0.60
2:B:543:ARG:HB3	2:B:679:ARG:HH12	1.66	0.60
2:B:79:GLN:HB3	2:B:82:THR:HB	1.83	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:1058:GLU:HA	2:B:1061:PHE:HD2	1.67	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
2:B:603:VAL:HG13	2:B:729:ARG:HD2	1.84	0.59
1:C:301:LYS:HD3	2:D:479:GLN:HB3	1.84	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
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:668:SER:HB2	2:B:672:PHE:HD2	1.67	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:587:MET:HG2	2:D:591:THR:HG21	1.85	0.59
2:D:693:GLU:HB3	2:D:697:PHE:CZ	2.38	0.59
2:D:798:LEU:HD23	2:D:801:ILE:HD12	1.83	0.59
2:B:164:PRO:HG2	2:B:195:ILE:HD13	1.83	0.59
2:B:838:ASP:O	2:B:842:VAL:N	2.36	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
1:C:304:LEU:HD22	1:C:305:PRO:HD2	1.85	0.58
2:D:247:ASN:HB3	2:D:263:LEU:HB2	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:B:453:ASN:O	2:B:457:LYS:HG3	2.03	0.58
2:D:776:LEU:HD13	2:D:797:SER:HA	1.85	0.58
2:B:71:GLN:HB3	2:B:93:LYS:HE2	1.85	0.58
2:D:830:GLN:HG3	2:D:831:LEU:HD23	1.85	0.58
2:D:835:LEU:HD21	2:D:841:ALA:HB1	1.85	0.58
2:B:628:ASP:HB3	2:B:631:TYR:HD2	1.67	0.58
2:D:1112:TYR:CE1	2:D:1116:LEU:HD21	2.38	0.58
1:A:44:CYS:HB2	1:A:61:LEU:HD11	1.85	0.58
2:B:482:PRO:HA	2:B:489:TYR:HA	1.85	0.58
2:B:548:ILE:HD13	2:B:687:LYS:HD2	1.86	0.58
2:D:71:GLN:HB3	2:D:93:LYS:HE2	1.86	0.58
2:B:1103:LEU:HD13	3:X:271:GLU:H	1.68	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:B:812:VAL:HG21	2:B:835:LEU:HB2	1.86	0.58
2:B:985:ASN:O	2:B:989:ASN:ND2	2.37	0.58
2:D:842:VAL:HG11	2:D:865:THR:HG21	1.85	0.58
2:B:708:TYR:HA	2:B:711:GLN:HG3	1.84	0.58
2:B:989:ASN:O	2:B:993:PRO:HD3	2.04	0.58
2:D:164:PRO:HB3	2:D:204:HIS:CD2	2.39	0.58
2:D:599:LEU:HD23	2:D:602:LEU:HD12	1.86	0.58
3:X:18:ASP:HB3	3:X:21:GLN:HB2	1.85	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
1:A:384:ARG:HH21	1:A:389:THR:HG21	1.67	0.57
2:B:167:PHE:HD2	2:B:172:PRO:HD3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:VAL:HG22	2:B:78:PHE:HB3	1.87	0.57
1:C:160:VAL:HB	1:C:187:GLY:HA3	1.85	0.57
1:C:44:CYS:HB2	1:C:61:LEU:HD11	1.86	0.57
2:D:535:TYR:HB2	2:D:538:LYS:O	2.05	0.57
2:D:68:LYS:HG3	2:D:121:GLU:HG2	1.85	0.57
2:D:314:LEU:HG	2:D:327:ILE:HG12	1.87	0.57
3:X:259:ILE:HG13	3:X:260:THR:HG23	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:D:741:LEU:HA	2:D:768:THR:HB	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:A:182:PRO:O	2:B:413:MET:HB2	2.04	0.57
1:C:166:LEU:HD22	1:C:202:VAL:HG21	1.86	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
1:A:166:LEU:HD22	1:A:202:VAL:HG21	1.87	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
2:B:917:GLU:O	2:B:920:LEU:HB2	2.04	0.56
2:D:996:ARG:HH11	2:D:1031:GLN:HG3	1.70	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:674:CYS:SG	2:D:767:ASN:ND2	2.77	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:B:770:LEU:O	2:B:773:PHE:N	2.39	0.56
2:D:1080:ASP:N	2:D:1101:LYS:HG2	2.21	0.56
2:B:956:VAL:O	2:B:960:VAL:HG23	2.04	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:D:912:TYR:CE2	2:D:947:ALA:HB1	2.41	0.56
1:A:242:LEU:HD13	1:A:305:PRO:HG3	1.88	0.55
2:B:237:ILE:HD13	2:B:251:MET:SD	2.46	0.55
2:B:734:LEU:HA	2:B:737:ASN:HB2	1.87	0.55
1:C:242:LEU:HD13	1:C:305:PRO:HG3	1.87	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:D:549:GLU:O	2:D:553:GLU:HG2	2.07	0.55
1:C:71:LEU:HD11	2:D:860:ARG:CZ	2.36	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
2:B:118:SER:OG	2:B:177:ALA:HB2	2.06	0.55
2:B:549:GLU:O	2:B:553:GLU:HG2	2.05	0.55
2:D:337:PRO:HG3	2:D:394:HIS:CE1	2.41	0.55
2:B:12:ASP:H	2:B:433:ILE:HG13	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
3:X:289:ARG:HH11	3:X:289:ARG:HG2	1.71	0.55
3:X:379:THR:HA	3:X:382:LEU:HG	1.88	0.55
2:D:810:ASP:O	2:D:813:THR:OG1	2.21	0.55
1:C:107:GLN:HA	2:D:860:ARG:CZ	2.36	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
2:D:177:ALA:HA	2:D:183:ILE:HG13	1.87	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: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:247:ASN:HB3	2:B:263:LEU:HB2	1.89	0.54
2:B:12:ASP:HB2	2:B:433:ILE:HG23	1.88	0.54
2:B:450:VAL:O	2:B:454:LYS:N	2.38	0.54
2:B:651:SER:O	2:B:655:ARG:HG3	2.07	0.54
1:C:21:TRP:CZ3	1:C:366:HIS:HD2	2.26	0.54
2:B:177:ALA:HA	2:B:183:ILE:HG13	1.89	0.54
1:C:384:ARG:HE	1:C:389:THR:HG21	1.71	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
2:B:313:LYS:HD2	2:B:351:LEU:HD21	1.88	0.54
2:B:669:PRO:HD2	2:B:672:PHE:CD2	2.43	0.54
1:C:384:ARG:HH21	1:C:389:THR:HG21	1.72	0.54
2:D:350:GLN:HG2	2:D:524:PHE:HB2	1.89	0.54
3:X:120:THR:O	3:X:121:THR:OG1	2.21	0.54
2:D:54:CYS:SG	2:D:55:VAL:N	2.80	0.54
1:C:55:GLY:H	1:C:384:ARG:NH1	2.06	0.54
2:D:1003:LEU:HD12	2:D:1028:TYR:CZ	2.43	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)
2:B:241:ILE:HG22	2:B:250:VAL:HB	1.89	0.54
2:B:548:ILE:HD11	2:B:687:LYS:HZ2	1.73	0.54
2:B:79:GLN:HG3	2:B:80:ASN:N	2.23	0.54
2:D:579:LEU:O	2:D:583:LEU:HG	2.08	0.54
3:X:86:SER:HB3	3:X:91:TYR:CZ	2.42	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
1:A:107:GLN:HA	2:B:860:ARG:NH2	2.22	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
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:167:PHE:HD2	2:D:172:PRO:HD3	1.72	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
2:B:185:VAL:HB	2:B:193:THR:HG22	1.91	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
3:X:267:THR:O	3:X:305:LEU:HG	2.08	0.53
1:A:11:PRO:HB2	1:A:14:VAL:HG23	1.90	0.53
2:D:12:ASP:H	2:D:433:ILE:HG13	1.73	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:B:972:LEU:HD21	2:B:1005:ARG:HD3	1.91	0.52
2:D:1109:VAL:O	2:D:1112:TYR:HB3	2.09	0.52
2:D:460:ALA:O	2:D:462:THR:N	2.41	0.52
2:B:13:LEU:HA	2:B:16:PHE:HD2	1.75	0.52
1:C:279:ARG:HB3	1:C:307:VAL:HG12	1.92	0.52
2:D:164:PRO:HG2	2:D:195:ILE:HD13	1.90	0.52
3:X:175:GLU:H	3:X:175:GLU:CD	2.13	0.52
1:A:138:ASN:HD22	1:A:161:GLY:HA2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:LEU:HD13	1:A:280:TRP:CE2	2.44	0.52
2:B:771:GLN:HB3	2:B:819:LEU:HD22	1.91	0.52
2:B:847:LEU:O	2:B:851:LYS:HG2	2.10	0.52
2:D:1066:TYR:CE1	2:D:1108:ILE:HB	2.44	0.52
3:X:23:GLU:N	3:X:23:GLU:OE1	2.43	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:B:462:THR:O	2:B:466:LEU:HG	2.09	0.52
2:D:332:ILE:HG12	2:D:388:PHE:CE2	2.44	0.52
2:D:912:TYR:CZ	2:D:947:ALA:HB1	2.44	0.52
2:B:306:HIS:ND1	2:B:308:SER:HB3	2.25	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: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:D:81:ARG:H	2:D:109:ASN:HB3	1.75	0.52
2:D:165:ILE:HD13	2:D:187:PHE:CE2	2.39	0.52
2:B:1102:LEU:HA	2:B:1105:LEU:HD12	1.91	0.52
2:B:81:ARG:H	2:B:109:ASN:HB3	1.74	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: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
1:A:83:GLU:HA	1:A:96:PRO:HA	1.92	0.52
2:B:926:LYS:NZ	2:B:930:ASP:H	2.08	0.52
2:B:953:ALA:O	2:B:955:HIS:N	2.43	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
2:B:4:LEU:HG	2:B:393:SER:OG	2.10	0.52
2:B:955:HIS:O	2:B:958:LEU:HB2	2.10	0.52
2:D:118:SER:OG	2:D:177:ALA:HB2	2.11	0.51
1:A:143:ALA:CB	1:A:192:PHE:HD2	2.23	0.51
2:D:478:ILE:HD11	2:D:501:GLU:HG2	1.91	0.51
3:X:196:GLY:O	3:X:207:ARG:NH2	2.43	0.51
2:B:164:PRO:HB3	2:B:204:HIS:NE2	2.26	0.51
2:B:650:ASP:OD1	2:B:651:SER:N	2.44	0.51
2:D:1060:THR:O	2:D:1063:ILE:HB	2.10	0.51
2:D:485:ASP:OD1	2:D:485:ASP:N	2.43	0.51
2:D:816:VAL:HG11	2:D:832:ILE:HD13	1.92	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)
1:A:130:LYS:O	1:A:134:HIS:NE2	2.41	0.51
1:A:264:ASP:OD1	1:A:264:ASP:N	2.40	0.51
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:377:LYS:HG2	2:B:393:SER:HB3	1.92	0.51
2:B:478:ILE:HD11	2:B:501:GLU:HG2	1.92	0.51
2:B:767:ASN:HB3	2:B:770:LEU:HD11	1.92	0.51
2:D:663:ASN:OD1	2:D:796:SER:OG	2.22	0.51
1:A:337:GLY:HA3	1:A:358:MET:O	2.11	0.51
1:C:264:ASP:OD1	1:C:264:ASP:N	2.42	0.51
2:D:13:LEU:HA	2:D:16:PHE:HD2	1.76	0.51
3:X:147:CYS:O	3:X:151:MET:HG2	2.11	0.51
1:A:240:LEU:HB3	1:A:241:PRO:HD3	1.92	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
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
1:A:55:GLY:H	1:A:384:ARG:NH1	2.09	0.51
2:B:1112:TYR:OH	2:D:1112:TYR:OH	2.22	0.51
2:B:1113:HIS:O	2:B:1117:LYS:HG3	2.10	0.51
2:D:998:ASP:O	2:D:1002:LEU:HG	2.11	0.51
2:D:313:LYS:HD2	2:D:351:LEU:HD21	1.93	0.51
2:B:524:PHE:CE1	2:B:531:THR:HA	2.45	0.51
