Full wwPDB X-ray Structure Validation Report

Aug 16, 2016 – 08:36 AM EDT

PDB ID	:	5IRO
Title	:	Crystal structure of a complex between the Human adenovirus type 4 E3-19K protein and MHC class molecule HLA-A2/TAX
Authors	:	Li, L.; Bouvier, M.
Deposited on	:	2016-03-14
Resolution	:	2.64 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

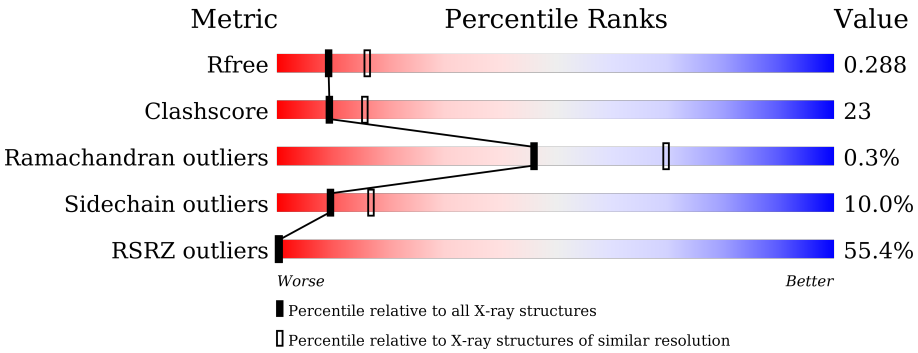
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.64 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3377 (2.68-2.60)
Clashscore	102246	3781 (2.68-2.60)
Ramachandran outliers	100387	3722 (2.68-2.60)
Sidechain outliers	100360	3722 (2.68-2.60)
RSRZ outliers	91569	3388 (2.68-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	275	43% 46% 44% 6% ·
1	E	275	48% 51% 41% 5% ·
1	I	275	38% 52% 35% 5% 8%
1	M	275	48% 46% 44% 6% ·
1	Q	275	76% 44% 43% 7% 6%
1	U	275	72% 46% 37% 6% 11%

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Mol	Chain	Length	Quality of chain
2	B	9	22% 22% 56% 22%
2	F	9	44% 22% 56% 22%
2	J	9	33% 44% 56%
2	N	9	44% 44% 56%
2	R	9	89% 44% 44% 11%
2	V	9	89% 22% 56% 22%
3	C	100	52% 62% 30%
3	G	100	36% 52% 41% 5%
3	K	100	25% 55% 38% 5%
3	O	100	46% 58% 35% 5%
3	S	100	79% 59% 33% 6%
3	W	100	83% 54% 41%
4	D	108	35% 59% 34% 6%
4	H	108	31% 69% 24% 5%
4	L	108	31% 68% 22% 6% 5%
4	P	108	33% 56% 36% 5%
4	T	108	79% 51% 41% 5%
4	X	108	78% 61% 30% 5% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23039 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 HLA class I histocompatibility antigen, A-2 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2144	1338	389	408	9			
1	E	268	Total	C	N	O	S	0	0	0
			2183	1363	398	413	9			
1	I	252	Total	C	N	O	S	0	0	0
			2053	1282	376	386	9			
1	M	265	Total	C	N	O	S	0	0	0
			2160	1351	392	408	9			
1	Q	259	Total	C	N	O	S	0	0	0
			2111	1315	385	402	9			
1	U	246	Total	C	N	O	S	0	0	0
			2007	1259	363	376	9			

- Molecule 2 is a protein called TAX protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	F	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	J	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	N	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	R	9	Total	C	N	O	0	0	0
			76	56	9	11			
2	V	9	Total	C	N	O	0	0	0
			76	56	9	11			

- Molecule 3 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	96	Total	C	N	O	S	0	0	0
			802	513	136	150	3			
3	G	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	K	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	O	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	S	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			
3	W	98	Total	C	N	O	S	0	0	0
			820	524	139	154	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
K	0	MET	-	initiating methionine	UNP P61769
O	0	MET	-	initiating methionine	UNP P61769
S	0	MET	-	initiating methionine	UNP P61769
W	0	MET	-	initiating methionine	UNP P61769

- Molecule 4 is a protein called E3 19 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	102	Total	C	N	O	S	0	0	0
			823	520	144	149	10			
4	H	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	L	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	P	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	T	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			
4	X	103	Total	C	N	O	S	0	0	0
			832	526	146	150	10			

- Molecule 5 is water.

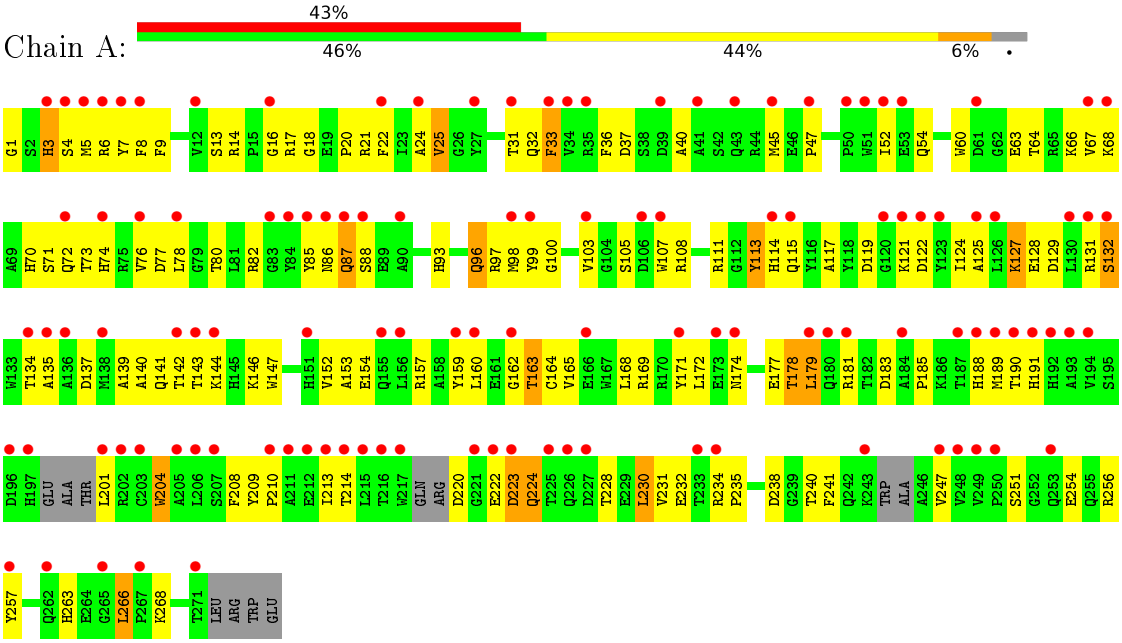
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	D	2	Total O 2 2	0	0
5	E	3	Total O 3 3	0	0
5	G	1	Total O 1 1	0	0
5	I	5	Total O 5 5	0	0
5	J	1	Total O 1 1	0	0
5	K	2	Total O 2 2	0	0
5	L	1	Total O 1 1	0	0
5	M	4	Total O 4 4	0	0
5	O	2	Total O 2 2	0	0
5	P	3	Total O 3 3	0	0
5	Q	3	Total O 3 3	0	0
5	S	3	Total O 3 3	0	0
5	T	3	Total O 3 3	0	0
5	U	3	Total O 3 3	0	0
5	W	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

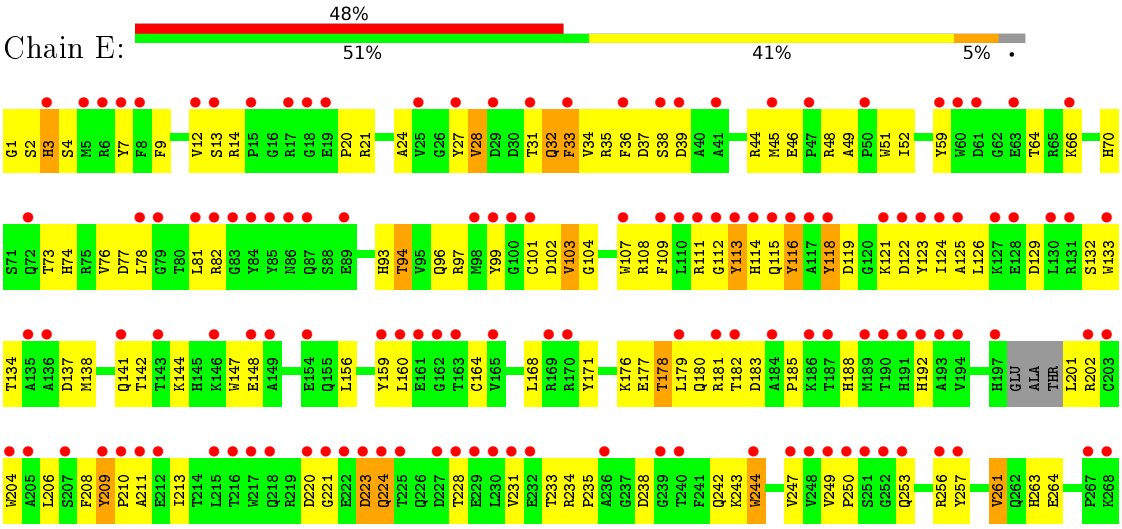
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

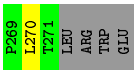
Chain A:



• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

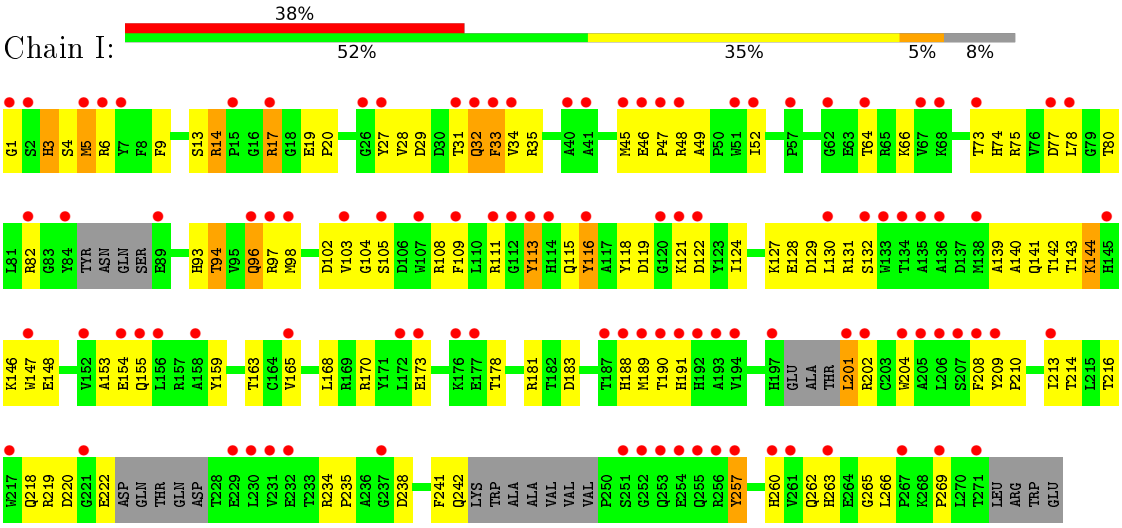
Chain E:





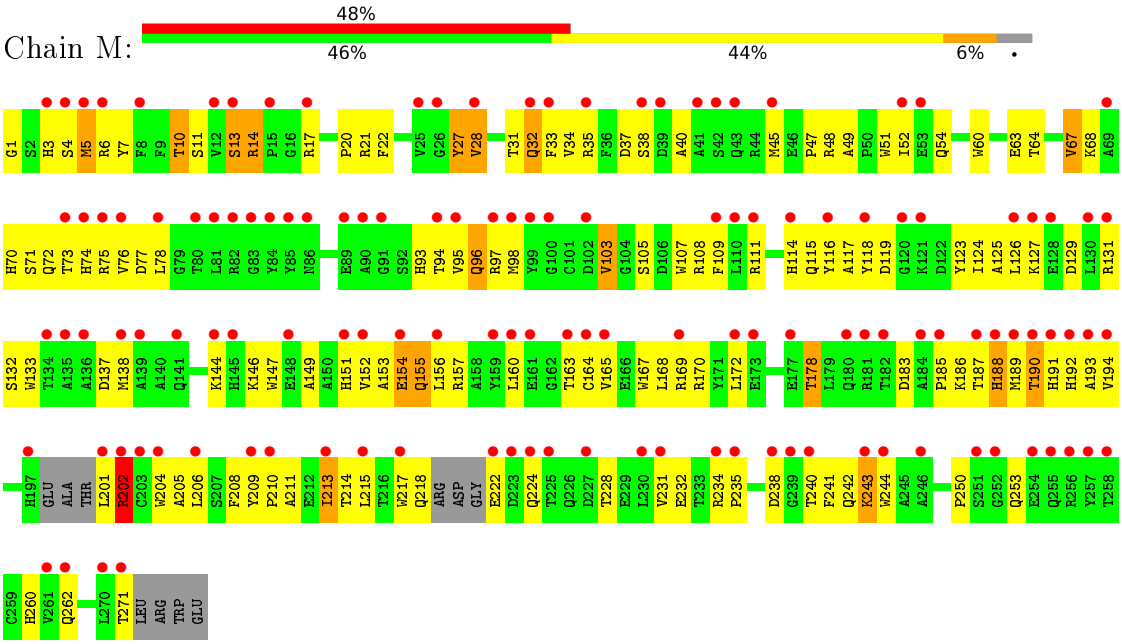
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain I:



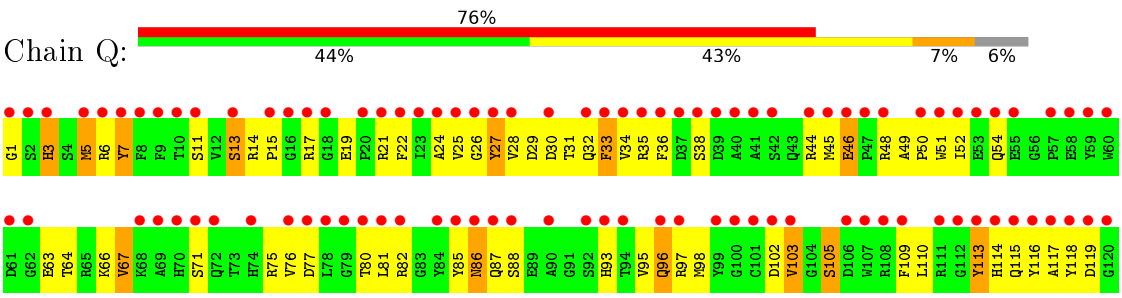
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

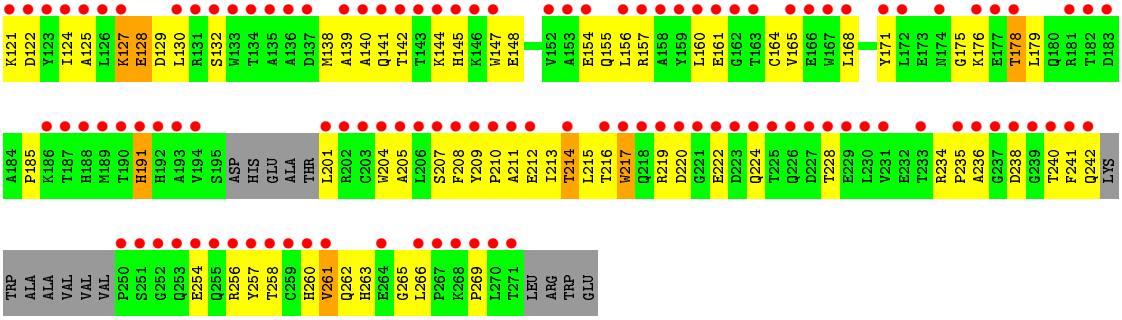
Chain M:



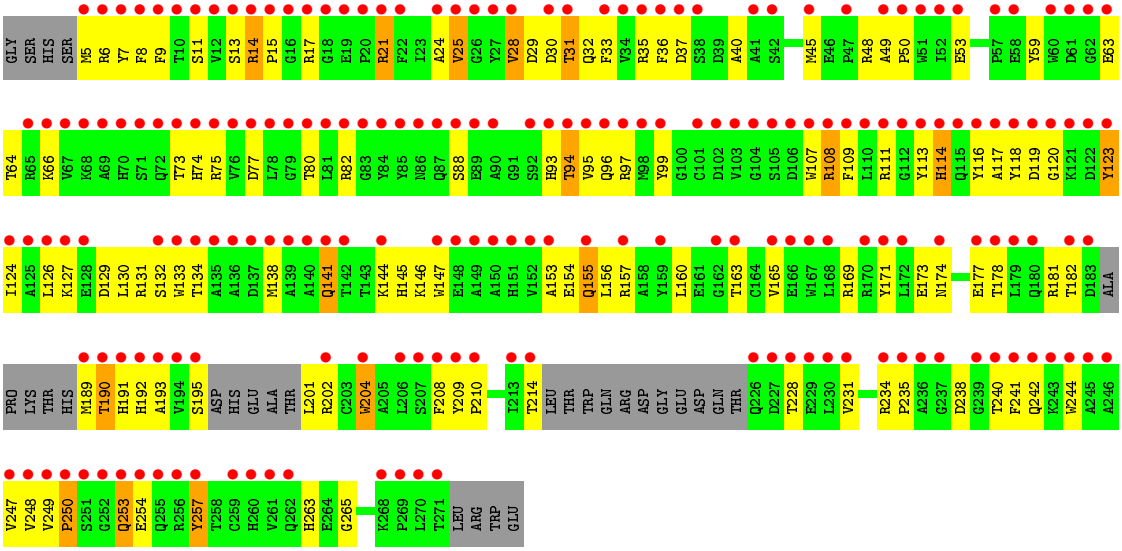
• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain

Chain Q:

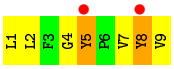




• Molecule 1: HLA class I histocompatibility antigen, A-2 alpha chain



• Molecule 2: TAX protein



• Molecule 2: TAX protein

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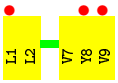
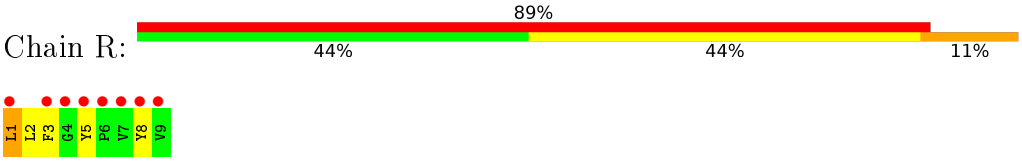


• Molecule 2: TAX protein

Chain N:

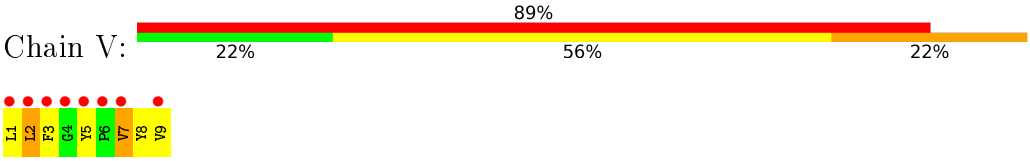
• Molecule 2: TAX protein

Chain R:



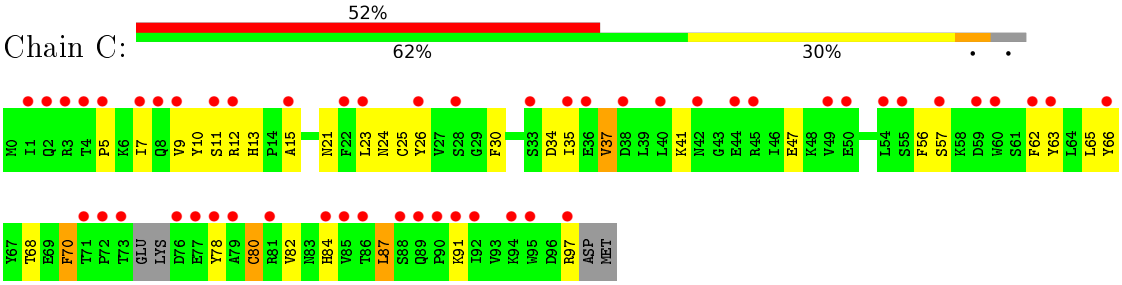
• Molecule 2: TAX protein

Chain V:



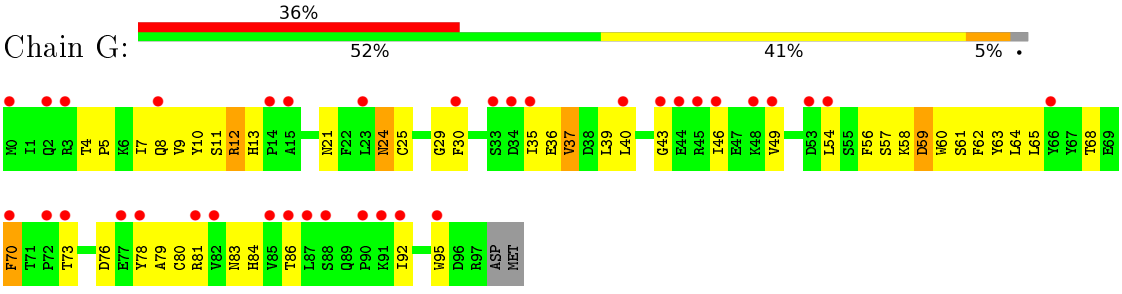
• Molecule 3: Beta-2-microglobulin

Chain C:



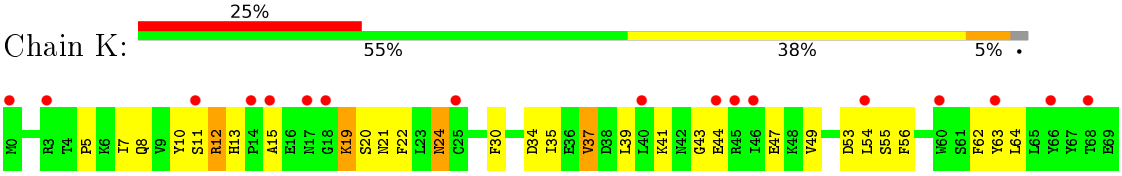
• Molecule 3: Beta-2-microglobulin

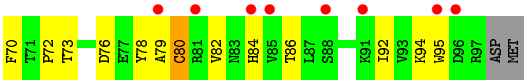
Chain G:



• Molecule 3: Beta-2-microglobulin

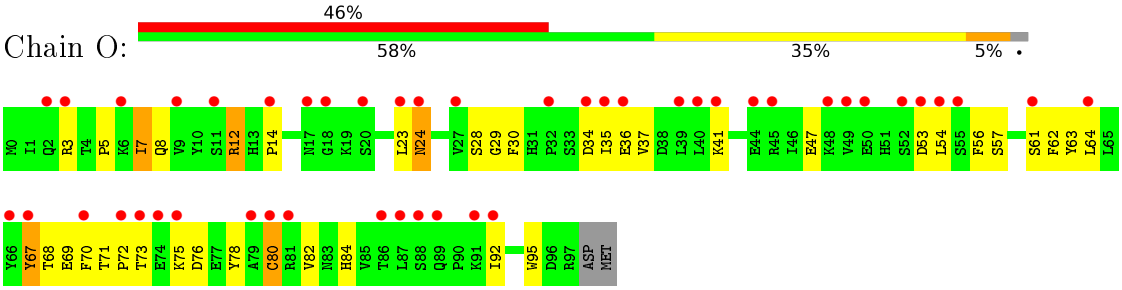
Chain K:





