Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2023 – 12:21 am GMT

PDB ID	:	2J4U
Title	:	E.coli OmpC - camel Lactoferrin complex
Authors	:	Baalaji, S.; Acharya, R.K.; Singh, T.P.; Krishnaswamy, S.
Deposited on	:	2006-09-06
Resolution	:	2.99 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

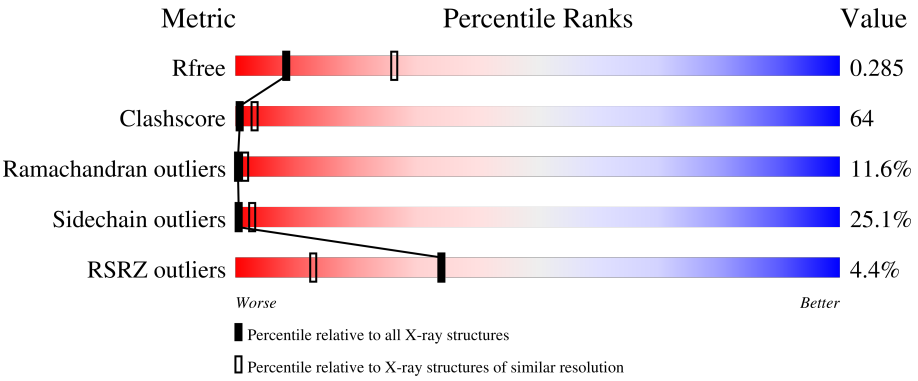
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.99 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	P	346	23% 42% 21% 12%
1	Q	346	22% 38% 26% 11%
1	R	346	19% 41% 26% 11%
1	U	346	20% 43% 22% 13%
1	V	346	22% 40% 25% 12%

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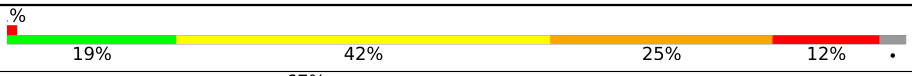
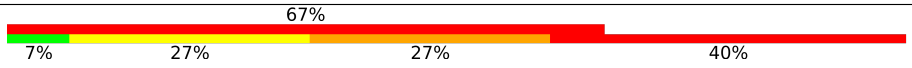
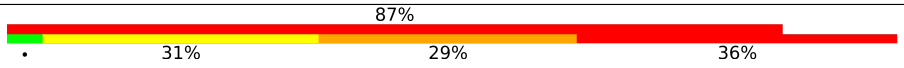
Mol	Chain	Length	Quality of chain
1	W	346	
2	S	45	
2	X	45	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16534 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 OUTER MEMBRANE PROTEIN C PRECURSOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			
1	Q	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			
1	R	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			
1	U	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			
1	V	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			
1	W	337	Total	C	N	O	S	0	0	0
			2636	1653	441	539	3			

- Molecule 2 is a protein called LACTOTRANSFERRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	45	Total	C	N	O	S	0	0	0
			359	221	72	61	5			
2	X	45	Total	C	N	O	S	0	0	0
			359	221	72	61	5			

There are 2 discrepancies between the modelled and reference sequences:

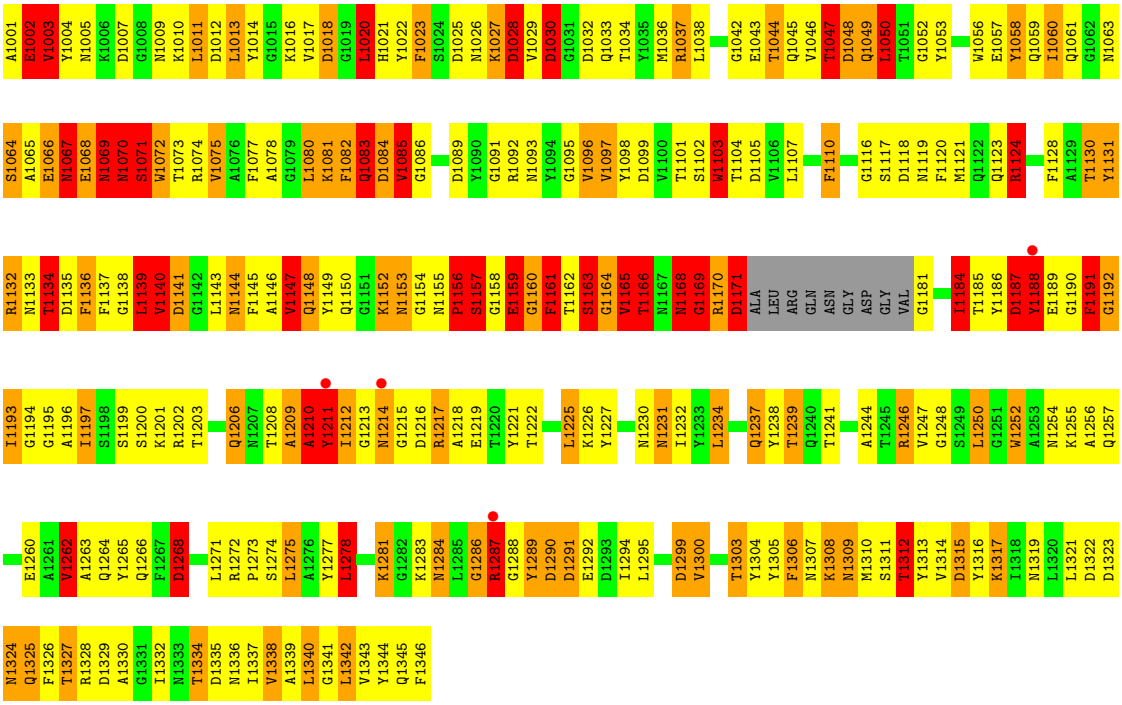
Chain	Residue	Modelled	Actual	Comment	Reference
S	1017	LYS	SER	conflict	UNP Q9TUM0
X	1017	LYS	SER	conflict	UNP Q9TUM0

3 Residue-property plots (i)

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

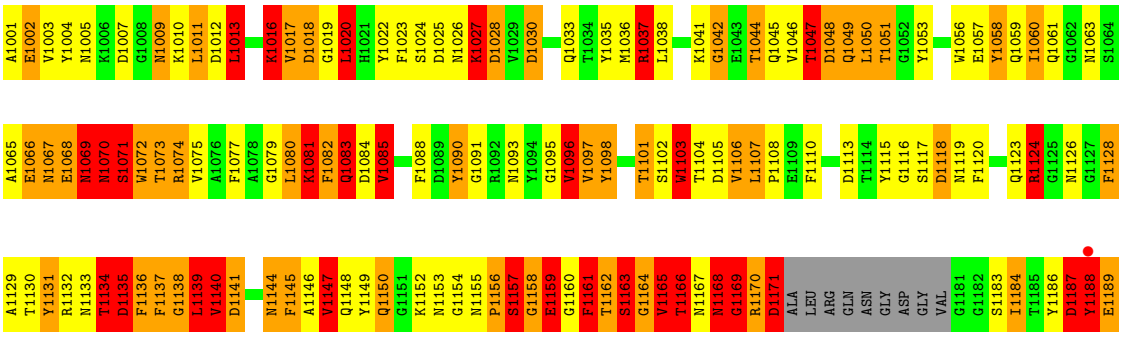
• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR

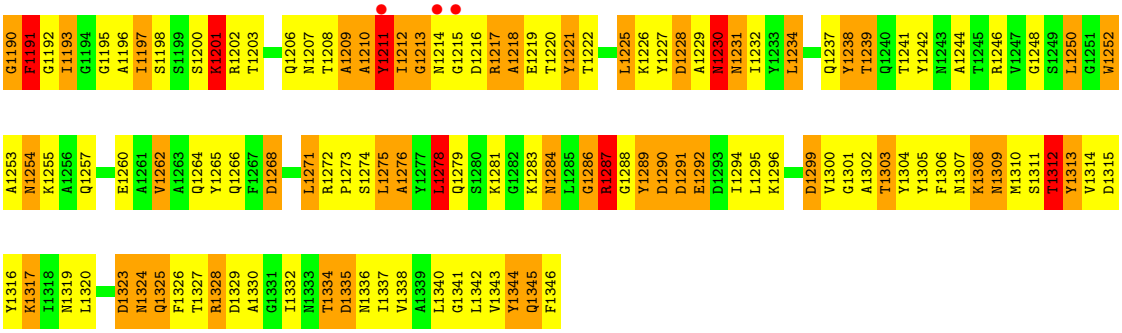
Chain P:



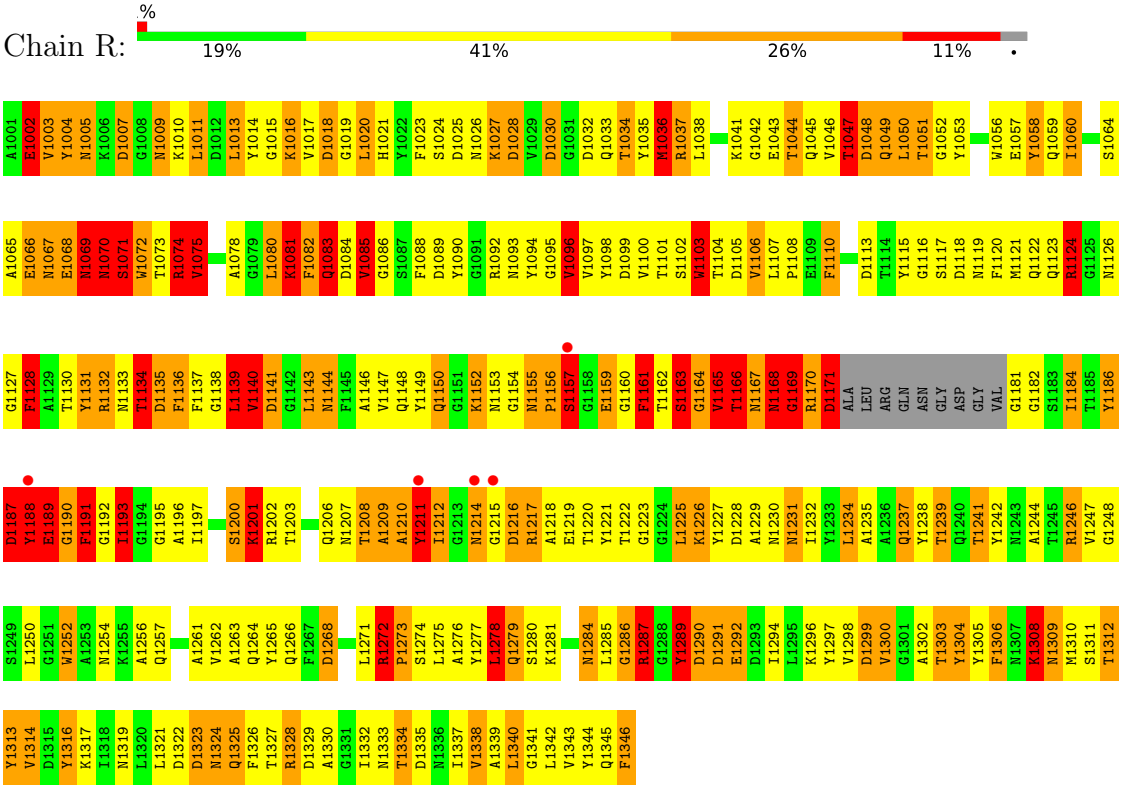
• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR

Chain Q:

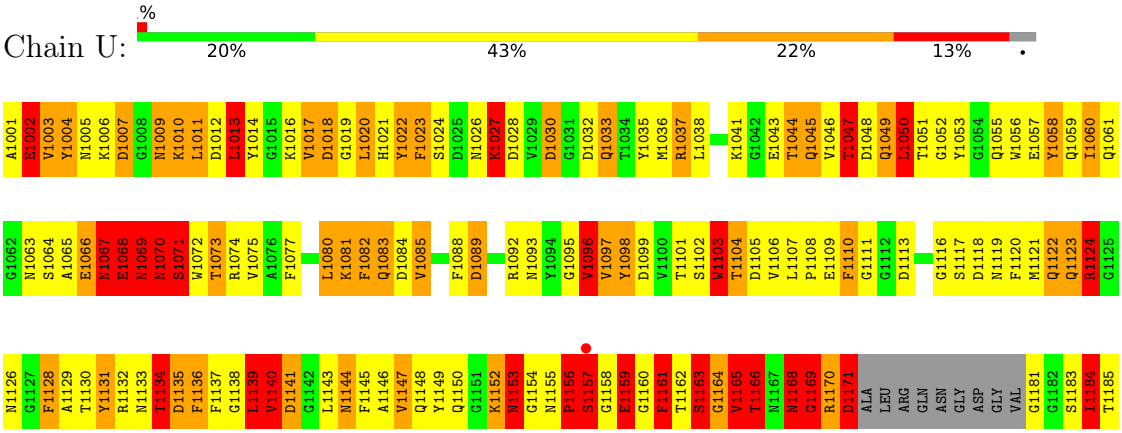


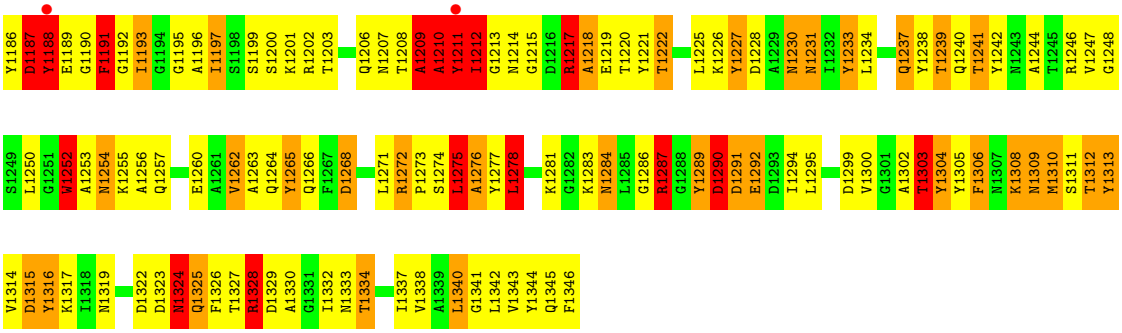


• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR



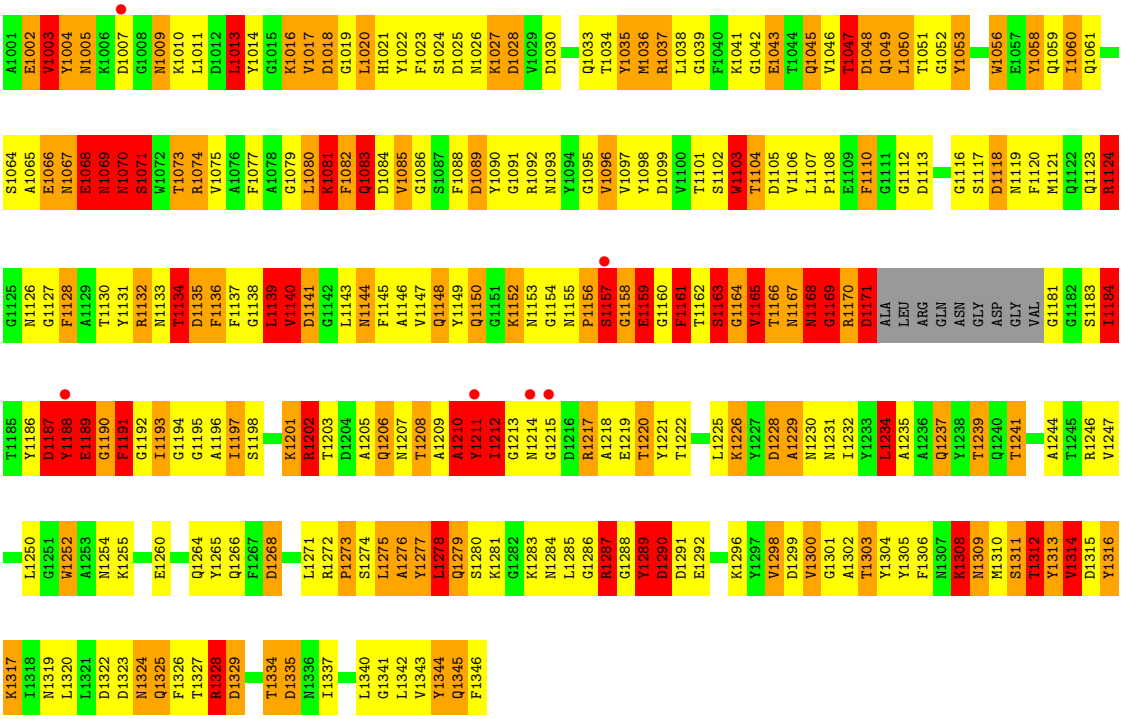
• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR





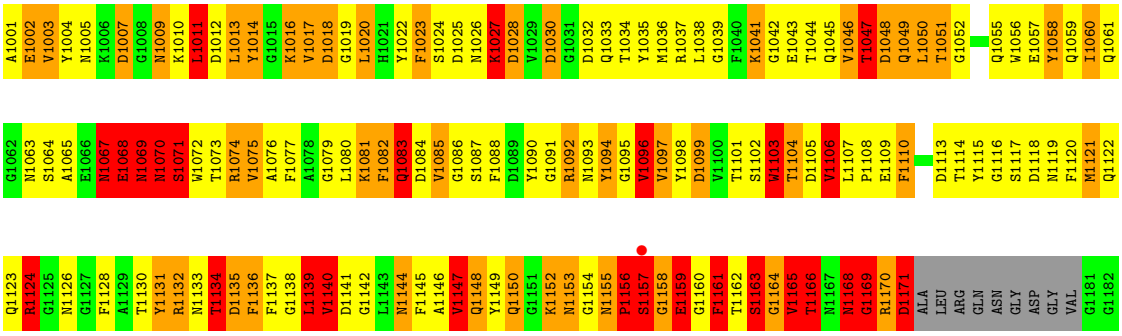
• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR

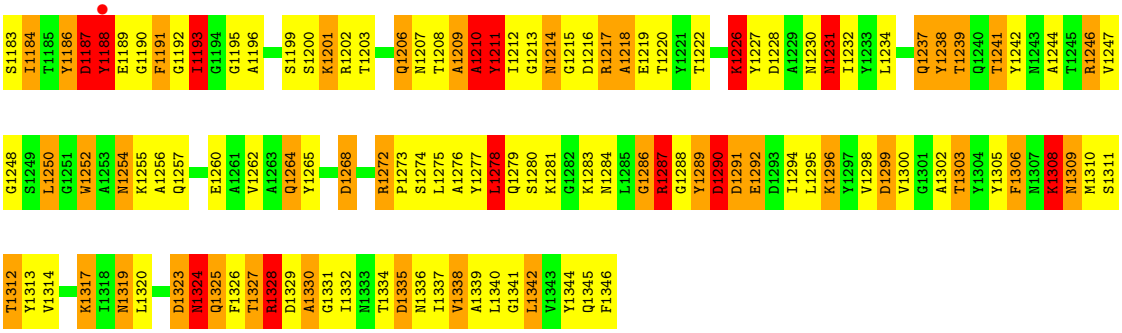
Chain V:



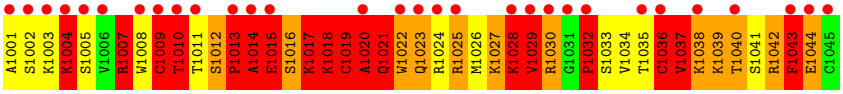
• Molecule 1: OUTER MEMBRANE PROTEIN C PRECURSOR

Chain W:

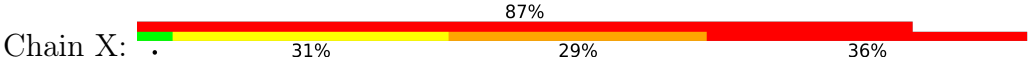


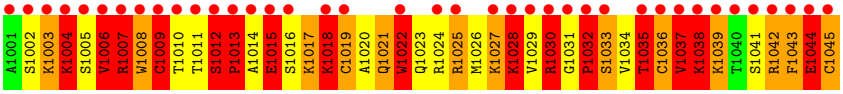


• Molecule 2: LACTOTRANSFERRIN



• Molecule 2: LACTOTRANSFERRIN





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	201.47Å 116.29Å 152.28Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	152.50 – 2.99 19.76 – 2.99	Depositor EDS
% Data completeness (in resolution range)	78.8 (152.50-2.99) 79.0 (19.76-2.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.282 0.216 , 0.285	Depositor DCC
R_{free} test set	2831 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.467 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.467 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.467 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.459 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.468 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16534	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.60% 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	P	2.31	98/2692 (3.6%)	1.99	100/3641 (2.7%)
1	Q	2.28	94/2692 (3.5%)	1.94	99/3641 (2.7%)
1	R	2.34	118/2692 (4.4%)	2.01	103/3641 (2.8%)
1	U	2.31	108/2692 (4.0%)	1.95	89/3641 (2.4%)
1	V	2.32	107/2692 (4.0%)	1.99	90/3641 (2.5%)
1	W	2.30	111/2692 (4.1%)	1.97	92/3641 (2.5%)
2	S	2.65	17/365 (4.7%)	1.80	5/485 (1.0%)
2	X	2.68	20/365 (5.5%)	1.87	8/485 (1.6%)
All	All	2.33	673/16882 (4.0%)	1.97	586/22816 (2.6%)

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	P	0	12
1	Q	1	9
1	R	1	8
1	U	1	11
1	V	1	8
1	W	0	10
2	S	0	2
2	X	0	5
All	All	4	65