1:C:7:GLN:NE2	2:D:983:LYS:HD2	2.26	0.51
2:D:65:ASN:HB2	2:D:75:TRP:CD1	2.46	0.51
2:D:828:CYS:HA	2:D:831:LEU:HB2	1.92	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:695:PHE:CE1	2:B:724:LEU:HB3	2.45	0.50
2:B:923:ASP:OD1	2:B:941:THR:OG1	2.18	0.50
1:C:162:ASP:HA	1:C:186:PRO:HB3	1.93	0.50
2:D:492:TYR:OH	2:D:496:ARG:NH2	2.45	0.50
3:X:416:HIS:CE1	3:X:432:ALA:HA	2.46	0.50
3:X:54:LEU:HD22	3:X:434:PHE:CE1	2.46	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
1:A:258:VAL:HG13	1:A:270:ALA:HB2	1.93	0.50
2:B:237:ILE:HG21	2:B:251:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:LYS:HD3	2:B:609:TYR:CE1	2.45	0.50
2:B:63:THR:OG1	2:B:521:SER:OG	2.29	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: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:546:TYR:HE1	2:B:791:HIS:CE1	2.29	0.50
2:B:859:VAL:HG12	2:B:863:LYS:HE3	1.93	0.50
1:C:40:ILE:HG23	1:C:73:LEU:HD11	1.93	0.50
2:D:642:LEU:HB3	2:D:645:PRO:HD3	1.92	0.50
2:D:723:SER:O	2:D:726:GLU:HB3	2.11	0.50
2:D:812:VAL:HG21	2:D:835:LEU:HB2	1.93	0.50
2:B:1060:THR:O	2:B:1063:ILE:HB	2.11	0.50
2:B:350:GLN:HG2	2:B:524:PHE:HB2	1.94	0.50
2:B:937:ILE:O	2:B:941:THR:OG1	2.29	0.50
2:D:422:TRP:CZ2	2:D:499:TYR:HA	2.46	0.50
2:D:636:ILE:HA	2:D:639:LEU:HD12	1.92	0.50
1:A:384:ARG:HE	1:A:389:THR:CG2	2.24	0.50
2:B:1112:TYR:HH	2:D:1112:TYR:HH	1.51	0.50
2:B:170:GLN:OE1	2:B:208:HIS:NE2	2.44	0.50
2:D:985:ASN:HA	2:D:988:LEU:HD12	1.93	0.50
1:C:258:VAL:HG13	1:C:270:ALA:HB2	1.93	0.50
2:D:676:SER:HB2	2:D:773:PHE:CE1	2.47	0.50
2:B:943:LYS:HG3	2:B:974:PHE:CZ	2.47	0.50
1:C:283:PHE:HB2	1:C:299:GLY:N	2.27	0.50
2:D:977:GLN:O	2:D:981:GLN:HG3	2.11	0.50
2:B:131:ILE:HG12	2:B:137:LEU:HD23	1.93	0.49
2:B:313:LYS:HB3	2:B:329:LYS:HD3	1.94	0.49
2:B:332:ILE:HG12	2:B:388:PHE:HE2	1.76	0.49
2:B:881:GLU:CB	2:B:901:HIS:HE1	2.25	0.49
1:C:252:ALA:HB2	2:D:826:ASN:HD22	1.77	0.49
2:D:1047:TYR:O	2:D:1050:THR:OG1	2.31	0.49
2:D:1119:VAL:O	2:D:1123:VAL:HG23	2.13	0.49
2:D:767:ASN:OD1	2:D:768:THR:N	2.44	0.49
2:D:742:LEU:HD22	2:D:826:ASN:HD21	1.77	0.49
2:B:50:PHE:CZ	2:B:442:SER:HA	2.48	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
1:C:231:ASN:ND2	2:D:491:TYR:OH	2.45	0.49
2:D:1073:LEU:HD11	2:D:1105:LEU:HD13	1.94	0.49
3:X:381:GLY:O	3:X:384:MET:HB2	2.11	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
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
3:X:83:GLN:HB3	3:X:91:TYR:CZ	2.48	0.49
1:A:283:PHE:HB2	1:A:299:GLY:N	2.27	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
3:X:363:GLY:O	3:X:422:GLN:NE2	2.35	0.49
1:A:280:TRP:CD1	1:A:305:PRO:HA	2.48	0.49
2:B:919:SER:HB2	2:B:941:THR:HG23	1.93	0.49
1:C:130:LYS:HE2	2:D:608:SER:HB3	1.95	0.49
2:D:629:PRO:HA	2:D:632:ILE:HD12	1.95	0.49
2:B:172:PRO:HA	2:B:187:PHE:HD1	1.78	0.49
2:D:1063:ILE:HG12	2:D:1112:TYR:HE1	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:115:VAL:O	2:B:116:ALA:HB3	2.12	0.49
2:B:178:ILE:HD11	2:B:182:GLU:HB2	1.95	0.49
2:B:905:LYS:O	2:B:909:GLU:HG3	2.12	0.49
2:D:939:HIS:O	2:D:942:LEU:HB2	2.12	0.49
2:D:982:GLY:O	2:D:984:ILE:N	2.46	0.49
1:A:162:ASP:HA	1:A:186:PRO:HB3	1.94	0.48
2:B:1063:ILE:HG12	2:B:1112:TYR:HE1	1.78	0.48
2:B:1120:ALA:HA	2:B:1123:VAL:HG23	1.94	0.48
2:B:422:TRP:CZ2	2:B:499:TYR:HA	2.48	0.48
2:D:524:PHE:CE1	2:D:531:THR:HA	2.47	0.48
2:B:188:PHE:O	2:B:236:THR:OG1	2.25	0.48
2:B:492:TYR:OH	2:B:496:ARG:NH2	2.46	0.48
2:B:9:VAL:HB	2:B:539:VAL:HG23	1.94	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
2:D:590:SER:O	2:D:594:GLU:HG2	2.12	0.48
1:C:12:LEU:HD22	2:D:951:PHE:HB3	1.96	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
2:D:170:GLN:OE1	2:D:208:HIS:NE2	2.46	0.48
2:D:86:PHE:HB3	2:D:101:ASN:ND2	2.22	0.48
3:X:222:MET:SD	3:X:365:LEU:HB3	2.53	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)
1:A:71:LEU:HD11	2:B:860:ARG:NH2	2.29	0.48
2:B:959:MET:SD	2:B:994:THR:HB	2.54	0.48
2:D:284:PHE:CD2	2:D:287:LEU:HD13	2.48	0.48
2:D:945:ALA:HB1	2:D:954:ALA:CB	2.43	0.48
3:X:332:ALA:HA	3:X:335:LEU:HD12	1.94	0.48
2:B:460:ALA:O	2:B:462:THR:N	2.42	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:D:492:TYR:O	2:D:495:LYS:HB3	2.14	0.48
2:B:1045:SER:HA	2:B:1048:ILE:HD12	1.96	0.48
2:B:1105:LEU:HA	2:B:1108:ILE:HG12	1.94	0.48
2:B:65:ASN:HB2	2:B:75:TRP:CD1	2.49	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
2:B:913:ILE:O	2:B:916:LEU:HB2	2.13	0.48
1:C:192:PHE:HE1	1:C:200:LEU:HD22	1.78	0.48
2:D:768:THR:O	2:D:770:LEU:N	2.47	0.48
3:X:43:PRO:O	3:X:47:GLN:NE2	2.38	0.48
2:B:1010:MET:O	2:B:1013:VAL:HG12	2.13	0.48
2:B:600:ARG:HG3	2:B:834:TRP:NE1	2.28	0.48
1:C:233:TRP:HD1	2:D:413:MET:SD	2.37	0.48
2:D:433:ILE:HG22	2:D:434:GLU:HG3	1.96	0.48
1:C:182:PRO:HB3	2:D:597:TYR:CZ	2.49	0.48
2:D:703:THR:HG23	2:D:704:SER:H	1.79	0.48
2:D:742:LEU:HB2	2:D:824:GLN:HG3	1.96	0.48
3:X:405:ILE:O	3:X:409:ILE:HG13	2.14	0.48
1:C:130:LYS:O	1:C:134:HIS:NE2	2.40	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: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:D:60:GLY:HA2	2:D:78:PHE:O	2.13	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
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:290:ASP:N	2:D:290:ASP:OD1	2.47	0.48
2:D:814:GLU:O	2:D:817:GLU:HB3	2.14	0.48
3:X:29:ARG:O	3:X:33:THR:OG1	2.18	0.48
2:B:763:LEU:HD21	2:B:774:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:975:VAL:HA	2:D:978:LEU:HB2	1.96	0.47
3:X:306:GLU:O	3:X:308:GLN:HG3	2.14	0.47
2:B:485:ASP:N	2:B:485:ASP:OD1	2.42	0.47
2:D:353:SER:HB2	2:D:361:PHE:CD2	2.49	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
1:A:40:ILE:HG23	1:A:73:LEU:HD11	1.96	0.47
2:B:1015:SER:HB3	2:B:1018:CYS:HB2	1.95	0.47
2:B:816:VAL:O	2:B:820:PHE:HB3	2.14	0.47
2:D:906:LEU:HD22	2:D:914:ASP:HB2	1.95	0.47
3:X:237:VAL:H	3:X:260:THR:HG1	1.55	0.47
2:B:207:GLN:HG3	2:B:207:GLN:O	2.14	0.47
2:B:419:SER:O	2:B:423:LEU:HD12	2.14	0.47
2:B:958:LEU:HD13	2:B:975:VAL:HG22	1.96	0.47
1:C:337:GLY:HA3	1:C:358:MET:O	2.13	0.47
2:B:1067:LEU:HD13	2:D:1116:LEU:HD22	1.95	0.47
2:B:1109:VAL:O	2:B:1112:TYR:HB3	2.14	0.47
2:B:293:THR:CG2	2:B:353:SER:H	2.27	0.47
2:B:548:ILE:CD1	2:B:687:LYS:HD2	2.44	0.47
1:C:156:VAL:HG21	1:C:214:TRP:CH2	2.50	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:636:ILE:HD13	2:D:639:LEU:HD12	1.95	0.47
2:D:935:ILE:CG2	2:D:967:LYS:HZ3	2.28	0.47
2:D:968:LYS:HA	2:D:971:LEU:HD12	1.96	0.47
1:A:39:GLY:HA2	1:A:66:THR:OG1	2.15	0.47
1:A:210:ARG:HH12	2:B:417:ASP:N	2.12	0.47
2:B:1101:LYS:O	2:B:1105:LEU:HG	2.14	0.47
2:B:284:PHE:HD2	2:B:287:LEU:HD13	1.80	0.47
2:B:632:ILE:O	2:B:636:ILE:HG12	2.14	0.47
2:D:339:ASP:O	2:D:342:ILE:HB	2.13	0.47
2:B:945:ALA:HB1	2:B:954:ALA:HB1	1.96	0.47
2:D:129:TYR:OH	2:D:180:THR:O	2.32	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:241:ILE:HG22	2:D:250:VAL:HB	1.95	0.47
2:D:826:ASN:N	2:D:826:ASN:OD1	2.43	0.47
2:D:859:VAL:HG13	2:D:918:PHE:HZ	1.79	0.47
1:A:182:PRO:HB3	2:B:597:TYR:CE2	2.49	0.47
1:A:244:ASN:HB3	1:A:246:CYS:SG	2.55	0.47
1:A:252:ALA:HB2	2:B:826:ASN:ND2	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HB3	1:A:307:VAL:HG12	1.96	0.47
2:B:673:LEU:O	2:B:677:VAL:HG23	2.15	0.47
2:D:196:ILE:HD13	2:D:205:TYR:HE2	1.80	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
1:A:195:SER:HB2	1:A:264:ASP:HA	1.96	0.47
1:A:216:LEU:HD12	1:A:216:LEU:HA	1.78	0.47
2:B:131:ILE:HG12	2:B:137:LEU:CD2	2.45	0.47
2:B:339:ASP:O	2:B:342:ILE:HB	2.15	0.47
2:B:705:GLN:O	2:B:709:GLU:HG3	2.15	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
3:X:199:LEU:HD23	3:X:203:GLY:O	2.15	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:B:284:PHE:CD2	2:B:287:LEU:HD13	2.50	0.46
2:B:466:LEU:O	2:B:470:VAL:HG23	2.14	0.46
2:B:652:LEU:HD23	2:B:655:ARG:NE	2.30	0.46
1:C:114:ILE:HG23	1:C:121:ILE:HG23	1.97	0.46
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
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: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
2:B:718:ASP:O	2:B:722:LEU:HG	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
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:B:1101:LYS:O	2:B:1104:THR:HG23	2.16	0.46
2:B:139:TYR:HB3	2:B:160:LEU:O	2.16	0.46
2:B:178:ILE:HG21	2:B:263:LEU:HD21	1.97	0.46
2:B:629:PRO:HA	2:B:632:ILE:HD12	1.98	0.46
2:B:815:LEU:HD22	2:B:819:LEU:HD11	1.97	0.46
2:B:995:LEU:O	2:B:999:VAL:HG23	2.15	0.46
1:C:192:PHE:CE1	1:C:200:LEU:HD22	2.50	0.46