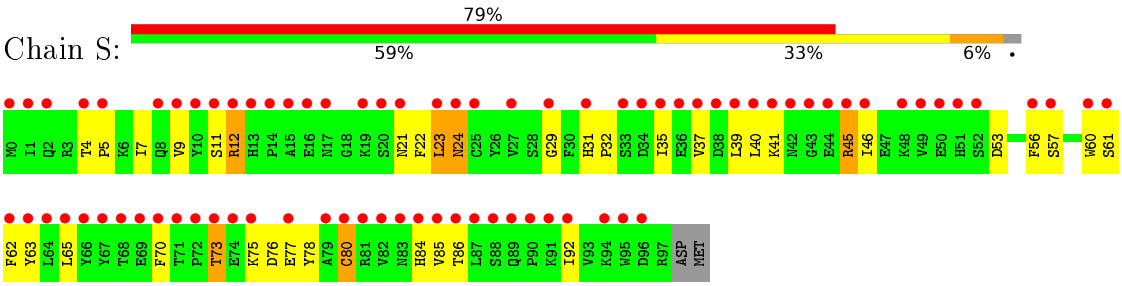
- Molecule 3: Beta-2-microglobulin

Chain O:



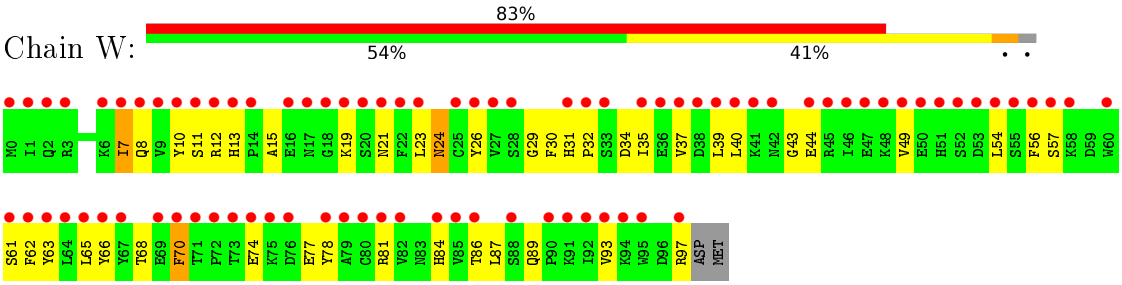
- Molecule 3: Beta-2-microglobulin

Chain S:



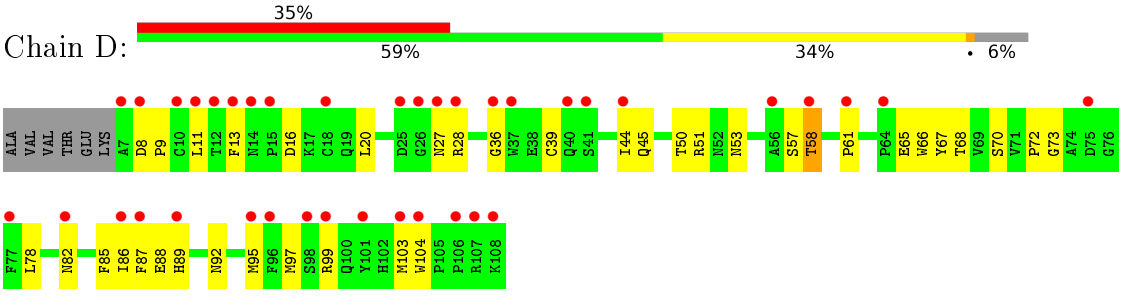
- Molecule 3: Beta-2-microglobulin

Chain W:



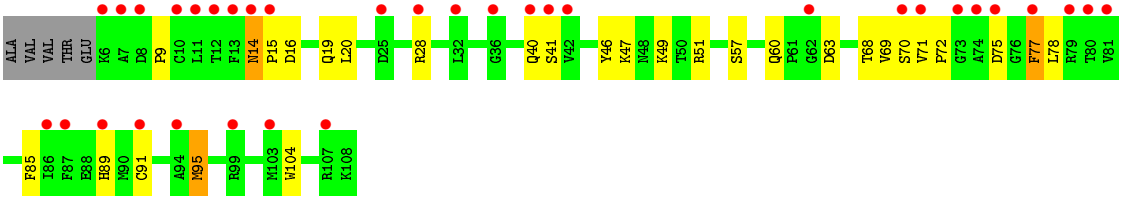
- Molecule 4: E3 19 kDa protein

Chain D:



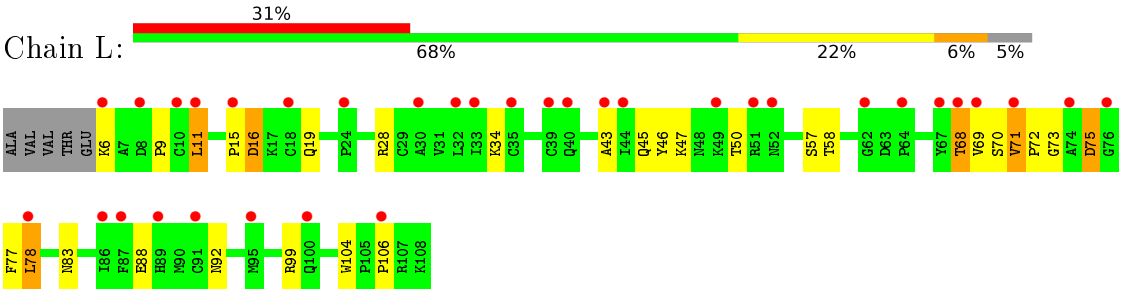
- Molecule 4: E3 19 kDa protein

Chain H:



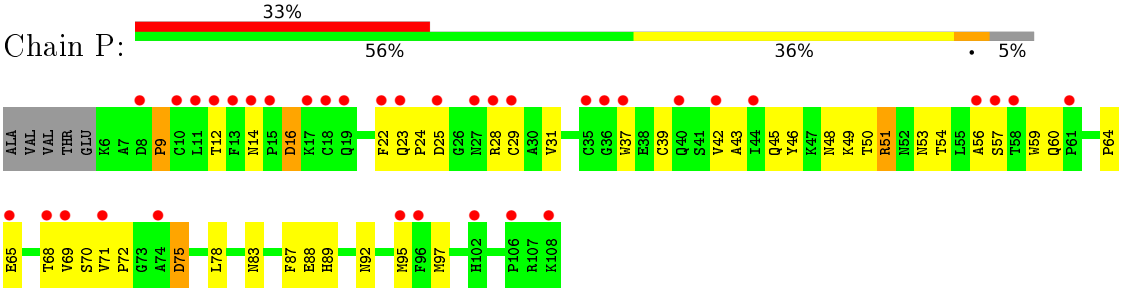
• Molecule 4: E3 19 kDa protein

Chain L:



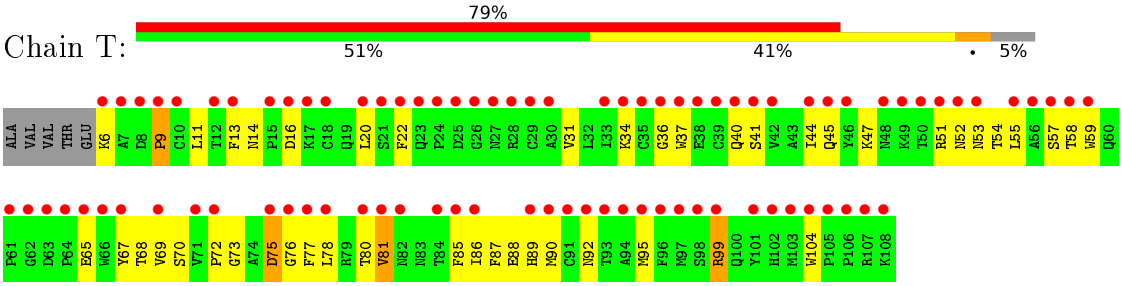
• Molecule 4: E3 19 kDa protein

Chain P:



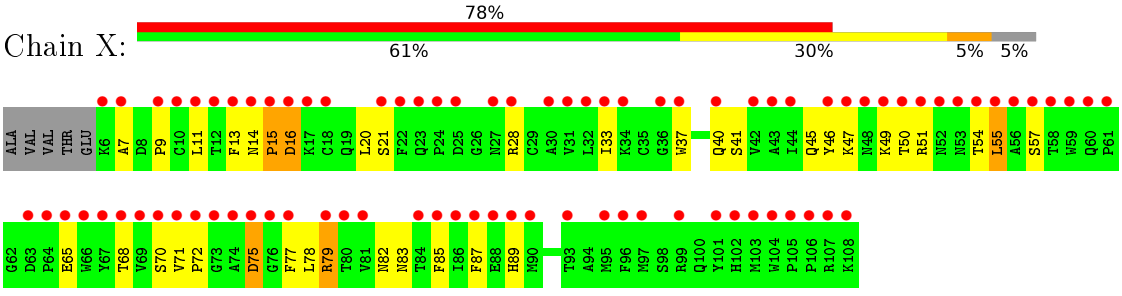
• Molecule 4: E3 19 kDa protein

Chain T:



• Molecule 4: E3 19 kDa protein

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	165.73Å 165.73Å 122.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.62 – 2.64 49.62 – 2.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.62-2.64) 99.3 (49.62-2.64)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.257 , 0.288 0.256 , 0.288	Depositor DCC
R_{free} test set	1970 reflections (1.79%)	DCC
Wilson B-factor (Å^2)	43.9	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	0.359 for -h,-k,l 0.389 for h,-h-k,-l 0.337 for -k,-h,-l	Xtriage
Reported twinning fraction	0.470 for -h,-k,l	Depositor
Outliers	0 of 110879 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	23039	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.38	1/2202 (0.0%)	0.60	0/2983
1	E	0.32	0/2245	0.59	0/3045
1	I	0.29	0/2109	0.57	0/2852
1	M	0.39	0/2221	0.75	3/3012 (0.1%)
1	Q	0.36	0/2169	0.69	1/2937 (0.0%)
1	U	0.34	0/2061	0.62	0/2791
2	B	0.46	0/79	0.66	0/108
2	F	0.48	0/79	0.79	0/108
2	J	0.32	0/79	0.47	0/108
2	N	0.37	0/79	0.45	0/108
2	R	0.33	0/79	0.48	0/108
2	V	0.47	0/79	0.89	1/108 (0.9%)
3	C	0.31	0/824	0.57	0/1115
3	G	0.28	0/843	0.57	0/1141
3	K	0.28	0/843	0.52	0/1141
3	O	0.28	0/843	0.54	0/1141
3	S	0.28	0/843	0.56	0/1141
3	W	0.30	0/843	0.59	0/1141
4	D	0.28	0/849	0.56	0/1154
4	H	0.34	0/858	0.63	0/1165
4	L	0.27	0/858	0.58	0/1165
4	P	0.31	0/858	0.57	0/1165
4	T	0.28	0/858	0.55	0/1165
4	X	0.29	0/858	0.64	1/1165 (0.1%)
All	All	0.33	1/23659 (0.0%)	0.61	6/32067 (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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	SER	CB-OG	-7.13	1.32	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	202	ARG	NE-CZ-NH2	-17.95	111.33	120.30
1	M	202	ARG	NE-CZ-NH1	8.67	124.64	120.30
2	V	2	LEU	CA-CB-CG	-5.83	101.89	115.30
1	Q	27	TYR	CA-CB-CG	5.74	124.31	113.40
1	M	190	THR	OG1-CB-CG2	-5.69	96.91	110.00
4	X	55	LEU	CA-CB-CG	5.30	127.49	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	189	MET	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	0	1999	131	1
1	E	2183	0	2037	105	0
1	I	2053	0	1916	103	0
1	M	2160	0	2016	150	0
1	Q	2111	0	1966	114	0
1	U	2007	0	1881	112	0
2	B	76	0	79	12	0
2	F	76	0	79	9	0
2	J	76	0	79	6	0
2	N	76	0	79	10	0
2	R	76	0	79	8	0
2	V	76	0	79	8	0
3	C	802	0	770	27	0
3	G	820	0	790	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	820	0	790	29	0
3	O	820	0	790	32	0
3	S	820	0	790	36	0
3	W	820	0	790	41	0
4	D	823	0	773	27	0
4	H	832	0	786	16	0
4	L	832	0	786	22	0
4	P	832	0	786	26	0
4	T	832	0	786	39	0
4	X	832	0	786	29	0
5	A	3	0	0	0	0
5	D	2	0	0	0	0
5	E	3	0	0	0	0
5	G	1	0	0	0	0
5	I	5	0	0	0	0
5	J	1	0	0	0	0
5	K	2	0	0	0	0
5	L	1	0	0	0	0
5	M	4	0	0	0	0
5	O	2	0	0	1	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
5	U	3	0	0	0	0
5	W	1	0	0	0	0
All	All	23039	0	21712	1015	1

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 23.