All (673) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1161	PHE	CB-CG	21.34	1.87	1.51
1	W	1161	PHE	CB-CG	20.92	1.86	1.51
1	U	1161	PHE	CB-CG	20.71	1.86	1.51
1	P	1161	PHE	CB-CG	20.63	1.86	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1161	PHE	CB-CG	19.21	1.84	1.51
1	Q	1161	PHE	CB-CG	18.95	1.83	1.51
1	V	1068	GLU	CG-CD	14.39	1.73	1.51
1	R	1068	GLU	CG-CD	13.95	1.72	1.51
1	Q	1157	SER	N-CA	13.78	1.74	1.46
1	W	1157	SER	N-CA	13.71	1.73	1.46
1	Q	1068	GLU	CG-CD	13.54	1.72	1.51
1	V	1157	SER	N-CA	13.28	1.73	1.46
1	V	1161	PHE	CD1-CE1	13.15	1.65	1.39
1	P	1252	TRP	CG-CD1	13.13	1.55	1.36
1	R	1157	SER	N-CA	13.02	1.72	1.46
2	S	1019	CYS	CB-SG	13.01	2.04	1.82
1	U	1157	SER	N-CA	12.97	1.72	1.46
1	W	1068	GLU	CG-CD	12.61	1.70	1.51
2	X	1045	CYS	CB-SG	12.32	2.03	1.82
1	P	1157	SER	N-CA	12.30	1.71	1.46
1	R	1081	LYS	CD-CE	12.13	1.81	1.51
1	Q	1161	PHE	CD1-CE1	11.59	1.62	1.39
1	R	1103	TRP	CB-CG	11.38	1.70	1.50
1	U	1161	PHE	CD1-CE1	11.36	1.61	1.39
1	V	1103	TRP	CB-CG	11.15	1.70	1.50
1	U	1161	PHE	CG-CD2	11.13	1.55	1.38
1	Q	1103	TRP	CB-CG	10.72	1.69	1.50
1	W	1252	TRP	CB-CG	10.68	1.69	1.50
1	P	1252	TRP	CB-CG	10.64	1.69	1.50
1	U	1161	PHE	CG-CD1	10.52	1.54	1.38
1	P	1161	PHE	CD1-CE1	10.49	1.60	1.39
1	U	1165	VAL	CA-CB	-10.46	1.32	1.54
1	W	1161	PHE	CD1-CE1	10.45	1.60	1.39
1	V	1081	LYS	CD-CE	10.44	1.77	1.51
1	R	1069	ASN	C-O	10.26	1.42	1.23
1	R	1268	ASP	CB-CG	10.17	1.73	1.51
1	U	1103	TRP	CB-CG	10.17	1.68	1.50
1	W	1188	TYR	CE2-CZ	10.05	1.51	1.38
1	V	1268	ASP	CB-CG	9.91	1.72	1.51
1	Q	1252	TRP	CG-CD1	9.82	1.50	1.36
1	U	1268	ASP	CB-CG	9.77	1.72	1.51
1	V	1149	TYR	CG-CD1	9.76	1.51	1.39
1	R	1252	TRP	CG-CD1	9.76	1.50	1.36
1	P	1068	GLU	CG-CD	9.71	1.66	1.51
1	P	1103	TRP	CB-CG	9.70	1.67	1.50
1	P	1165	VAL	CA-CB	-9.61	1.34	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1149	TYR	CB-CG	9.61	1.66	1.51
1	W	1081	LYS	CD-CE	9.59	1.75	1.51
1	R	1161	PHE	CD2-CE2	9.53	1.58	1.39
1	P	1188	TYR	CD2-CE2	9.48	1.53	1.39
1	W	1069	ASN	C-O	9.46	1.41	1.23
1	Q	1161	PHE	CG-CD2	9.39	1.52	1.38
1	Q	1165	VAL	CA-CB	-9.37	1.35	1.54
1	U	1252	TRP	CG-CD1	9.37	1.49	1.36
1	V	1161	PHE	CG-CD2	9.36	1.52	1.38
1	U	1276	ALA	CA-CB	-9.36	1.32	1.52
2	S	1036	CYS	CB-SG	9.24	1.98	1.82
1	W	1161	PHE	CG-CD1	9.23	1.52	1.38
1	V	1188	TYR	CG-CD2	9.20	1.51	1.39
1	V	1323	ASP	CB-CG	-9.17	1.32	1.51
2	X	1019	CYS	CB-SG	9.16	1.97	1.82
1	V	1161	PHE	CG-CD1	9.15	1.52	1.38
1	R	1161	PHE	CD1-CE1	9.12	1.57	1.39
1	W	1103	TRP	CB-CG	9.09	1.66	1.50
1	P	1058	TYR	CD2-CE2	9.09	1.52	1.39
1	V	1069	ASN	C-O	9.09	1.40	1.23
1	U	1014	TYR	CD1-CE1	8.97	1.52	1.39
1	V	1120	PHE	CD2-CE2	8.96	1.57	1.39
1	Q	1161	PHE	CD2-CE2	8.95	1.57	1.39
1	R	1161	PHE	CG-CD1	8.95	1.52	1.38
1	P	1188	TYR	CE2-CZ	8.93	1.50	1.38
1	W	1165	VAL	CA-CB	-8.89	1.36	1.54
1	V	1068	GLU	CB-CG	8.88	1.69	1.52
1	U	1188	TYR	CD1-CE1	8.86	1.52	1.39
1	Q	1081	LYS	CD-CE	8.83	1.73	1.51
1	V	1169	GLY	CA-C	8.82	1.66	1.51
1	U	1188	TYR	CD2-CE2	8.81	1.52	1.39
1	Q	1268	ASP	CB-CG	8.78	1.70	1.51
1	Q	1191	PHE	CE1-CZ	8.76	1.53	1.37
1	R	1014	TYR	CD1-CE1	8.76	1.52	1.39
1	P	1068	GLU	CB-CG	8.75	1.68	1.52
1	R	1289	TYR	CE1-CZ	8.74	1.50	1.38
1	W	1188	TYR	CG-CD2	8.73	1.50	1.39
1	Q	1211	TYR	CB-CG	8.72	1.64	1.51
1	U	1211	TYR	CB-CG	8.71	1.64	1.51
1	W	1110	PHE	CE2-CZ	8.68	1.53	1.37
1	R	1316	TYR	CB-CG	-8.67	1.38	1.51
1	R	1068	GLU	CB-CG	8.66	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	1115	TYR	CD2-CE2	8.64	1.52	1.39
1	W	1134	THR	CB-CG2	8.60	1.80	1.52
1	U	1068	GLU	CG-CD	8.57	1.64	1.51
1	Q	1334	THR	CA-CB	8.56	1.75	1.53
1	U	1305	TYR	CG-CD1	-8.56	1.28	1.39
1	U	1014	TYR	CD2-CE2	8.55	1.52	1.39
1	P	1213	GLY	CA-C	8.52	1.65	1.51
1	U	1313	TYR	CE2-CZ	8.51	1.49	1.38
1	Q	1068	GLU	CD-OE2	8.51	1.35	1.25
1	V	1191	PHE	CD1-CE1	8.50	1.56	1.39
1	V	1149	TYR	CE1-CZ	8.43	1.49	1.38
1	R	1211	TYR	CB-CG	8.40	1.64	1.51
1	U	1149	TYR	CG-CD1	8.40	1.50	1.39
1	R	1186	TYR	CD1-CE1	-8.39	1.26	1.39
1	Q	1069	ASN	C-O	8.38	1.39	1.23
1	P	1161	PHE	CG-CD2	8.38	1.51	1.38
1	R	1323	ASP	CB-CG	-8.36	1.34	1.51
1	R	1004	TYR	CD2-CE2	8.33	1.51	1.39
1	P	1149	TYR	CB-CG	8.32	1.64	1.51
1	W	1289	TYR	CE1-CZ	8.31	1.49	1.38
1	W	1082	PHE	CB-CG	8.26	1.65	1.51
1	R	1306	PHE	CE1-CZ	8.24	1.53	1.37