2:D:1062:ILE:HG22	2:D:1066:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:289:SER:O	2:D:299:LEU:HB2	2.14	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: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
2:B:243:LEU:HD21	2:B:292:THR:HG21	1.97	0.46
1:C:143:ALA:CB	1:C:192:PHE:HD2	2.29	0.46
1:C:191:GLN:OE1	1:C:259:ARG:HD2	2.16	0.46
2:D:172:PRO:HA	2:D:187:PHE:HD1	1.80	0.46
2:D:241:ILE:CG2	2:D:250:VAL:HB	2.46	0.46
1:A:170:ARG:HD3	1:A:214:TRP:CZ3	2.51	0.46
2:B:1017:PRO:HA	2:B:1020:TYR:HD2	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: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
1:A:283:PHE:C	2:B:487:THR:HB	2.35	0.46
2:B:353:SER:HB2	2:B:361:PHE:CD2	2.51	0.46
2:B:690:VAL:O	2:B:693:GLU:HB2	2.16	0.46
1:C:11:PRO:HB2	1:C:14:VAL:HG23	1.98	0.46
1:C:384:ARG:HE	1:C:389:THR:CG2	2.29	0.46
2:D:340:GLU:HB3	2:D:342:ILE:HD13	1.98	0.46
1:C:130:LYS:HD3	2:D:609:TYR:CE1	2.51	0.46
2:D:742:LEU:HD12	2:D:827:ALA:HB2	1.98	0.46
1:A:134:HIS:HB3	2:B:605:ASP:OD1	2.16	0.46
2:B:198:ASN:HB3	2:B:201:ASP:HB3	1.96	0.46
2:B:162:TYR:HE2	2:B:204:HIS:CE1	2.34	0.46
2:B:875:GLN:HB2	2:B:879:LEU:HG	1.98	0.46
2:D:1019:TRP:CZ2	2:D:1048:ILE:HD11	2.51	0.46
2:D:1112:TYR:O	2:D:1116:LEU:HG	2.15	0.46
2:D:450:VAL:O	2:D:454:LYS:N	2.37	0.46
2:D:466:LEU:O	2:D:470:VAL:HG23	2.15	0.46
2:D:697:PHE:O	2:D:701:LEU:HG	2.16	0.46
2:D:828:CYS:O	2:D:832:ILE:HB	2.16	0.46
2:D:948:ALA:O	2:D:950:LYS:HG2	2.16	0.46
2:D:1025:SER:O	2:D:1029:LYS:HG2	2.15	0.46
2:D:1034:ARG:HH21	2:D:1076:LEU:HD22	1.81	0.46
2:D:178:ILE:HG21	2:D:263:LEU:HD21	1.97	0.46
2:D:50:PHE:CZ	2:D:442:SER:HA	2.50	0.46
2:D:512:LEU:HA	2:D:512:LEU:HD22	1.86	0.46
2:D:671:LEU:HD12	2:D:672:PHE:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:708:TYR:OH	2:D:713:LYS:HD2	2.15	0.46
2:B:832:ILE:HG13	2:B:835:LEU:HD22	1.97	0.45
1:C:322:HIS:HA	1:C:323:PRO:HD3	1.84	0.45
2:D:198:ASN:HB3	2:D:201:ASP:HB3	1.97	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:919:SER:HB2	2:D:941:THR:OG1	2.16	0.45
3:X:333:HIS:NE2	3:X:358:LEU:HD11	2.30	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:284:PHE:HD2	2:D:287:LEU:HD13	1.81	0.45
2:D:329:LYS:HB3	2:D:329:LYS:HZ2	1.82	0.45
1:A:156:VAL:HG21	1:A:214:TRP:CH2	2.51	0.45
2:B:5:LYS:HE2	2:B:549:GLU:HG3	1.97	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:815:LEU:O	2:B:819:LEU:HG	2.16	0.45
1:C:102:LEU:O	1:C:113:LEU:HD12	2.16	0.45
2:D:1104:THR:O	2:D:1108:ILE:HG23	2.17	0.45
3:X:85:SER:O	3:X:126:GLY:N	2.48	0.45
2:B:1028:TYR:O	2:B:1031:GLN:HB3	2.15	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
2:D:377:LYS:HG2	2:D:393:SER:HB3	1.97	0.45
2:D:768:THR:C	2:D:770:LEU:H	2.19	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
3:X:83:GLN:HB3	3:X:91:TYR:CE1	2.51	0.45
1:A:11:PRO:HB2	1:A:14:VAL:CG2	2.47	0.45
2:B:1044:LEU:O	2:B:1048:ILE:HG13	2.17	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
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: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
2:B:1010:MET:SD	2:B:1021:ASN:HB3	2.57	0.45
1:C:130:LYS:HD3	2:D:609:TYR:HE1	1.81	0.45
1:C:160:VAL:HG11	1:C:202:VAL:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:ILE:HG12	2:D:137:LEU:HD23	1.98	0.45
2:D:276:GLN:HB3	2:D:279:LEU:HD23	1.99	0.45
3:X:279:LEU:O	3:X:283:ILE:HG13	2.17	0.45
1:A:243:VAL:O	1:A:245:THR:OG1	2.35	0.45
2:B:81:ARG:HA	2:B:109:ASN:HA	1.98	0.45
2:D:158:TRP:H	2:D:158:TRP:HE3	1.64	0.45
2:D:668:SER:HB2	2:D:672:PHE:HD2	1.82	0.45
1:A:107:GLN:HE22	2:B:860:ARG:HG2	1.80	0.45
2:B:417:ASP:HB2	2:B:418:ILE:H	1.52	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:B:75:TRP:CE3	2:B:539:VAL:HG13	2.51	0.44
2:B:881:GLU:HB3	2:B:901:HIS:HE1	1.82	0.44
2:D:1058:GLU:O	2:D:1062:ILE:HG13	2.17	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
3:X:206:ILE:HD11	3:X:395:ALA:HB1	1.99	0.44
2:B:1103:LEU:CD1	3:X:271:GLU:H	2.29	0.44
1:A:21:TRP:CZ2	1:A:373:ALA:HB2	2.52	0.44
1:A:53:SER:O	1:A:384:ARG:HD3	2.17	0.44
2:B:340:GLU:HB3	2:B:342:ILE:HD13	2.00	0.44
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.81	0.44
1:C:212:PHE:HE1	1:C:233:TRP:CE3	2.34	0.44
2:D:28:ALA:HB1	2:D:107:PRO:HB3	1.98	0.44
2:D:12:ASP:HB2	2:D:433:ILE:CG2	2.45	0.44
2:D:436:ILE:O	2:D:440:LEU:HG	2.18	0.44
2:D:474:ILE:HG12	2:D:502:TRP:CZ2	2.52	0.44
2:D:595:ILE:HD13	2:D:696:ILE:HD11	1.98	0.44
2:B:1023:LEU:O	2:B:1026:TRP:HB3	2.18	0.44
2:B:382:LEU:HD21	2:B:389:SER:H	1.82	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:1082:TRP:CH2	2:B:1100:GLN:HG3	2.52	0.44
2:B:579:LEU:O	2:B:583:LEU:HG	2.17	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:D:196:ILE:HD13	2:D:205:TYR:CE2	2.52	0.44
2:D:97:LEU:HD21	2:D:762:ALA:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:77:ILE:HB	2:D:84:THR:OG1	2.18	0.44
2:D:940:GLU:O	2:D:944:THR:HG23	2.17	0.44
1:A:210:ARG:NH1	2:B:417:ASP:OD1	2.50	0.44
2:B:1060:THR:HG22	2:B:1063:ILE:HD12	2.00	0.44
2:B:622:HIS:O	2:B:627:VAL:HG21	2.16	0.44
1:C:280:TRP:CE2	1:C:305:PRO:HB3	2.53	0.44
1:C:236:THR:HG21	2:D:417:ASP:OD1	2.18	0.44
2:D:533:ILE:HD12	2:D:535:TYR:HE1	1.83	0.44
2:D:838:ASP:O	2:D:842:VAL:N	2.43	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:436:ILE:O	2:B:440:LEU:HG	2.17	0.44
2:B:600:ARG:HG3	2:B:834:TRP:HE1	1.82	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:1039:ILE:HG23	2:B:1083:ILE:HG13	2.00	0.44
2:B:844:LEU:HA	2:B:844:LEU:HD23	1.63	0.44
2:D:1115:GLN:O	2:D:1119:VAL:HG23	2.17	0.44
2:B:1013:VAL:HG13	2:B:1015:SER:H	1.83	0.44
2:B:385:ASP:HB3	2:B:387:SER:HB3	2.00	0.44
2:B:88:VAL:HB	2:B:671:LEU:HD23	1.99	0.44
1:C:280:TRP:CD1	1:C:305:PRO:HA	2.53	0.44
2:D:207:GLN:O	2:D:207:GLN:HG3	2.18	0.44
2:D:243:LEU:HD21	2:D:292:THR:HG21	2.00	0.44
2:D:914:ASP:O	2:D:918:PHE:HD1	2.01	0.44
3:X:205:LEU:C	3:X:207:ARG:H	2.21	0.44
3:X:245:GLN:O	3:X:248:ILE:HB	2.17	0.44
3:X:261:ALA:O	3:X:267:THR:HG23	2.18	0.44
2:B:66:LYS:CG	2:B:119:PHE:HB2	2.43	0.43
2:B:543:ARG:HB3	2:B:679:ARG:HH22	1.82	0.43
2:B:703:THR:HG23	2:B:704:SER:H	1.83	0.43
2:B:798:LEU:HA	2:B:801:ILE:HD12	2.00	0.43
2:B:871:SER:H	2:B:883:GLN:HG2	1.83	0.43
1:C:25:SER:HB2	1:C:77:SER:HA	2.00	0.43
2:D:249:LEU:HB2	2:D:261:LEU:HB3	2.00	0.43
3:X:289:ARG:HH11	3:X:289:ARG:CG	2.30	0.43
3:X:379:THR:HA	3:X:382:LEU:CG	2.48	0.43
3:X:36:TRP:HA	3:X:39:LEU:HD12	2.00	0.43
2:B:4:LEU:HA	2:B:4:LEU:HD23	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: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
1:C:252:ALA:HB2	2:D:826:ASN:HB3	2.00	0.43
2:D:301:TYR:HA	2:D:302:PRO:HD3	1.88	0.43
2:D:417:ASP:OD1	2:D:417:ASP:N	2.50	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:933:LEU:O	2:B:937:ILE:HG13	2.17	0.43
2:B:945:ALA:HB1	2:B:954:ALA:CB	2.48	0.43
2:B:955:HIS:HE1	2:B:978:LEU:HD13	1.81	0.43
2:D:131:ILE:HG12	2:D:137:LEU:CD2	2.47	0.43
2:D:651:SER:O	2:D:655:ARG:HG3	2.18	0.43
1:A:10:LEU:HG	1:A:379:SER:HA	2.01	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:178:ILE:HG13	2:B:179:SER:N	2.33	0.43
2:B:290:ASP:OD1	2:B:290:ASP:N	2.51	0.43
2:B:279:LEU:HD21	2:B:303:ASP:HA	2.00	0.43
2:B:889:TYR:CG	2:B:933:LEU:HD13	2.53	0.43
2:D:1030:HIS:HA	2:D:1034:ARG:CG	2.48	0.43
2:D:362:LEU:HD12	2:D:378:CYS:O	2.18	0.43
3:X:266:GLY:HA3	3:X:305:LEU:O	2.19	0.43
1:A:25:SER:HB2	1:A:77:SER:HA	2.01	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
2:D:173:ASP:HB2	2:D:188:PHE:CE1	2.53	0.43
2:D:978:LEU:O	2:D:982:GLY:N	2.50	0.43
1:A:322:HIS:HA	1:A:323:PRO:HD3	1.84	0.43
2:B:445:ASN:OD1	2:B:446:SER:N	2.51	0.43
2:B:988:LEU:O	2:B:991:SER:OG	2.26	0.43
1:C:39:GLY:HA2	1:C:66:THR:OG1	2.19	0.43
1:C:69:PRO:HD2	1:C:107:GLN:HB2	2.01	0.43
2:D:812:VAL:CG2	2:D:835:LEU:HB2	2.48	0.43
3:X:109:LEU:HD23	3:X:109:LEU:HA	1.88	0.43
3:X:277:GLU:H	3:X:277:GLU:CD	2.21	0.43
2:B:991:SER:O	2:B:994:THR:OG1	2.37	0.43
2:D:198:ASN:HB3	2:D:201:ASP:CB	2.49	0.43
2:D:287:LEU:HD12	2:D:346:LEU:O	2.19	0.43
2:D:329:LYS:HB3	2:D:329:LYS:NZ	2.33	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:B:245:THR:HG23	2:B:246:TYR:HD1	1.84	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:D:75:TRP:CE3	2:D:539:VAL:HG13	2.53	0.43
3:X:157:HIS:O	3:X:158:LEU:HD23	2.18	0.43
2:B:12:ASP:HB2	2:B:433:ILE:CG2	2.48	0.43
2:B:23:ALA:HA	2:B:103:LYS:O	2.18	0.43
2:D:1073:LEU:HD21	2:D:1105:LEU:HD13	2.00	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
1:A:19:THR:HG22	1:A:362:ASP:HB3	2.01	0.42
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