All (1015) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLN:HB2	1:I:48:ARG:HH12	1.24	1.01
1:M:205:ALA:HB3	1:M:243:LYS:HE2	1.45	0.99
1:Q:5:MET:HG3	1:Q:6:ARG:HG3	1.47	0.96
1:U:250:PRO:O	1:U:253:GLN:NE2	2.01	0.93
1:E:59:TYR:HH	1:E:171:TYR:HH	1.12	0.91
3:W:15:ALA:HB3	3:W:97:ARG:HH12	1.33	0.89
1:E:77:ASP:OD2	1:E:97:ARG:NH2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:MET:HG2	1:A:6:ARG:HG2	1.58	0.86
1:A:14:ARG:HB3	1:A:17:ARG:HB3	1.58	0.85
1:U:82:ARG:NH2	1:U:88:SER:O	2.10	0.85
3:C:12:ARG:NH2	4:D:97:MET:SD	2.49	0.84
1:A:224:GLN:HE22	1:A:228:THR:H	1.23	0.84
1:Q:77:ASP:OD2	1:Q:97:ARG:NH2	2.10	0.83
1:M:77:ASP:OD2	1:M:97:ARG:NH2	2.13	0.82
1:Q:217:TRP:HD1	1:Q:217:TRP:H	1.25	0.82
4:T:44:ILE:HD13	4:T:55:LEU:HB2	1.60	0.82
1:U:93:HIS:ND1	1:U:119:ASP:OD2	2.12	0.81
1:M:21:ARG:NH1	1:M:22:PHE:H	1.77	0.81
3:C:47:GLU:O	3:W:89:GLN:NE2	2.14	0.80
1:Q:141:GLN:OE1	1:Q:144:LYS:NZ	2.14	0.80
1:E:223:ASP:OD1	1:E:223:ASP:N	2.13	0.80
1:U:173:GLU:O	4:X:51:ARG:NH2	2.14	0.80
1:M:190:THR:O	1:M:202:ARG:HG2	1.82	0.80
1:A:17:ARG:HD3	3:W:44:GLU:HB2	1.63	0.80
1:A:127:LYS:NZ	1:A:132:SER:OG	2.11	0.80
3:G:35:ILE:HD11	3:G:84:HIS:CD2	2.17	0.80
3:C:37:VAL:HB	3:C:82:VAL:HG22	1.61	0.79
1:A:177:GLU:O	4:D:28:ARG:NH1	2.15	0.79
1:I:32:GLN:HB2	1:I:48:ARG:NH1	1.96	0.79
1:A:99:TYR:HB3	1:A:114:HIS:HD2	1.48	0.79
1:M:205:ALA:CB	1:M:243:LYS:HE2	2.13	0.79
1:M:188:HIS:HB2	1:M:204:TRP:HZ2	1.49	0.78
4:T:70:SER:HB3	4:T:78:LEU:HD21	1.66	0.78
1:E:201:LEU:N	1:E:247:VAL:O	2.17	0.78
3:G:39:LEU:HB2	3:G:49:VAL:HG11	1.66	0.77
4:T:92:ASN:HA	4:T:99:ARG:NH2	1.99	0.77
1:M:6:ARG:HH22	1:M:115:GLN:HG3	1.50	0.77
1:Q:262:GLN:HE22	1:Q:269:PRO:HB3	1.50	0.76
3:G:54:LEU:HG	3:G:64:LEU:HD11	1.66	0.76
4:X:77:PHE:O	4:X:79:ARG:NH1	2.18	0.76
1:I:6:ARG:NH1	1:I:98:MET:SD	2.58	0.76
1:Q:21:ARG:NH1	1:Q:38:SER:OG	2.18	0.76
1:A:9:PHE:HB2	1:A:97:ARG:HB2	1.67	0.76
3:K:56:PHE:HA	3:K:62:PHE:HA	1.68	0.76
1:I:77:ASP:OD2	1:I:97:ARG:NH2	2.18	0.76
1:U:77:ASP:OD2	1:U:97:ARG:NH2	2.20	0.75
1:M:147:TRP:NE1	2:N:8:TYR:O	2.19	0.75
1:U:14:ARG:HG2	1:U:17:ARG:HB2	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:PHE:HA	3:C:62:PHE:HA	1.69	0.74
4:T:69:VAL:HG23	4:T:81:VAL:HG13	1.70	0.74
1:M:21:ARG:NH2	1:M:37:ASP:HA	2.01	0.74
1:Q:219:ARG:HB2	1:Q:257:TYR:CZ	2.23	0.74
3:S:31:HIS:HD2	3:S:32:PRO:HA	1.51	0.74
4:T:72:PRO:HA	4:T:78:LEU:HA	1.70	0.74
1:Q:5:MET:HG2	1:Q:27:TYR:HE2	1.52	0.74
3:S:56:PHE:HA	3:S:62:PHE:HA	1.69	0.74
4:L:16:ASP:O	4:L:83:ASN:ND2	2.22	0.73
1:Q:238:ASP:OD2	3:S:12:ARG:NH1	2.20	0.73
3:S:73:THR:OG1	3:S:75:LYS:HG2	1.89	0.73
3:G:81:ARG:HG2	3:G:92:ILE:HG12	1.69	0.73
1:I:218:GLN:HB3	1:I:260:HIS:HD2	1.54	0.73
4:T:92:ASN:HA	4:T:99:ARG:HH22	1.54	0.72
3:W:56:PHE:HA	3:W:62:PHE:HA	1.69	0.72
1:E:209:TYR:H	1:E:209:TYR:HD2	1.36	0.72
3:K:54:LEU:HG	3:K:64:LEU:HD11	1.72	0.72
1:Q:14:ARG:HB3	1:Q:17:ARG:HB2	1.70	0.72
1:M:231:VAL:HG21	1:M:244:TRP:HE3	1.55	0.72
3:G:84:HIS:ND1	3:G:86:THR:HG23	2.05	0.71
1:M:250:PRO:O	1:M:253:GLN:NE2	2.23	0.71
1:M:97:ARG:HG2	1:M:116:TYR:HD1	1.55	0.71
3:G:43:GLY:HA2	1:Q:17:ARG:HH11	1.55	0.71
1:U:109:PHE:O	1:U:111:ARG:NH2	2.22	0.71
1:A:4:SER:HB3	1:A:103:VAL:HG22	1.71	0.71
1:A:8:PHE:HB2	1:A:25:VAL:HG13	1.72	0.71
1:A:73:THR:HG23	1:A:97:ARG:HH22	1.55	0.71
1:E:250:PRO:O	1:E:253:GLN:NE2	2.23	0.71
1:E:21:ARG:NH1	1:E:38:SER:OG	2.20	0.70
1:U:120:GLY:N	1:U:123:TYR:OH	2.24	0.70
1:U:9:PHE:HB3	1:U:74:HIS:HE1	1.55	0.70
1:A:223:ASP:OD1	1:A:223:ASP:N	2.24	0.70
3:C:11:SER:OG	3:C:21:ASN:ND2	2.23	0.70
1:A:13:SER:HB3	1:A:93:HIS:H	1.56	0.70
1:I:235:PRO:O	3:K:10:TYR:OH	2.07	0.70
1:Q:35:ARG:HG3	1:Q:46:GLU:HG3	1.74	0.70
3:W:44:GLU:OE2	3:W:81:ARG:NH2	2.22	0.70
1:M:109:PHE:O	1:M:111:ARG:NH2	2.24	0.70
3:K:24:ASN:OD1	3:K:24:ASN:N	2.24	0.70
3:K:19:LYS:HE2	3:K:20:SER:H	1.57	0.69
1:E:45:MET:H	1:E:64:THR:HG22	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:13:PHE:HE1	4:T:73:GLY:HA2	1.57	0.69
1:U:13:SER:HB3	1:U:93:HIS:H	1.56	0.69
1:I:27:TYR:HA	1:I:32:GLN:HA	1.75	0.69
1:I:147:TRP:NE1	2:J:8:TYR:O	2.23	0.69
1:I:73:THR:OG1	2:J:7:VAL:O	2.11	0.69
3:S:84:HIS:ND1	3:S:86:THR:HG23	2.07	0.69
1:A:45:MET:H	1:A:64:THR:HG22	1.57	0.69
1:I:124:ILE:HD11	1:I:140:ALA:HA	1.75	0.69
4:H:72:PRO:HA	4:H:78:LEU:HA	1.74	0.68
1:A:124:ILE:HG21	1:A:147:TRP:HZ3	1.58	0.68
1:I:219:ARG:N	1:I:222:GLU:OE2	2.25	0.68
1:M:45:MET:H	1:M:64:THR:HG22	1.57	0.68
1:Q:28:VAL:O	1:Q:31:THR:OG1	2.09	0.68
4:X:70:SER:HB3	4:X:78:LEU:HD21	1.73	0.68
1:M:232:GLU:OE1	3:O:28:SER:OG	2.09	0.68
1:A:201:LEU:N	1:A:247:VAL:O	2.27	0.68
3:G:24:ASN:OD1	3:G:24:ASN:N	2.26	0.68
1:M:37:ASP:HB3	1:M:40:ALA:HB2	1.76	0.68
3:C:5:PRO:HB3	3:C:30:PHE:HB3	1.76	0.68
1:E:109:PHE:O	1:E:111:ARG:NH2	2.26	0.68
1:I:218:GLN:NE2	1:I:220:ASP:O	2.25	0.68
1:I:4:SER:HB3	1:I:168:LEU:HD21	1.74	0.68
1:M:13:SER:HA	1:M:20:PRO:HB3	1.76	0.68
1:A:162:GLY:H	1:A:165:VAL:HG22	1.58	0.67
1:U:24:ALA:HB3	1:U:36:PHE:HB3	1.75	0.67
1:E:24:ALA:HB3	1:E:36:PHE:HB3	1.76	0.67
3:G:56:PHE:HA	3:G:62:PHE:HA	1.75	0.67
1:E:235:PRO:HB2	3:G:65:LEU:HD22	1.77	0.67
1:Q:5:MET:HG2	1:Q:27:TYR:CE2	2.29	0.67
3:O:24:ASN:N	3:O:24:ASN:OD1	2.27	0.67
3:O:56:PHE:HA	3:O:62:PHE:HA	1.75	0.67
1:I:4:SER:OG	1:I:102:ASP:OD1	2.12	0.67
4:H:89:HIS:NE2	4:L:19:GLN:OE1	2.27	0.67
1:M:108:ARG:HA	1:M:169:ARG:HH21	1.60	0.67
1:Q:3:HIS:O	1:Q:3:HIS:ND1	2.27	0.67
1:M:6:ARG:NH1	1:M:98:MET:SD	2.68	0.67
4:X:50:THR:O	4:X:51:ARG:HD3	1.95	0.67
1:U:124:ILE:HD11	1:U:133:TRP:HB3	1.75	0.66
4:T:36:GLY:O	4:T:53:ASN:ND2	2.26	0.66
3:G:13:HIS:H	3:G:21:ASN:HD21	1.44	0.66
1:U:189:MET:HG3	1:U:201:LEU:HD23	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:21:ARG:NH1	1:M:38:SER:OG	2.29	0.66
1:U:13:SER:OG	1:U:82:ARG:NH1	2.27	0.66
1:U:131:ARG:HD3	1:U:153:ALA:HB3	1.76	0.66
1:A:24:ALA:HB3	1:A:36:PHE:HB3	1.77	0.66
1:U:181:ARG:HH21	4:X:28:ARG:HH11	1.44	0.66
3:W:26:TYR:HB2	3:W:65:LEU:HD13	1.78	0.65
1:Q:217:TRP:CD1	1:Q:217:TRP:N	2.64	0.65
3:G:40:LEU:HD11	3:G:79:ALA:HB3	1.78	0.65
1:A:54:GLN:O	4:D:51:ARG:NH2	2.30	0.65
4:L:43:ALA:HB3	4:L:70:SER:HB2	1.77	0.65
1:I:238:ASP:OD2	3:K:12:ARG:NH1	2.29	0.65
1:M:20:PRO:HG2	1:M:75:ARG:HD3	1.78	0.65
1:A:66:LYS:HE3	2:B:2:LEU:HB3	1.77	0.65
3:W:24:ASN:OD1	3:W:24:ASN:N	2.30	0.65
1:Q:147:TRP:NE1	2:R:8:TYR:O	2.30	0.64
3:O:54:LEU:HG	3:O:64:LEU:HD11	1.78	0.64
1:A:213:ILE:HG12	1:A:263:HIS:HD2	1.62	0.64
1:U:45:MET:H	1:U:64:THR:HG22	1.62	0.64
1:E:211:ALA:HB1	1:E:233:THR:HG21	1.79	0.64
1:A:13:SER:OG	1:A:82:ARG:NH1	2.30	0.64
4:P:88:GLU:O	4:P:92:ASN:ND2	2.31	0.64
1:Q:263:HIS:CD2	1:Q:265:GLY:H	2.16	0.64
1:A:93:HIS:ND1	1:A:119:ASP:OD2	2.31	0.64
3:K:30:PHE:CE1	3:K:62:PHE:HB2	2.33	0.64
1:M:231:VAL:HG21	1:M:244:TRP:CE3	2.33	0.64
1:A:157:ARG:HA	1:A:160:LEU:HD12	1.80	0.63
4:P:16:ASP:O	4:P:83:ASN:ND2	2.31	0.63
1:Q:82:ARG:NH2	1:Q:88:SER:O	2.31	0.63
1:A:85:TYR:OH	1:A:137:ASP:OD2	2.11	0.63
1:E:129:ASP:HB2	1:E:132:SER:OG	1.98	0.63
1:Q:157:ARG:HA	1:Q:160:LEU:HD12	1.79	0.63
3:W:13:HIS:H	3:W:21:ASN:HD21	1.43	0.63
1:M:191:HIS:HE1	1:M:193:ALA:HB2	1.62	0.63
1:E:124:ILE:HG23	1:E:133:TRP:CH2	2.34	0.63
3:G:5:PRO:HB3	3:G:30:PHE:HB3	1.81	0.63
2:R:1:LEU:HD23	2:R:2:LEU:HD12	1.81	0.62
3:S:24:ASN:OD1	3:S:24:ASN:N	2.32	0.62
1:M:54:GLN:O	4:P:51:ARG:NH2	2.32	0.62
1:U:191:HIS:CD2	1:U:201:LEU:HD12	2.34	0.62
4:D:28:ARG:NH2	4:D:58:THR:OG1	2.32	0.62
1:M:95:VAL:HG13	1:M:116:TYR:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:234:ARG:HE	1:U:242:GLN:HB2	1.63	0.62
1:U:73:THR:OG1	2:V:7:VAL:O	2.15	0.62
4:X:16:ASP:O	4:X:83:ASN:ND2	2.32	0.62
4:P:43:ALA:HB3	4:P:70:SER:HB2	1.81	0.62
1:U:37:ASP:HB3	1:U:40:ALA:HB2	1.82	0.62
1:A:82:ARG:HD2	1:A:93:HIS:HB2	1.82	0.62
4:P:42:VAL:HG22	4:P:71:VAL:HG12	1.81	0.62
1:I:13:SER:HA	1:I:20:PRO:HB3	1.81	0.61
1:M:35:ARG:HD2	3:O:53:ASP:HB2	1.80	0.61
3:K:79:ALA:HB2	3:K:94:LYS:HG2	1.82	0.61
1:E:234:ARG:HD3	3:G:8:GLN:NE2	2.16	0.61
4:T:92:ASN:O	4:T:99:ARG:NH1	2.33	0.61
1:A:188:HIS:HB3	1:A:204:TRP:HZ2	1.64	0.61
1:I:9:PHE:HB3	1:I:74:HIS:HE1	1.65	0.61
1:U:14:ARG:NH1	1:U:21:ARG:HB2	2.16	0.61
1:A:188:HIS:CD2	1:A:189:MET:H	2.19	0.61
1:A:235:PRO:O	3:C:10:TYR:OH	2.17	0.61
1:A:99:TYR:HB3	1:A:114:HIS:CD2	2.32	0.61
3:S:11:SER:OG	3:S:21:ASN:ND2	2.34	0.61
1:I:131:ARG:NH2	1:I:154:GLU:OE1	2.34	0.61
1:E:102:ASP:OD2	1:E:113:TYR:OH	2.16	0.60
3:G:36:GLU:HB3	3:G:83:ASN:ND2	2.16	0.60
1:I:45:MET:H	1:I:64:THR:HG22	1.65	0.60
3:S:29:GLY:HA2	3:S:61:SER:HB2	1.83	0.60
1:U:174:ASN:OD1	4:X:51:ARG:NH1	2.34	0.60
1:I:131:ARG:HD3	1:I:153:ALA:HB3	1.83	0.60
1:U:202:ARG:HG3	1:U:204:TRP:CZ3	2.37	0.60
3:O:73:THR:OG1	3:O:75:LYS:HG2	2.01	0.60
4:P:72:PRO:HA	4:P:78:LEU:HA	1.83	0.60
1:A:141:GLN:N	1:A:141:GLN:OE1	2.33	0.60
1:A:98:MET:HB3	1:A:115:GLN:HG3	1.82	0.60
1:E:112:GLY:HA3	1:E:160:LEU:HD11	1.83	0.60
1:M:71:SER:O	1:M:75:ARG:HG2	2.01	0.60
1:Q:144:LYS:HA	1:Q:147:TRP:CE3	2.37	0.60
4:T:34:LYS:HA	4:T:54:THR:HG22	1.82	0.60
1:Q:124:ILE:HD11	1:Q:140:ALA:HA	1.83	0.60
1:E:116:TYR:N	1:E:124:ILE:O	2.18	0.59
1:M:28:VAL:O	1:M:31:THR:OG1	2.18	0.59
4:D:72:PRO:HA	4:D:78:LEU:HA	1.82	0.59
3:O:7:ILE:HD11	3:O:80:CYS:HB3	1.84	0.59
1:U:249:VAL:HG12	1:U:253:GLN:NE2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:15:PRO:HG2	4:H:71:VAL:HG11	1.83	0.59
1:M:191:HIS:HB2	1:M:201:LEU:HG	1.84	0.59
1:E:21:ARG:CZ	1:E:39:ASP:HB2	2.33	0.59
3:G:36:GLU:HB3	3:G:83:ASN:HD21	1.67	0.59
4:P:49:LYS:NZ	4:P:56:ALA:O	2.29	0.59
4:X:72:PRO:HA	4:X:78:LEU:HA	1.84	0.59
1:I:262:GLN:HG2	1:I:269:PRO:HB3	1.83	0.59
1:M:21:ARG:NH2	1:M:22:PHE:O	2.36	0.59
1:A:82:ARG:HH21	1:A:87:GLN:HG3	1.66	0.59
1:M:137:ASP:OD1	1:M:138:MET:N	2.28	0.59
1:Q:212:GLU:N	1:Q:212:GLU:OE1	2.36	0.59
1:I:27:TYR:HH	3:K:63:TYR:HH	1.43	0.59
1:Q:35:ARG:HE	1:Q:48:ARG:HD3	1.68	0.59
3:C:24:ASN:HB3	3:C:65:LEU:HD11	1.83	0.59
1:E:182:THR:HA	1:E:209:TYR:CZ	2.38	0.59
4:L:72:PRO:HA	4:L:78:LEU:HA	1.85	0.59
3:K:19:LYS:HE2	3:K:20:SER:N	2.18	0.59
1:Q:44:ARG:HA	1:Q:64:THR:HG23	1.85	0.59
1:I:181:ARG:HH21	4:L:28:ARG:HH11	1.50	0.58
1:A:201:LEU:HD22	1:A:257:TYR:OH	2.04	0.58
1:M:157:ARG:HA	1:M:160:LEU:HD12	1.84	0.58
1:M:235:PRO:HA	1:M:241:PHE:HD1	1.69	0.58
1:Q:154:GLU:HA	1:Q:157:ARG:HB3	1.85	0.58
4:T:75:ASP:N	4:T:75:ASP:OD1	2.35	0.58
1:U:5:MET:HG2	1:U:6:ARG:HG2	1.86	0.58
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.38	0.58
3:O:72:PRO:HB3	3:O:95:TRP:HH2	1.67	0.58
1:Q:154:GLU:HG3	1:Q:157:ARG:HD3	1.84	0.58
1:A:63:GLU:OE1	2:B:2:LEU:HB2	2.04	0.58
1:E:159:TYR:OH	2:F:1:LEU:O	2.14	0.58
3:G:29:GLY:HA2	3:G:61:SER:HB2	1.84	0.58
3:G:59:ASP:N	3:G:59:ASP:OD1	2.37	0.58
1:M:22:PHE:HB2	1:M:75:ARG:HH12	1.68	0.57
1:M:73:THR:HG23	1:M:97:ARG:HH12	1.69	0.57
1:A:191:HIS:CE1	1:A:201:LEU:HD21	2.38	0.57
4:D:70:SER:HB3	4:D:78:LEU:HD21	1.86	0.57
1:E:209:TYR:CD1	1:E:210:PRO:HD3	2.39	0.57
1:M:4:SER:OG	1:M:103:VAL:N	2.35	0.57
1:M:204:TRP:HZ3	1:M:206:LEU:HB2	1.69	0.57
1:A:3:HIS:ND1	1:A:3:HIS:O	2.32	0.57
1:E:13:SER:HA	1:E:20:PRO:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:213:ILE:HD12	1:Q:263:HIS:HB2	1.87	0.57
1:Q:235:PRO:HB2	3:S:65:LEU:HD22	1.86	0.57
1:U:253:GLN:NE2	1:U:253:GLN:H	2.02	0.57
1:U:77:ASP:O	1:U:80:THR:OG1	2.18	0.57
3:G:35:ILE:HG22	3:G:37:VAL:HG12	1.86	0.57
1:I:213:ILE:HB	1:I:263:HIS:HD2	1.70	0.57
1:Q:116:TYR:HE1	1:Q:147:TRP:CH2	2.23	0.57
4:D:92:ASN:HA	4:D:99:ARG:NH2	2.20	0.57
1:E:133:TRP:CD1	1:E:144:LYS:HD3	2.40	0.57
1:M:107:TRP:O	1:M:169:ARG:NE	2.32	0.57
1:M:1:GLY:O	1:M:3:HIS:ND1	2.38	0.57
1:M:250:PRO:HB2	1:M:253:GLN:HE22	1.70	0.57
1:Q:102:ASP:OD2	1:Q:113:TYR:OH	2.22	0.57
1:E:114:HIS:HD1	1:E:126:LEU:HB2	1.70	0.56
4:T:37:TRP:HZ2	4:T:54:THR:HG1	1.53	0.56
1:A:99:TYR:HA	1:A:114:HIS:HA	1.87	0.56
1:M:213:ILE:HB	1:M:243:LYS:HZ2	1.69	0.56
1:E:76:VAL:HG23	2:F:8:TYR:HE1	1.69	0.56
1:Q:185:PRO:HB3	1:Q:208:PHE:CZ	2.40	0.56
1:U:177:GLU:OE1	4:X:49:LYS:NZ	2.39	0.56
1:I:98:MET:HE2	3:K:56:PHE:HE1	1.71	0.56
1:M:124:ILE:HG21	1:M:147:TRP:HZ3	1.70	0.56
1:Q:205:ALA:HB1	1:Q:208:PHE:CE2	2.40	0.56
1:U:174:ASN:HA	4:X:51:ARG:HH12	1.69	0.56
1:M:21:ARG:HH22	1:M:37:ASP:HA	1.70	0.56
1:M:95:VAL:HG13	1:M:116:TYR:HE1	1.69	0.56
1:M:190:THR:HB	1:M:202:ARG:HE	1.71	0.56
1:U:238:ASP:OD2	3:W:12:ARG:NH1	2.38	0.56
1:A:20:PRO:HG3	1:A:78:LEU:HD21	1.86	0.56
1:E:147:TRP:NE1	2:F:8:TYR:O	2.38	0.56
4:P:28:ARG:NH1	4:P:59:TRP:O	2.37	0.56
1:Q:219:ARG:HG3	1:Q:222:GLU:HB2	1.88	0.56
1:U:201:LEU:N	1:U:247:VAL:O	2.39	0.56
1:A:54:GLN:NE2	1:A:174:ASN:O	2.39	0.56
4:D:27:ASN:ND2	4:D:103:MET:HG2	2.21	0.56
1:E:3:HIS:ND1	1:E:3:HIS:O	2.39	0.56
1:E:156:LEU:HA	2:F:3:PHE:CE1	2.40	0.56
1:I:111:ARG:NH1	1:I:111:ARG:HB2	2.20	0.56
4:D:61:PRO:HD3	4:D:104:TRP:CH2	2.41	0.56
1:M:131:ARG:HH22	1:M:151:HIS:CD2	2.24	0.56
3:W:11:SER:OG	3:W:21:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:54:LEU:HD11	3:W:62:PHE:CD1	2.41	0.56
3:G:40:LEU:HB2	3:G:43:GLY:O	2.06	0.55
1:M:146:LYS:HZ1	2:N:8:TYR:HB3	1.71	0.55
3:S:45:ARG:NH1	3:S:46:ILE:HG22	2.21	0.55
3:W:31:HIS:HD2	3:W:32:PRO:HA	1.71	0.55
1:A:21:ARG:NH2	1:A:37:ASP:OD2	2.39	0.55
1:I:3:HIS:ND1	1:I:3:HIS:O	2.39	0.55
4:L:11:LEU:HD12	4:L:11:LEU:H	1.70	0.55
1:Q:86:ASN:N	1:Q:86:ASN:OD1	2.37	0.55
1:E:70:HIS:O	1:E:74:HIS:ND1	2.38	0.55
1:A:177:GLU:HG3	4:D:57:SER:HA	1.89	0.55
1:E:20:PRO:HG3	1:E:78:LEU:HD21	1.88	0.55
1:Q:30:ASP:OD2	1:Q:211:ALA:N	2.31	0.55
4:X:75:ASP:N	4:X:75:ASP:OD1	2.40	0.55
1:E:94:THR:OG1	1:E:96:GLN:OE1	2.24	0.55
3:K:13:HIS:H	3:K:21:ASN:HD21	1.55	0.55
1:A:107:TRP:O	1:A:169:ARG:NE	2.35	0.55
1:A:220:ASP:OD2	1:A:256:ARG:NH2	2.39	0.55
3:C:11:SER:OG	3:C:13:HIS:O	2.23	0.55
4:H:70:SER:HB3	4:H:78:LEU:HD21	1.88	0.55
3:O:69:GLU:OE2	3:W:19:LYS:NZ	2.29	0.55
1:U:154:GLU:HG2	1:U:157:ARG:HD3	1.89	0.55
1:A:188:HIS:CG	1:A:189:MET:H	2.25	0.55
3:K:35:ILE:HG22	3:K:37:VAL:HG12	1.89	0.55
1:E:144:LYS:O	1:E:148:GLU:HG3	2.05	0.55
1:I:147:TRP:HZ2	2:J:9:VAL:HG12	1.72	0.55
1:U:181:ARG:HH21	4:X:28:ARG:NH1	2.04	0.55
4:X:37:TRP:HE1	4:X:54:THR:HG1	1.52	0.55
1:A:224:GLN:HE22	1:A:228:THR:N	1.97	0.55
1:I:218:GLN:HB3	1:I:260:HIS:CD2	2.38	0.55
4:X:37:TRP:NE1	4:X:54:THR:OG1	2.37	0.54
1:A:263:HIS:HB3	1:A:266:LEU:HB2	1.90	0.54
1:I:13:SER:HB3	1:I:93:HIS:H	1.73	0.54
4:T:45:GLN:NE2	4:T:47:LYS:O	2.40	0.54
1:U:6:ARG:HD2	1:U:8:PHE:CE2	2.41	0.54
1:A:147:TRP:HZ2	2:B:9:VAL:HG12	1.71	0.54
1:E:33:PHE:CE2	1:E:52:ILE:HB	2.42	0.54
1:M:14:ARG:HB3	1:M:17:ARG:HG2	1.88	0.54
3:K:37:VAL:HB	3:K:82:VAL:HG22	1.90	0.54
1:M:115:GLN:HA	1:M:125:ALA:HA	1.90	0.54
1:U:114:HIS:CD2	1:U:156:LEU:HD21	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:201:LEU:HD13	1:U:257:TYR:OH	2.07	0.54
1:I:257:TYR:H	1:I:257:TYR:HD2	1.55	0.54
1:U:202:ARG:HG3	1:U:204:TRP:CE3	2.42	0.54
1:E:118:TYR:H	1:E:118:TYR:HD2	1.56	0.54
1:M:78:LEU:HB3	1:M:95:VAL:HG21	1.88	0.54
1:Q:13:SER:HB2	1:Q:93:HIS:H	1.72	0.54
1:Q:208:PHE:O	1:Q:240:THR:HA	2.07	0.54
1:E:115:GLN:HA	1:E:125:ALA:HA	1.89	0.54
1:E:185:PRO:HG3	1:E:208:PHE:HB3	1.88	0.54
1:I:77:ASP:O	1:I:80:THR:OG1	2.19	0.54
1:Q:216:THR:O	1:Q:260:HIS:N	2.40	0.54
1:M:28:VAL:HG11	1:M:51:TRP:HH2	1.73	0.54
1:E:28:VAL:O	1:E:31:THR:OG1	2.23	0.53
1:E:238:ASP:OD2	3:G:12:ARG:NH1	2.41	0.53
1:M:108:ARG:NH1	1:M:169:ARG:HH22	2.06	0.53
1:M:217:TRP:CZ2	1:M:224:GLN:HB2	2.43	0.53
1:E:261:VAL:HG13	1:E:270:LEU:HB2	1.89	0.53
3:W:23:LEU:HG	3:W:70:PHE:CG	2.44	0.53
4:P:75:ASP:OD1	4:P:75:ASP:N	2.41	0.53
3:W:30:PHE:HB2	3:W:84:HIS:NE2	2.24	0.53
1:M:103:VAL:HG13	1:M:107:TRP:HA	1.91	0.53
1:M:94:THR:OG1	1:M:96:GLN:OE1	2.25	0.53
1:Q:127:LYS:HG3	1:Q:128:GLU:N	2.23	0.53
3:G:56:PHE:HB3	3:G:62:PHE:CD1	2.43	0.53
1:M:238:ASP:OD1	1:M:240:THR:OG1	2.23	0.53
1:M:33:PHE:HD1	1:M:34:VAL:HG23	1.74	0.53
1:Q:139:ALA:HA	1:Q:142:THR:HG22	1.90	0.53
4:D:45:GLN:HB3	4:D:68:THR:OG1	2.08	0.53
1:Q:121:LYS:HG3	1:Q:122:ASP:H	1.72	0.53
1:U:11:SER:HA	1:U:21:ARG:O	2.09	0.53
1:U:7:TYR:C	1:U:8:PHE:HD2	2.12	0.53
1:A:73:THR:OG1	2:B:7:VAL:O	2.21	0.53
3:C:21:ASN:HB3	3:C:70:PHE:CE2	2.43	0.53
4:H:95:MET:HE1	4:H:104:TRP:CG	2.44	0.53
1:I:48:ARG:HG2	1:I:48:ARG:HH21	1.74	0.53
3:O:12:ARG:HH21	4:P:97:MET:HB3	1.74	0.53
4:P:28:ARG:NH2	4:P:60:GLN:HB3	2.24	0.53
1:A:17:ARG:C	3:W:44:GLU:HB3	2.29	0.53
1:I:19:GLU:OE1	1:I:20:PRO:HD2	2.09	0.53
1:M:1:GLY:HA2	1:M:105:SER:HA	1.90	0.53
4:X:45:GLN:HB3	4:X:68:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:TRP:CZ2	2:J:9:VAL:HG12	2.44	0.52
1:M:208:PHE:CE1	1:M:241:PHE:HB2	2.44	0.52
1:M:74:HIS:NE2	1:M:97:ARG:HG3	2.24	0.52
4:H:46:TYR:CE2	4:H:47:LYS:HE3	2.44	0.52
1:M:14:ARG:HD2	1:M:21:ARG:HB2	1.90	0.52
1:Q:219:ARG:HB2	1:Q:257:TYR:CE1	2.45	0.52
1:U:204:TRP:HZ2	1:U:244:TRP:CD2	2.27	0.52
1:A:66:LYS:HD2	2:B:4:GLY:HA2	1.91	0.52
1:E:124:ILE:HG23	1:E:133:TRP:CZ2	2.44	0.52
1:Q:216:THR:N	1:Q:260:HIS:O	2.42	0.52
3:S:56:PHE:HB3	3:S:62:PHE:CD1	2.44	0.52
3:W:31:HIS:CD2	3:W:32:PRO:HA	2.43	0.52
1:E:73:THR:OG1	2:F:7:VAL:O	2.24	0.52
3:O:30:PHE:CE1	3:O:62:PHE:HB2	2.45	0.52
1:Q:14:ARG:NE	1:Q:19:GLU:O	2.42	0.52
4:X:20:LEU:HD11	4:X:85:PHE:CD1	2.44	0.52
3:S:35:ILE:CD1	3:S:84:HIS:HD2	2.23	0.52
4:T:65:GLU:HA	4:T:87:PHE:CD2	2.45	0.52
1:U:235:PRO:O	3:W:10:TYR:OH	2.22	0.52
1:E:141:GLN:HA	1:E:144:LYS:HG2	1.91	0.52
3:S:31:HIS:CD2	3:S:32:PRO:HA	2.38	0.52
1:U:191:HIS:HE1	1:U:193:ALA:HB2	1.74	0.52
1:U:263:HIS:CD2	1:U:265:GLY:H	2.28	0.52
3:C:30:PHE:HB2	3:C:84:HIS:HE2	1.74	0.52
3:K:39:LEU:HB2	3:K:49:VAL:HG11	1.90	0.52
1:Q:209:TYR:HB3	1:Q:210:PRO:HD3	1.90	0.52
1:Q:22:PHE:CE2	1:Q:24:ALA:HB2	2.45	0.52
3:S:41:LYS:HB2	3:S:45:ARG:CZ	2.39	0.52
3:W:40:LEU:HG	3:W:43:GLY:O	2.10	0.52
1:Q:63:GLU:OE1	2:R:2:LEU:HD13	2.10	0.52
3:C:11:SER:HG	3:C:21:ASN:HD21	1.57	0.52
1:M:14:ARG:CZ	1:M:17:ARG:HH21	2.22	0.52
3:W:7:ILE:HD11	3:W:93:VAL:HB	1.91	0.52
4:X:49:LYS:HE3	4:X:51:ARG:CZ	2.39	0.52
1:U:250:PRO:C	1:U:253:GLN:HE22	2.06	0.51
3:G:57:SER:OG	3:G:58:LYS:N	2.43	0.51
1:M:93:HIS:ND1	1:M:119:ASP:OD2	2.35	0.51
3:O:29:GLY:HA2	3:O:61:SER:HB2	1.91	0.51
4:P:39:CYS:O	4:P:53:ASN:ND2	2.29	0.51
1:A:115:GLN:HA	1:A:125:ALA:HA	1.92	0.51
4:H:49:LYS:HE3	4:H:51:ARG:HH21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:PRO:O	3:G:10:TYR:OH	2.17	0.51
1:I:14:ARG:HG2	1:I:17:ARG:HB3	1.93	0.51
1:M:215:LEU:HD21	1:M:243:LYS:HE3	1.92	0.51
1:A:230:LEU:H	1:A:230:LEU:HD23	1.74	0.51
1:E:234:ARG:HE	1:E:242:GLN:HB2	1.75	0.51
1:I:121:LYS:HG3	1:I:122:ASP:H	1.75	0.51
1:U:129:ASP:CG	1:U:130:LEU:H	2.14	0.51
1:A:6:ARG:HG3	1:A:8:PHE:CE2	2.46	0.51
1:I:109:PHE:CZ	1:I:111:ARG:HA	2.46	0.51
1:Q:171:TYR:HE1	2:R:1:LEU:HD13	1.75	0.51
1:A:121:LYS:HG3	1:A:122:ASP:H	1.76	0.51
1:A:137:ASP:O	1:A:141:GLN:NE2	2.43	0.51
1:I:218:GLN:NE2	1:I:222:GLU:H	2.07	0.51
4:T:22:PHE:CD2	4:T:90:MET:HB3	2.46	0.51
1:M:73:THR:OG1	2:N:7:VAL:O	2.28	0.51
4:X:33:ILE:HB	4:X:55:LEU:HG	1.93	0.51
1:A:82:ARG:NH2	1:A:88:SER:O	2.43	0.51
3:G:35:ILE:HD11	3:G:84:HIS:HD2	1.71	0.51
1:A:1:GLY:HA2	1:A:105:SER:HA	1.92	0.51
1:A:177:GLU:HG2	4:D:28:ARG:HH22	1.76	0.51
1:E:27:TYR:OH	1:E:32:GLN:NE2	2.44	0.51
1:I:93:HIS:ND1	1:I:119:ASP:OD2	2.33	0.51
3:S:84:HIS:CE1	3:S:86:THR:HG23	2.46	0.51
4:H:14:ASN:O	4:H:16:ASP:N	2.42	0.50
1:I:109:PHE:CE2	1:I:111:ARG:HA	2.46	0.50
1:I:127:LYS:HD3	1:I:128:GLU:N	2.27	0.50
3:K:84:HIS:ND1	3:K:86:THR:OG1	2.33	0.50
1:Q:164:CYS:O	1:Q:168:LEU:HB2	2.11	0.50
1:Q:11:SER:OG	1:Q:95:VAL:O	2.26	0.50
1:A:108:ARG:HA	1:A:169:ARG:HH21	1.74	0.50
3:G:21:ASN:HB3	3:G:70:PHE:CE2	2.47	0.50
1:I:97:ARG:HD3	1:I:116:TYR:CD2	2.46	0.50
1:Q:145:HIS:ND1	1:Q:148:GLU:OE1	2.30	0.50
1:Q:33:PHE:CE2	1:Q:52:ILE:HB	2.46	0.50
4:L:73:GLY:N	4:L:77:PHE:O	2.41	0.50
1:M:124:ILE:HG21	1:M:147:TRP:CZ3	2.45	0.50
1:M:97:ARG:HG2	1:M:116:TYR:CD1	2.42	0.50
1:Q:1:GLY:H2	1:Q:105:SER:HA	1.76	0.50
1:Q:109:PHE:CD1	1:Q:161:GLU:HG2	2.46	0.50
1:U:108:ARG:HA	1:U:169:ARG:HH21	1.76	0.50
1:A:171:TYR:CE1	2:B:1:LEU:HD22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:ILE:HG23	4:D:89:HIS:HB2	1.93	0.50
1:E:209:TYR:CG	1:E:210:PRO:CD	2.95	0.50
1:U:35:ARG:HD2	1:U:48:ARG:HG3	1.92	0.50
1:U:94:THR:OG1	1:U:96:GLN:OE1	2.27	0.50
1:I:170:ARG:O	1:I:173:GLU:HG2	2.12	0.50
3:K:5:PRO:HB3	3:K:30:PHE:HB3	1.92	0.50
1:I:234:ARG:HD3	3:K:8:GLN:NE2	2.27	0.50
1:M:116:TYR:CE2	1:M:123:TYR:HD2	2.29	0.50
1:Q:262:GLN:HA	1:Q:266:LEU:HD11	1.93	0.50
1:Q:262:GLN:NE2	1:Q:269:PRO:HB3	2.22	0.50
1:U:97:ARG:HD3	1:U:116:TYR:HD1	1.75	0.50
1:M:191:HIS:ND1	1:M:192:HIS:N	2.59	0.50
1:M:209:TYR:HB3	1:M:210:PRO:HD3	1.93	0.50
1:M:72:GLN:O	1:M:76:VAL:HG22	2.10	0.50
4:D:68:THR:HG22	4:D:82:ASN:OD1	2.11	0.50
1:E:231:VAL:HG11	1:E:244:TRP:CB	2.41	0.50
1:U:177:GLU:HG3	4:X:57:SER:HA	1.94	0.50
3:C:30:PHE:HB2	3:C:84:HIS:NE2	2.27	0.50
1:M:260:HIS:HE1	1:M:271:THR:HG22	1.76	0.50
4:T:73:GLY:N	4:T:77:PHE:O	2.40	0.50
1:U:254:GLU:HB3	1:U:257:TYR:OH	2.12	0.50
3:K:34:ASP:C	3:K:35:ILE:HD12	2.32	0.50
1:Q:93:HIS:ND1	1:Q:119:ASP:OD2	2.45	0.50
1:U:126:LEU:HG	1:U:127:LYS:O	2.11	0.50
3:W:56:PHE:HB3	3:W:62:PHE:CD1	2.47	0.50
1:A:224:GLN:NE2	1:A:228:THR:H	2.01	0.49
1:E:164:CYS:O	1:E:168:LEU:HB2	2.11	0.49
1:E:28:VAL:HG11	1:E:51:TRP:HH2	1.77	0.49
2:V:3:PHE:CE2	2:V:5:TYR:HB2	2.47	0.49
3:S:12:ARG:HB3	3:S:22:PHE:HB2	1.94	0.49
1:M:47:PRO:HB3	1:M:60:TRP:CH2	2.47	0.49
1:U:208:PHE:HB2	1:U:263:HIS:CE1	2.47	0.49
3:C:30:PHE:CE1	3:C:62:PHE:HB2	2.47	0.49
1:M:218:GLN:NE2	1:M:222:GLU:O	2.34	0.49
1:M:250:PRO:C	1:M:253:GLN:HE22	2.13	0.49
4:D:57:SER:OG	4:D:58:THR:N	2.44	0.49
1:E:177:GLU:HG3	4:H:57:SER:HA	1.93	0.49
1:I:139:ALA:HA	1:I:142:THR:HG22	1.93	0.49
1:Q:7:TYR:CZ	1:Q:26:GLY:HA3	2.47	0.49
1:A:33:PHE:HE1	1:A:171:TYR:CD1	2.31	0.49
4:T:14:ASN:O	4:T:16:ASP:N	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:8:PHE:HB2	1:U:25:VAL:HG12	1.93	0.49
1:U:73:THR:HG23	1:U:97:ARG:HH12	1.77	0.49
1:A:152:VAL:HG13	2:B:5:TYR:OH	2.13	0.49
4:D:44:ILE:HD11	4:D:67:TYR:HD1	1.77	0.49
1:I:111:ARG:NH2	1:I:128:GLU:OE2	2.45	0.49
1:M:114:HIS:O	1:M:126:LEU:N	2.41	0.49
1:M:35:ARG:NH1	3:O:53:ASP:OD2	2.40	0.49