1	R	1252	TRP	CB-CG	8.23	1.65	1.50
1	R	1103	TRP	CG-CD1	8.23	1.48	1.36
1	V	1165	VAL	CA-CB	-8.21	1.37	1.54
1	W	1268	ASP	CB-CG	8.19	1.69	1.51
1	W	1188	TYR	CD2-CE2	8.19	1.51	1.39
1	V	1188	TYR	CD2-CE2	8.15	1.51	1.39
1	V	1276	ALA	CA-CB	-8.15	1.35	1.52
1	W	1289	TYR	CD1-CE1	8.12	1.51	1.39
1	V	1120	PHE	CB-CG	-8.11	1.37	1.51
1	W	1041	LYS	CE-NZ	8.11	1.69	1.49
1	U	1302	ALA	CA-CB	-8.11	1.35	1.52
1	W	1161	PHE	CG-CD2	8.10	1.50	1.38
1	Q	1188	TYR	CD2-CE2	8.05	1.51	1.39
1	P	1149	TYR	CG-CD1	8.02	1.49	1.39
1	W	1068	GLU	CD-OE1	8.01	1.34	1.25
1	P	1268	ASP	CB-CG	8.00	1.68	1.51
1	Q	1161	PHE	CG-CD1	7.99	1.50	1.38
1	W	1188	TYR	CE1-CZ	7.98	1.49	1.38
1	U	1188	TYR	CG-CD2	7.98	1.49	1.39
1	V	1103	TRP	CG-CD1	7.97	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1191	PHE	CD1-CE1	7.97	1.55	1.39
1	Q	1188	TYR	CG-CD2	7.97	1.49	1.39
1	Q	1211	TYR	CA-C	7.97	1.73	1.52
1	P	1300	VAL	CB-CG2	7.97	1.69	1.52
1	W	1188	TYR	CD1-CE1	7.97	1.51	1.39
1	R	1110	PHE	CE2-CZ	7.92	1.52	1.37
1	Q	1149	TYR	CB-CG	7.82	1.63	1.51
1	Q	1171	ASP	C-O	7.79	1.38	1.23
1	R	1188	TYR	CE2-CZ	7.79	1.48	1.38
1	U	1188	TYR	CG-CD1	7.78	1.49	1.39
1	W	1161	PHE	CD2-CE2	7.75	1.54	1.39
1	Q	1035	TYR	CE1-CZ	-7.74	1.28	1.38
1	R	1149	TYR	CG-CD1	7.73	1.49	1.39
1	R	1169	GLY	CA-C	7.73	1.64	1.51
2	X	1009	CYS	CB-SG	7.72	1.95	1.82
1	U	1171	ASP	CB-CG	7.72	1.68	1.51
1	V	1017	VAL	CA-CB	-7.71	1.38	1.54
1	R	1211	TYR	CG-CD1	7.70	1.49	1.39
1	R	1134	THR	CB-CG2	7.69	1.77	1.52
1	R	1168	ASN	CB-CG	-7.68	1.33	1.51
1	W	1211	TYR	CA-C	7.63	1.72	1.52
1	U	1291	ASP	CB-CG	7.63	1.67	1.51
1	U	1211	TYR	CG-CD2	7.61	1.49	1.39
2	X	1022	TRP	CB-CG	7.60	1.64	1.50
1	P	1191	PHE	CG-CD1	7.60	1.50	1.38
1	P	1211	TYR	CB-CG	7.59	1.63	1.51
1	P	1068	GLU	CD-OE2	7.56	1.33	1.25
1	U	1161	PHE	CD2-CE2	7.55	1.54	1.39
1	Q	1018	ASP	CB-CG	-7.55	1.35	1.51
1	P	1092	ARG	CZ-NH1	7.54	1.42	1.33
1	W	1287	ARG	CG-CD	7.53	1.70	1.51
1	Q	1323	ASP	CB-CG	-7.49	1.36	1.51
1	R	1276	ALA	CA-CB	-7.47	1.36	1.52
1	P	1306	PHE	CE1-CZ	7.45	1.51	1.37
1	U	1004	TYR	CD2-CE2	7.44	1.50	1.39
2	S	1029	VAL	CA-CB	7.43	1.70	1.54
1	W	1191	PHE	CD1-CE1	7.42	1.54	1.39
1	W	1004	TYR	CD2-CE2	7.42	1.50	1.39
1	V	1149	TYR	CB-CG	7.41	1.62	1.51
1	P	1014	TYR	CD2-CE2	7.41	1.50	1.39
1	V	1335	ASP	CB-CG	-7.40	1.36	1.51
1	V	1171	ASP	C-O	7.39	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	1037	VAL	CA-CB	7.36	1.70	1.54
1	Q	1188	TYR	CD1-CE1	7.35	1.50	1.39
1	P	1014	TYR	CD1-CE1	7.35	1.50	1.39
1	Q	1120	PHE	CE2-CZ	7.35	1.51	1.37
1	V	1134	THR	CB-CG2	7.34	1.76	1.52
1	U	1058	TYR	CB-CG	-7.32	1.40	1.51
1	W	1323	ASP	CB-CG	-7.31	1.36	1.51
1	R	1161	PHE	CG-CD2	7.31	1.49	1.38
1	U	1211	TYR	CG-CD1	7.31	1.48	1.39
1	U	1103	TRP	CG-CD1	7.31	1.47	1.36
1	V	1022	TYR	CD2-CE2	-7.26	1.28	1.39
1	V	1150	GLN	CB-CG	-7.24	1.32	1.52
1	U	1171	ASP	C-O	7.23	1.37	1.23
2	S	1014	ALA	N-CA	7.20	1.60	1.46
1	U	1023	PHE	C-O	7.20	1.37	1.23
1	U	1169	GLY	CA-C	7.18	1.63	1.51
1	U	1068	GLU	CD-OE2	7.18	1.33	1.25
2	X	1044	GLU	CB-CG	7.17	1.65	1.52
1	U	1058	TYR	CD1-CE1	7.15	1.50	1.39
1	V	1161	PHE	CD2-CE2	7.14	1.53	1.39
1	W	1171	ASP	C-O	7.14	1.36	1.23
1	R	1165	VAL	CA-CB	-7.13	1.39	1.54
1	P	1334	THR	CA-CB	7.11	1.71	1.53
1	V	1211	TYR	CB-CG	7.10	1.62	1.51
1	P	1161	PHE	CG-CD1	7.09	1.49	1.38
1	P	1188	TYR	CD1-CE1	7.09	1.50	1.39
1	V	1252	TRP	CG-CD1	7.08	1.46	1.36
1	U	1277	TYR	CD1-CE1	7.06	1.50	1.39
1	U	1316	TYR	CB-CG	-7.05	1.41	1.51
1	V	1305	TYR	CG-CD1	-7.03	1.30	1.39
1	V	1056	TRP	CG-CD1	7.02	1.46	1.36
1	W	1211	TYR	CB-CG	6.99	1.62	1.51
1	R	1186	TYR	CD2-CE2	-6.96	1.28	1.39
1	U	1314	VAL	CB-CG1	-6.95	1.38	1.52
1	V	1068	GLU	CD-OE2	6.93	1.33	1.25
1	U	1289	TYR	CE1-CZ	6.92	1.47	1.38
1	U	1218	ALA	CA-CB	-6.91	1.38	1.52
1	W	1302	ALA	CA-CB	-6.91	1.38	1.52
2	S	1032	PRO	N-CA	6.89	1.58	1.47
1	R	1004	TYR	CE2-CZ	6.88	1.47	1.38
1	R	1090	TYR	CD1-CE1	-6.86	1.29	1.39
2	S	1010	THR	CA-CB	6.85	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1110	PHE	CE2-CZ	6.83	1.50	1.37
1	P	1161	PHE	CA-CB	6.83	1.69	1.53
1	V	1191	PHE	CE1-CZ	6.83	1.50	1.37
1	P	1023	PHE	CD2-CE2	6.81	1.52	1.39
1	R	1171	ASP	C-O	6.81	1.36	1.23
1	R	1149	TYR	CE1-CZ	6.80	1.47	1.38
1	R	1188	TYR	CG-CD2	6.80	1.48	1.39
1	W	1211	TYR	CG-CD1	6.79	1.48	1.39