1:C:115:ILE:HB	1:C:123:THR:HB	2.00	0.42
2:D:11:ILE:HA	2:D:14:GLN:CD	2.40	0.42
3:X:198:GLY:O	3:X:203:GLY:N	2.52	0.42
1:A:328:TYR:CE1	1:A:343:ASN:HB2	2.54	0.42
1:A:69:PRO:HD2	1:A:107:GLN:HB2	2.00	0.42
2:B:1038:ALA:O	2:B:1041:TYR:HB2	2.18	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
2:B:380:LEU:HD23	2:B:389:SER:O	2.19	0.42
2:B:635:LEU:O	2:B:639:LEU:HG	2.19	0.42
2:D:767:ASN:HB3	2:D:770:LEU:HD21	2.01	0.42
3:X:61:ILE:O	3:X:80:TRP:HA	2.19	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:B:923:ASP:OD1	2:B:937:ILE:HG22	2.20	0.42
1:C:19:THR:HG22	1:C:362:ASP:HB3	2.01	0.42
1:C:302:ASN:O	1:C:303:LEU:HD23	2.20	0.42
2:D:235:ASN:O	2:D:235:ASN:ND2	2.47	0.42
2:D:340:GLU:HG3	2:D:340:GLU:O	2.20	0.42
2:D:603:VAL:HG13	2:D:729:ARG:HD2	2.01	0.42
2:D:79:GLN:HG3	2:D:80:ASN:N	2.35	0.42
2:D:75:TRP:O	2:D:85:ILE:HG13	2.20	0.42
2:D:98:SER:O	2:D:99:LYS:HD3	2.19	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:B:1014:GLU:HG3	2:B:1014:GLU:O	2.18	0.42
2:B:276:GLN:HB3	2:B:279:LEU:HD23	2.00	0.42
2:B:421:ILE:H	2:B:421:ILE:HG13	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:PRO:HB3	2:B:597:TYR:CZ	2.55	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
2:D:59:ALA:O	2:D:536:ALA:HB1	2.20	0.42
3:X:429:ALA:O	3:X:432:ALA:N	2.52	0.42
3:X:93:GLY:HA3	3:X:127:GLY:O	2.18	0.42
2:B:1113:HIS:HA	2:B:1116:LEU:CD1	2.50	0.42
2:B:162:TYR:HE2	2:B:204:HIS:HE1	1.66	0.42
2:B:797:SER:OG	2:B:798:LEU:N	2.52	0.42
2:D:1068:ILE:O	2:D:1072:THR:HG23	2.19	0.42
2:D:81:ARG:HA	2:D:109:ASN:HA	2.01	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
1:A:299:GLY:N	2:B:489:TYR:HH	2.18	0.42
2:B:823:LYS:HB3	2:B:824:GLN:H	1.62	0.42
1:C:21:TRP:CZ2	1:C:373:ALA:HB2	2.54	0.42
2:D:178:ILE:HD11	2:D:182:GLU:HB2	2.01	0.42
3:X:134:ASP:HA	3:X:135:PRO:HD3	1.88	0.42
3:X:217:TYR:O	3:X:220:GLU:HB3	2.19	0.42
2:B:233:SER:O	2:B:235:ASN:N	2.51	0.42
2:B:698:LEU:HD23	2:B:698:LEU:HA	1.91	0.42
2:B:6:HIS:CE1	2:B:375:ILE:HD12	2.55	0.42
2:B:926:LYS:HZ3	2:B:930:ASP:HB2	1.85	0.42
2:D:1069:VAL:O	2:D:1073:LEU:HG	2.19	0.42
2:D:143:SER:O	2:D:146:TRP:HB3	2.20	0.42
2:D:956:VAL:O	2:D:960:VAL:HG23	2.19	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
2:B:271:THR:C	2:B:272:ILE:HD12	2.40	0.42
2:B:731:VAL:O	2:B:734:LEU:HB2	2.19	0.42
2:D:1056:LYS:HE2	2:D:1122:GLN:OE1	2.19	0.42
2:D:423:LEU:HD11	2:D:471:LEU:HG	2.01	0.42
2:D:681:LEU:HD12	2:D:738:SER:OG	2.20	0.42
3:X:281:ARG:NE	3:X:299:GLU:OE2	2.53	0.42
2:B:798:LEU:HD23	2:B:801:ILE:HD12	2.01	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: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
2:D:279:LEU:HD11	2:D:303:ASP:H	1.83	0.42
3:X:192:CYS:HB2	3:X:387:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:292:ARG:HB2	3:X:295:ASP:CG	2.40	0.42
3:X:297:ALA:HA	3:X:302:LEU:HB2	2.02	0.42
1:A:107:GLN:HA	2:B:860:ARG:CZ	2.50	0.41
2:B:100:PHE:CE1	2:B:147:PHE:HA	2.45	0.41
2:B:367:TRP:O	2:B:373:THR:HG23	2.20	0.41
2:B:420:GLU:O	2:B:424:GLN:HG3	2.20	0.41
2:B:768:THR:OG1	2:B:769:ALA:N	2.53	0.41
1:C:237:LEU:HD13	1:C:280:TRP:CD2	2.55	0.41
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:D:521:SER:O	2:D:534:ASN:HB2	2.20	0.41
2:B:106:PHE:HB3	2:B:107:PRO:HD2	2.02	0.41
2:B:1107:ALA:O	2:B:1110:ALA:HB3	2.20	0.41
2:B:1111:GLU:HA	2:B:1114:LEU:HD12	2.02	0.41
2:B:1112:TYR:O	2:B:1116:LEU:HG	2.20	0.41
2:B:990:TYR:O	2:B:993:PRO:HD2	2.20	0.41
1:C:143:ALA:HB3	1:C:192:PHE:HD2	1.85	0.41
1:C:326:MET:HB3	1:C:326:MET:HE2	1.89	0.41
2:D:581:ARG:HG3	2:D:693:GLU:OE2	2.19	0.41
3:X:20:ASN:O	3:X:22:THR:N	2.50	0.41
3:X:21:GLN:HB3	3:X:24:PHE:HB3	2.01	0.41
3:X:50:LEU:O	3:X:53:ARG:HB2	2.19	0.41
3:X:97:PHE:CE2	3:X:146:PHE:HE2	2.38	0.41
1:A:160:VAL:HG11	1:A:202:VAL:HG13	2.01	0.41
2:B:1100:GLN:HB3	2:B:1104:THR:CG2	2.50	0.41
2:B:1112:TYR:CZ	2:B:1116:LEU:HD21	2.56	0.41
2:B:961:LEU:HA	2:B:961:LEU:HD22	1.85	0.41
1:C:53:SER:O	1:C:384:ARG:HD3	2.19	0.41
2:D:1064:GLU:HA	2:D:1067:LEU:HG	2.01	0.41
3:X:260:THR:HG21	3:X:310:PRO:HB3	2.02	0.41
2:B:1082:TRP:CZ2	3:X:305:LEU:HD22	2.50	0.41
2:B:1081:THR:O	2:B:1101:LYS:NZ	2.54	0.41
2:B:481:GLU:HB3	2:B:493:GLU:OE1	2.20	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:1042:GLU:O	2:D:1045:SER:OG	2.21	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:B:196:ILE:HD13	2:B:205:TYR:HE2	1.84	0.41
2:B:329:LYS:NZ	2:B:329:LYS:HB3	2.35	0.41
2:B:847:LEU:O	2:B:850:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:5:LYS:HE2	2:D:549:GLU:HG3	2.01	0.41
2:D:602:LEU:HD22	2:D:606:LEU:HD22	2.03	0.41
2:D:772:PHE:HD1	2:D:815:LEU:HD21	1.86	0.41
2:B:143:SER:O	2:B:146:TRP:HB3	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
3:X:286:LYS:HA	3:X:286:LYS:HD2	1.72	0.41
1:A:191:GLN:O	1:A:201:ILE:HG22	2.21	0.41
2:B:1063:ILE:HG12	2:B:1112:TYR:CE1	2.56	0.41
2:B:279:LEU:HD11	2:B:303:ASP:H	1.84	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
1:A:236:THR:HG21	2:B:417:ASP:OD1	2.20	0.41
2:B:423:LEU:HD11	2:B:471:LEU:HG	2.02	0.41
2:B:708:TYR:HA	2:B:711:GLN:CG	2.50	0.41
1:C:64:ILE:HG12	1:C:119:GLU:HA	2.02	0.41
1:C:210:ARG:HH12	2:D:417:ASP:H	1.68	0.41
1:C:244:ASN:HB3	1:C:246:CYS:SG	2.61	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: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:407:PHE:CG	2:B:422:TRP:CH2	3.09	0.41
2:D:242:PHE:HD1	2:D:249:LEU:HD13	1.85	0.41
2:D:4:LEU:HA	2:D:4:LEU:HD23	1.91	0.41
3:X:216:VAL:O	3:X:230:PHE:HE2	2.03	0.41
3:X:98:HIS:CG	3:X:99:PRO:HD2	2.55	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:718:ASP:O	2:D:722:LEU:HG	2.21	0.41
2:D:847:LEU:HA	2:D:847:LEU:HD23	1.89	0.41
2:D:471:LEU:HD23	2:D:471:LEU:HA	1.75	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
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
2:B:846:ALA:HB1	2:B:862:PHE:CZ	2.56	0.41
2:B:83:LEU:HG	2:B:84:THR:N	2.36	0.41
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:D:84:THR:HG22	2:D:103:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:199:LEU:HD23	3:X:203:GLY:C	2.41	0.41
3:X:245:GLN:HG3	3:X:245:GLN:H	1.62	0.41
1:A:143:ALA:HB3	1:A:192:PHE:CD2	2.57	0.40
1:A:51:PRO:O	1:A:53:SER:N	2.45	0.40
2:B:1112:TYR:CE2	2:B:1116:LEU:HD11	2.57	0.40
2:B:875:GLN:OE1	2:B:879:LEU:HG	2.21	0.40
1:C:182:PRO:O	2:D:413:MET:HB2	2.22	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:B:362:LEU:HD12	2:B:378:CYS:O	2.21	0.40
2:D:165:ILE:HG21	2:D:187:PHE:HZ	1.85	0.40
2:D:724:LEU:O	2:D:727:ASP:HB2	2.21	0.40
2:D:849:TYR:HB3	2:D:858:ALA:HB2	2.03	0.40
3:X:333:HIS:O	3:X:336:ILE:HB	2.20	0.40
3:X:416:HIS:HB2	3:X:428:GLY:HA2	2.02	0.40
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.97	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
1:C:200:LEU:HD23	1:C:214:TRP:CD1	2.57	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:C:182:PRO:HB3	2:D:597:TYR:CE2	2.57	0.40
1:A:127:LEU:HD23	1:A:127:LEU:HA	1.94	0.40
2:B:548:ILE:O	2:B:552:ASP:HB2	2.21	0.40
2:B:733:PHE:HA	2:B:834:TRP:CZ3	2.56	0.40
2:B:926:LYS:NZ	2:B:933:LEU:HD23	2.35	0.40
2:B:962:SER:HB3	2:B:971:LEU:HD11	2.03	0.40
2:B:995:LEU:HA	2:B:995:LEU:HD23	1.87	0.40
2:D:178:ILE:HG13	2:D:179:SER:N	2.36	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:7:LEU:O	3:X:10:PHE:HB3	2.22	0.40
3:X:257:ARG:HG3	3:X:257:ARG:O	2.20	0.40
3:X:26:GLN:O	3:X:30:GLU:HG3	2.20	0.40
1:A:212:PHE:CE1	1:A:233:TRP:CE3	3.08	0.40
1:A:56:LEU:HB2	1:A:371:HIS:NE2	2.37	0.40
2:B:1105:LEU:O	2:B:1108:ILE:HG12	2.22	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:102:ASN:OD1	3:X:105:ILE:N	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:X:289:ARG:HB3	3:X:290:ASP:H	1.51	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%)	41	77
1	C	336/394 (85%)	319 (95%)	16 (5%)	1 (0%)	41	77
2	B	1006/1139 (88%)	869 (86%)	117 (12%)	20 (2%)	7	38
2	D	951/1139 (84%)	821 (86%)	108 (11%)	22 (2%)	6	34
3	X	440/450 (98%)	420 (96%)	17 (4%)	3 (1%)	22	63
All	All	3068/3516 (87%)	2744 (89%)	277 (9%)	47 (2%)	10	46

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%)	15	40
1	C	300/345 (87%)	280 (93%)	20 (7%)	16	41
2	B	940/1050 (90%)	859 (91%)	81 (9%)	10	32
2	D	897/1050 (85%)	828 (92%)	69 (8%)	13	37
3	X	347/354 (98%)	330 (95%)	17 (5%)	25	50
All	All	2783/3144 (88%)	2575 (92%)	208 (8%)	13	38

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%)	3.79	268 (78%) 0 0	358, 705, 903, 929	0
1	C	344/394 (87%)	7.37	315 (91%) 0 0	5, 817, 978, 997	0
2	B	1022/1139 (89%)	2.96	650 (63%) 0 0	273, 650, 901, 955	0