1:Q:77:ASP:O	1:Q:80:THR:OG1	2.22	0.49
4:T:95:MET:O	4:T:99:ARG:NH1	2.45	0.49
1:U:21:ARG:NH1	1:U:37:ASP:OD1	2.46	0.49
1:A:146:LYS:HE2	2:B:8:TYR:HE2	1.78	0.49
4:D:88:GLU:O	4:D:92:ASN:ND2	2.46	0.49
1:I:159:TYR:OH	2:J:1:LEU:O	2.25	0.49
1:M:5:MET:HB2	1:M:6:ARG:H	1.46	0.49
1:M:146:LYS:NZ	2:N:8:TYR:HB3	2.27	0.49
4:L:78:LEU:N	4:P:48:ASN:OD1	2.34	0.49
1:E:250:PRO:C	1:E:253:GLN:HE22	2.14	0.49
1:I:127:LYS:C	1:I:129:ASP:H	2.16	0.49
4:L:45:GLN:HB3	4:L:68:THR:OG1	2.13	0.49
1:M:49:ALA:O	1:M:52:ILE:HG22	2.13	0.49
1:M:147:TRP:HZ2	2:N:9:VAL:HG12	1.77	0.49
1:Q:76:VAL:HG13	4:X:7:ALA:O	2.12	0.49
1:I:4:SER:CB	1:I:168:LEU:HD21	2.41	0.48
1:M:116:TYR:CG	1:M:117:ALA:N	2.81	0.48
4:T:22:PHE:CE2	4:T:90:MET:HB3	2.48	0.48
4:L:15:PRO:HG2	4:L:71:VAL:HG11	1.93	0.48
1:M:98:MET:HE2	3:O:56:PHE:HE1	1.78	0.48
1:Q:118:TYR:CG	1:Q:119:ASP:N	2.79	0.48
1:E:27:TYR:HH	3:G:63:TYR:HH	1.60	0.48
1:E:28:VAL:HG11	1:E:51:TRP:CH2	2.48	0.48
1:I:201:LEU:HD13	1:I:257:TYR:OH	2.13	0.48
1:U:114:HIS:O	1:U:114:HIS:ND1	2.46	0.48
3:G:9:VAL:HG22	3:G:25:CYS:SG	2.54	0.48
1:I:234:ARG:HE	1:I:242:GLN:HB2	1.77	0.48
1:M:183:ASP:HB2	1:M:209:TYR:N	2.27	0.48
1:M:190:THR:HB	1:M:202:ARG:NE	2.26	0.48
3:O:41:LYS:HG3	3:O:78:TYR:CE1	2.49	0.48
3:O:37:VAL:HG12	3:O:82:VAL:HG22	1.94	0.48
1:Q:234:ARG:HE	1:Q:242:GLN:HB2	1.78	0.48
4:X:65:GLU:HA	4:X:87:PHE:CD2	2.49	0.48
1:A:232:GLU:O	1:A:234:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ASP:HB3	1:A:40:ALA:HB2	1.96	0.48
1:Q:103:VAL:HA	1:Q:110:LEU:H	1.77	0.48
3:S:35:ILE:HD11	3:S:84:HIS:HD2	1.78	0.48
4:H:91:CYS:O	4:H:95:MET:HG3	2.14	0.48
1:I:129:ASP:HB2	1:I:132:SER:OG	2.14	0.48
1:I:32:GLN:N	1:I:32:GLN:OE1	2.40	0.48
4:T:40:GLN:O	4:T:41:SER:OG	2.29	0.48
1:U:127:LYS:C	1:U:129:ASP:H	2.16	0.48
1:A:171:TYR:HE1	2:B:1:LEU:HD22	1.79	0.48
1:A:82:ARG:NH2	1:A:87:GLN:HG3	2.29	0.48
1:Q:85:TYR:HB2	1:Q:87:GLN:HE22	1.79	0.48
1:U:114:HIS:NE2	1:U:126:LEU:HB2	2.29	0.48
1:U:28:VAL:O	1:U:31:THR:HG23	2.14	0.48
3:K:30:PHE:HB2	3:K:84:HIS:NE2	2.29	0.48
1:M:250:PRO:HB2	1:M:253:GLN:NE2	2.28	0.48
1:U:171:TYR:CE1	2:V:1:LEU:HD22	2.48	0.48
1:U:191:HIS:HD2	1:U:201:LEU:HD12	1.79	0.48
3:G:43:GLY:HA3	1:Q:17:ARG:HG2	1.94	0.48
1:U:231:VAL:HG11	1:U:244:TRP:HB3	1.95	0.48
1:E:27:TYR:CZ	1:E:32:GLN:HG3	2.48	0.48
3:K:43:GLY:O	3:K:44:GLU:HG3	2.14	0.48
1:U:96:GLN:HG2	1:U:117:ALA:HB3	1.95	0.48
1:A:154:GLU:HA	1:A:157:ARG:HB3	1.94	0.47
3:G:73:THR:OG1	3:G:76:ASP:HB2	2.14	0.47
1:M:191:HIS:CD2	1:M:201:LEU:HD12	2.49	0.47
1:Q:235:PRO:HA	1:Q:241:PHE:CD1	2.49	0.47
1:A:124:ILE:HG21	1:A:147:TRP:CZ3	2.43	0.47
1:E:14:ARG:HG3	1:E:20:PRO:HA	1.96	0.47
1:M:108:ARG:HD2	1:M:169:ARG:NH2	2.30	0.47
1:A:111:ARG:HD2	1:A:128:GLU:O	2.14	0.47
1:A:185:PRO:HD2	1:A:266:LEU:HD23	1.96	0.47
1:E:66:LYS:HD2	2:F:4:GLY:HA2	1.96	0.47
4:H:72:PRO:HA	4:H:77:PHE:O	2.14	0.47
1:I:209:TYR:HB3	1:I:210:PRO:HD3	1.96	0.47
1:I:94:THR:OG1	1:I:96:GLN:OE1	2.32	0.47
1:M:156:LEU:HA	2:N:3:PHE:CE1	2.50	0.47
4:P:28:ARG:HH22	4:P:59:TRP:C	2.16	0.47
1:U:234:ARG:HH22	1:U:244:TRP:HZ3	1.60	0.47
1:A:17:ARG:HA	3:W:44:GLU:N	2.29	0.47
1:E:35:ARG:HE	1:E:48:ARG:HD3	1.79	0.47
1:E:35:ARG:HG3	1:E:46:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:19:LYS:O	3:K:72:PRO:HD2	2.13	0.47
1:M:234:ARG:HD3	3:O:8:GLN:NE2	2.28	0.47
4:T:44:ILE:HD11	4:T:51:ARG:O	2.15	0.47
4:T:57:SER:OG	4:T:58:THR:N	2.47	0.47
1:U:249:VAL:HG12	1:U:253:GLN:HE21	1.79	0.47
4:D:36:GLY:O	4:D:53:ASN:ND2	2.41	0.47
1:E:231:VAL:HG11	1:E:244:TRP:HB2	1.96	0.47
1:I:208:PHE:CE1	1:I:241:PHE:HB2	2.49	0.47
3:K:15:ALA:HB2	3:K:95:TRP:HZ2	1.79	0.47
1:A:17:ARG:CZ	3:W:40:LEU:HD11	2.44	0.47
4:D:95:MET:O	4:D:99:ARG:NE	2.47	0.47
1:E:21:ARG:HD2	1:E:37:ASP:OD1	2.15	0.47
1:Q:213:ILE:HD11	1:Q:261:VAL:HG23	1.97	0.47
4:T:22:PHE:HE1	4:T:31:VAL:HG13	1.78	0.47
3:W:57:SER:H	3:W:63:TYR:HE2	1.62	0.47
1:A:14:ARG:O	1:A:16:GLY:N	2.45	0.47
1:E:209:TYR:CD2	1:E:210:PRO:HD2	2.49	0.47
1:M:214:THR:CG2	1:M:262:GLN:HB2	2.45	0.47
1:M:34:VAL:HG11	1:M:45:MET:HE1	1.96	0.47
1:A:188:HIS:HD2	1:A:190:THR:HG23	1.79	0.47
1:I:190:THR:O	1:I:201:LEU:HG	2.15	0.47
1:M:27:TYR:H	1:M:33:PHE:HE2	1.62	0.47
3:O:80:CYS:O	3:O:92:ILE:HA	2.15	0.47
1:Q:34:VAL:HG21	1:Q:45:MET:SD	2.54	0.47
1:U:118:TYR:CG	1:U:119:ASP:N	2.75	0.47
1:U:238:ASP:OD1	1:U:240:THR:OG1	2.26	0.47
1:M:164:CYS:O	1:M:168:LEU:HB2	2.15	0.47
1:M:188:HIS:HB2	1:M:204:TRP:CZ2	2.38	0.47
1:Q:24:ALA:HB3	1:Q:36:PHE:HB3	1.95	0.47
1:U:204:TRP:HZ2	1:U:244:TRP:CE2	2.33	0.47
1:A:147:TRP:CZ2	2:B:9:VAL:HG12	2.50	0.47
1:E:51:TRP:CD1	1:E:178:THR:HG21	2.50	0.47
3:O:5:PRO:HB3	3:O:30:PHE:HB3	1.96	0.47
4:P:46:TYR:OH	4:P:59:TRP:HD1	1.98	0.47
1:U:29:ASP:CG	1:U:30:ASP:H	2.18	0.47
1:E:256:ARG:HG3	1:E:257:TYR:HD1	1.80	0.46
1:I:188:HIS:CD2	1:I:189:MET:H	2.34	0.46
1:I:1:GLY:HA2	1:I:105:SER:HA	1.96	0.46
1:M:116:TYR:N	1:M:124:ILE:O	2.40	0.46
4:X:40:GLN:O	4:X:41:SER:OG	2.30	0.46
1:A:127:LYS:C	1:A:129:ASP:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:SER:HB3	1:A:168:LEU:HD21	1.96	0.46
1:M:154:GLU:HA	1:M:157:ARG:HB3	1.97	0.46
1:M:51:TRP:HE1	1:M:178:THR:HG1	1.63	0.46
4:D:20:LEU:HD11	4:D:85:PHE:CD1	2.50	0.46
3:G:78:TYR:O	3:G:95:TRP:N	2.44	0.46
1:I:118:TYR:CG	1:I:119:ASP:N	2.81	0.46
1:I:109:PHE:HD1	1:I:165:VAL:HG21	1.80	0.46
1:I:33:PHE:CE2	1:I:52:ILE:HB	2.50	0.46
1:M:5:MET:HG3	1:M:27:TYR:HB3	1.97	0.46
1:M:6:ARG:HH22	1:M:115:GLN:CG	2.25	0.46
3:W:24:ASN:CB	3:W:65:LEU:HD11	2.45	0.46
1:I:257:TYR:N	1:I:257:TYR:CD2	2.84	0.46
3:O:73:THR:HG23	3:O:76:ASP:H	1.79	0.46
1:Q:205:ALA:HB1	1:Q:208:PHE:HE2	1.80	0.46
1:M:108:ARG:HA	1:M:108:ARG:HD2	1.64	0.46
1:M:224:GLN:OE1	1:M:228:THR:OG1	2.24	0.46
1:M:235:PRO:HA	1:M:241:PHE:CD1	2.48	0.46
1:M:54:GLN:HB3	4:P:51:ARG:NH2	2.31	0.46
4:X:49:LYS:HE3	4:X:51:ARG:NH2	2.31	0.46
1:A:100:GLY:O	1:A:113:TYR:N	2.36	0.46
1:Q:129:ASP:HB2	1:Q:132:SER:OG	2.15	0.46
1:Q:109:PHE:HD1	1:Q:165:VAL:HG21	1.80	0.46
1:Q:235:PRO:HA	1:Q:241:PHE:HD1	1.79	0.46
1:M:206:LEU:HD11	3:O:14:PRO:HD3	1.96	0.46
1:M:20:PRO:HG2	1:M:75:ARG:CD	2.44	0.46
1:Q:256:ARG:HG3	1:Q:257:TYR:CD1	2.51	0.46
3:S:80:CYS:O	3:S:92:ILE:HA	2.15	0.46
1:A:127:LYS:HG2	1:A:132:SER:OG	2.15	0.46
1:A:154:GLU:HG2	1:A:157:ARG:HD3	1.98	0.46
1:A:164:CYS:O	1:A:168:LEU:HB2	2.16	0.46
3:C:9:VAL:HG22	3:C:25:CYS:SG	2.55	0.46
3:C:87:LEU:HD11	3:C:91:LYS:HE3	1.98	0.46
3:K:73:THR:OG1	3:K:76:ASP:HB2	2.15	0.46
1:Q:44:ARG:HG3	1:Q:64:THR:OG1	2.15	0.46
4:X:14:ASN:OD1	4:X:15:PRO:HD3	2.15	0.46
1:E:14:ARG:HH11	1:E:21:ARG:HB2	1.81	0.46
4:L:99:ARG:HD2	4:L:104:TRP:O	2.16	0.46
1:M:21:ARG:NH2	1:M:37:ASP:OD1	2.48	0.46
3:S:56:PHE:HD1	3:S:60:TRP:HA	1.81	0.46
1:M:76:VAL:HG23	2:N:8:TYR:HE1	1.81	0.45
1:Q:178:THR:O	1:Q:209:TYR:OH	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:31:HIS:HD2	3:S:32:PRO:CA	2.26	0.45
3:K:13:HIS:O	3:K:21:ASN:ND2	2.49	0.45
1:M:127:LYS:HB3	1:M:132:SER:OG	2.16	0.45
1:E:249:VAL:HG21	1:E:257:TYR:HE2	1.81	0.45
1:I:257:TYR:N	1:I:257:TYR:HD2	2.15	0.45
1:I:5:MET:HB3	1:I:6:ARG:H	1.56	0.45
1:Q:214:THR:HG23	1:Q:262:GLN:HB2	1.97	0.45
1:U:123:TYR:CD2	1:U:123:TYR:N	2.83	0.45
1:A:108:ARG:HH11	1:A:169:ARG:HH22	1.65	0.45
1:I:141:GLN:OE1	1:I:144:LYS:NZ	2.41	0.45
4:L:70:SER:HB3	4:L:78:LEU:HD11	1.98	0.45
3:S:23:LEU:HD23	3:S:39:LEU:HD22	1.99	0.45
1:U:114:HIS:CD2	1:U:126:LEU:HB2	2.51	0.45
1:U:155:GLN:O	1:U:155:GLN:HG2	2.15	0.45
3:G:46:ILE:O	3:G:49:VAL:HG13	2.16	0.45
1:I:219:ARG:HG2	1:I:257:TYR:HB2	1.98	0.45
4:T:6:LYS:HE2	1:U:75:ARG:NH2	2.32	0.45
1:I:6:ARG:HH22	1:I:115:GLN:HG2	1.81	0.45
1:M:108:ARG:HH11	1:M:169:ARG:HH22	1.63	0.45
1:U:190:THR:HG23	1:U:202:ARG:HD3	1.99	0.45
4:X:45:GLN:OE1	4:X:50:THR:HG22	2.16	0.45
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.24	0.45
1:E:224:GLN:NE2	1:E:228:THR:H	2.14	0.45
1:E:49:ALA:O	1:E:52:ILE:HG22	2.16	0.45
1:M:208:PHE:CD1	1:M:213:ILE:HD11	2.51	0.45
1:E:96:GLN:HG3	3:G:60:TRP:HE3	1.82	0.45
4:L:88:GLU:O	4:L:92:ASN:ND2	2.49	0.45
1:M:14:ARG:NE	1:M:17:ARG:HE	2.15	0.45
1:M:215:LEU:HD11	1:M:243:LYS:CD	2.46	0.45
4:T:86:ILE:HD11	4:T:88:GLU:HB3	1.98	0.45
4:T:9:PRO:HD2	2:V:8:TYR:OH	2.15	0.45
4:X:14:ASN:O	4:X:16:ASP:N	2.49	0.45
4:X:50:THR:OG1	4:X:50:THR:O	2.31	0.45
1:A:178:THR:OG1	1:A:178:THR:O	2.33	0.45
3:C:37:VAL:HG13	3:C:66:TYR:CE1	2.51	0.45
1:E:213:ILE:HB	1:E:263:HIS:HD2	1.82	0.45
4:L:77:PHE:CZ	4:P:64:PRO:HD3	2.52	0.45
1:Q:201:LEU:HD13	1:Q:254:GLU:OE1	2.17	0.45
3:S:11:SER:HG	3:S:21:ASN:ND2	2.15	0.45
1:U:99:TYR:HA	1:U:114:HIS:HA	1.98	0.45
1:E:44:ARG:HB3	1:E:64:THR:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ARG:NE	1:I:113:TYR:HD1	2.15	0.45
1:I:66:LYS:HE3	2:J:2:LEU:HB2	1.98	0.45
1:M:118:TYR:HD2	1:M:123:TYR:HB2	1.82	0.45
1:M:21:ARG:CZ	1:M:38:SER:H	2.29	0.45
1:M:147:TRP:CZ2	2:N:9:VAL:HG12	2.51	0.45
1:Q:220:ASP:O	1:Q:222:GLU:N	2.49	0.45
3:W:37:VAL:HG21	3:W:66:TYR:CD1	2.52	0.45
1:E:209:TYR:CG	1:E:210:PRO:HD3	2.52	0.44
1:E:208:PHE:HZ	1:E:243:LYS:HG3	1.82	0.44
4:L:6:LYS:NZ	4:L:6:LYS:HA	2.32	0.44
1:Q:236:ALA:O	3:S:12:ARG:HD2	2.17	0.44
1:A:47:PRO:HB3	1:A:60:TRP:CH2	2.53	0.44
3:C:9:VAL:CG2	3:C:80:CYS:HB2	2.47	0.44
1:I:183:ASP:HB2	1:I:209:TYR:N	2.33	0.44
1:M:186:LYS:HA	1:M:186:LYS:HD2	1.79	0.44
1:M:211:ALA:HB2	1:M:241:PHE:CE2	2.52	0.44
3:S:73:THR:HG1	3:S:75:LYS:H	1.64	0.44
1:U:49:ALA:HA	1:U:50:PRO:HD3	1.74	0.44
3:W:23:LEU:HG	3:W:70:PHE:CD2	2.52	0.44
3:W:86:THR:OG1	3:W:87:LEU:N	2.50	0.44
3:C:23:LEU:HB2	3:C:68:THR:HG22	1.99	0.44
4:D:8:ASP:OD1	4:D:11:LEU:HG	2.16	0.44
1:E:178:THR:HG23	1:E:179:LEU:HD12	1.98	0.44
1:M:116:TYR:CD2	1:M:123:TYR:HD2	2.36	0.44
1:U:107:TRP:O	1:U:169:ARG:NH2	2.49	0.44
3:W:34:ASP:C	3:W:35:ILE:HD12	2.38	0.44
1:A:66:LYS:HG2	2:B:2:LEU:HD23	1.99	0.44
1:I:144:LYS:O	1:I:148:GLU:HG3	2.17	0.44
1:I:6:ARG:HG3	1:I:113:TYR:HE1	1.82	0.44
1:M:32:GLN:CD	1:M:32:GLN:H	2.21	0.44
1:M:6:ARG:HD3	1:M:98:MET:HG2	2.00	0.44
1:Q:21:ARG:HH11	1:Q:38:SER:HG	1.62	0.44
1:A:77:ASP:O	1:A:80:THR:OG1	2.21	0.44
3:K:11:SER:OG	3:K:21:ASN:ND2	2.50	0.44
4:L:19:GLN:O	4:L:34:LYS:N	2.49	0.44
1:M:107:TRP:CH2	1:M:172:LEU:HB3	2.53	0.44
1:Q:127:LYS:C	1:Q:129:ASP:H	2.20	0.44
3:S:46:ILE:O	3:S:46:ILE:HG23	2.17	0.44
1:U:154:GLU:HA	1:U:157:ARG:HB3	1.99	0.44
3:W:30:PHE:CE1	3:W:62:PHE:HB2	2.53	0.44
1:E:124:ILE:HG23	1:E:133:TRP:HH2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:190:THR:O	1:I:202:ARG:HB2	2.17	0.44
1:M:108:ARG:HH11	1:M:169:ARG:NH2	2.15	0.44
1:M:204:TRP:CZ3	1:M:206:LEU:HB2	2.51	0.44
1:Q:127:LYS:NZ	1:Q:129:ASP:OD1	2.38	0.44
1:A:45:MET:SD	1:A:67:VAL:HG21	2.58	0.44
1:A:235:PRO:HB2	3:C:65:LEU:HD22	1.99	0.44
4:H:28:ARG:NH2	4:H:60:GLN:HB3	2.33	0.44
1:M:160:LEU:O	1:M:165:VAL:HG23	2.17	0.44
1:Q:176:LYS:HA	1:Q:179:LEU:HG	2.00	0.44
1:Q:115:GLN:HA	1:Q:125:ALA:HA	1.99	0.44
1:Q:49:ALA:HA	1:Q:50:PRO:HD3	1.84	0.44
1:U:204:TRP:CZ2	1:U:244:TRP:CD2	3.06	0.44
2:B:2:LEU:HD12	2:B:2:LEU:HA	1.89	0.44
1:E:108:ARG:HD2	1:E:108:ARG:HA	1.76	0.44
1:E:138:MET:O	1:E:141:GLN:HG2	2.18	0.44
3:G:30:PHE:CE1	3:G:62:PHE:HB2	2.53	0.44
3:O:3:ARG:NH1	5:O:101:HOH:O	2.50	0.44
1:U:156:LEU:HA	2:V:3:PHE:HE1	1.83	0.44
1:U:234:ARG:HD3	3:W:8:GLN:NE2	2.33	0.44
1:U:50:PRO:O	1:U:53:GLU:HG2	2.17	0.44
1:U:6:ARG:HD2	1:U:8:PHE:CZ	2.53	0.44
3:W:39:LEU:HA	3:W:39:LEU:HD23	1.91	0.44
4:D:65:GLU:HA	4:D:87:PHE:CD2	2.53	0.43
1:E:2:SER:HB2	1:E:264:GLU:OE2	2.18	0.43
1:I:127:LYS:HB3	1:I:132:SER:OG	2.18	0.43
3:O:35:ILE:HG13	3:O:84:HIS:HD2	1.83	0.43
4:P:9:PRO:O	4:P:12:THR:OG1	2.36	0.43
1:A:18:GLY:N	3:W:44:GLU:HB3	2.33	0.43
1:A:254:GLU:C	1:A:257:TYR:HE2	2.22	0.43
1:A:68:LYS:O	1:A:72:GLN:HG2	2.19	0.43
1:E:103:VAL:HG13	1:E:107:TRP:HA	1.99	0.43
1:Q:49:ALA:O	1:Q:52:ILE:HG22	2.17	0.43
1:Q:63:GLU:O	1:Q:67:VAL:HG22	2.18	0.43
3:W:77:GLU:HG2	3:W:78:TYR:N	2.33	0.43
3:W:35:ILE:HD11	3:W:84:HIS:CD2	2.53	0.43
1:M:215:LEU:HD11	1:M:243:LYS:CE	2.49	0.43
3:W:31:HIS:HD2	3:W:32:PRO:CA	2.32	0.43
1:A:4:SER:CB	1:A:168:LEU:HD21	2.48	0.43
1:E:121:LYS:HG3	1:E:122:ASP:H	1.82	0.43
1:I:181:ARG:HH21	4:L:28:ARG:NH1	2.15	0.43
1:I:191:HIS:HB2	1:I:201:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:75:ASP:HB2	4:L:77:PHE:CD2	2.53	0.43
4:P:28:ARG:HH11	4:P:29:CYS:H	1.66	0.43
4:T:65:GLU:OE2	4:T:88:GLU:HB2	2.19	0.43
1:U:114:HIS:CE1	1:U:126:LEU:HB2	2.53	0.43
1:U:208:PHE:CE1	1:U:241:PHE:HB2	2.53	0.43
3:C:34:ASP:C	3:C:35:ILE:HD12	2.39	0.43
1:E:66:LYS:HE3	2:F:2:LEU:HB2	2.01	0.43
1:I:1:GLY:N	1:I:104:GLY:O	2.46	0.43
1:Q:114:HIS:CG	1:Q:156:LEU:HD21	2.54	0.43
1:Q:54:GLN:HA	4:T:54:THR:OG1	2.19	0.43
2:R:3:PHE:CE2	2:R:5:TYR:HB2	2.53	0.43
3:S:9:VAL:HG22	3:S:80:CYS:HB2	1.99	0.43
1:U:97:ARG:HD3	1:U:116:TYR:CD1	2.52	0.43
1:A:172:LEU:HD22	1:A:179:LEU:HD22	2.00	0.43
3:K:80:CYS:O	3:K:92:ILE:HA	2.18	0.43
3:O:7:ILE:HD12	3:O:82:VAL:HG21	2.00	0.43
1:M:234:ARG:HG3	1:M:242:GLN:HB2	1.99	0.43
1:M:60:TRP:O	1:M:64:THR:HG23	2.18	0.43
3:S:45:ARG:HH11	3:S:45:ARG:HG3	1.84	0.43
4:T:59:TRP:CD1	4:T:87:PHE:HB2	2.53	0.43
1:U:204:TRP:CZ2	1:U:244:TRP:CG	3.07	0.43
1:A:208:PHE:CG	1:A:213:ILE:HD11	2.54	0.43
3:C:57:SER:H	3:C:63:TYR:HE2	1.67	0.43
3:C:23:LEU:HG	3:C:70:PHE:CD2	2.54	0.43
4:D:65:GLU:HA	4:D:87:PHE:CE2	2.54	0.43
1:Q:7:TYR:CE1	2:R:2:LEU:HD11	2.54	0.43
1:U:191:HIS:ND1	1:U:192:HIS:N	2.66	0.43
1:A:234:ARG:HA	1:A:235:PRO:HD3	1.84	0.43
1:A:33:PHE:CE2	1:A:52:ILE:HB	2.54	0.43
1:E:118:TYR:CD2	1:E:123:TYR:HB2	2.53	0.43
1:E:177:GLU:CD	1:E:177:GLU:H	2.22	0.43
1:I:188:HIS:CG	1:I:189:MET:H	2.37	0.43
1:U:141:GLN:HG3	1:U:145:HIS:CE1	2.54	0.43
1:U:209:TYR:HB3	1:U:210:PRO:HD3	2.01	0.43
1:E:133:TRP:CG	1:E:134:THR:N	2.86	0.43
1:E:256:ARG:HG3	1:E:257:TYR:CD1	2.54	0.43
1:E:82:ARG:HD2	1:E:93:HIS:HB2	2.00	0.43
1:M:238:ASP:OD2	3:O:12:ARG:NH1	2.52	0.43
3:O:71:THR:HA	3:O:72:PRO:HD2	1.87	0.43
1:Q:219:ARG:HB2	1:Q:257:TYR:CE2	2.53	0.43
4:T:44:ILE:HG22	4:T:69:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:114:HIS:CD2	1:U:126:LEU:HD22	2.54	0.43
1:U:96:GLN:HB2	3:W:56:PHE:CE2	2.53	0.43
1:A:87:GLN:CD	1:A:88:SER:H	2.21	0.42
1:M:95:VAL:HG13	1:M:116:TYR:OH	2.19	0.42
1:M:11:SER:HA	1:M:21:ARG:O	2.19	0.42
1:Q:201:LEU:HB2	1:Q:254:GLU:CD	2.40	0.42
4:T:20:LEU:HD11	4:T:85:PHE:CD1	2.54	0.42
3:C:35:ILE:HG22	3:C:37:VAL:HG12	2.01	0.42
1:I:35:ARG:CZ	1:I:48:ARG:HD3	2.49	0.42
1:I:74:HIS:NE2	1:I:97:ARG:HG3	2.34	0.42
3:O:57:SER:H	3:O:63:TYR:HE2	1.66	0.42
1:Q:66:LYS:HD2	2:R:3:PHE:O	2.19	0.42
3:C:26:TYR:HB2	3:C:65:LEU:HD13	2.00	0.42
2:F:1:LEU:HD12	2:F:2:LEU:N	2.33	0.42
3:G:11:SER:OG	3:G:21:ASN:ND2	2.52	0.42
1:M:260:HIS:CE1	1:M:271:THR:HA	2.54	0.42
1:Q:51:TRP:CE3	1:Q:175:GLY:HA3	2.54	0.42
4:T:22:PHE:CZ	4:T:87:PHE:HD1	2.37	0.42
1:A:251:SER:HA	1:A:254:GLU:OE2	2.20	0.42
1:M:127:LYS:C	1:M:129:ASP:H	2.23	0.42
1:M:253:GLN:H	1:M:253:GLN:NE2	2.16	0.42
3:O:34:ASP:C	3:O:35:ILE:HD12	2.40	0.42
4:P:65:GLU:HA	4:P:87:PHE:CD2	2.55	0.42
1:U:6:ARG:HB2	1:U:8:PHE:HE2	1.85	0.42
1:A:63:GLU:O	1:A:67:VAL:HG23	2.20	0.42
1:E:1:GLY:N	1:E:104:GLY:O	2.50	0.42
1:I:49:ALA:O	1:I:52:ILE:HG22	2.20	0.42
1:M:129:ASP:HB2	1:M:132:SER:OG	2.19	0.42
4:P:45:GLN:HB3	4:P:68:THR:OG1	2.19	0.42
1:Q:22:PHE:CD2	1:Q:71:SER:HB2	2.55	0.42
4:T:44:ILE:HG13	4:T:52:ASN:O	2.20	0.42
1:A:204:TRP:N	1:A:204:TRP:CE3	2.87	0.42
1:A:204:TRP:HE3	1:A:204:TRP:N	2.18	0.42
1:M:191:HIS:O	1:M:202:ARG:NH1	2.53	0.42
1:Q:66:LYS:HE3	2:R:2:LEU:HB2	2.01	0.42
3:S:35:ILE:HG22	3:S:37:VAL:HG13	2.01	0.42
3:W:29:GLY:HA2	3:W:61:SER:HB2	2.01	0.42
1:A:177:GLU:HG2	4:D:28:ARG:NH2	2.35	0.42
1:E:181:ARG:HB3	1:E:183:ASP:OD2	2.19	0.42
3:K:41:LYS:HG3	3:K:78:TYR:CE1	2.54	0.42
1:M:149:ALA:O	1:M:151:HIS:ND1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ARG:NH1	1:A:169:ARG:HH22	2.17	0.42
1:I:108:ARG:HA	1:I:108:ARG:HD2	1.82	0.42
1:I:46:GLU:HA	1:I:47:PRO:HD3	1.71	0.42
1:Q:144:LYS:HE2	1:Q:148:GLU:OE2	2.19	0.42
1:Q:30:ASP:OD2	1:Q:210:PRO:HA	2.20	0.42
1:Q:85:TYR:HB2	1:Q:87:GLN:OE1	2.18	0.42
4:T:45:GLN:O	4:T:67:TYR:HB2	2.20	0.42
1:U:124:ILE:HA	1:U:134:THR:O	2.19	0.42
3:W:23:LEU:HB2	3:W:68:THR:HG22	2.02	0.42
1:A:22:PHE:CD2	1:A:71:SER:HB2	2.54	0.42
1:A:85:TYR:HB3	1:A:86:ASN:H	1.64	0.42
1:Q:191:HIS:HB2	1:Q:201:LEU:HD12	2.02	0.42
4:D:66:TRP:HZ3	4:D:68:THR:HG23	1.84	0.42
1:E:234:ARG:HA	1:E:235:PRO:HD3	1.82	0.42
1:I:3:HIS:HB2	1:I:29:ASP:OD2	2.19	0.42
1:M:191:HIS:HD2	1:M:201:LEU:HD12	1.84	0.42
1:U:141:GLN:HG3	1:U:145:HIS:HE1	1.84	0.42
1:U:171:TYR:OH	2:V:1:LEU:HD22	2.20	0.42
1:A:188:HIS:O	1:A:189:MET:HG2	2.20	0.41
1:M:167:TRP:CE3	1:M:170:ARG:HD3	2.55	0.41
1:M:185:PRO:CB	1:M:205:ALA:HB1	2.49	0.41
4:P:37:TRP:NE1	4:P:54:THR:OG1	2.52	0.41
1:Q:3:HIS:HB2	1:Q:29:ASP:CG	2.41	0.41
3:S:57:SER:H	3:S:63:TYR:HE2	1.68	0.41
4:T:76:GLY:HA2	1:U:146:LYS:HG3	2.01	0.41
1:A:96:GLN:HG2	1:A:117:ALA:HB3	2.02	0.41
1:E:137:ASP:CG	1:E:138:MET:H	2.23	0.41
1:I:111:ARG:NH1	1:I:128:GLU:HG2	2.34	0.41
1:I:31:THR:HG21	1:I:209:TYR:OH	2.19	0.41
4:L:28:ARG:CD	4:L:106:PRO:HG3	2.50	0.41
1:M:70:HIS:CE1	2:N:2:LEU:HD22	2.55	0.41
3:S:40:LEU:HA	3:S:45:ARG:HH12	1.85	0.41
3:S:4:THR:HA	3:S:5:PRO:HD3	1.84	0.41
1:A:131:ARG:HD3	1:A:153:ALA:HB3	2.01	0.41
1:A:135:ALA:HB1	1:A:140:ALA:HB1	2.02	0.41
1:A:18:GLY:HA3	3:W:44:GLU:OE1	2.20	0.41
1:I:33:PHE:HA	1:I:33:PHE:HD2	1.73	0.41
1:I:48:ARG:NH2	1:I:48:ARG:HG2	2.34	0.41
1:M:155:GLN:HG2	1:M:155:GLN:O	2.21	0.41
1:M:63:GLU:O	1:M:67:VAL:HG22	2.19	0.41
4:P:45:GLN:HG3	4:P:46:TYR:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:21:ASN:HB3	3:W:70:PHE:CE2	2.56	0.41
1:E:66:LYS:HE2	1:E:66:LYS:HB2	1.85	0.41
4:H:40:GLN:O	4:H:41:SER:OG	2.33	0.41
1:I:13:SER:OG	1:I:82:ARG:NH1	2.53	0.41
1:A:127:LYS:HZ2	1:A:132:SER:HG	1.53	0.41
1:A:168:LEU:O	1:A:172:LEU:HG	2.21	0.41
1:A:76:VAL:O	1:A:80:THR:HG23	2.21	0.41
3:G:13:HIS:N	3:G:21:ASN:HD21	2.15	0.41
4:H:60:GLN:HG2	4:H:63:ASP:OD2	2.20	0.41
1:Q:25:VAL:HG13	1:Q:48:ARG:NH1	2.35	0.41
1:Q:96:GLN:HG2	1:Q:117:ALA:HB3	2.02	0.41
1:U:156:LEU:HA	2:V:3:PHE:CE1	2.55	0.41
1:A:70:HIS:HA	1:A:73:THR:HG22	2.03	0.41
1:I:4:SER:HB3	1:I:103:VAL:HG22	2.01	0.41
1:Q:15:PRO:HD2	1:Q:17:ARG:HG3	2.03	0.41
1:Q:219:ARG:NH1	1:Q:257:TYR:OH	2.48	0.41
1:A:220:ASP:O	1:A:222:GLU:N	2.54	0.41
1:A:33:PHE:HA	1:A:33:PHE:HD2	1.69	0.41
1:E:101:CYS:HB3	1:E:160:LEU:HD12	2.03	0.41
1:I:127:LYS:HD3	1:I:128:GLU:H	1.85	0.41
1:I:14:ARG:HE	1:I:17:ARG:HD2	1.86	0.41
1:I:181:ARG:NH2	4:L:106:PRO:HB3	2.35	0.41
3:O:41:LYS:HE3	3:O:78:TYR:OH	2.21	0.41
4:P:29:CYS:HB2	4:P:95:MET:HG3	2.02	0.41
3:S:12:ARG:CB	3:S:22:PHE:HB2	2.50	0.41
3:S:77:GLU:HG2	3:S:78:TYR:N	2.36	0.41
1:U:141:GLN:O	1:U:145:HIS:ND1	2.54	0.41
1:E:176:LYS:O	1:E:180:GLN:N	2.54	0.41
4:H:20:LEU:HD11	4:H:85:PHE:CD1	2.56	0.41
1:I:143:THR:O	1:I:146:LYS:HB2	2.21	0.41
3:K:12:ARG:HB3	3:K:22:PHE:HB2	2.02	0.41
1:Q:3:HIS:HB2	1:Q:29:ASP:OD2	2.20	0.41
1:Q:80:THR:OG1	1:Q:81:LEU:N	2.54	0.41
4:T:65:GLU:HA	4:T:87:PHE:HD2	1.85	0.41
1:U:14:ARG:HA	1:U:15:PRO:HD3	1.94	0.41
1:U:59:TYR:O	1:U:63:GLU:HB2	2.21	0.41
1:A:45:MET:H	1:A:64:THR:CG2	2.30	0.41
1:E:206:LEU:HD23	1:E:206:LEU:HA	1.78	0.41
3:G:21:ASN:HB3	3:G:70:PHE:HE2	1.83	0.41
1:I:20:PRO:HG3	1:I:78:LEU:HD21	2.01	0.41
1:M:147:TRP:HB3	1:M:152:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:201:LEU:HB3	1:M:202:ARG:H	1.52	0.41
4:T:68:THR:HB	4:T:80:THR:CG2	2.50	0.41
1:U:129:ASP:HB3	1:U:132:SER:OG	2.21	0.41
1:A:159:TYR:CD1	1:A:163:THR:HB	2.55	0.41
1:A:6:ARG:CZ	1:A:8:PHE:HZ	2.33	0.41
1:E:250:PRO:HB2	1:E:253:GLN:OE1	2.21	0.41
1:I:189:MET:HG3	1:I:201:LEU:CD2	2.51	0.41
1:I:214:THR:CG2	1:I:262:GLN:HB2	2.51	0.41
1:I:33:PHE:CE1	1:I:52:ILE:HD13	2.55	0.41
1:U:147:TRP:CH2	2:V:9:VAL:HG12	2.56	0.41
1:U:160:LEU:O	1:U:165:VAL:HG23	2.21	0.41
1:U:95:VAL:HA	1:U:117:ALA:O	2.21	0.41
1:A:1:GLY:H2	1:A:105:SER:HA	1.85	0.41
1:A:231:VAL:HG22	1:A:234:ARG:CZ	2.50	0.41
4:D:13:PHE:HE1	4:D:73:GLY:HA2	1.85	0.41
1:E:35:ARG:HG3	1:E:35:ARG:O	2.21	0.41
1:I:201:LEU:HD23	1:I:202:ARG:H	1.86	0.41
1:M:64:THR:O	1:M:68:LYS:HG3	2.21	0.41
4:P:22:PHE:CE1	4:P:31:VAL:HG13	2.56	0.41
3:S:73:THR:HG21	3:S:76:ASP:HB2	2.02	0.41
1:A:266:LEU:HD12	1:A:268:LYS:O	2.22	0.40
1:E:123:TYR:CD2	1:E:124:ILE:HG12	2.56	0.40
1:E:181:ARG:HD3	1:E:181:ARG:HA	1.84	0.40
1:E:99:TYR:HB3	1:E:114:HIS:HD2	1.86	0.40
1:M:10:THR:HG21	3:O:62:PHE:HE1	1.87	0.40
1:Q:266:LEU:HD12	1:Q:266:LEU:O	2.20	0.40
4:D:27:ASN:HD22	4:D:103:MET:HG2	1.87	0.40
4:H:72:PRO:HD3	4:H:78:LEU:HD12	2.02	0.40
3:O:23:LEU:O	3:O:67:TYR:HA	2.21	0.40
4:P:23:GLN:HA	4:P:24:PRO:HD3	1.92	0.40
4:T:99:ARG:HH21	4:T:104:TRP:HE1	1.69	0.40
1:U:9:PHE:HB3	1:U:74:HIS:CE1	2.45	0.40
1:A:139:ALA:O	1:A:142:THR:HG22	2.21	0.40
1:A:188:HIS:HB3	1:A:204:TRP:CZ2	2.52	0.40
3:C:41:LYS:HE3	3:C:78:TYR:OH	2.21	0.40
1:E:250:PRO:HB2	1:E:253:GLN:HE22	1.86	0.40
4:L:57:SER:OG	4:L:58:THR:N	2.51	0.40
1:Q:115:GLN:C	1:Q:116:TYR:HD2	2.25	0.40
1:Q:127:LYS:HG2	1:Q:132:SER:OG	2.21	0.40
1:Q:213:ILE:HD11	1:Q:261:VAL:CG2	2.51	0.40
4:T:22:PHE:HZ	4:T:87:PHE:CD1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:66:LYS:HE2	1:U:66:LYS:HB2	1.91	0.40
4:X:68:THR:HG22	4:X:82:ASN:OD1	2.21	0.40
1:A:209:TYR:HB3	1:A:210:PRO:HD3	2.02	0.40
1:E:4:SER:HB2	1:E:102:ASP:HA	2.04	0.40
1:E:220:ASP:HB3	1:E:221:GLY:H	1.76	0.40
1:E:249:VAL:HG12	1:E:253:GLN:HE21	1.87	0.40
1:E:27:TYR:OH	3:G:63:TYR:OH	2.33	0.40
4:L:46:TYR:CE2	4:L:47:LYS:HE3	2.56	0.40
1:M:6:ARG:NH2	1:M:115:GLN:HG3	2.28	0.40
1:M:156:LEU:HA	2:N:3:PHE:HE1	1.86	0.40
3:S:84:HIS:CG	3:S:85:VAL:H	2.40	0.40
1:U:118:TYR:N	1:U:123:TYR:CE2	2.87	0.40
1:U:191:HIS:CE1	1:U:193:ALA:HB2	2.55	0.40
4:X:46:TYR:CE2	4:X:47:LYS:HE3	2.57	0.40
1:A:181:ARG:HB3	1:A:183:ASP:OD1	2.20	0.40
3:C:15:ALA:HB3	3:C:97:ARG:NH1	2.37	0.40
1:E:9:PHE:HZ	2:F:2:LEU:HD21	1.85	0.40
1:I:234:ARG:HA	1:I:235:PRO:HD3	1.81	0.40
1:I:263:HIS:CE1	1:I:265:GLY:H	2.39	0.40
1:M:133:TRP:CZ2	1:M:153:ALA:HB2	2.57	0.40
3:O:36:GLU:N	3:O:36:GLU:OE1	2.55	0.40
1:Q:33:PHE:HA	1:Q:33:PHE:HD2	1.72	0.40
3:S:9:VAL:CG2	3:S:80:CYS:HB2	2.51	0.40
1:U:118:TYR:HB3	1:U:123:TYR:CZ	2.56	0.40