1	R	1221	TYR	CB-CG	-6.79	1.41	1.51
1	V	1304	TYR	CG-CD1	6.78	1.48	1.39
1	W	1068	GLU	CD-OE2	6.78	1.33	1.25
1	R	1308	LYS	CD-CE	6.78	1.68	1.51
2	S	1043	PHE	CB-CG	6.77	1.62	1.51
1	W	1149	TYR	CG-CD1	6.75	1.48	1.39
1	P	1191	PHE	CD1-CE1	6.74	1.52	1.39
1	W	1131	TYR	CG-CD1	6.74	1.48	1.39
1	R	1188	TYR	CD1-CE1	6.73	1.49	1.39
1	P	1277	TYR	CD1-CE1	6.73	1.49	1.39
1	P	1335	ASP	CB-CG	-6.73	1.37	1.51
1	V	1277	TYR	CD1-CE1	6.73	1.49	1.39
1	U	1161	PHE	CE2-CZ	6.72	1.50	1.37
1	Q	1189	GLU	CG-CD	6.71	1.62	1.51
1	Q	1056	TRP	CG-CD1	6.71	1.46	1.36
1	V	1211	TYR	CA-C	6.71	1.70	1.52
1	U	1035	TYR	CE2-CZ	-6.70	1.29	1.38
1	U	1022	TYR	CB-CG	-6.70	1.41	1.51
1	U	1191	PHE	CD1-CE1	6.69	1.52	1.39
1	Q	1211	TYR	CG-CD2	6.68	1.47	1.39
1	W	1046	VAL	CB-CG2	-6.68	1.38	1.52
1	Q	1134	THR	CB-CG2	6.67	1.74	1.52
2	X	1035	THR	CA-CB	6.66	1.70	1.53
1	P	1191	PHE	CE2-CZ	6.66	1.50	1.37
1	Q	1082	PHE	CB-CG	6.66	1.62	1.51
1	Q	1115	TYR	CZ-OH	6.66	1.49	1.37
2	S	1043	PHE	N-CA	6.66	1.59	1.46
1	V	1298	VAL	CB-CG1	6.65	1.66	1.52
1	W	1017	VAL	CB-CG1	6.64	1.66	1.52
1	W	1131	TYR	CG-CD2	6.64	1.47	1.39
1	R	1289	TYR	CD1-CE1	6.64	1.49	1.39
1	W	1070	ASN	CA-C	6.63	1.70	1.52
1	Q	1149	TYR	CG-CD1	6.63	1.47	1.39
1	W	1067	ASN	CB-CG	-6.62	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1191	PHE	CD2-CE2	6.61	1.52	1.39
1	U	1069	ASN	CB-CG	6.61	1.66	1.51
1	U	1149	TYR	CD1-CE1	6.60	1.49	1.39
1	U	1252	TRP	CB-CG	6.58	1.62	1.50
1	W	1161	PHE	CE2-CZ	6.58	1.49	1.37
1	Q	1041	LYS	CD-CE	6.57	1.67	1.51
1	U	1161	PHE	CA-CB	6.56	1.68	1.53
1	W	1252	TRP	CG-CD1	6.56	1.46	1.36
1	P	1018	ASP	CB-CG	-6.54	1.38	1.51
1	P	1110	PHE	CE2-CZ	6.54	1.49	1.37
2	S	1014	ALA	CA-CB	6.54	1.66	1.52
1	W	1305	TYR	CG-CD1	-6.54	1.30	1.39
1	Q	1252	TRP	CB-CG	6.53	1.61	1.50
1	P	1323	ASP	CB-CG	-6.52	1.38	1.51
1	U	1265	TYR	CZ-OH	-6.52	1.26	1.37
1	V	1120	PHE	CD1-CE1	6.51	1.52	1.39
1	R	1306	PHE	CD2-CE2	6.50	1.52	1.39
1	W	1210	ALA	C-O	6.50	1.35	1.23
1	Q	1287	ARG	CG-CD	6.49	1.68	1.51
1	R	1305	TYR	CG-CD1	-6.49	1.30	1.39
1	W	1289	TYR	CD2-CE2	6.46	1.49	1.39
1	R	1018	ASP	CB-CG	-6.46	1.38	1.51
1	V	1188	TYR	CE2-CZ	6.46	1.47	1.38
1	P	1161	PHE	CD2-CE2	6.44	1.52	1.39
1	Q	1276	ALA	CA-CB	-6.44	1.39	1.52
1	Q	1169	GLY	CA-C	6.42	1.62	1.51
1	U	1213	GLY	CA-C	6.42	1.62	1.51
1	U	1273	PRO	C-O	6.41	1.36	1.23
1	U	1211	TYR	CA-C	6.41	1.69	1.52
1	P	1188	TYR	CG-CD1	6.39	1.47	1.39
1	Q	1313	TYR	CE2-CZ	6.39	1.46	1.38
1	Q	1305	TYR	CG-CD1	-6.39	1.30	1.39
1	P	1147	VAL	N-CA	-6.39	1.33	1.46
1	P	1211	TYR	CA-C	6.39	1.69	1.52
1	R	1273	PRO	C-O	6.37	1.35	1.23
1	Q	1254	ASN	CG-ND2	6.37	1.48	1.32
1	V	1004	TYR	CE1-CZ	6.36	1.46	1.38
1	U	1147	VAL	C-O	6.36	1.35	1.23
1	U	1149	TYR	CB-CG	6.36	1.61	1.51
1	P	1081	LYS	CD-CE	6.36	1.67	1.51
1	V	1188	TYR	CD1-CE1	6.33	1.48	1.39
1	R	1313	TYR	CE2-CZ	6.32	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1008	TRP	CB-CG	6.31	1.61	1.50
1	U	1018	ASP	CB-CG	-6.31	1.38	1.51
1	R	1103	TRP	CD2-CE2	6.31	1.49	1.41
1	P	1058	TYR	CD1-CE1	6.31	1.48	1.39
1	P	1188	TYR	CG-CD2	6.31	1.47	1.39
1	U	1023	PHE	CB-CG	-6.28	1.40	1.51
1	R	1305	TYR	CE1-CZ	-6.28	1.30	1.38
1	V	1058	TYR	CB-CG	-6.28	1.42	1.51
1	R	1188	TYR	CD2-CE2	6.28	1.48	1.39
1	U	1323	ASP	CB-CG	-6.28	1.38	1.51
1	W	1166	THR	CB-CG2	6.28	1.73	1.52
1	U	1188	TYR	CE2-CZ	6.27	1.46	1.38
1	U	1057	GLU	CD-OE1	-6.27	1.18	1.25
1	W	1022	TYR	CB-CG	-6.26	1.42	1.51
1	V	1308	LYS	CD-CE	6.25	1.66	1.51
1	U	1104	THR	CA-CB	-6.25	1.37	1.53
1	U	1227	TYR	CD1-CE1	-6.25	1.29	1.39
2	S	1019	CYS	N-CA	6.24	1.58	1.46
1	P	1161	PHE	CA-C	6.23	1.69	1.52
1	Q	1213	GLY	CA-C	6.23	1.61	1.51
1	W	1149	TYR	CB-CG	6.23	1.60	1.51
1	W	1305	TYR	CD1-CE1	-6.23	1.30	1.39
1	R	1191	PHE	CE2-CZ	6.22	1.49	1.37
1	R	1214	ASN	CB-CG	6.22	1.65	1.51
1	U	1191	PHE	CE1-CZ	6.20	1.49	1.37
1	W	1109	GLU	CD-OE1	-6.20	1.18	1.25
1	V	1191	PHE	CE2-CZ	6.20	1.49	1.37
1	W	1191	PHE	CE1-CZ	6.19	1.49	1.37
1	Q	1072	TRP	CB-CG	6.18	1.61	1.50
1	V	1234	LEU	C-O	6.18	1.35	1.23
1	U	1120	PHE	CE2-CZ	6.17	1.49	1.37
1	W	1314	VAL	CB-CG2	6.16	1.65	1.52
1	R	1227	TYR	CE2-CZ	6.16	1.46	1.38
1	P	1131	TYR	CG-CD2	6.16	1.47	1.39
1	R	1014	TYR	CD2-CE2	6.16	1.48	1.39
1	R	1131	TYR	CG-CD2	6.15	1.47	1.39
1	V	1047	THR	CB-CG2	-6.15	1.32	1.52