2	D	977/1139 (85%)	2.77	500 (51%) 0 1	298, 714, 927, 984	0
3	X	442/450 (98%)	1.53	121 (27%) 0 2	219, 451, 760, 881	0
All	All	3128/3516 (88%)	3.27	1854 (59%) 0 0	5, 667, 929, 997	0

All (1854) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	ILE	29.6
1	C	33	ALA	22.1
1	C	102	LEU	21.8
1	C	65	GLN	21.3
1	C	66	THR	20.2
1	C	40	ILE	19.4
1	C	321	PRO	19.3
1	C	64	ILE	18.9
2	D	715	ALA	18.2
1	C	62	PHE	18.2
2	D	716	GLY	18.1
1	C	20	THR	18.1
1	C	320	CYS	17.8
1	C	32	LEU	17.8
1	C	63	THR	17.2
1	C	34	ILE	17.0
1	C	171	LEU	16.9
1	C	155	GLN	16.8
2	B	487	THR	16.7
1	C	167	ILE	16.2

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Mol	Chain	Res	Type	RSRZ
1	C	41	THR	16.1
1	C	172	THR	15.9
2	D	1080	ASP	15.9
1	C	113	LEU	15.9
1	C	43	TYR	15.7
1	C	364	CYS	15.5
1	C	60	GLU	15.0
2	D	706	GLN	15.0
1	C	45	ALA	14.9
1	C	19	THR	14.8
1	C	262	GLY	14.6
1	C	83	GLU	14.6
1	C	96	PRO	14.5
1	C	159	SER	14.3
1	A	299	GLY	14.3
1	C	173	ASP	14.2
1	C	261	ILE	14.1
2	D	288	THR	14.1
1	C	67	GLY	14.0
2	B	928	THR	13.8
1	C	363	PHE	13.8
2	D	717	CYS	13.5
1	C	7	GLN	13.3
1	C	21	TRP	13.0
1	C	61	LEU	13.0
1	C	44	CYS	12.9
1	C	322	HIS	12.9
2	D	700	SER	12.9
1	C	358	MET	12.7
2	D	1038	ALA	12.5
1	C	98	TYR	12.4
1	C	143	ALA	12.4
2	B	172	PRO	12.4
1	C	124	GLN	12.3
1	C	170	ARG	12.3
1	C	100	LEU	12.2
1	C	42	ILE	12.2
1	C	118	ASN	12.2
2	D	704	SER	12.2
1	C	24	GLN	12.2
1	C	50	THR	12.2
1	C	79	CYS	12.2

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Mol	Chain	Res	Type	RSRZ
2	D	705	GLN	12.2
1	C	125	HIS	12.1
1	C	77	SER	12.1
2	D	1076	LEU	12.0
1	C	56	LEU	12.0
1	C	46	SER	12.0
1	C	47	GLU	12.0
1	C	144	ASP	11.9
1	C	357	GLY	11.8
2	B	488	GLY	11.7
2	D	487	THR	11.7
1	C	259	ARG	11.6
1	C	48	GLU	11.6
1	C	154	GLU	11.6
2	D	646	MET	11.4
1	A	253	SER	11.4
1	C	359	PRO	11.4
2	D	107	PRO	11.4
1	C	30	ASN	11.4
1	C	5	SER	11.3
2	B	335	SER	11.3
1	C	382	LEU	11.3
1	A	300	PRO	11.2
1	C	373	ALA	11.1
1	C	74	SER	11.0
1	A	82	SER	11.0
1	C	179	ALA	11.0
1	C	57	THR	10.9
2	D	718	ASP	10.8
1	C	264	ASP	10.8
1	C	51	PRO	10.8
1	C	53	SER	10.7
2	B	930	ASP	10.7
1	C	52	GLY	10.6
1	C	101	PHE	10.6
1	C	82	SER	10.6
2	B	87	ASP	10.6
2	B	537	ASN	10.5
1	C	76	SER	10.5
2	D	1039	ILE	10.4
2	D	949	GLY	10.4
1	C	59	GLN	10.3

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Mol	Chain	Res	Type	RSRZ
1	C	168	ILE	10.2
1	C	362	ASP	10.2
2	D	417	ASP	10.2
2	D	410	PRO	10.2
1	C	175	GLY	10.1
2	B	180	THR	10.1
2	D	983	LYS	10.1
2	D	240	MET	10.1
1	C	6	ASN	10.0
1	C	97	VAL	10.0
1	A	30	ASN	10.0
2	D	239	SER	10.0
1	C	269	LEU	10.0
2	D	1041	TYR	9.9
1	C	202	VAL	9.9
1	C	374	ILE	9.9
1	C	78	SER	9.9
1	C	177	ILE	9.8
1	C	81	TYR	9.8
2	D	986	GLN	9.8
1	C	11	PRO	9.8
2	D	1035	ASP	9.7
1	C	239	THR	9.7
1	C	55	GLY	9.7
2	D	707	ASP	9.7
2	D	1040	ILE	9.7
1	C	58	LEU	9.7
2	D	1075	LEU	9.6
2	D	698	LEU	9.6
1	C	103	ALA	9.5
2	D	1037	ALA	9.5
1	C	176	PRO	9.5
2	B	448	SER	9.5
2	B	867	LEU	9.5
1	C	323	PRO	9.5
1	C	119	GLU	9.5
2	D	1074	GLU	9.4
1	C	112	ARG	9.4
1	A	23	SER	9.4
1	C	156	VAL	9.4
1	C	104	CYS	9.4
1	C	209	ILE	9.3

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Mol	Chain	Res	Type	RSRZ
1	A	302	ASN	9.3
1	C	361	VAL	9.3
2	B	8	VAL	9.3
1	A	98	TYR	9.3
2	B	238	ILE	9.3
1	C	325	TYR	9.3
1	A	81	TYR	9.3
1	C	180	GLY	9.3
2	B	50	PHE	9.2
1	C	383	THR	9.2
2	D	647	ARG	9.2
2	D	1042	GLU	9.2
2	B	926	LYS	9.2
1	C	330	ALA	9.1
1	C	75	PHE	9.1
2	B	705	GLN	9.1
2	B	113	ASP	9.1
2	D	1079	GLU	9.1
1	C	365	TRP	9.1
2	D	711	GLN	9.0
1	C	166	LEU	9.0
1	C	49	GLN	8.9
1	C	360	ILE	8.9
1	C	115	ILE	8.9
1	C	381	LEU	8.8
2	B	893	ASN	8.8
1	C	145	VAL	8.8
2	B	536	ALA	8.8
1	C	157	ILE	8.8
1	C	212	PHE	8.8
1	C	267	GLY	8.7
2	B	706	GLN	8.7
1	A	173	ASP	8.6
1	C	263	SER	8.6
2	D	1026	TRP	8.5
1	C	80	SER	8.5
2	D	946	CYS	8.5
1	C	376	THR	8.5
2	B	447	SER	8.5
2	D	703	THR	8.4
1	C	158	ALA	8.4
2	D	1044	LEU	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	31	LEU	8.4
1	C	372	LEU	8.4
1	A	24	GLN	8.4
1	C	16	PRO	8.3
2	B	449	GLN	8.3
1	C	377	GLU	8.3
2	B	489	TYR	8.3
1	C	54	THR	8.3
2	D	1073	LEU	8.3
2	D	712	SER	8.3
1	C	253	SER	8.3
1	C	238	ASN	8.3
2	D	696	ILE	8.3
2	B	950	LYS	8.2
2	D	702	ILE	8.2
2	B	173	ASP	8.2
2	D	955	HIS	8.2
2	D	1072	THR	8.2
1	C	25	SER	8.2
1	C	174	GLU	8.2
2	D	29	LEU	8.2
2	D	713	LYS	8.2
2	D	1003	LEU	8.2
1	A	96	PRO	8.2
1	A	83	GLU	8.1
1	A	97	VAL	8.1
2	B	208	HIS	8.1
2	D	991	SER	8.1
1	C	326	MET	8.1
2	B	482	PRO	8.1
2	D	287	LEU	8.0
2	D	28	ALA	8.0
2	D	1019	TRP	8.0
2	B	450	VAL	8.0
2	D	701	LEU	8.0
2	D	627	VAL	8.0
1	C	317	LEU	8.0
1	C	9	GLN	8.0
1	A	43	TYR	8.0
1	A	281	ASN	8.0
1	C	197	PRO	7.9
1	C	319	ALA	7.9

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Mol	Chain	Res	Type	RSRZ
1	C	141	ASP	7.9
2	D	709	GLU	7.9
2	B	477	THR	7.9
1	A	118	ASN	7.9
2	B	929	ASP	7.9
1	A	29	SER	7.9
1	C	270	ALA	7.9
2	D	947	ALA	7.9
1	C	194	PRO	7.9
2	D	648	ASP	7.8
2	D	645	PRO	7.8
2	D	1077	PRO	7.8
1	C	123	THR	7.8
2	B	520	LEU	7.8
2	B	114	GLY	7.8
1	C	39	GLY	7.8
1	C	249	SER	7.8
2	B	266	ASN	7.8
2	B	481	GLU	7.8
2	D	958	LEU	7.8
1	C	152	LEU	7.8
1	C	107	GLN	7.7
2	B	6	HIS	7.7
1	C	151	ARG	7.7
1	A	301	LYS	7.7
1	A	141	ASP	7.7
2	D	1071	ASN	7.7
1	C	195	SER	7.6
1	C	237	LEU	7.6
1	C	149	ASP	7.6
2	B	991	SER	7.6
2	D	605	ASP	7.6
1	C	371	HIS	7.6
2	D	1022	ILE	7.6
1	C	375	ALA	7.6
2	B	789	PRO	7.6
2	B	7	ALA	7.5
1	C	356	LEU	7.5
2	D	1043	LYS	7.5
2	B	72	THR	7.5
2	D	1064	GLU	7.5
2	D	27	PRO	7.5

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Mol	Chain	Res	Type	RSRZ
2	D	1021	ASN	7.5
1	C	10	LEU	7.4
1	C	268	ILE	7.4
2	B	955	HIS	7.4
1	C	71	LEU	7.4
2	B	334	PRO	7.4
2	D	1020	TYR	7.4
1	C	99	SER	7.4
2	B	866	SER	7.3
2	D	708	TYR	7.3
1	C	142	ILE	7.3
2	B	59	ALA	7.3
2	D	347	SER	7.3
1	C	126	VAL	7.3
1	C	366	HIS	7.3
1	C	153	ALA	7.3
2	B	552	ASP	7.3
1	A	107	GLN	7.3
1	C	169	TRP	7.2
2	B	241	ILE	7.2
2	D	286	TYR	7.2
1	C	15	ARG	7.2
2	B	587	MET	7.2
2	D	626	ASN	7.2
1	C	150	ASN	7.2
2	B	485	ASP	7.1
1	C	117	LYS	7.1
1	C	213	ASP	7.1
1	C	324	ARG	7.1
1	C	13	ASN	7.1
2	B	282	GLN	7.0
1	C	210	ARG	7.0
1	A	358	MET	7.0
1	C	252	ALA	7.0
2	D	176	ALA	7.0
1	A	74	SER	7.0
1	C	214	TRP	7.0
1	A	261	ILE	7.0
2	D	714	PHE	7.0
2	B	337	PRO	7.0
1	C	250	GLY	7.0
1	A	34	ILE	7.0

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Mol	Chain	Res	Type	RSRZ
2	B	889	TYR	7.0
2	B	74	ARG	7.0
2	D	950	LYS	6.9
2	B	517	ASP	6.9
2	B	239	SER	6.9
1	C	380	VAL	6.9
2	B	242	PHE	6.9
2	B	338	ASP	6.9
2	B	451	SER	6.9
2	B	71	GLN	6.9
1	C	23	SER	6.9
2	D	174	LEU	6.9
2	D	710	LEU	6.8
2	B	142	LEU	6.8
1	C	211	ILE	6.8
2	D	476	SER	6.8
1	A	205	ARG	6.8
1	A	174	GLU	6.8
1	C	266	SER	6.8
2	D	628	ASP	6.8
3	X	293	VAL	6.8
1	C	116	THR	6.7
1	A	388	PHE	6.7
2	D	185	VAL	6.7
1	A	357	GLY	6.7
1	A	366	HIS	6.7
2	B	515	PHE	6.7
1	C	203	GLY	6.7
2	B	539	VAL	6.7
2	B	700	SER	6.7
2	D	1000	ASP	6.7
1	C	178	LEU	6.7
2	B	86	PHE	6.6
2	D	186	SER	6.6
1	A	239	THR	6.6
2	D	649	ILE	6.6
2	B	375	ILE	6.6
2	D	289	SER	6.6
1	C	281	ASN	6.5
1	C	384	ARG	6.5
1	C	231	ASN	6.5
1	C	316	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	368	ASP	6.5
2	B	376	GLN	6.5
1	C	205	ARG	6.5
2	D	721	PHE	6.5
2	D	1031	GLN	6.5
1	A	144	ASP	6.5
1	C	329	PHE	6.5
2	B	479	GLN	6.5
2	B	572	GLU	6.5
2	B	1080	ASP	6.5
1	A	329	PHE	6.5
1	C	260	TRP	6.5
2	D	609	TYR	6.5
2	D	845	LYS	6.4
2	B	540	ALA	6.4
2	B	457	LYS	6.4
1	C	38	THR	6.4
1	C	378	GLY	6.4
1	C	18	THR	6.4
1	A	283	PHE	6.4
1	C	201	ILE	6.4
2	B	152	ALA	6.4
2	B	516	GLY	6.4
3	X	302	LEU	6.3
2	B	1019	TRP	6.3
2	B	670	SER	6.3
2	B	525	ASP	6.3
2	D	1025	SER	6.3
2	D	134	ALA	6.3
1	C	111	VAL	6.3
2	B	788	SER	6.3
2	D	1067	LEU	6.3
1	A	254	SER	6.3
2	B	454	LYS	6.3
1	A	262	GLY	6.3
1	C	12	LEU	6.3
1	C	73	LEU	6.3
2	B	486	LEU	6.3
2	B	63	THR	6.2
2	B	347	SER	6.2
3	X	344	ALA	6.2
1	C	181	TYR	6.2

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Mol	Chain	Res	Type	RSRZ
2	B	927	GLU	6.2
2	D	1036	ALA	6.2
3	X	310	PRO	6.2
2	D	1004	GLU	6.2
1	C	146	TYR	6.2
2	B	374	VAL	6.2
2	B	126	THR	6.2
2	D	988	LEU	6.2
2	B	519	ILE	6.2
1	C	215	THR	6.1
1	A	28	CYS	6.1
1	A	150	ASN	6.1
1	A	45	ALA	6.1
2	D	945	ALA	6.1
2	D	948	ALA	6.1
2	B	252	LEU	6.1
2	D	1069	VAL	6.1
2	D	418	ILE	6.1
2	B	23	ALA	6.1
1	A	152	LEU	6.1
1	A	25	SER	6.1
1	C	22	CYS	6.1
1	A	234	LEU	6.1
2	D	695	PHE	6.1
2	B	493	GLU	6.1
2	D	184	CYS	6.1
1	A	104	CYS	6.1
1	A	374	ILE	6.1
2	D	251	MET	6.1
2	D	942	LEU	6.1
2	B	88	VAL	6.0
2	B	570	LEU	6.0
2	B	97	LEU	6.0
2	B	432	SER	6.0
2	B	151	ASP	6.0
1	A	367	GLN	6.0
3	X	303	VAL	6.0
1	C	234	LEU	6.0
1	C	8	TYR	6.0
1	A	72	HIS	6.0
1	A	322	HIS	6.0
1	A	31	LEU	6.0