All (1) 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)
1:A:105:SER:OG	1:A:129:ASP:OD1[3_555]	2.13	0.07

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	256/275 (93%)	229 (90%)	27 (10%)	0	100	100
1	E	264/275 (96%)	233 (88%)	31 (12%)	0	100	100
1	I	242/275 (88%)	216 (89%)	26 (11%)	0	100	100
1	M	259/275 (94%)	230 (89%)	29 (11%)	0	100	100
1	Q	253/275 (92%)	225 (89%)	27 (11%)	1 (0%)	39	63
1	U	238/275 (86%)	214 (90%)	23 (10%)	1 (0%)	39	63
2	B	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	J	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	N	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
2	V	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	C	92/100 (92%)	82 (89%)	10 (11%)	0	100	100
3	G	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
3	K	96/100 (96%)	84 (88%)	12 (12%)	0	100	100
3	O	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	S	96/100 (96%)	86 (90%)	10 (10%)	0	100	100
3	W	96/100 (96%)	85 (88%)	11 (12%)	0	100	100
4	D	100/108 (93%)	88 (88%)	11 (11%)	1 (1%)	19	37
4	H	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	L	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	P	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	T	101/108 (94%)	89 (88%)	11 (11%)	1 (1%)	19	37
4	X	101/108 (94%)	89 (88%)	10 (10%)	2 (2%)	9	16
All	All	2731/2952 (92%)	2424 (89%)	298 (11%)	9 (0%)	46	70