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Mol	Chain	Res	Type	RSRZ
2	B	112	LYS	6.0
2	B	240	MET	6.0
2	B	996	ARG	6.0
2	D	1023	LEU	6.0
1	A	365	TRP	6.0
2	D	912	TYR	6.0
1	A	55	GLY	5.9
2	D	419	SER	5.9
2	B	870	TYR	5.9
1	A	356	LEU	5.9
1	C	280	TRP	5.9
1	A	350	ASN	5.9
2	D	833	GLY	5.9
2	D	1070	LEU	5.9
1	A	50	THR	5.9
2	D	408	ASP	5.9
1	A	340	GLN	5.9
2	B	62	TYR	5.9
2	D	1028	TYR	5.9
2	B	518	GLU	5.9
2	D	1045	SER	5.9
1	A	33	ALA	5.8
1	A	32	LEU	5.8
2	B	395	SER	5.8
2	B	484	SER	5.8
2	D	1007	ALA	5.8
2	D	1078	LYS	5.8
2	B	1076	LEU	5.8
2	D	173	ASP	5.8
3	X	268	VAL	5.8
2	B	175	MET	5.8
1	C	17	TYR	5.8
1	C	200	LEU	5.8
2	B	93	LYS	5.8
2	B	237	ILE	5.8
2	D	957	ALA	5.8
2	D	1046	ARG	5.8
2	D	921	LEU	5.8
2	D	954	ALA	5.8
2	B	1082	TRP	5.8
1	A	100	LEU	5.8
2	B	61	VAL	5.7

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Mol	Chain	Res	Type	RSRZ
2	D	963	THR	5.7
2	B	535	TYR	5.7
1	C	236	THR	5.7
1	C	131	SER	5.7
1	C	127	LEU	5.7
2	D	241	ILE	5.7
2	D	1034	ARG	5.7
1	C	105	VAL	5.7
2	D	990	TYR	5.7
2	B	933	LEU	5.7
2	B	171	LYS	5.7
2	D	356	GLY	5.7
1	C	72	HIS	5.7
2	B	1035	ASP	5.7
1	C	265	GLY	5.7
1	A	308	GLN	5.7
2	B	170	GLN	5.7
2	B	169	ASN	5.6
1	C	368	ASP	5.6
1	C	29	SER	5.6
2	B	886	ALA	5.6
2	B	532	TYR	5.6
1	C	130	LYS	5.6
2	B	146	TRP	5.6
2	D	1100	GLN	5.6
2	B	431	THR	5.6
1	A	56	LEU	5.6
1	A	362	ASP	5.6
2	B	554	GLU	5.6
1	A	143	ALA	5.6
2	D	486	LEU	5.6
1	C	35	GLY	5.6
1	A	377	GLU	5.6
3	X	274	PHE	5.5
2	D	26	VAL	5.5
1	A	369	GLY	5.5
2	D	193	THR	5.5
1	C	258	VAL	5.5
2	B	135	ARG	5.5
1	A	58	LEU	5.5
2	B	584	HIS	5.5
2	D	1124	THR	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	344	THR	5.5
2	B	26	VAL	5.5
2	D	1047	TYR	5.5
2	D	1048	ILE	5.4
1	C	14	VAL	5.4
2	B	183	ILE	5.4
2	B	998	ASP	5.4
1	A	279	ARG	5.4
2	B	453	ASN	5.4
2	B	1034	ARG	5.4
3	X	271	GLU	5.4
1	A	52	GLY	5.4
1	A	341	LEU	5.4
1	C	379	SER	5.4
2	D	657	ARG	5.4
2	D	856	VAL	5.4
1	C	208	ASN	5.4
2	B	54	CYS	5.4
2	B	882	PHE	5.4
2	B	446	SER	5.4
2	B	1071	ASN	5.4
1	A	26	PRO	5.4
2	D	1006	LYS	5.4
1	A	269	LEU	5.4
1	C	232	PRO	5.4
3	X	367	ALA	5.4
1	A	60	GLU	5.3
1	A	252	ALA	5.3
2	D	1126	GLU	5.3
1	A	145	VAL	5.3
1	C	283	PHE	5.3
2	B	1081	THR	5.3
2	D	195	ILE	5.3
2	D	520	LEU	5.3
2	D	285	PRO	5.3
1	A	266	SER	5.3
1	C	389	THR	5.3
1	C	28	CYS	5.3
1	A	211	ILE	5.3
2	B	410	PRO	5.2
2	B	195	ILE	5.2
2	D	488	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	650	ASP	5.2
2	B	527	SER	5.2
2	B	704	SER	5.2
2	D	953	ALA	5.2
1	C	70	THR	5.2
1	C	385	LEU	5.2
1	C	251	ILE	5.2
2	B	280	PRO	5.2
1	A	140	ILE	5.2
2	B	514	HIS	5.2
2	B	528	ASN	5.2
2	B	553	GLU	5.2
1	A	99	SER	5.2
1	A	307	VAL	5.2
1	A	325	TYR	5.2
1	A	51	PRO	5.1
2	B	176	ALA	5.1
2	B	247	ASN	5.1
2	B	286	TYR	5.1
2	D	668	SER	5.1
2	D	172	PRO	5.1
2	B	586	CYS	5.1
1	A	282	LEU	5.1
1	A	375	ALA	5.1
2	D	854	GLU	5.1
2	B	70	SER	5.1
3	X	260	THR	5.1
2	B	263	LEU	5.1
2	D	1032	ASN	5.1
1	A	112	ARG	5.1
2	D	992	MET	5.1
2	B	473	SER	5.1
2	B	834	TRP	5.1
2	D	519	ILE	5.1
1	A	15	ARG	5.1
2	B	709	GLU	5.1
2	D	1002	LEU	5.1
1	A	151	ARG	5.0
1	A	116	THR	5.0
1	A	263	SER	5.0
2	D	1068	ILE	5.0
2	D	348	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	344	TRP	5.0
2	D	175	MET	5.0
2	D	151	ASP	5.0
1	A	342	ILE	5.0
2	B	668	SER	5.0
1	A	21	TRP	5.0
2	B	3	GLU	5.0
2	B	1079	GLU	5.0
1	C	134	HIS	5.0
2	D	1063	ILE	5.0
2	B	60	GLY	5.0
2	D	1024	PHE	5.0
3	X	300	PHE	5.0
2	B	144	LYS	5.0
2	B	948	ALA	5.0
2	B	251	MET	5.0
1	A	319	ALA	4.9
3	X	226	HIS	4.9
2	B	150	PRO	4.9
2	B	174	LEU	4.9
2	D	939	HIS	4.9
2	B	444	GLN	4.9
1	A	106	CYS	4.9
2	B	533	ILE	4.9
1	A	328	TYR	4.9
2	B	125	THR	4.9
2	B	397	ASP	4.9
2	D	968	LYS	4.9
1	C	128	GLY	4.9
2	D	525	ASP	4.9
2	B	386	GLU	4.9
2	D	97	LEU	4.9
1	C	386	MET	4.9
1	C	354	ILE	4.9
2	B	949	GLY	4.9
2	B	440	LEU	4.9
2	D	759	THR	4.9
2	D	719	LYS	4.9
1	A	249	SER	4.9
1	C	216	LEU	4.9
2	B	954	ALA	4.9
2	D	1011	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
2	D	989	ASN	4.9
2	B	181	SER	4.8
3	X	368	PRO	4.8
1	A	175	GLY	4.8
1	C	132	GLY	4.8
2	B	1024	PHE	4.8
2	B	133	HIS	4.8
2	D	415	SER	4.8
2	B	483	ASN	4.8
2	B	932	ASP	4.8
2	D	938	THR	4.8
2	B	394	HIS	4.8
2	D	985	ASN	4.8
1	A	138	ASN	4.8
2	B	994	THR	4.8
2	D	832	ILE	4.8
2	D	1065	HIS	4.8
2	B	478	ILE	4.8
1	C	191	GLN	4.8
2	B	367	TRP	4.8
2	B	946	CYS	4.8
1	C	279	ARG	4.8
2	B	19	GLU	4.8
2	B	1075	LEU	4.8
2	B	707	ASP	4.8
2	B	1100	GLN	4.8
3	X	258	VAL	4.7
2	B	109	ASN	4.7
3	X	371	ALA	4.7
1	A	131	SER	4.7
1	A	353	PRO	4.7
2	D	263	LEU	4.7
2	B	438	VAL	4.7
2	D	964	THR	4.7
3	X	257	ARG	4.7
1	A	306	ASN	4.7
1	A	326	MET	4.7
1	A	142	ILE	4.7
2	B	1031	GLN	4.7
2	D	444	GLN	4.7
2	D	485	ASP	4.7
2	D	1066	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	161	CYS	4.7
2	B	141	ARG	4.7
2	B	189	ASN	4.7
2	B	434	GLU	4.7
2	B	909	GLU	4.7
2	D	922	ALA	4.7
2	D	943	LYS	4.7
2	B	153	ARG	4.7
3	X	343	VAL	4.7
1	C	106	CYS	4.7
2	B	951	PHE	4.7
2	D	1030	HIS	4.7
2	D	135	ARG	4.7
2	D	608	SER	4.7
1	A	327	ASP	4.6
2	D	72	THR	4.6
1	A	137	VAL	4.6
2	B	590	SER	4.6
1	A	22	CYS	4.6
1	A	387	GLY	4.6
1	C	165	THR	4.6
2	B	387	SER	4.6
2	B	1026	TRP	4.6
1	A	351	SER	4.6
2	D	259	LYS	4.6
2	D	1033	TYR	4.6
1	C	120	THR	4.6
2	B	249	LEU	4.6
2	D	699	LEU	4.6
2	D	763	LEU	4.6
2	B	538	LYS	4.6
2	B	445	ASN	4.6
3	X	425	TYR	4.6
2	B	521	SER	4.6
2	B	892	GLN	4.6
1	C	302	ASN	4.6
2	B	626	ASN	4.6
2	B	696	ILE	4.6
1	A	264	ASP	4.6
2	B	963	THR	4.5
2	B	829	MET	4.5
2	D	177	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	555	PRO	4.5
2	B	103	LYS	4.5
2	D	1112	TYR	4.5
2	B	408	ASP	4.5
2	B	107	PRO	4.5
2	B	947	ALA	4.5
1	C	198	ASN	4.5
1	A	385	LEU	4.5
3	X	261	ALA	4.5
1	A	376	THR	4.5
1	A	371	HIS	4.5
2	B	184	CYS	4.5
1	C	147	SER	4.5
1	C	140	ILE	4.5
1	A	71	LEU	4.5
2	D	416	GLY	4.5
1	A	280	TRP	4.5
2	B	403	GLU	4.5
1	C	109	ASN	4.5
2	B	443	PHE	4.5
2	D	163	ARG	4.5
2	B	480	ILE	4.5
2	D	452	LYS	4.5
1	C	139	ASP	4.5
2	B	336	LEU	4.5
1	C	328	TYR	4.4
2	B	551	PHE	4.4
2	B	90	LEU	4.4
2	B	1002	LEU	4.4
2	B	22	LEU	4.4
1	A	339	ILE	4.4
1	A	278	LEU	4.4
1	A	166	LEU	4.4
1	A	363	PHE	4.4
2	B	774	SER	4.4
2	B	790	LEU	4.4
1	A	27	SER	4.4
1	A	172	THR	4.4
2	B	758	ASN	4.4
2	D	426	ILE	4.4
2	B	348	ASP	4.4
2	B	833	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	167	PHE	4.4
1	A	146	TYR	4.4
1	A	77	SER	4.4
2	B	701	LEU	4.4
2	D	340	GLU	4.4
2	B	385	ASP	4.4
2	D	1102	LEU	4.4
1	A	41	THR	4.4
1	C	27	SER	4.4
1	A	102	LEU	4.4
2	B	585	SER	4.4
2	B	923	ASP	4.3
2	D	507	LYS	4.3
2	B	474	ILE	4.3
1	A	268	ILE	4.3
3	X	296	TYR	4.3
1	C	36	HIS	4.3
2	B	21	THR	4.3
1	C	257	ASN	4.3
2	B	194	LYS	4.3
2	B	999	VAL	4.3
2	D	180	THR	4.3
3	X	294	ALA	4.3
2	B	435	SER	4.3
2	D	1029	LYS	4.3
1	A	80	SER	4.3
1	A	331	THR	4.3
2	D	342	ILE	4.3
2	D	1062	ILE	4.3
2	B	108	SER	4.3
3	X	370	LYS	4.3
1	A	304	LEU	4.3
3	X	297	ALA	4.3
2	D	860	ARG	4.3
2	D	855	ALA	4.3
2	D	998	ASP	4.3
1	A	305	PRO	4.3
1	C	196	ASN	4.3
2	B	523	ASN	4.3
1	A	352	ILE	4.2
2	B	101	ASN	4.2
2	B	894	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	277	TRP	4.2
1	C	233	TRP	4.2
2	B	836	ASN	4.2
2	B	138	TYR	4.2
2	B	53	GLU	4.2
1	C	121	ILE	4.2
1	C	137	VAL	4.2
2	B	9	VAL	4.2
3	X	269	VAL	4.2
1	C	148	ALA	4.2
1	C	129	GLY	4.2
3	X	366	PHE	4.2
2	B	925	SER	4.2
2	D	108	SER	4.2
2	B	200	LYS	4.2
2	B	143	SER	4.2
2	B	140	ILE	4.2
2	B	912	TYR	4.2
2	B	115	VAL	4.2
1	C	350	ASN	4.2
1	C	69	PRO	4.2
2	B	117	PHE	4.2
1	A	372	LEU	4.2
1	C	278	LEU	4.2
1	A	132	GLY	4.2
1	A	57	THR	4.2
2	D	1001	ASN	4.2
2	B	522	ILE	4.1
2	D	801	ILE	4.1
1	C	370	SER	4.1
2	B	629	PRO	4.1
1	C	68	LEU	4.1
2	D	183	ILE	4.1
2	B	124	ASP	4.1
2	B	490	ASP	4.1
2	B	350	GLN	4.1
2	B	534	ASN	4.1
2	B	958	LEU	4.1
2	D	71	GLN	4.1
1	A	332	ALA	4.1
1	C	235	LEU	4.1
2	D	984	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
3	X	309	GLN	4.1
1	A	330	ALA	4.1
2	B	111	MET	4.1
2	B	494	TYR	4.1
2	B	436	ILE	4.1
1	A	267	GLY	4.1
1	C	242	LEU	4.1
2	B	5	LYS	4.1
2	B	119	PHE	4.1
2	B	934	SER	4.1
2	D	404	LYS	4.1
2	B	24	LEU	4.1
1	A	5	SER	4.1
2	D	669	PRO	4.1
2	D	897	CYS	4.1
3	X	66	VAL	4.1
1	C	282	LEU	4.1
2	D	472	SER	4.1
1	A	255	LEU	4.1
2	D	1101	LYS	4.1
1	C	331	THR	4.1
1	C	186	PRO	4.1
1	A	338	LEU	4.0
3	X	346	GLY	4.0
2	B	526	PRO	4.0
2	D	290	ASP	4.0
1	C	207	GLY	4.0
2	B	77	ILE	4.0
1	C	133	HIS	4.0
1	C	254	SER	4.0
2	B	862	PHE	4.0
2	B	75	TRP	4.0
2	B	1	MET	4.0
2	B	163	ARG	4.0
1	A	103	ALA	4.0
1	A	133	HIS	4.0
2	D	504	ARG	4.0
1	A	114	ILE	4.0
1	A	321	PRO	4.0
1	C	108	ASP	4.0
1	C	192	PHE	4.0
2	D	515	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	625	PRO	4.0
1	A	303	LEU	4.0
2	B	261	LEU	4.0
2	D	93	LYS	4.0
2	D	208	HIS	4.0
1	C	308	GLN	4.0
2	D	87	ASP	4.0
1	A	14	VAL	4.0
1	A	259	ARG	4.0
2	D	54	CYS	4.0
2	D	323	LEU	4.0
1	C	341	LEU	4.0
2	D	335	SER	4.0
1	A	111	VAL	4.0
2	D	896	SER	4.0
2	B	571	ILE	4.0
2	D	653	ILE	4.0
2	D	325	VAL	4.0
1	A	209	ILE	3.9
2	B	897	CYS	3.9
2	D	242	PHE	3.9
1	C	367	GLN	3.9
2	B	137	LEU	3.9
2	B	419	SER	3.9
2	B	1067	LEU	3.9
2	B	913	ILE	3.9
2	B	91	ASN	3.9
2	B	164	PRO	3.9
2	B	121	GLU	3.9
2	B	962	SER	3.9
2	D	494	TYR	3.9
2	D	720	LEU	3.9
2	D	1125	ALA	3.9
1	A	214	TRP	3.9
2	D	1117	LYS	3.9
2	B	1022	ILE	3.9
2	B	323	LEU	3.9
2	D	1059	ARG	3.9
1	A	157	ILE	3.9
2	D	951	PHE	3.9
2	D	261	LEU	3.9
2	B	985	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	965	PRO	3.9
2	D	249	LEU	3.9
2	D	512	LEU	3.9
2	B	399	PHE	3.9
2	B	678	ALA	3.9
1	C	388	PHE	3.9
2	B	501	GLU	3.9
1	C	122	ILE	3.9
2	B	134	ALA	3.9
1	A	246	CYS	3.9
2	D	829	MET	3.9
1	C	110	THR	3.8
2	B	967	LYS	3.8
2	D	1018	CYS	3.8
1	A	235	LEU	3.8
2	B	253	SER	3.8
2	B	988	LEU	3.8
2	B	504	ARG	3.8
2	D	411	THR	3.8
2	B	549	GLU	3.8
2	B	51	LYS	3.8
1	A	42	ILE	3.8
2	B	628	ASP	3.8
1	A	195	SER	3.8
2	D	987	LEU	3.8
2	D	1012	ASN	3.8
2	B	524	PHE	3.8
3	X	447	ILE	3.8
2	B	1124	THR	3.8
1	A	310	ILE	3.8
2	D	853	LYS	3.8
2	D	192	LEU	3.8
1	A	159	SER	3.8
1	A	183	LEU	3.8
1	C	188	ILE	3.8
2	B	885	ILE	3.8
2	D	697	PHE	3.8
2	B	12	ASP	3.8
2	D	527	SER	3.8
2	D	972	LEU	3.8
2	D	604	GLN	3.8
2	B	582	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	247	HIS	3.8
2	D	383	ASP	3.8
2	D	923	ASP	3.8
3	X	240	SER	3.7
1	C	369	GLY	3.7
2	D	528	ASN	3.7
2	D	996	ARG	3.7
2	D	952	ASP	3.7
2	B	1040	ILE	3.7
1	A	73	LEU	3.7
1	C	138	ASN	3.7
2	D	940	GLU	3.7
2	B	69	GLY	3.7
2	D	516	GLY	3.7
2	B	1030	HIS	3.7
2	D	606	LEU	3.7
2	B	277	THR	3.7
1	A	139	ASP	3.7
2	D	194	LYS	3.7
2	B	476	SER	3.7
2	B	1032	ASN	3.7
2	B	492	TYR	3.7
2	D	812	VAL	3.7
1	A	312	LEU	3.7
2	D	1111	GLU	3.7
3	X	320	PRO	3.7
3	X	308	GLN	3.7
2	B	235	ASN	3.7
2	B	952	ASP	3.7
1	C	353	PRO	3.7
1	C	335	GLN	3.7
3	X	345	GLU	3.7
2	B	275	SER	3.7
2	B	268	CYS	3.7
3	X	225	ARG	3.7
2	D	936	ALA	3.7
2	D	1060	THR	3.7
1	A	309	GLY	3.7
2	B	439	ALA	3.7
2	D	999	VAL	3.7
2	B	377	LYS	3.7
2	D	53	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	199	GLN	3.6
2	B	106	PHE	3.6
2	B	513	ASP	3.6
2	B	392	TRP	3.6
1	A	79	CYS	3.6
1	C	334	SER	3.6
1	C	193	ARG	3.6
1	C	309	GLY	3.6
3	X	341	LYS	3.6
2	B	841	ALA	3.6
1	A	171	LEU	3.6
2	B	604	GLN	3.6
2	B	371	LEU	3.6
1	A	359	PRO	3.6
2	B	122	HIS	3.6
2	D	802	PHE	3.6
2	B	875	GLN	3.6
2	B	4	LEU	3.6
2	B	497	LEU	3.6
2	B	1020	TYR	3.6
2	B	452	LYS	3.6
3	X	238	SER	3.6
1	C	241	PRO	3.6
2	B	914	ASP	3.6
2	D	944	THR	3.6
1	A	324	ARG	3.6
1	A	158	ALA	3.6
1	A	346	GLU	3.6
2	D	725	LEU	3.6
2	B	207	GLN	3.6
2	B	639	LEU	3.6
2	D	423	LEU	3.6
3	X	237	VAL	3.6
2	B	1083	ILE	3.6
2	B	65	ASN	3.6
3	X	365	LEU	3.6
2	B	98	SER	3.6
2	B	96	PRO	3.6
1	A	389	THR	3.6
2	B	583	LEU	3.6
2	D	118	SER	3.6
2	D	852	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	366	ALA	3.5
2	B	472	SER	3.5
2	B	541	PHE	3.5
2	B	1003	LEU	3.5
1	A	360	ILE	3.5
3	X	313	VAL	3.5
1	C	318	GLY	3.5
1	A	7	GLN	3.5
2	B	393	SER	3.5
1	A	354	ILE	3.5
2	D	457	LYS	3.5
2	D	316	ALA	3.5
3	X	423	THR	3.5
1	C	305	PRO	3.5
2	D	811	LEU	3.5
2	B	185	VAL	3.5
2	B	68	LYS	3.5
2	B	1021	ASN	3.5
3	X	292	ARG	3.5
1	A	54	THR	3.5
1	A	348	ASP	3.5
2	B	771	GLN	3.5
2	D	357	SER	3.5
1	A	197	PRO	3.5
3	X	127	GLY	3.5
2	D	454	LYS	3.5
2	D	1049	SER	3.5
2	D	629	PRO	3.5
2	B	1023	LEU	3.5
2	D	250	VAL	3.5
2	D	967	LYS	3.5
2	D	91	ASN	3.5
2	D	152	ALA	3.5
2	D	997	GLN	3.5
2	B	279	LEU	3.5
2	B	943	LYS	3.5
2	B	145	THR	3.5
1	C	274	SER	3.5
1	C	303	LEU	3.5
1	A	379	SER	3.5
2	B	762	ALA	3.4
1	A	386	MET	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	458	PHE	3.4
2	B	505	PHE	3.4
2	B	243	LEU	3.4
1	A	194	PRO	3.4
2	B	333	PRO	3.4
2	B	1033	TYR	3.4
2	D	475	VAL	3.4
1	A	16	PRO	3.4
2	B	857	LYS	3.4
2	B	692	ILE	3.4
2	D	1108	ILE	3.4
1	A	383	THR	3.4
2	B	675	ALA	3.4
2	D	437	GLN	3.4
2	B	832	ILE	3.4
2	B	937	ILE	3.4
2	D	1122	GLN	3.4
1	A	318	GLY	3.4
1	C	189	SER	3.4
3	X	64	ARG	3.4
3	X	301	GLY	3.4
1	A	49	GLN	3.4
2	B	761	GLU	3.4
2	B	856	VAL	3.4
2	B	99	LYS	3.4
2	B	682	ASP	3.4
2	D	420	GLU	3.4
2	D	252	LEU	3.4
2	D	956	VAL	3.4
2	B	365	ILE	3.4
2	B	110	VAL	3.4
2	B	591	THR	3.4
2	B	878	VAL	3.4
2	B	1044	LEU	3.4
2	D	153	ARG	3.4
2	D	1005	ARG	3.4
1	A	260	TRP	3.4
2	D	343	PRO	3.4
2	D	1105	LEU	3.4
2	D	491	TYR	3.4
1	A	53	SER	3.3
2	B	673	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLN	3.3
2	B	898	TYR	3.3
1	A	155	GLN	3.3
1	A	244	ASN	3.3
1	A	343	ASN	3.3
2	D	65	ASN	3.3
2	D	498	LEU	3.3
2	D	644	ASN	3.3
1	A	44	CYS	3.3
2	B	843	TYR	3.3
1	A	345	TYR	3.3
2	B	603	VAL	3.3
2	B	491	TYR	3.3
2	D	386	GLU	3.3
2	D	920	LEU	3.3
2	B	627	VAL	3.3
2	D	129	TYR	3.3
2	B	78	PHE	3.3
3	X	262	SER	3.3
2	B	964	THR	3.3
3	X	406	MET	3.3
1	C	26	PRO	3.3
2	B	130	ALA	3.3
1	A	381	LEU	3.3
2	B	246	TYR	3.3
1	C	204	GLU	3.3
2	D	1017	PRO	3.3
1	C	304	LEU	3.3
2	D	914	ASP	3.3
2	D	941	THR	3.3
1	A	188	ILE	3.3
2	B	66	LYS	3.3
2	B	248	VAL	3.3
2	D	106	PHE	3.3
2	D	1027	ARG	3.3
2	B	837	SER	3.3
2	B	702	ILE	3.3
2	D	70	SER	3.3
2	B	851	LYS	3.3
2	B	364	ILE	3.3
2	D	899	TYR	3.3
2	B	1039	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	437	GLN	3.3
2	B	688	PHE	3.2
2	D	722	LEU	3.2
1	A	156	VAL	3.2
2	B	530	VAL	3.2
2	B	669	PRO	3.2
1	C	162	ASP	3.2
2	B	58	ASP	3.2
2	B	89	SER	3.2
2	B	418	ILE	3.2
2	D	500	ASN	3.2
2	D	1010	MET	3.2
2	D	586	CYS	3.2
1	A	317	LEU	3.2
2	D	762	ALA	3.2
2	B	102	VAL	3.2
1	C	135	ASN	3.2
1	A	186	PRO	3.2
2	B	128	ILE	3.2
2	D	237	ILE	3.2
1	A	212	PHE	3.2
2	D	324	ASN	3.2
2	D	830	GLN	3.2
2	B	965	PRO	3.2
2	B	234	PRO	3.2
1	C	273	LYS	3.2
2	B	922	ALA	3.2
2	D	962	SER	3.2
2	B	830	GLN	3.2
1	A	75	PHE	3.2
1	C	327	ASP	3.2
2	B	674	CYS	3.2
2	B	860	ARG	3.2
2	D	247	ASN	3.2
1	A	17	TYR	3.2
2	B	990	TYR	3.2
2	B	1062	ILE	3.2
2	B	64	SER	3.2
1	A	323	PRO	3.2
2	B	939	HIS	3.2
2	B	512	LEU	3.2
2	D	1050	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	1027	ARG	3.2
2	D	849	TYR	3.2
2	D	86	PHE	3.2
1	C	240	LEU	3.2
2	B	877	ALA	3.2
2	D	670	SER	3.2
2	D	88	VAL	3.2
2	B	944	THR	3.2
2	B	984	ILE	3.2
2	D	961	LEU	3.2
2	D	508	LEU	3.2
2	D	917	GLU	3.2
2	B	987	LEU	3.2
2	B	1041	TYR	3.2
2	B	264	SER	3.1
2	B	177	ALA	3.1
3	X	218	PHE	3.1
2	B	430	ASN	3.1
2	D	238	ILE	3.1
1	A	245	THR	3.1
1	C	344	THR	3.1
2	B	636	ILE	3.1
2	D	181	SER	3.1
2	D	971	LEU	3.1
2	B	1029	LYS	3.1
2	D	1056	LYS	3.1
2	D	935	ILE	3.1
3	X	299	GLU	3.1
2	D	114	GLY	3.1
2	D	834	TRP	3.1
2	B	507	LYS	3.1
2	B	404	LYS	3.1
2	B	961	LEU	3.1
2	D	1104	THR	3.1
2	D	306	HIS	3.1
2	D	511	TYR	3.1
2	B	1025	SER	3.1
3	X	272	SER	3.1
2	B	471	LEU	3.1
2	D	74	ARG	3.1
1	A	313	PHE	3.1
1	A	181	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
3	X	17	ARG	3.1
2	D	692	ILE	3.1
2	D	656	LEU	3.1
2	D	1058	GLU	3.1
2	B	801	ILE	3.1
3	X	229	GLY	3.1
2	D	98	SER	3.1
1	C	255	LEU	3.1
2	B	10	PRO	3.1
3	X	219	THR	3.1
3	X	259	ILE	3.1
2	B	942	LEU	3.1
3	X	18	ASP	3.1
2	D	959	MET	3.1
3	X	230	PHE	3.1
1	A	167	ILE	3.1
1	C	277	TRP	3.1
2	B	372	ASN	3.1
3	X	107	LYS	3.1
2	D	1123	VAL	3.1
1	C	339	ILE	3.1
1	A	105	VAL	3.1
2	B	888	LYS	3.0
2	B	2	ASN	3.0
2	D	503	GLU	3.0
1	A	247	HIS	3.0
2	D	1118	ASP	3.0
1	C	336	HIS	3.0
2	B	542	ILE	3.0
2	D	69	GLY	3.0
2	D	484	SER	3.0
2	B	940	GLU	3.0
2	D	305	SER	3.0
2	B	767	ASN	3.0
3	X	446	VAL	3.0
1	C	315	SER	3.0
1	C	187	GLY	3.0
2	D	601	GLU	3.0
3	X	65	VAL	3.0
2	D	161	CYS	3.0
1	A	108	ASP	3.0
2	B	230	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	840	ILE	3.0
1	A	206	ASN	3.0
3	X	273	GLY	3.0
2	D	1008	PHE	3.0
1	A	370	SER	3.0
1	A	210	ARG	3.0
2	B	589	PHE	3.0
2	B	708	TYR	3.0
2	B	236	THR	3.0
2	B	667	GLN	3.0
1	A	361	VAL	3.0
1	C	352	ILE	3.0
2	D	438	VAL	3.0
2	B	193	THR	3.0
2	D	376	GLN	3.0
2	B	838	ASP	3.0
2	D	119	PHE	3.0
2	D	57	TYR	3.0
2	B	1120	ALA	3.0
1	A	168	ILE	3.0
2	B	910	SER	3.0
2	B	409	VAL	3.0
2	B	85	ILE	2.9
2	B	429	HIS	2.9
2	D	532	TYR	2.9
2	B	588	SER	2.9
1	A	274	SER	2.9
1	C	355	GLN	2.9
2	B	267	GLN	2.9
2	B	759	THR	2.9
2	D	337	PRO	2.9
2	D	521	SER	2.9
1	A	265	GLY	2.9
2	B	129	TYR	2.9
2	B	259	LYS	2.9
2	B	116	ALA	2.9
2	B	1038	ALA	2.9
2	D	164	PRO	2.9
3	X	267	THR	2.9
3	X	342	ALA	2.9
2	D	434	GLU	2.9
1	A	176	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	811	LEU	2.9
2	B	188	PHE	2.9
2	D	850	LEU	2.9
2	B	276	GLN	2.9
2	B	737	ASN	2.9
2	B	373	THR	2.9
2	B	531	THR	2.9
2	B	689	GLN	2.9
3	X	270	ASP	2.9
2	D	432	SER	2.9
3	X	304	TYR	2.9
2	B	197	LEU	2.9
2	B	1006	LYS	2.9
2	B	1028	TYR	2.9
1	A	136	PHE	2.9
2	D	284	PHE	2.9
2	B	975	VAL	2.9
2	D	317	ASN	2.9