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	L	9	PRO
4	P	9	PRO
4	X	9	PRO
4	H	9	PRO

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Mol	Chain	Res	Type
4	T	9	PRO
4	D	9	PRO
1	Q	128	GLU
1	U	250	PRO
4	X	15	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	222/231 (96%)	199 (90%)	23 (10%)	9 15
1	E	225/231 (97%)	200 (89%)	25 (11%)	8 13
1	I	211/231 (91%)	188 (89%)	23 (11%)	8 13
1	M	223/231 (96%)	200 (90%)	23 (10%)	9 15
1	Q	218/231 (94%)	188 (86%)	30 (14%)	4 7
1	U	206/231 (89%)	179 (87%)	27 (13%)	5 8
2	B	8/8 (100%)	6 (75%)	2 (25%)	1 1
2	F	8/8 (100%)	5 (62%)	3 (38%)	0 0
2	J	8/8 (100%)	8 (100%)	0	100 100
2	N	8/8 (100%)	8 (100%)	0	100 100
2	R	8/8 (100%)	7 (88%)	1 (12%)	6 10
2	V	8/8 (100%)	6 (75%)	2 (25%)	1 1
3	C	91/95 (96%)	86 (94%)	5 (6%)	27 49
3	G	93/95 (98%)	84 (90%)	9 (10%)	10 18
3	K	93/95 (98%)	83 (89%)	10 (11%)	8 14
3	O	93/95 (98%)	85 (91%)	8 (9%)	13 24
3	S	93/95 (98%)	84 (90%)	9 (10%)	10 18
3	W	93/95 (98%)	88 (95%)	5 (5%)	27 50
4	D	91/96 (95%)	87 (96%)	4 (4%)	35 61
4	H	92/96 (96%)	85 (92%)	7 (8%)	16 30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	L	92/96 (96%)	84 (91%)	8 (9%)	13 23
4	P	92/96 (96%)	83 (90%)	9 (10%)	10 18
4	T	92/96 (96%)	87 (95%)	5 (5%)	27 50
4	X	92/96 (96%)	84 (91%)	8 (9%)	13 23
All	All	2460/2580 (95%)	2214 (90%)	246 (10%)	9 17

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	7	TYR
1	A	25	VAL
1	A	31	THR
1	A	32	GLN
1	A	33	PHE
1	A	74	HIS
1	A	87	GLN
1	A	96	GLN
1	A	113	TYR
1	A	127	LYS
1	A	134	THR
1	A	143	THR
1	A	144	LYS
1	A	163	THR
1	A	178	THR
1	A	179	LEU
1	A	204	TRP
1	A	214	THR
1	A	223	ASP
1	A	224	GLN
1	A	230	LEU
1	A	266	LEU
2	B	5	TYR
2	B	8	TYR
3	C	7	ILE
3	C	37	VAL
3	C	70	PHE
3	C	80	CYS
3	C	87	LEU
4	D	16	ASP
4	D	39	CYS

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Mol	Chain	Res	Type
4	D	50	THR
4	D	58	THR
1	E	3	HIS
1	E	7	TYR
1	E	12	VAL
1	E	28	VAL
1	E	32	GLN
1	E	33	PHE
1	E	34	VAL
1	E	81	LEU
1	E	94	THR
1	E	103	VAL
1	E	113	TYR
1	E	116	TYR
1	E	118	TYR
1	E	119	ASP
1	E	142	THR
1	E	178	THR
1	E	188	HIS
1	E	192	HIS
1	E	202	ARG
1	E	204	TRP
1	E	209	TYR
1	E	223	ASP
1	E	224	GLN
1	E	244	TRP
1	E	261	VAL
2	F	1	LEU
2	F	7	VAL
2	F	9	VAL
3	G	4	THR
3	G	7	ILE
3	G	12	ARG
3	G	24	ASN
3	G	37	VAL
3	G	59	ASP
3	G	68	THR
3	G	70	PHE
3	G	80	CYS
4	H	14	ASN
4	H	19	GLN
4	H	68	THR

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Mol	Chain	Res	Type
4	H	69	VAL
4	H	75	ASP
4	H	77	PHE
4	H	95	MET
1	I	3	HIS
1	I	5	MET
1	I	14	ARG
1	I	17	ARG
1	I	28	VAL
1	I	32	GLN
1	I	33	PHE
1	I	34	VAL
1	I	75	ARG
1	I	94	THR
1	I	96	GLN
1	I	113	TYR
1	I	116	TYR
1	I	130	LEU
1	I	144	LYS
1	I	155	GLN
1	I	163	THR
1	I	178	THR
1	I	201	LEU
1	I	204	TRP
1	I	216	THR
1	I	257	TYR
1	I	266	LEU
3	K	7	ILE
3	K	12	ARG
3	K	19	LYS
3	K	24	ASN
3	K	37	VAL
3	K	47	GLU
3	K	53	ASP
3	K	55	SER
3	K	70	PHE
3	K	80	CYS
4	L	11	LEU
4	L	16	ASP
4	L	50	THR
4	L	68	THR
4	L	69	VAL

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Mol	Chain	Res	Type
4	L	71	VAL
4	L	75	ASP
4	L	78	LEU
1	M	5	MET
1	M	7	TYR
1	M	10	THR
1	M	13	SER
1	M	14	ARG
1	M	27	TYR
1	M	28	VAL
1	M	32	GLN
1	M	48	ARG
1	M	67	VAL
1	M	96	GLN
1	M	103	VAL
1	M	144	LYS
1	M	154	GLU
1	M	155	GLN
1	M	163	THR
1	M	178	THR
1	M	187	THR
1	M	188	HIS
1	M	194	VAL
1	M	202	ARG
1	M	213	ILE
1	M	243	LYS
3	O	7	ILE
3	O	12	ARG
3	O	24	ASN
3	O	47	GLU
3	O	67	TYR
3	O	68	THR
3	O	70	PHE
3	O	80	CYS
4	P	14	ASN
4	P	16	ASP
4	P	25	ASP
4	P	50	THR
4	P	51	ARG
4	P	57	SER
4	P	69	VAL
4	P	75	ASP

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Mol	Chain	Res	Type
4	P	89	HIS
1	Q	3	HIS
1	Q	5	MET
1	Q	7	TYR
1	Q	13	SER
1	Q	32	GLN
1	Q	33	PHE
1	Q	46	GLU
1	Q	67	VAL
1	Q	75	ARG
1	Q	86	ASN
1	Q	96	GLN
1	Q	98	MET
1	Q	103	VAL
1	Q	105	SER
1	Q	113	TYR
1	Q	127	LYS
1	Q	130	LEU
1	Q	138	MET
1	Q	155	GLN
1	Q	178	THR
1	Q	191	HIS
1	Q	204	TRP
1	Q	207	SER
1	Q	214	THR
1	Q	215	LEU
1	Q	217	TRP
1	Q	224	GLN
1	Q	228	THR
1	Q	258	THR
1	Q	261	VAL
2	R	1	LEU
3	S	7	ILE
3	S	12	ARG
3	S	23	LEU
3	S	24	ASN
3	S	45	ARG
3	S	53	ASP
3	S	70	PHE
3	S	73	THR
3	S	80	CYS
4	T	11	LEU

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Mol	Chain	Res	Type
4	T	75	ASP
4	T	81	VAL
4	T	89	HIS
4	T	99	ARG
1	U	14	ARG
1	U	21	ARG
1	U	25	VAL
1	U	28	VAL
1	U	31	THR
1	U	32	GLN
1	U	33	PHE
1	U	94	THR
1	U	108	ARG
1	U	113	TYR
1	U	114	HIS
1	U	123	TYR
1	U	138	MET
1	U	141	GLN
1	U	144	LYS
1	U	155	GLN
1	U	163	THR
1	U	178	THR
1	U	182	THR
1	U	190	THR
1	U	195	SER
1	U	204	TRP
1	U	214	THR
1	U	228	THR
1	U	248	VAL
1	U	253	GLN
1	U	257	TYR
2	V	2	LEU
2	V	7	VAL
3	W	7	ILE
3	W	24	ASN
3	W	49	VAL
3	W	70	PHE
3	W	74	GLU
4	X	11	LEU
4	X	13	PHE
4	X	16	ASP
4	X	21	SER

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Mol	Chain	Res	Type
4	X	71	VAL
4	X	75	ASP
4	X	79	ARG
4	X	89	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	HIS
1	A	188	HIS
1	A	224	GLN
4	D	27	ASN
1	E	115	GLN
1	E	253	GLN
1	I	54	GLN
1	I	114	HIS
1	I	188	HIS
1	I	260	HIS
4	L	92	ASN
1	M	96	GLN
1	M	253	GLN
3	O	8	GLN
4	P	92	ASN
1	Q	224	GLN
1	Q	260	HIS
1	Q	262	GLN
1	Q	263	HIS
3	S	31	HIS
4	T	92	ASN
1	U	114	HIS
1	U	253	GLN
3	W	31	HIS
4	X	19	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	264/275 (96%)	2.18	118 (44%)	0	0	20, 49, 98, 218	0
1	E	268/275 (97%)	2.51	133 (49%)	0	0	18, 49, 126, 173	0
1	I	252/275 (91%)	2.06	104 (41%)	0	0	14, 41, 85, 176	0
1	M	265/275 (96%)	2.55	132 (49%)	0	0	18, 51, 117, 161	0
1	Q	259/275 (94%)	4.72	210 (81%)	0	0	22, 61, 134, 238	0
1	U	246/275 (89%)	4.95	199 (80%)	0	0	27, 59, 131, 224	0
2	B	9/9 (100%)	2.16	2 (22%)	1	0	29, 33, 52, 58	0
2	F	9/9 (100%)	2.19	4 (44%)	0	0	34, 53, 82, 85	0
2	J	9/9 (100%)	2.06	3 (33%)	0	0	22, 33, 49, 83	0
2	N	9/9 (100%)	2.16	4 (44%)	0	0	20, 39, 61, 77	0
2	R	9/9 (100%)	4.52	8 (88%)	0	0	33, 41, 70, 75	0
2	V	9/9 (100%)	4.30	8 (88%)	0	0	41, 51, 77, 80	0
3	C	96/100 (96%)	2.31	52 (54%)	0	0	30, 54, 130, 166	0
3	G	98/100 (98%)	1.97	36 (36%)	0	0	16, 42, 73, 218	0
3	K	98/100 (98%)	1.62	25 (25%)	1	0	15, 40, 74, 180	0
3	O	98/100 (98%)	2.28	46 (46%)	0	0	26, 48, 121, 147	0
3	S	98/100 (98%)	5.05	79 (80%)	0	0	23, 57, 142, 203	0
3	W	98/100 (98%)	4.93	83 (84%)	0	0	20, 57, 115, 187	0
4	D	102/108 (94%)	1.87	38 (37%)	0	0	15, 42, 79, 193	0
4	H	103/108 (95%)	1.95	34 (33%)	0	0	22, 38, 76, 132	0
4	L	103/108 (95%)	1.77	34 (33%)	0	0	17, 36, 81, 129	0
4	P	103/108 (95%)	1.99	36 (34%)	0	0	16, 44, 115, 147	0
4	T	103/108 (95%)	4.48	85 (82%)	0	0	19, 54, 114, 160	0
4	X	103/108 (95%)	3.98	84 (81%)	0	0	18, 49, 92, 186	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	2811/2952 (95%)	3.01	1557 (55%)	0	0	14, 49, 118, 238	0

All (1557) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	33	PHE	22.2
1	E	227	ASP	22.0
3	W	9	VAL	21.8
3	W	93	VAL	20.9
1	U	83	GLY	19.9
3	S	9	VAL	19.9
1	M	189	MET	19.7
1	U	112	GLY	18.6
1	Q	190	THR	17.7
4	X	7	ALA	17.6
1	Q	172	LEU	17.4
1	Q	188	HIS	17.3
4	T	97	MET	16.7
1	Q	16	GLY	16.2
1	U	61	ASP	16.1
1	Q	239	GLY	16.0
3	S	42	ASN	15.4
3	W	1	ILE	15.3
3	S	15	ALA	15.2
1	U	136	ALA	14.9
4	X	74	ALA	14.5
3	O	44	GLU	14.1
4	T	103	MET	14.1
1	U	150	ALA	13.9
1	U	152	VAL	13.8
1	Q	8	PHE	13.7
1	A	190	THR	13.6
1	E	135	ALA	13.6
1	Q	256	ARG	13.6
1	Q	111	ARG	13.4
1	Q	18	GLY	13.3
1	U	269	PRO	13.3
1	U	194	VAL	13.2
3	S	90	PRO	13.2
3	S	8	GLN	12.9
4	T	52	ASN	12.8
3	S	10	TYR	12.6

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Mol	Chain	Res	Type	RSRZ
1	Q	230	LEU	12.5
1	M	193	ALA	12.4
1	U	25	VAL	12.2
1	Q	183	ASP	12.2
1	Q	93	HIS	12.1
4	T	21	SER	12.1
1	U	178	THR	12.0
3	S	39	LEU	11.8
3	S	40	LEU	11.8
1	Q	118	TYR	11.8
1	U	261	VAL	11.8
1	E	15	PRO	11.8
4	T	15	PRO	11.8
1	U	107	TRP	11.7
3	W	84	HIS	11.7
1	Q	27	TYR	11.7
4	T	35	CYS	11.6
1	U	208	PHE	11.6
1	U	111	ARG	11.6
4	P	11	LEU	11.2
1	U	74	HIS	11.2
1	U	15	PRO	11.2
3	W	78	TYR	11.1
1	U	18	GLY	11.0
1	Q	116	TYR	10.8
1	E	190	THR	10.8
3	S	1	ILE	10.8
1	U	271	THR	10.7
1	E	193	ALA	10.6
1	Q	177	GLU	10.6
3	G	44	GLU	10.5
1	U	127	LYS	10.3
1	U	119	ASP	10.3
1	U	9	PHE	10.3
1	M	188	HIS	10.3
4	X	31	VAL	10.2
1	E	223	ASP	10.2
1	Q	192	HIS	10.1
4	T	98	SER	10.0
1	Q	41	ALA	9.9
1	Q	226	GLN	9.9
1	Q	71	SER	9.9

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Mol	Chain	Res	Type	RSRZ
2	V	5	TYR	9.8
1	E	182	THR	9.8
3	W	35	ILE	9.8
1	M	90	ALA	9.7
4	T	16	ASP	9.6
1	Q	133	TRP	9.6
1	Q	254	GLU	9.6
4	L	8	ASP	9.5
1	Q	143	THR	9.5
1	A	188	HIS	9.5
4	X	13	PHE	9.5
3	S	66	TYR	9.5
1	U	93	HIS	9.3
4	T	80	THR	9.3
1	U	204	TRP	9.3
4	T	18	CYS	9.3
1	U	248	VAL	9.2
1	U	24	ALA	9.1
1	Q	194	VAL	9.1
3	W	2	GLN	9.1
1	U	151	HIS	9.0
1	M	251	SER	8.9
4	X	33	ILE	8.8
1	Q	15	PRO	8.8
1	U	6	ARG	8.8
1	Q	109	PHE	8.8
1	M	217	TRP	8.8
1	Q	62	GLY	8.8
1	U	190	THR	8.8
3	G	88	SER	8.8
1	U	247	VAL	8.7
1	M	252	GLY	8.7
4	X	71	VAL	8.7
4	X	77	PHE	8.7
1	Q	70	HIS	8.7
1	U	270	LEU	8.7
1	U	90	ALA	8.7
1	U	47	PRO	8.6
3	S	89	GLN	8.6
4	T	7	ALA	8.6
4	T	9	PRO	8.5
4	X	57	SER	8.5

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Mol	Chain	Res	Type	RSRZ
1	Q	139	ALA	8.5
4	P	18	CYS	8.5
3	S	60	TRP	8.4
1	Q	236	ALA	8.4
1	I	221	GLY	8.4
4	X	56	ALA	8.3
2	R	9	VAL	8.3
4	T	89	HIS	8.3
1	A	223	ASP	8.3
1	U	192	HIS	8.3
1	Q	233	THR	8.3
1	U	241	PHE	8.3
3	W	32	PRO	8.2
3	S	25	CYS	8.2
1	Q	227	ASP	8.2
4	X	24	PRO	8.2
1	U	67	VAL	8.2
1	M	111	ARG	8.2
3	S	84	HIS	8.2
1	E	131	ARG	8.2
3	W	47	GLU	8.2
1	Q	9	PHE	8.2
4	T	58	THR	8.2
3	S	21	ASN	8.1
1	A	180	GLN	8.1
3	S	69	GLU	8.1
3	S	14	PRO	8.1
3	W	67	TYR	8.1
1	Q	229	GLU	8.1
1	U	239	GLY	8.1
4	X	16	ASP	8.1
3	W	57	SER	8.1
1	Q	142	THR	8.1
3	W	63	TYR	8.0
1	Q	208	PHE	8.0
4	H	13	PHE	8.0
1	Q	42	SER	8.0
4	X	85	PHE	8.0
1	Q	126	LEU	8.0
1	U	249	VAL	8.0
1	Q	60	TRP	7.9
1	U	259	CYS	7.9