2	D	530	VAL	2.9
2	B	57	TYR	2.9
2	B	576	ILE	2.9
2	B	936	ALA	2.9
2	B	592	LEU	2.9
2	B	812	VAL	2.9
1	A	251	ILE	2.9
2	D	375	ILE	2.9
2	B	895	LEU	2.9
2	D	836	ASN	2.9
2	B	250	VAL	2.8
2	B	262	ASP	2.8
2	B	896	SER	2.8
2	D	902	LEU	2.8
2	B	721	PHE	2.8
2	B	891	HIS	2.8
1	A	311	SER	2.8
2	B	869	LEU	2.8
2	B	986	GLN	2.8
2	B	441	LEU	2.8
1	A	101	PHE	2.8
2	B	643	GLU	2.8
1	A	250	GLY	2.8
2	B	1065	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	365	ILE	2.8
1	A	62	PHE	2.8
2	B	876	PHE	2.8
2	B	970	CYS	2.8
2	D	960	VAL	2.8
1	A	384	ARG	2.8
3	X	326	GLU	2.8
2	B	1042	GLU	2.8
2	D	816	VAL	2.8
2	B	1121	VAL	2.8
2	D	346	LEU	2.8
2	D	798	LEU	2.8
2	B	511	TYR	2.8
2	B	123	SER	2.8
2	B	703	THR	2.8
2	B	1072	THR	2.8
2	D	774	SER	2.8
1	A	135	ASN	2.8
2	B	136	VAL	2.8
2	B	763	LEU	2.8
2	B	1007	ALA	2.8
2	B	578	ASP	2.8
2	B	384	GLN	2.8
2	B	908	GLU	2.8
2	D	6	HIS	2.8
1	C	307	VAL	2.8
2	B	938	THR	2.8
1	A	20	THR	2.8
1	A	380	VAL	2.8
2	B	147	PHE	2.8
2	D	837	SER	2.8
2	D	517	ASP	2.8
2	B	332	ILE	2.8
2	B	685	LEU	2.8
1	C	256	ALA	2.7
2	D	777	ASN	2.7
1	A	203	GLY	2.7
2	B	396	LEU	2.7
1	C	340	GLN	2.7
2	B	475	VAL	2.7
3	X	239	GLY	2.7
2	D	24	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	X	305	LEU	2.7
3	X	248	ILE	2.7
2	B	199	PRO	2.7
2	D	272	ILE	2.7
1	A	125	HIS	2.7
2	B	442	SER	2.7
2	B	917	GLU	2.7
2	B	1066	TYR	2.7
2	D	916	LEU	2.7
2	D	1116	LEU	2.7
2	D	441	LEU	2.7
2	B	791	HIS	2.7
3	X	222	MET	2.7
1	A	127	LEU	2.7
2	B	158	TRP	2.7
2	B	581	ARG	2.7
2	B	1036	ALA	2.7
2	D	12	ASP	2.7
3	X	179	MET	2.7
2	B	890	HIS	2.7
2	B	671	LEU	2.7
2	B	698	LEU	2.7
2	B	711	GLN	2.7
2	D	150	PRO	2.7
1	A	46	SER	2.7
1	A	207	GLY	2.7
2	B	325	VAL	2.7
2	D	909	GLU	2.7
2	B	695	PHE	2.7
2	D	113	ASP	2.7
2	D	473	SER	2.7
2	D	729	ARG	2.7
2	D	724	LEU	2.7
2	D	524	PHE	2.7
1	A	19	THR	2.7
1	A	109	ASN	2.7
2	B	182	GLU	2.7
2	B	835	LEU	2.7
2	D	90	LEU	2.7
2	B	1014	GLU	2.7
2	B	67	SER	2.7
2	B	456	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	505	PHE	2.6
2	B	854	GLU	2.6
2	B	605	ASP	2.6
1	A	242	LEU	2.6
2	B	995	LEU	2.6
2	B	1074	GLU	2.6
2	B	255	ASP	2.6
2	B	291	HIS	2.6
2	D	62	TYR	2.6
2	D	138	TYR	2.6
3	X	413	CYS	2.6
1	C	310	ILE	2.6
2	B	52	LYS	2.6
2	D	370	ASN	2.6
2	D	413	MET	2.6
2	B	11	ILE	2.6
2	B	852	SER	2.6
2	B	992	MET	2.6
2	B	1112	TYR	2.6
2	D	248	VAL	2.6
1	A	123	THR	2.6
3	X	55	VAL	2.6
3	X	319	LEU	2.6
2	B	911	ALA	2.6
2	D	810	ASP	2.6
2	D	772	PHE	2.6
2	B	979	THR	2.6
2	B	307	GLY	2.6
2	D	117	PHE	2.6
2	B	983	LYS	2.6
2	D	536	ALA	2.6
3	X	422	GLN	2.6
2	B	318	ALA	2.6
1	A	271	MET	2.6
1	A	355	GLN	2.6
2	B	600	ARG	2.6
1	C	184	SER	2.6
1	C	387	GLY	2.6
2	B	132	THR	2.6
2	B	916	LEU	2.6
2	B	502	TRP	2.6
2	D	268	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	366	ALA	2.6
2	D	518	GLU	2.6
2	D	848	ILE	2.6
1	A	69	PRO	2.6
3	X	314	PRO	2.6
2	B	798	LEU	2.6
2	B	496	ARG	2.6
1	A	204	GLU	2.6
2	B	710	LEU	2.6
2	D	8	VAL	2.6
2	B	968	LYS	2.6
2	D	133	HIS	2.6
2	D	523	ASN	2.6
2	D	1115	GLN	2.6
2	B	398	SER	2.6
2	D	246	TYR	2.5
1	A	373	ALA	2.5
2	D	341	PHE	2.5
2	B	13	LEU	2.5
2	B	154	LEU	2.5
2	B	849	TYR	2.5
2	B	816	VAL	2.5
2	B	256	TYR	2.5
2	B	1037	ALA	2.5
2	B	324	ASN	2.5
2	B	787	ILE	2.5
2	B	368	LYS	2.5
2	B	871	SER	2.5
2	D	913	ILE	2.5
2	B	105	HIS	2.5
2	B	736	GLU	2.5
2	D	167	PHE	2.5
2	D	270	GLU	2.5
3	X	430	ASN	2.5
3	X	21	GLN	2.5
2	B	844	LEU	2.5
2	D	966	LEU	2.5
3	X	87	ALA	2.5
1	A	12	LEU	2.5
2	B	508	LEU	2.5
2	B	863	LYS	2.5
2	D	901	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	265	THR	2.5
2	D	1013	VAL	2.5
2	B	974	PHE	2.5
2	B	717	CYS	2.5
2	D	788	SER	2.5
1	A	378	GLY	2.5
1	C	190	VAL	2.5
2	B	346	LEU	2.5
1	C	342	ILE	2.5
2	B	632	ILE	2.5
2	B	646	MET	2.5
2	B	257	LYS	2.5
2	B	575	GLN	2.5
2	B	924	ALA	2.5
3	X	82	VAL	2.5
2	D	758	ASN	2.5
2	D	264	SER	2.5
1	C	160	VAL	2.5
1	A	6	ASN	2.5
2	D	501	GLU	2.5
2	D	50	PHE	2.5
2	D	260	VAL	2.4
2	D	652	LEU	2.4
1	A	47	GLU	2.4
2	B	378	CYS	2.4
2	B	853	LYS	2.4
2	B	1048	ILE	2.4
2	D	489	TYR	2.4
3	X	32	MET	2.4
1	C	183	LEU	2.4
2	B	573	GLY	2.4
1	A	59	GLN	2.4
2	B	127	ILE	2.4
3	X	286	LYS	2.4
3	X	194	PHE	2.4
1	A	270	ALA	2.4
3	X	282	LEU	2.4
2	D	314	LEU	2.4
2	D	496	ARG	2.4
2	D	126	THR	2.4
2	B	413	MET	2.4
2	B	831	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	514	HIS	2.4
2	D	742	LEU	2.4
3	X	410	HIS	2.4
2	B	900	LEU	2.4
3	X	374	ALA	2.4
2	B	131	ILE	2.4
3	X	372	ALA	2.4
2	D	981	GLN	2.4
2	B	1123	VAL	2.4
2	D	480	ILE	2.4
1	C	243	VAL	2.4
2	D	63	THR	2.4
2	B	899	TYR	2.4
2	D	142	LEU	2.4
2	D	1061	PHE	2.4
1	A	162	ASP	2.4
1	A	243	VAL	2.4
2	D	502	TRP	2.4
2	B	793	THR	2.4
1	A	119	GLU	2.4
2	B	260	VAL	2.4
2	B	300	TYR	2.4
2	B	817	GLU	2.4
2	B	956	VAL	2.4
1	A	192	PHE	2.4
2	B	290	ASP	2.4
2	D	266	ASN	2.4
2	D	824	GLN	2.4
2	B	73	LEU	2.4
2	B	681	LEU	2.4
2	D	318	ALA	2.4
3	X	196	GLY	2.4
2	B	1011	ILE	2.3
3	X	317	ILE	2.3
2	D	666	ALA	2.3
2	B	579	LEU	2.3
2	B	402	ILE	2.3
2	B	714	PHE	2.3
3	X	351	THR	2.3
2	B	1068	ILE	2.3
2	D	364	ILE	2.3
2	B	802	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
3	X	318	ALA	2.3
2	D	651	SER	2.3
1	A	191	GLN	2.3
1	A	48	GLU	2.3
1	C	306	ASN	2.3
2	B	25	TRP	2.3
2	D	101	ASN	2.3
2	D	469	ALA	2.3
3	X	235	VAL	2.3
3	X	59	ARG	2.3
1	A	333	HIS	2.3
3	X	327	LEU	2.3
2	D	537	ASN	2.3
1	A	320	CYS	2.3
2	B	1070	LEU	2.3
2	D	900	LEU	2.3
2	B	601	GLU	2.3
2	B	470	VAL	2.3
2	D	994	THR	2.3
2	B	855	ALA	2.3
2	B	813	THR	2.3
2	D	49	LEU	2.3
2	B	20	GLY	2.3
2	B	772	PHE	2.3
2	B	292	THR	2.3
2	B	971	LEU	2.3
2	B	1104	THR	2.3
2	B	309	PHE	2.3
2	B	80	ASN	2.3
2	B	640	VAL	2.3
2	D	468	ASN	2.3
2	B	510	ALA	2.3
3	X	180	ALA	2.3
2	D	414	SER	2.3
1	A	257	ASN	2.3
2	B	941	THR	2.3
2	B	848	ILE	2.2
3	X	322	ALA	2.2
1	A	193	ARG	2.2
3	X	76	VAL	2.2
3	X	348	ASN	2.2
2	B	320	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	64	SER	2.2
3	X	311	TRP	2.2
3	X	312	SER	2.2
2	B	822	PHE	2.2
3	X	254	PHE	2.2
2	B	593	SER	2.2
2	D	191	GLY	2.2
2	B	95	GLU	2.2
2	B	594	GLU	2.2
2	D	631	TYR	2.2
2	D	895	LEU	2.2
2	B	270	GLU	2.2
3	X	409	ILE	2.2
1	A	213	ASP	2.2
2	B	1117	LYS	2.2
2	D	412	ASN	2.2
3	X	281	ARG	2.2
3	X	167	GLY	2.2
2	D	301	TYR	2.2
2	D	182	GLU	2.2
2	D	334	PRO	2.2
2	D	857	LYS	2.2
2	D	397	ASP	2.2
2	B	388	PHE	2.2
2	D	974	PHE	2.2
2	D	761	GLU	2.2
3	X	83	GLN	2.2
2	D	933	LEU	2.2
2	B	959	MET	2.2
2	D	931	GLU	2.2
1	C	136	PHE	2.2
2	D	674	CYS	2.2
2	D	302	PRO	2.2
2	D	732	SER	2.2
2	D	844	LEU	2.2
2	D	23	ALA	2.2
2	D	338	ASP	2.2
2	D	409	VAL	2.2
3	X	228	MET	2.2
3	X	298	LYS	2.2
2	B	192	LEU	2.2
2	D	471	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	1118	ASP	2.2
1	A	241	PRO	2.2
1	A	237	LEU	2.2
2	B	1077	PRO	2.2
2	B	269	VAL	2.2
3	X	373	ASN	2.2
2	B	82	THR	2.2
2	B	931	GLU	2.2
2	D	19	GLU	2.2
2	D	339	ASP	2.2
2	D	765	SER	2.2
3	X	182	MET	2.2
3	X	434	PHE	2.2
2	B	550	SER	2.2
3	X	176	VAL	2.2
2	B	847	LEU	2.2
2	D	1016	GLN	2.2
2	D	937	ILE	2.2
2	B	976	ASN	2.1
2	B	304	ASN	2.1
2	D	425	HIS	2.1
2	D	407	PHE	2.1
3	X	188	ASN	2.1
1	A	40	ILE	2.1
3	X	321	CYS	2.1
2	B	104	ILE	2.1
2	B	642	LEU	2.1
1	C	185	SER	2.1
3	X	137	GLY	2.1
1	C	206	ASN	2.1
2	B	343	PRO	2.1
2	B	500	ASN	2.1
2	B	645	PRO	2.1
2	D	526	PRO	2.1
1	A	154	GLU	2.1
2	B	271	THR	2.1
2	B	905	LYS	2.1
3	X	212	GLY	2.1
1	A	11	PRO	2.1
2	D	622	HIS	2.1
2	D	797	SER	2.1
1	A	238	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	117	LYS	2.1
3	X	166	ALA	2.1
2	B	162	TYR	2.1
1	A	364	CYS	2.1
2	B	281	LEU	2.1
3	X	128	LYS	2.1
2	B	879	LEU	2.1
2	B	1064	GLU	2.1
2	D	371	LEU	2.1
3	X	233	MET	2.1
3	X	359	PHE	2.1
2	B	139	TYR	2.1
2	B	401	LEU	2.1
3	X	150	LEU	2.1
2	D	22	LEU	2.1
2	D	767	ASN	2.1
2	B	1078	LYS	2.1
1	A	18	THR	2.1
2	B	168	LEU	2.1
2	D	831	LEU	2.1
1	A	232	PRO	2.1
2	D	445	ASN	2.1
2	B	258	LEU	2.1
2	B	957	ALA	2.1
2	D	456	ASP	2.1
2	D	630	ASP	2.1
2	D	295	SER	2.1
2	B	160	LEU	2.1
2	B	289	SER	2.1
2	B	498	LEU	2.1
1	C	37	ASP	2.1
2	D	458	PHE	2.1
1	A	273	LYS	2.1
2	D	99	LYS	2.1
2	D	907	PHE	2.1
2	B	55	VAL	2.1
2	B	904	LYS	2.1
1	C	271	MET	2.0
2	B	1010	MET	2.0
2	D	982	GLY	2.0
3	X	151	MET	2.0
1	A	170	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	244	SER	2.0
2	B	342	ILE	2.0
2	D	975	VAL	2.0
2	B	935	ILE	2.0
2	D	273	GLU	2.0
2	B	845	LYS	2.0
3	X	285	ILE	2.0
2	D	835	LEU	2.0
1	A	236	THR	2.0
2	D	387	SER	2.0
2	D	903	SER	2.0
2	D	197	LEU	2.0
2	B	810	ASP	2.0
2	D	513	ASP	2.0
2	B	284	PHE	2.0
3	X	175	GLU	2.0
1	A	347	LYS	2.0
2	B	574	TYR	2.0
2	D	320	SER	2.0
2	D	910	SER	2.0
2	D	919	SER	2.0
2	D	970	CYS	2.0
2	D	128	ILE	2.0
2	B	1043	LYS	2.0
1	A	76	SER	2.0
2	B	305	SER	2.0
2	D	906	LEU	2.0
2	B	794	VAL	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.