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Mol	Chain	Res	Type	RSRZ
1	M	192	HIS	7.9
1	Q	160	LEU	7.9
4	T	85	PHE	7.8
1	U	214	THR	7.8
1	Q	88	SER	7.8
1	Q	132	SER	7.8
3	W	10	TYR	7.8
1	Q	161	GLU	7.8
1	Q	235	PRO	7.8
1	E	18	GLY	7.7
3	W	20	SER	7.7
3	S	41	LYS	7.7
1	U	115	GLN	7.7
3	S	73	THR	7.7
1	Q	103	VAL	7.6
1	Q	250	PRO	7.6
1	I	194	VAL	7.6
1	I	197	HIS	7.6
1	U	12	VAL	7.6
1	U	257	TYR	7.5
1	Q	231	VAL	7.5
4	H	15	PRO	7.5
1	Q	228	THR	7.5
1	Q	61	ASP	7.5
3	S	85	VAL	7.5
1	U	250	PRO	7.4
1	U	101	CYS	7.4
1	U	94	THR	7.4
3	W	37	VAL	7.4
3	W	72	PRO	7.4
3	O	49	VAL	7.4
3	G	35	ILE	7.3
3	S	63	TYR	7.3
1	E	133	TRP	7.3
1	M	194	VAL	7.3
1	U	117	ALA	7.3
1	U	105	SER	7.3
1	E	194	VAL	7.3
3	S	64	LEU	7.3
1	Q	259	CYS	7.3
3	S	65	LEU	7.2
4	X	69	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
3	S	43	GLY	7.2
1	M	15	PRO	7.2
1	U	231	VAL	7.2
1	A	189	MET	7.2
1	E	160	LEU	7.1
3	W	49	VAL	7.1
1	I	192	HIS	7.1
4	T	24	PRO	7.1
1	M	225	THR	7.1
1	Q	222	GLU	7.1
1	U	195	SER	7.1
3	W	80	CYS	7.1
1	Q	225	THR	7.1
1	Q	33	PHE	7.0
1	U	135	ALA	7.0
3	W	51	HIS	7.0
3	W	38	ASP	7.0
1	M	3	HIS	7.0
4	T	105	PRO	7.0
1	U	26	GLY	7.0
1	U	244	TRP	6.9
1	I	201	LEU	6.9
1	U	109	PHE	6.9
3	S	52	SER	6.9
1	U	163	THR	6.9
4	T	26	GLY	6.9
1	I	138	MET	6.9
1	U	69	ALA	6.9
3	S	34	ASP	6.9
3	W	54	LEU	6.8
1	U	116	TYR	6.8
1	U	230	LEU	6.8
3	C	9	VAL	6.8
1	U	124	ILE	6.8
4	T	12	THR	6.8
3	W	79	ALA	6.8
4	H	86	ILE	6.8
1	Q	84	TYR	6.8
1	Q	30	ASP	6.8
3	W	31	HIS	6.8
1	U	210	PRO	6.7
1	Q	258	THR	6.7

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Mol	Chain	Res	Type	RSRZ
1	U	140	ALA	6.7
1	M	254	GLU	6.7
1	E	257	TYR	6.7
3	S	72	PRO	6.7
3	S	20	SER	6.7
1	Q	261	VAL	6.7
1	Q	39	ASP	6.6
3	S	81	ARG	6.6
1	M	209	TYR	6.6
1	U	180	GLN	6.6
1	I	193	ALA	6.6
1	Q	219	ARG	6.6
2	R	4	GLY	6.6
1	U	22	PHE	6.6
1	Q	217	TRP	6.6
3	C	72	PRO	6.5
3	O	88	SER	6.5
1	U	177	GLU	6.5
4	H	11	LEU	6.5
1	U	31	THR	6.5
4	T	93	THR	6.5
1	A	217	TRP	6.5
1	Q	187	THR	6.5
1	Q	253	GLN	6.4
1	I	98	MET	6.4
1	I	47	PRO	6.4
4	T	102	HIS	6.4
3	W	56	PHE	6.4
2	V	9	VAL	6.4
1	U	114	HIS	6.4
1	M	17	ARG	6.4
1	Q	125	ALA	6.4
3	O	74	GLU	6.4
4	X	55	LEU	6.4
1	M	256	ARG	6.4
4	X	96	PHE	6.3
1	U	75	ARG	6.3
1	E	247	VAL	6.3
1	M	206	LEU	6.3
1	E	252	GLY	6.3
1	U	193	ALA	6.3
1	U	254	GLU	6.3

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Mol	Chain	Res	Type	RSRZ
3	O	72	PRO	6.3
4	P	28	ARG	6.3
1	Q	76	VAL	6.3
1	U	174	ASN	6.3
1	U	227	ASP	6.3
1	E	230	LEU	6.3
1	A	193	ALA	6.3
1	U	82	ARG	6.3
3	O	45	ARG	6.3
1	Q	214	THR	6.3
4	T	42	VAL	6.2
3	W	91	LYS	6.2
3	K	54	LEU	6.2
1	A	90	ALA	6.2
1	U	17	ARG	6.2
1	I	15	PRO	6.2
4	X	15	PRO	6.2
4	X	75	ASP	6.2
1	U	191	HIS	6.2
1	U	260	HIS	6.2
3	W	65	LEU	6.2
1	M	224	GLN	6.2
1	U	179	LEU	6.2
4	X	52	ASN	6.2
1	U	27	TYR	6.2
4	T	17	LYS	6.2
1	E	205	ALA	6.2
3	S	46	ILE	6.1
1	Q	6	ARG	6.1
1	M	83	GLY	6.1
1	Q	45	MET	6.1
1	Q	36	PHE	6.1
1	U	182	THR	6.1
3	W	73	THR	6.1
1	U	255	GLN	6.1
1	I	217	TRP	6.1
1	E	181	ARG	6.1
1	Q	124	ILE	6.1
3	W	85	VAL	6.1
1	Q	162	GLY	6.1
4	X	89	HIS	6.1
3	W	16	GLU	6.0

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Mol	Chain	Res	Type	RSRZ
1	Q	48	ARG	6.0
3	S	74	GLU	6.0
4	T	107	ARG	6.0
3	S	31	HIS	6.0
3	S	91	LYS	6.0
3	S	49	VAL	6.0
4	T	78	LEU	6.0
1	M	271	THR	6.0
3	W	45	ARG	6.0
1	Q	117	ALA	5.9
4	H	41	SER	5.9
1	A	122	ASP	5.9
1	Q	174	ASN	5.9
3	S	35	ILE	5.9
1	M	172	LEU	5.9
1	Q	7	TYR	5.9
4	T	50	THR	5.9
1	U	106	ASP	5.9
3	K	88	SER	5.9
3	W	52	SER	5.9
1	Q	241	PHE	5.9
1	M	89	GLU	5.9
1	A	248	VAL	5.9
4	X	106	PRO	5.9
1	I	116	TYR	5.9
1	I	254	GLU	5.9
3	W	41	LYS	5.9
1	E	127	LYS	5.8
1	U	240	THR	5.8
3	W	11	SER	5.8
1	U	16	GLY	5.8
4	X	84	THR	5.8
1	E	116	TYR	5.8
4	T	30	ALA	5.8
1	U	8	PHE	5.8
1	U	243	LYS	5.8
4	T	56	ALA	5.8
1	U	65	ARG	5.8
4	T	37	TRP	5.8
4	X	37	TRP	5.8
1	M	187	THR	5.7
1	U	36	PHE	5.7

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Mol	Chain	Res	Type	RSRZ
4	X	103	MET	5.7
3	S	95	TRP	5.7
1	Q	120	GLY	5.6
1	M	136	ALA	5.6
1	Q	140	ALA	5.6
1	M	197	HIS	5.6
4	T	55	LEU	5.6
1	A	210	PRO	5.6
2	F	8	TYR	5.6
1	Q	17	ARG	5.6
1	U	137	ASP	5.6
1	U	120	GLY	5.6
3	W	86	THR	5.6
1	Q	223	ASP	5.6
1	U	148	GLU	5.6
3	S	82	VAL	5.5
4	T	99	ARG	5.5
3	W	17	ASN	5.5
1	E	187	THR	5.5
1	M	231	VAL	5.5
1	Q	165	VAL	5.5
1	A	247	VAL	5.5
1	U	113	TYR	5.5
1	M	120	GLY	5.5
4	T	27	ASN	5.5
4	X	48	ASN	5.5
4	P	106	PRO	5.5
2	B	5	TYR	5.5
1	Q	85	TYR	5.4
1	U	76	VAL	5.4
1	Q	189	MET	5.4
1	U	142	THR	5.4
1	U	7	TYR	5.4
1	U	133	TRP	5.4
1	M	223	ASP	5.4
1	Q	112	GLY	5.4
3	W	69	GLU	5.4
1	U	34	VAL	5.4
3	S	23	LEU	5.4
1	U	165	VAL	5.3
4	X	30	ALA	5.3
1	Q	136	ALA	5.3

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Mol	Chain	Res	Type	RSRZ
3	S	67	TYR	5.3
3	C	86	THR	5.3
1	E	189	MET	5.3
1	E	118	TYR	5.3
1	A	234	ARG	5.3
1	I	136	ALA	5.3
1	Q	13	SER	5.3
1	M	227	ASP	5.2
1	Q	28	VAL	5.2
1	Q	47	PRO	5.2
3	S	79	ALA	5.2
4	L	11	LEU	5.2
2	B	8	TYR	5.2
1	Q	269	PRO	5.2
1	U	86	ASN	5.2
1	A	267	PRO	5.2
1	E	204	TRP	5.2
3	W	3	ARG	5.2
1	U	141	GLN	5.2
4	H	75	ASP	5.1
1	Q	242	GLN	5.1
3	G	0	MET	5.1
1	E	41	ALA	5.1
3	S	83	ASN	5.1
1	Q	266	LEU	5.1
3	O	92	ILE	5.1
1	U	11	SER	5.1
3	S	50	GLU	5.1
3	W	42	ASN	5.1
1	A	206	LEU	5.1
3	C	35	ILE	5.1
3	K	14	PRO	5.1
4	X	46	TYR	5.0
4	X	12	THR	5.0
1	I	78	LEU	5.0
1	U	126	LEU	5.0
1	Q	50	PRO	5.0
4	T	71	VAL	5.0
1	A	6	ARG	5.0
1	Q	193	ALA	5.0
3	S	62	PHE	5.0
4	T	96	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	U	228	THR	5.0
1	Q	260	HIS	5.0
4	T	94	ALA	5.0
1	M	262	GLN	5.0
1	U	62	GLY	5.0
2	R	5	TYR	5.0
3	C	66	TYR	5.0
1	Q	90	ALA	5.0
1	A	162	GLY	5.0
1	M	243	LYS	5.0
1	Q	78	LEU	5.0
1	E	221	GLY	4.9
1	U	35	ARG	4.9
1	U	229	GLU	4.9
3	W	60	TRP	4.9
1	Q	182	THR	4.9
1	U	167	TRP	4.9
4	X	108	LYS	4.9
1	I	46	GLU	4.9
1	I	209	TYR	4.9
4	T	39	CYS	4.9
1	M	13	SER	4.9
1	Q	237	GLY	4.9
4	D	108	LYS	4.9
4	D	10	CYS	4.9
4	H	6	LYS	4.9
3	G	40	LEU	4.8
3	W	74	GLU	4.8
4	T	41	SER	4.8
1	Q	25	VAL	4.8
2	N	8	TYR	4.8
3	W	50	GLU	4.8
4	X	93	THR	4.8
1	Q	79	GLY	4.8
1	U	42	SER	4.8
4	T	25	ASP	4.8
3	W	81	ARG	4.8
1	Q	207	SER	4.8
1	M	82	ARG	4.8
1	Q	152	VAL	4.8
1	Q	212	GLU	4.8
1	I	251	SER	4.8

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Mol	Chain	Res	Type	RSRZ
3	S	77	GLU	4.8
4	X	42	VAL	4.8
1	Q	176	LYS	4.7
3	W	94	LYS	4.7
3	S	38	ASP	4.7
1	U	71	SER	4.7
4	T	36	GLY	4.7
4	T	101	TYR	4.7
1	Q	141	GLN	4.7
4	D	103	MET	4.7
4	D	11	LEU	4.7
1	Q	2	SER	4.7
1	Q	257	TYR	4.7
3	K	45	ARG	4.7
1	Q	178	THR	4.7
1	A	222	GLU	4.7
1	U	53	GLU	4.7
1	Q	119	ASP	4.7
1	U	84	TYR	4.7
1	I	256	ARG	4.7
1	A	213	ILE	4.7
3	W	25	CYS	4.7
1	U	21	ARG	4.7
1	A	106	ASP	4.7
3	K	46	ILE	4.7
4	T	86	ILE	4.7
1	Q	127	LYS	4.7
3	S	70	PHE	4.7
1	U	226	GLN	4.7
1	Q	210	PRO	4.6
4	H	42	VAL	4.6
1	E	84	TYR	4.6
1	Q	206	LEU	4.6
1	U	19	GLU	4.6
1	U	37	ASP	4.6
1	Q	74	HIS	4.6
1	I	206	LEU	4.6
4	P	15	PRO	4.6
3	O	36	GLU	4.6
2	R	1	LEU	4.6
3	W	0	MET	4.6
3	W	27	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	U	110	LEU	4.6
4	T	22	PHE	4.6
3	S	37	VAL	4.6
4	X	67	TYR	4.6
1	M	201	LEU	4.6
1	A	262	GLN	4.6
4	X	43	ALA	4.6
3	K	17	ASN	4.6
1	E	192	HIS	4.5
4	D	86	ILE	4.5
1	U	237	GLY	4.5
1	I	205	ALA	4.5
1	Q	156	LEU	4.5
1	U	68	LYS	4.5
1	U	132	SER	4.5
3	W	6	LYS	4.5
4	H	74	ALA	4.5
4	L	100	GLN	4.5
3	K	81	ARG	4.5
1	Q	240	THR	4.5
3	O	87	LEU	4.5
3	W	40	LEU	4.5
1	U	95	VAL	4.5
4	H	80	THR	4.5
1	U	123	TYR	4.5
1	E	229	GLU	4.5
1	Q	38	SER	4.5
1	Q	137	ASP	4.5
4	P	13	PHE	4.5
3	C	78	TYR	4.5
3	S	4	THR	4.5
1	I	252	GLY	4.5
4	L	40	GLN	4.4
1	M	257	TYR	4.4
2	R	8	TYR	4.4
1	Q	186	LYS	4.4
1	U	81	LEU	4.4
4	T	46	TYR	4.4
3	S	92	ILE	4.4
3	W	62	PHE	4.4
4	H	77	PHE	4.4
1	E	217	TRP	4.4

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Mol	Chain	Res	Type	RSRZ
3	S	17	ASN	4.4
4	L	78	LEU	4.4
1	U	28	VAL	4.4
3	O	86	THR	4.4
3	W	88	SER	4.3
3	O	3	ARG	4.3
1	U	209	TYR	4.3
1	A	225	THR	4.3
1	Q	271	THR	4.3
1	M	53	GLU	4.3
3	W	36	GLU	4.3
1	E	244	TRP	4.3
1	E	82	ARG	4.3
1	U	85	TYR	4.3
1	A	212	GLU	4.3
4	D	96	PHE	4.3
1	M	204	TRP	4.3
4	X	70	SER	4.3
1	I	189	MET	4.3
3	W	64	LEU	4.3
2	V	7	VAL	4.3
3	C	90	PRO	4.3
4	T	81	VAL	4.3
1	I	31	THR	4.3
1	A	243	LYS	4.3
3	S	96	ASP	4.3
4	D	25	ASP	4.3
4	T	61	PRO	4.3
4	D	89	HIS	4.3
1	M	185	PRO	4.3
1	M	118	TYR	4.3
3	G	73	THR	4.3
1	U	256	ARG	4.2
4	X	105	PRO	4.2
2	V	4	GLY	4.2
1	Q	106	ASP	4.2
1	A	194	VAL	4.2
3	G	53	ASP	4.2
1	U	149	ALA	4.2
1	Q	20	PRO	4.2
4	P	69	VAL	4.2
1	M	128	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	244	TRP	4.2
1	Q	121	LYS	4.2
1	U	30	ASP	4.2
1	U	97	ARG	4.2
3	C	54	LEU	4.2
3	C	3	ARG	4.2
1	E	130	LEU	4.2
1	U	41	ALA	4.2
3	W	53	ASP	4.2
4	X	22	PHE	4.2
1	E	17	ARG	4.1
1	E	220	ASP	4.1
1	M	116	TYR	4.1
4	P	27	ASN	4.1
3	W	33	SER	4.1
3	O	40	LEU	4.1
3	G	90	PRO	4.1
1	Q	22	PHE	4.1
4	D	28	ARG	4.1
1	Q	92	SER	4.1
3	S	88	SER	4.1
1	I	1	GLY	4.1
1	E	128	GLU	4.1
1	U	170	ARG	4.1
4	X	99	ARG	4.1
1	I	84	TYR	4.1
1	E	61	ASP	4.1
2	R	3	PHE	4.1
1	E	146	LYS	4.1
1	E	267	PRO	4.1
1	M	130	LEU	4.0
1	U	168	LEU	4.0
1	U	207	SER	4.0
1	Q	221	GLY	4.0
4	X	10	CYS	4.0
3	C	49	VAL	4.0
1	A	136	ALA	4.0
1	U	73	THR	4.0
1	A	86	ASN	4.0
1	U	172	LEU	4.0
3	O	39	LEU	4.0
1	M	141	GLN	4.0

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Mol	Chain	Res	Type	RSRZ
4	X	28	ARG	4.0
1	A	22	PHE	4.0
1	E	117	ALA	4.0
1	Q	268	LYS	4.0
1	Q	163	THR	4.0
1	Q	52	ILE	4.0
1	E	6	ARG	4.0
3	C	73	THR	4.0
1	U	246	ALA	4.0
1	A	51	TRP	4.0
1	E	162	GLY	4.0
3	C	5	PRO	4.0
1	E	165	VAL	4.0
1	U	96	GLN	4.0
4	X	23	GLN	4.0
1	E	98	MET	4.0
1	Q	267	PRO	4.0
1	U	50	PRO	4.0
3	O	27	VAL	4.0
1	I	260	HIS	3.9
1	Q	216	THR	3.9
3	W	66	TYR	3.9
1	U	213	ILE	3.9
1	M	239	GLY	3.9
4	P	10	CYS	3.9
1	Q	35	ARG	3.9
1	I	187	THR	3.9
1	U	72	GLN	3.9
3	C	85	VAL	3.9
1	U	118	TYR	3.9
4	T	106	PRO	3.9
1	Q	1	GLY	3.9
1	U	122	ASP	3.9
1	M	191	HIS	3.9
4	H	89	HIS	3.9
3	G	48	LYS	3.9
1	E	211	ALA	3.9
1	Q	115	GLN	3.9
4	L	71	VAL	3.9
4	X	17	LYS	3.9
1	E	154	GLU	3.9
4	D	82	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	Q	224	GLN	3.9
1	A	271	THR	3.9
1	I	120	GLY	3.9
4	D	44	ILE	3.9
1	A	160	LEU	3.8
1	M	4	SER	3.8
1	U	63	GLU	3.8
1	E	159	TYR	3.8
4	X	51	ARG	3.8
3	S	27	VAL	3.8
4	T	92	ASN	3.8
4	T	104	TRP	3.8
1	I	271	THR	3.8
1	M	121	LYS	3.8
1	A	257	TYR	3.8
1	Q	97	ARG	3.8
1	E	109	PHE	3.8
3	C	15	ALA	3.8
3	W	39	LEU	3.8
1	Q	202	ARG	3.8
4	T	48	ASN	3.8
1	Q	58	GLU	3.8
1	A	205	ALA	3.8
1	I	176	LYS	3.8
1	I	230	LEU	3.8
1	U	251	SER	3.8
1	Q	21	ARG	3.8
1	U	102	ASP	3.8
1	U	234	ARG	3.8
3	W	21	ASN	3.8
4	P	74	ALA	3.8
4	X	61	PRO	3.8
4	T	10	CYS	3.8
1	E	111	ARG	3.8
1	E	87	GLN	3.8
4	H	40	GLN	3.7
1	Q	99	TYR	3.7
1	Q	204	TRP	3.7
3	C	22	PHE	3.7
3	K	79	ALA	3.7
1	A	249	VAL	3.7
1	Q	144	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
4	X	73	GLY	3.7
1	E	191	HIS	3.7
4	P	102	HIS	3.7
3	S	80	CYS	3.7
1	E	3	HIS	3.7
4	P	44	ILE	3.7
1	A	5	MET	3.7
1	M	26	GLY	3.7
1	Q	102	ASP	3.7
4	P	25	ASP	3.7
1	I	40	ALA	3.7
3	K	44	GLU	3.7
4	L	52	ASN	3.7
1	I	257	TYR	3.7
1	M	84	TYR	3.6
3	O	89	GLN	3.6
1	U	45	MET	3.6
1	A	227	ASP	3.6
1	Q	100	GLY	3.6
1	E	222	GLU	3.6
3	C	7	ILE	3.6
3	W	7	ILE	3.6
4	P	42	VAL	3.6
1	U	77	ASP	3.6
1	I	105	SER	3.6
3	G	78	TYR	3.6
4	H	12	THR	3.6
1	E	78	LEU	3.6
1	U	58	GLU	3.6
4	X	87	PHE	3.6
3	G	49	VAL	3.6
3	G	72	PRO	3.6
4	X	9	PRO	3.6
1	M	94	THR	3.6
1	E	86	ASN	3.6
1	U	162	GLY	3.6
4	D	95	MET	3.6
1	M	75	ARG	3.6
1	U	60	TRP	3.6
1	U	92	SER	3.6
1	U	10	THR	3.6
1	Q	171	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	181	ARG	3.6
1	Q	191	HIS	3.6
1	Q	80	THR	3.6
4	P	12	THR	3.6
1	A	201	LEU	3.6
1	M	109	PHE	3.5
4	X	107	ARG	3.5
3	K	11	SER	3.5
3	S	94	LYS	3.5
1	A	233	THR	3.5
3	G	23	LEU	3.5
1	A	192	HIS	3.5
1	I	191	HIS	3.5
3	S	56	PHE	3.5
4	D	8	ASP	3.5
2	R	7	VAL	3.5
1	Q	81	LEU	3.5
3	W	23	LEU	3.5
1	Q	264	GLU	3.5
3	C	77	GLU	3.5
2	V	2	LEU	3.5
1	Q	159	TYR	3.5
4	T	67	TYR	3.5
1	M	45	MET	3.5
1	A	43	GLN	3.5
1	Q	157	ARG	3.5
1	M	28	VAL	3.5
4	P	36	GLY	3.5
4	X	40	GLN	3.5
3	C	60	TRP	3.5
1	M	165	VAL	3.5
1	A	156	LEU	3.5
4	T	13	PHE	3.5
2	J	8	TYR	3.5
1	U	103	VAL	3.5
3	G	91	LYS	3.4
1	M	98	MET	3.4
1	A	121	LYS	3.4
1	U	157	ARG	3.4
3	S	87	LEU	3.4
4	X	32	LEU	3.4
1	I	204	TRP	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	209	TYR	3.4
3	C	38	ASP	3.4
1	E	231	VAL	3.4
1	A	265	GLY	3.4
1	M	33	PHE	3.4
1	E	113	TYR	3.4
3	K	0	MET	3.4
4	X	90	MET	3.4
3	C	97	ARG	3.4
4	D	26	GLY	3.4
3	C	91	LYS	3.4
1	A	135	ALA	3.4
3	C	71	THR	3.4
3	G	86	THR	3.4
4	T	69	VAL	3.4
4	L	33	ILE	3.4
1	E	60	TRP	3.4
3	C	33	SER	3.4
3	C	81	ARG	3.4
1	Q	211	ALA	3.4
3	S	0	MET	3.4
1	E	225	THR	3.4
4	T	38	GLU	3.4
2	V	1	LEU	3.4
1	E	228	THR	3.4
1	M	52	ILE	3.4
1	Q	54	GLN	3.4
1	Q	87	GLN	3.4
4	L	51	ARG	3.4
1	U	206	LEU	3.4
1	U	242	GLN	3.4
1	I	190	THR	3.3
1	Q	203	CYS	3.3
1	A	8	PHE	3.3
1	E	124	ILE	3.3
3	G	33	SER	3.3
1	Q	26	GLY	3.3
4	D	40	GLN	3.3
1	U	253	GLN	3.3
3	W	82	VAL	3.3
4	D	75	ASP	3.3
1	E	19	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	89	GLU	3.3
1	Q	255	GLN	3.3
4	D	99	ARG	3.3
1	E	250	PRO	3.3
3	C	63	TYR	3.3
3	K	68	THR	3.3
1	U	128	GLU	3.3
3	C	44	GLU	3.3
3	K	95	TRP	3.3
1	Q	77	ASP	3.3
3	O	61	SER	3.3
1	M	164	CYS	3.3
1	A	250	PRO	3.3
1	Q	5	MET	3.3
3	G	34	ASP	3.3
1	A	207	SER	3.3
1	Q	59	TYR	3.3
4	X	50	THR	3.3
4	X	101	TYR	3.3
4	H	62	GLY	3.3
1	M	156	LEU	3.3
1	E	13	SER	3.3
4	T	84	THR	3.3
1	E	224	GLN	3.3
1	I	45	MET	3.3
3	O	2	GLN	3.3
1	M	86	ASN	3.2
1	A	107	TRP	3.2
1	U	20	PRO	3.2
1	U	159	TYR	3.2
3	S	19	LYS	3.2
4	X	34	LYS	3.2
4	H	7	ALA	3.2
1	E	122	ASP	3.2
1	Q	130	LEU	3.2
1	M	42	SER	3.2
4	H	36	GLY	3.2
4	P	29	CYS	3.2
1	M	131	ARG	3.2
1	M	135	ALA	3.2
1	Q	32	GLN	3.2
1	Q	69	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	51	TRP	3.2
3	O	54	LEU	3.2
4	X	104	TRP	3.2
1	Q	114	HIS	3.2
3	S	86	THR	3.2
1	I	173	GLU	3.2
3	S	61	SER	3.2
4	X	14	ASN	3.2
3	W	22	PHE	3.2
4	D	41	SER	3.2
1	E	197	HIS	3.2
1	I	64	THR	3.2
1	I	134	THR	3.2
3	K	25	CYS	3.2
3	C	45	ARG	3.2
3	O	48	LYS	3.2
1	U	87	GLN	3.2
4	X	97	MET	3.2
1	Q	10	THR	3.2
1	M	69	ALA	3.2
1	A	215	LEU	3.2
1	Q	168	LEU	3.2
3	K	40	LEU	3.2
1	M	180	GLN	3.2
4	H	99	ARG	3.2
4	P	19	GLN	3.2
1	U	189	MET	3.1
4	T	59	TRP	3.1
3	O	73	THR	3.1
3	O	79	ALA	3.1
4	X	44	ILE	3.1
1	A	221	GLY	3.1
3	W	8	GLN	3.1
4	L	95	MET	3.1
1	M	182	THR	3.1
3	S	71	THR	3.1
1	M	246	ALA	3.1
1	U	125	ALA	3.1
3	W	26	TYR	3.1
4	D	107	ARG	3.1
1	E	45	MET	3.1
1	E	143	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	72	GLN	3.1
1	I	269	PRO	3.1
1	Q	113	TYR	3.1
3	C	95	TRP	3.1
1	I	111	ARG	3.1
1	M	255	GLN	3.1
4	T	44	ILE	3.1
2	V	6	PRO	3.1
4	X	59	TRP	3.1
1	E	50	PRO	3.1
1	U	52	ILE	3.1
3	C	88	SER	3.1
1	M	39	ASP	3.1
1	Q	123	TYR	3.1
1	Q	209	TYR	3.1
1	Q	145	HIS	3.1
1	Q	107	TRP	3.1
3	G	77	GLU	3.1
3	C	4	THR	3.1
3	W	19	LYS	3.1
1	E	207	SER	3.1
1	Q	238	ASP	3.1
1	I	48	ARG	3.1
4	X	79	ARG	3.1
4	X	95	MET	3.1
1	I	156	LEU	3.1
1	Q	40	ALA	3.1
2	R	6	PRO	3.1
4	X	86	ILE	3.1
1	M	25	VAL	3.0
1	Q	251	SER	3.0
1	E	268	LYS	3.0
1	U	245	ALA	3.0
3	S	16	GLU	3.0
4	D	27	ASN	3.0
4	P	14	ASN	3.0
4	P	108	LYS	3.0
1	Q	270	LEU	3.0
4	X	21	SER	3.0
1	U	236	ALA	3.0
1	A	74	HIS	3.0
4	H	91	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	216	THR	3.0
4	P	56	ALA	3.0
1	A	131	ARG	3.0
1	E	256	ARG	3.0
4	T	91	CYS	3.0
1	E	12	VAL	3.0
1	E	29	ASP	3.0
1	U	38	SER	3.0
1	U	183	ASP	3.0
4	T	57	SER	3.0
4	X	25	ASP	3.0
1	I	172	LEU	3.0
1	A	211	ALA	3.0
2	F	6	PRO	3.0
1	M	160	LEU	3.0
2	N	1	LEU	3.0
4	T	49	LYS	3.0
1	A	197	HIS	3.0
1	M	169	ARG	3.0
3	S	13	HIS	3.0
4	T	82	ASN	3.0
1	E	7	TYR	3.0
3	W	58	LYS	3.0
4	T	66	TRP	3.0
3	W	18	GLY	3.0
1	A	27	TYR	3.0
1	A	159	TYR	3.0
1	E	123	TYR	3.0
1	U	98	MET	3.0
1	Q	153	ALA	3.0
1	A	115	GLN	2.9
4	D	87	PHE	2.9
1	A	134	THR	2.9
4	H	8	ASP	2.9
1	A	33	PHE	2.9
1	A	166	GLU	2.9
4	D	13	PHE	2.9
1	M	78	LEU	2.9
1	M	230	LEU	2.9
3	C	40	LEU	2.9
1	E	25	VAL	2.9
4	P	95	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	218	GLN	2.9
1	M	43	GLN	2.9
3	G	2	GLN	2.9
4	D	104	TRP	2.9
4	T	64	PRO	2.9
1	A	52	ILE	2.9
1	M	202	ARG	2.9
1	Q	134	THR	2.9
4	D	12	THR	2.9
2	F	7	VAL	2.9
4	H	81	VAL	2.9
4	L	69	VAL	2.9
4	P	8	ASP	2.9
3	W	92	ILE	2.9
3	O	18	GLY	2.9
2	J	1	LEU	2.9
1	Q	34	VAL	2.9
1	E	125	ALA	2.9
3	C	1	ILE	2.9
1	A	78	LEU	2.9
1	I	130	LEU	2.9
2	J	9	VAL	2.9
1	U	51	TRP	2.9
3	W	95	TRP	2.9
4	X	63	ASP	2.9
3	C	11	SER	2.9
3	C	28	SER	2.9
3	K	63	TYR	2.9
1	A	35	ARG	2.9
1	E	202	ARG	2.9
4	T	72	PRO	2.9
3	W	61	SER	2.9
1	A	173	GLU	2.9
1	E	27	TYR	2.9
1	I	267	PRO	2.9
1	U	49	ALA	2.9
1	I	229	GLU	2.8
3	W	13	HIS	2.8
4	T	33	ILE	2.8
3	O	81	ARG	2.8
4	P	58	THR	2.8
4	X	58	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	U	104	GLY	2.8
1	M	145	HIS	2.8
4	P	96	PHE	2.8
3	W	12	ARG	2.8
3	W	76	ASP	2.8
2	N	9	VAL	2.8
1	E	251	SER	2.8
3	C	92	ILE	2.8
1	E	141	GLN	2.8
4	T	8	ASP	2.8
3	S	36	GLU	2.8
4	T	6	LYS	2.8
3	C	55	SER	2.8
4	X	102	HIS	2.8
4	X	36	GLY	2.8
1	A	138	MET	2.8
1	I	158	ALA	2.8
1	A	132	SER	2.8
3	W	55	SER	2.8
4	P	37	TRP	2.8
1	E	72	GLN	2.8
4	T	77	PHE	2.8
1	E	83	GLY	2.8
1	E	149	ALA	2.8
1	E	186	LYS	2.8
1	M	114	HIS	2.8
1	A	155	GLN	2.8
1	I	177	GLU	2.8
1	U	262	GLN	2.8
1	A	39	ASP	2.8
1	E	179	LEU	2.8
4	X	27	ASN	2.8
1	I	152	VAL	2.8
1	M	12	VAL	2.8
4	D	56	ALA	2.8
4	D	61	PRO	2.8
4	H	79	ARG	2.8
3	K	84	HIS	2.8
3	O	55	SER	2.8
4	H	10	CYS	2.8
3	C	36	GLU	2.7
4	T	45	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
4	T	108	LYS	2.7
1	I	6	ARG	2.7
1	U	89	GLU	2.7
1	E	210	PRO	2.7
1	I	202	ARG	2.7
1	Q	108	ARG	2.7
3	S	45	ARG	2.7
4	T	28	ARG	2.7
1	I	89	GLU	2.7
4	X	65	GLU	2.7
1	A	253	GLN	2.7
1	E	101	CYS	2.7
3	S	75	LYS	2.7
4	T	63	ASP	2.7
4	T	75	ASP	2.7
4	T	95	MET	2.7
1	A	120	GLY	2.7
1	M	126	LEU	2.7
3	K	66	TYR	2.7
1	Q	72	GLN	2.7
3	G	92	ILE	2.7
3	S	5	PRO	2.7
3	S	57	SER	2.7
1	I	122	ASP	2.7
1	Q	122	ASP	2.7
1	M	5	MET	2.7
1	E	63	GLU	2.7
1	U	80	THR	2.7
1	E	236	ALA	2.7
1	M	41	ALA	2.7
4	L	24	PRO	2.7
4	X	64	PRO	2.7
4	H	107	ARG	2.7
4	L	35	CYS	2.7
1	U	171	TYR	2.7
1	A	191	HIS	2.7
1	I	96	GLN	2.7
4	T	90	MET	2.7
1	M	81	LEU	2.7
1	M	99	TYR	2.7
3	C	12	ARG	2.7
1	I	188	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	261	VAL	2.7
1	Q	86	ASN	2.7
1	Q	51	TRP	2.7
4	T	51	ARG	2.7
4	T	40	GLN	2.6
4	X	72	PRO	2.6
1	Q	3	HIS	2.6
3	C	84	HIS	2.6
3	K	85	VAL	2.6
1	E	5	MET	2.6
1	A	203	CYS	2.6
4	L	10	CYS	2.6
4	L	91	CYS	2.6
4	P	40	GLN	2.6
3	G	45	ARG	2.6
4	P	23	GLN	2.6
1	I	52	ILE	2.6
1	I	133	TRP	2.6
1	I	213	ILE	2.6
1	M	139	ALA	2.6
1	Q	46	GLU	2.6
1	U	66	LYS	2.6
3	S	48	LYS	2.6
1	A	181	ARG	2.6
1	M	215	LEU	2.6
3	G	54	LEU	2.6
1	A	226	GLN	2.6
3	S	2	GLN	2.6
2	F	5	TYR	2.6
3	W	14	PRO	2.6
1	I	17	ARG	2.6
1	I	231	VAL	2.6
3	C	8	GLN	2.6
3	C	59	ASP	2.6
1	Q	147	TRP	2.6
4	X	88	GLU	2.6
1	I	145	HIS	2.6
4	L	87	PHE	2.6
4	L	15	PRO	2.6
4	L	68	THR	2.6
4	L	86	ILE	2.6
1	I	113	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	85	TYR	2.6
4	L	89	HIS	2.6
2	N	7	VAL	2.6
3	C	2	GLN	2.6
1	E	66	LYS	2.6
3	G	87	LEU	2.6
3	S	44	GLU	2.6
4	T	62	GLY	2.6
1	A	88	SER	2.6
3	G	3	ARG	2.6
3	C	79	ALA	2.6
3	S	51	HIS	2.6
4	P	71	VAL	2.6
1	E	215	LEU	2.6
1	E	239	GLY	2.6
1	I	62	GLY	2.6
1	A	41	ALA	2.5
1	M	91	GLY	2.5
1	I	82	ARG	2.5
3	W	28	SER	2.5
3	C	94	LYS	2.5
3	C	89	GLN	2.5
3	W	71	THR	2.5
1	A	61	ASP	2.5
1	U	70	HIS	2.5
1	A	179	LEU	2.5
1	I	237	GLY	2.5
1	U	202	ARG	2.5
1	E	33	PHE	2.5
1	M	203	CYS	2.5
4	L	76	GLY	2.5
1	M	144	LYS	2.5
1	A	98	MET	2.5
1	I	33	PHE	2.5
1	M	138	MET	2.5
1	Q	218	GLN	2.5
3	O	20	SER	2.5
1	M	210	PRO	2.5
1	U	57	PRO	2.5
3	O	80	CYS	2.5
4	X	68	THR	2.5
1	E	81	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	26	TYR	2.5
3	G	82	VAL	2.5
4	H	71	VAL	2.5
1	U	166	GLU	2.5
4	H	70	SER	2.5
1	A	24	ALA	2.5
1	I	263	HIS	2.5
1	M	97	ARG	2.5
1	Q	131	ARG	2.5
1	U	14	ARG	2.5
1	U	134	THR	2.5
1	A	84	TYR	2.5
3	S	33	SER	2.5
1	I	121	LYS	2.5
1	M	235	PRO	2.5
1	I	41	ALA	2.5
4	L	32	LEU	2.5
1	E	59	TYR	2.5
4	L	6	LYS	2.5
1	M	35	ARG	2.5
3	S	12	ARG	2.5
4	D	15	PRO	2.5
1	E	31	THR	2.5
1	M	270	LEU	2.5
3	C	23	LEU	2.5
1	E	107	TRP	2.5
1	A	216	THR	2.4
1	I	114	HIS	2.4
1	U	153	ALA	2.4
3	W	46	ILE	2.4
4	T	20	LEU	2.4
4	H	87	PHE	2.4
4	L	18	CYS	2.4
4	T	29	CYS	2.4
3	O	91	LYS	2.4
3	W	48	LYS	2.4
1	Q	57	PRO	2.4
1	E	38	SER	2.4
3	G	81	ARG	2.4
4	X	81	VAL	2.4
1	E	8	PHE	2.4
3	K	96	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
4	D	77	PHE	2.4
4	H	32	LEU	2.4
1	A	87	GLN	2.4
1	I	109	PHE	2.4
1	M	238	ASP	2.4
1	Q	37	ASP	2.4
1	I	7	TYR	2.4
1	I	27	TYR	2.4
1	A	3	HIS	2.4
1	A	31	THR	2.4
1	E	148	GLU	2.4
1	E	161	GLU	2.4
3	O	23	LEU	2.4
4	P	57	SER	2.4
1	Q	167	TRP	2.4
4	D	14	ASN	2.4
4	H	25	ASP	2.4
4	P	22	PHE	2.4
3	W	97	ARG	2.4
1	Q	146	LYS	2.4
4	D	18	CYS	2.4
1	I	77	ASP	2.4
3	K	18	GLY	2.4
3	K	60	TRP	2.4
3	C	50	GLU	2.4
1	U	139	ALA	2.4
4	P	35	CYS	2.4
4	H	14	ASN	2.4
4	L	44	ILE	2.4
1	U	79	GLY	2.4
1	E	36	PHE	2.4
1	M	173	GLU	2.4
3	O	50	GLU	2.4
1	U	99	TYR	2.4
1	Q	158	ALA	2.4
4	X	54	THR	2.4
1	M	213	ILE	2.4
4	D	36	GLY	2.4
4	T	34	LYS	2.4
4	X	18	CYS	2.4
1	E	169	ARG	2.4
1	M	8	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	62	PHE	2.4
1	U	147	TRP	2.4
1	A	171	TYR	2.3
1	I	32	GLN	2.3
4	D	58	THR	2.3
4	H	94	ALA	2.3
1	U	144	LYS	2.3
1	A	174	ASN	2.3
1	U	108	ARG	2.3
1	E	248	VAL	2.3
1	M	76	VAL	2.3
1	E	253	GLN	2.3
4	T	23	GLN	2.3
1	A	99	TYR	2.3
1	Q	220	ASP	2.3
1	A	187	THR	2.3
1	E	79	GLY	2.3
1	E	184	ALA	2.3
4	X	11	LEU	2.3
1	E	115	GLN	2.3
3	O	66	TYR	2.3
1	M	181	ARG	2.3
4	X	76	GLY	2.3
3	S	24	ASN	2.3
1	Q	96	GLN	2.3
3	G	95	TRP	2.3
3	S	29	GLY	2.3
1	E	240	THR	2.3
4	P	68	THR	2.3
3	O	9	VAL	2.3
1	E	212	GLU	2.3
1	I	147	TRP	2.3
1	M	73	THR	2.3
1	Q	68	LYS	2.3
3	G	66	TYR	2.3
3	O	17	ASN	2.3
4	D	7	ALA	2.3
4	T	65	GLU	2.3
1	U	88	SER	2.3
4	D	106	PRO	2.3
4	L	49	LYS	2.3
1	A	123	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	135	ALA	2.3
4	L	67	TYR	2.3
1	A	34	VAL	2.3
1	I	67	VAL	2.3
1	M	95	VAL	2.3
1	M	110	LEU	2.3
3	W	90	PRO	2.3
4	L	64	PRO	2.3
4	L	106	PRO	2.3
3	K	15	ALA	2.3
4	L	74	ALA	2.3
1	E	99	TYR	2.3
1	M	6	ARG	2.3
4	X	6	LYS	2.3
1	A	45	MET	2.2
1	E	110	LEU	2.2
4	L	43	ALA	2.2
1	M	134	THR	2.2
1	Q	94	THR	2.2
1	I	103	VAL	2.2
1	I	253	GLN	2.2
1	A	114	HIS	2.2
1	E	47	PRO	2.2
1	U	78	LEU	2.2
4	T	53	ASN	2.2
1	A	125	ALA	2.2
3	O	6	LYS	2.2
1	A	7	TYR	2.2
1	I	208	PHE	2.2
1	A	76	VAL	2.2
3	G	8	GLN	2.2
3	O	35	ILE	2.2
4	X	60	GLN	2.2
1	I	154	GLU	2.2
1	I	2	SER	2.2
4	P	17	LYS	2.2
1	M	234	ARG	2.2
1	Q	44	ARG	2.2
4	D	37	TRP	2.2
4	X	80	THR	2.2
3	C	76	ASP	2.2
1	I	68	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	57	PRO	2.2
1	A	83	GLY	2.2
1	E	85	TYR	2.2
4	X	47	LYS	2.2
1	I	34	VAL	2.2
1	Q	82	ARG	2.2
1	Q	201	LEU	2.2
4	L	39	CYS	2.2
1	I	5	MET	2.2
1	I	255	GLN	2.2
1	Q	205	ALA	2.2
4	H	103	MET	2.2
1	M	240	THR	2.2
1	Q	166	GLU	2.2
3	K	91	LYS	2.2
3	O	41	LYS	2.2
1	M	261	VAL	2.2
1	E	121	LYS	2.2
1	A	16	GLY	2.2
1	E	136	ALA	2.2
1	A	214	THR	2.2
1	E	163	THR	2.2
3	G	46	ILE	2.2
1	A	126	LEU	2.2
3	O	75	LYS	2.2
3	W	75	LYS	2.2
1	M	32	GLN	2.2
1	U	155	GLN	2.2
1	U	235	PRO	2.2
4	P	61	PRO	2.2
1	Q	135	ALA	2.2
1	Q	252	GLY	2.2
3	O	34	ASP	2.2
1	A	4	SER	2.1
4	X	53	ASN	2.1
1	A	67	VAL	2.1
1	Q	55	GLU	2.1
1	A	130	LEU	2.1
3	O	64	LEU	2.1
1	E	100	GLY	2.1
3	K	3	ARG	2.1
1	Q	53	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	74	HIS	2.1
3	G	14	PRO	2.1
1	M	258	THR	2.1
4	X	66	TRP	2.1
3	W	44	GLU	2.1
1	E	203	CYS	2.1
1	M	152	VAL	2.1
1	A	50	PRO	2.1
1	M	151	HIS	2.1
1	A	144	LYS	2.1
1	E	170	ARG	2.1
4	D	64	PRO	2.1
4	H	28	ARG	2.1
4	T	76	GLY	2.1
3	G	15	ALA	2.1
4	L	30	ALA	2.1
1	M	190	THR	2.1
1	U	138	MET	2.1
3	C	57	SER	2.1
1	I	165	VAL	2.1
1	E	114	HIS	2.1
1	Q	23	ILE	2.1
1	U	252	GLY	2.1
3	O	14	PRO	2.1
1	I	73	THR	2.1
1	U	13	SER	2.1
4	H	73	GLY	2.1
1	M	222	GLU	2.1
3	O	67	TYR	2.1
1	A	184	ALA	2.1
1	I	107	TRP	2.1
1	M	163	THR	2.1
2	V	3	PHE	2.1
3	O	52	SER	2.1
3	S	11	SER	2.1
4	L	62	GLY	2.1
1	M	154	GLU	2.1
1	Q	154	GLU	2.1
4	D	101	TYR	2.1
3	O	24	ASN	2.1
1	A	202	ARG	2.1
1	E	112	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	102	ASP	2.1
3	O	70	PHE	2.1
1	A	103	VAL	2.1
3	G	85	VAL	2.1
1	A	68	LYS	2.1
1	M	127	LYS	2.1
4	X	49	LYS	2.1
3	C	42	ASN	2.1
1	A	143	THR	2.1
1	M	161	GLU	2.1
1	Q	11	SER	2.1
1	U	5	MET	2.1
3	S	68	THR	2.1
1	I	112	GLY	2.1
3	G	43	GLY	2.1
3	W	70	PHE	2.1
1	U	268	LYS	2.0
1	I	97	ARG	2.0
1	M	148	GLU	2.0
4	P	65	GLU	2.0
1	E	39	ASP	2.0
1	I	26	GLY	2.0
1	I	207	SER	2.0
3	O	11	SER	2.0
3	O	53	ASP	2.0
3	G	70	PHE	2.0
1	A	47	PRO	2.0
1	E	249	VAL	2.0
1	E	232	GLU	2.0
1	M	184	ALA	2.0
1	A	196	ASP	2.0
1	I	132	SER	2.0
1	M	38	SER	2.0
1	M	100	GLY	2.0
4	D	98	SER	2.0
1	I	155	GLN	2.0
3	G	30	PHE	2.0
1	A	53	GLU	2.0
1	A	85	TYR	2.0
1	M	159	TYR	2.0
1	Q	24	ALA	2.0
1	U	121	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	142	THR	2.0
1	M	80	THR	2.0
1	Q	101	CYS	2.0
1	A	151	HIS	2.0
1	I	232	GLU	2.0
1	M	177	GLU	2.0
1	A	12	VAL	2.0
3	O	32	PRO	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.