1	V	1070	ASN	C-O	6.13	1.35	1.23
1	R	1161	PHE	CA-C	6.13	1.68	1.52
1	V	1300	VAL	CB-CG2	6.12	1.65	1.52
1	Q	1131	TYR	CG-CD2	6.11	1.47	1.39
1	P	1120	PHE	CE2-CZ	6.11	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	1334	THR	CA-CB	6.08	1.69	1.53
1	Q	1103	TRP	CG-CD1	6.08	1.45	1.36
1	R	1334	THR	CA-CB	6.07	1.69	1.53
1	P	1082	PHE	CB-CG	6.07	1.61	1.51
1	W	1291	ASP	CB-CG	6.06	1.64	1.51
1	R	1096	VAL	CB-CG1	-6.06	1.40	1.52
1	R	1100	VAL	CB-CG2	6.06	1.65	1.52
1	U	1099	ASP	CB-CG	-6.05	1.39	1.51
2	S	1004	LYS	N-CA	6.05	1.58	1.46
1	R	1279	GLN	CB-CG	-6.05	1.36	1.52
1	V	1071	SER	N-CA	6.04	1.58	1.46
1	U	1109	GLU	CD-OE1	-6.04	1.19	1.25
1	Q	1071	SER	CA-CB	6.04	1.62	1.52
1	W	1238	TYR	CE2-CZ	-6.04	1.30	1.38
1	P	1171	ASP	CG-OD1	6.04	1.39	1.25
1	P	1305	TYR	CG-CD1	-6.03	1.31	1.39
1	W	1068	GLU	CB-CG	6.03	1.63	1.52
1	P	1069	ASN	CB-CG	6.03	1.65	1.51
2	S	1010	THR	N-CA	6.03	1.58	1.46
1	Q	1301	GLY	C-O	6.01	1.33	1.23
1	V	1211	TYR	CG-CD1	6.01	1.47	1.39
1	R	1189	GLU	CG-CD	6.00	1.60	1.51
2	S	1015	GLU	CG-CD	6.00	1.60	1.51
1	W	1081	LYS	N-CA	6.00	1.58	1.46
1	P	1166	THR	CA-CB	5.99	1.69	1.53
1	R	1286	GLY	CA-C	5.99	1.61	1.51
1	P	1132	ARG	CG-CD	5.98	1.66	1.51
1	P	1188	TYR	CE1-CZ	5.98	1.46	1.38
1	V	1221	TYR	C-O	5.98	1.34	1.23
1	V	1317	LYS	CD-CE	5.97	1.66	1.51
1	U	1304	TYR	CE1-CZ	-5.97	1.30	1.38
1	Q	1289	TYR	CE1-CZ	5.97	1.46	1.38
1	U	1287	ARG	CG-CD	5.96	1.66	1.51
1	W	1317	LYS	CD-CE	5.95	1.66	1.51
1	Q	1156	PRO	C-N	5.95	1.47	1.34
1	Q	1273	PRO	C-O	5.94	1.35	1.23
1	R	1304	TYR	CE2-CZ	5.93	1.46	1.38
1	W	1319	ASN	N-CA	-5.92	1.34	1.46
1	R	1223	GLY	C-O	5.92	1.33	1.23
1	U	1081	LYS	CE-NZ	5.92	1.63	1.49
1	V	1127	GLY	N-CA	5.91	1.54	1.46
1	Q	1073	THR	C-O	5.91	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1082	PHE	CE2-CZ	5.90	1.48	1.37
1	Q	1069	ASN	CB-CG	5.90	1.64	1.51
1	U	1171	ASP	CG-OD1	5.89	1.39	1.25
1	W	1103	TRP	CD2-CE2	5.89	1.48	1.41
1	U	1014	TYR	CE2-CZ	5.89	1.46	1.38
1	W	1081	LYS	CG-CD	5.89	1.72	1.52
1	P	1273	PRO	C-O	5.88	1.35	1.23
1	W	1305	TYR	CE2-CZ	-5.88	1.30	1.38
1	U	1069	ASN	C-O	5.88	1.34	1.23
1	W	1106	VAL	CB-CG1	5.88	1.65	1.52
1	R	1201	LYS	CD-CE	5.88	1.66	1.51
1	V	1210	ALA	C-O	5.88	1.34	1.23
1	V	1221	TYR	N-CA	5.87	1.58	1.46
1	W	1041	LYS	CD-CE	5.87	1.66	1.51
1	V	1188	TYR	CG-CD1	5.87	1.46	1.39
1	P	1058	TYR	CB-CG	-5.87	1.42	1.51
1	W	1104	THR	CA-CB	-5.87	1.38	1.53
1	U	1241	THR	N-CA	-5.86	1.34	1.46
1	R	1211	TYR	CA-C	5.86	1.68	1.52
1	P	1070	ASN	C-O	5.86	1.34	1.23
1	W	1339	ALA	CA-CB	-5.86	1.40	1.52
1	Q	1211	TYR	CG-CD1	5.85	1.46	1.39
1	R	1164	GLY	CA-C	-5.85	1.42	1.51
1	R	1072	TRP	CE2-CZ2	-5.85	1.29	1.39
1	W	1279	GLN	CB-CG	-5.85	1.36	1.52
2	X	1030	ARG	N-CA	5.85	1.58	1.46
1	W	1188	TYR	CG-CD1	5.85	1.46	1.39
1	U	1070	ASN	C-O	5.85	1.34	1.23
1	V	1189	GLU	CG-CD	5.84	1.60	1.51
1	P	1027	LYS	CD-CE	5.84	1.65	1.51
1	Q	1317	LYS	CD-CE	5.84	1.65	1.51
2	X	1044	GLU	CG-CD	5.84	1.60	1.51
1	P	1082	PHE	CG-CD2	5.83	1.47	1.38
1	P	1103	TRP	CG-CD1	5.82	1.44	1.36
1	U	1022	TYR	CD1-CE1	5.82	1.48	1.39
1	W	1070	ASN	C-O	5.81	1.34	1.23
1	Q	1161	PHE	CA-CB	5.81	1.66	1.53
1	U	1022	TYR	CE1-CZ	5.81	1.46	1.38
1	U	1068	GLU	CB-CG	5.81	1.63	1.52
1	U	1103	TRP	CD2-CE2	5.81	1.48	1.41
1	P	1017	VAL	CA-CB	-5.79	1.42	1.54
1	R	1081	LYS	CE-NZ	5.79	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1053	TYR	CD2-CE2	5.78	1.48	1.39
2	X	1018	LYS	CA-C	5.78	1.68	1.52
1	U	1027	LYS	CB-CG	5.78	1.68	1.52
1	V	1127	GLY	C-O	5.78	1.32	1.23
1	Q	1171	ASP	CB-CG	5.78	1.63	1.51
1	R	1161	PHE	CA-CB	5.77	1.66	1.53
1	R	1057	GLU	CD-OE2	5.77	1.31	1.25
1	U	1213	GLY	N-CA	5.77	1.54	1.46
1	P	1287	ARG	CG-CD	5.77	1.66	1.51
1	Q	1302	ALA	CA-CB	-5.77	1.40	1.52
1	U	1210	ALA	C-O	5.76	1.34	1.23
2	X	1037	VAL	CB-CG2	5.76	1.65	1.52
1	R	1182	GLY	N-CA	5.76	1.54	1.46
1	R	1191	PHE	CE1-CZ	5.76	1.48	1.37
1	Q	1201	LYS	CB-CG	5.75	1.68	1.52
1	V	1290	ASP	CB-CG	-5.75	1.39	1.51
1	Q	1335	ASP	CB-CG	-5.74	1.39	1.51
2	X	1012	SER	CA-C	5.74	1.67	1.52
1	P	1157	SER	CA-CB	5.74	1.61	1.52
2	X	1006	VAL	CA-CB	5.74	1.66	1.54
1	V	1081	LYS	CE-NZ	5.74	1.63	1.49
1	P	1137	PHE	CD1-CE1	5.74	1.50	1.39
1	U	1134	THR	CB-CG2	5.73	1.71	1.52
1	Q	1188	TYR	CG-CD1	5.73	1.46	1.39
1	Q	1304	TYR	CE1-CZ	-5.72	1.31	1.38
1	R	1072	TRP	CE3-CZ3	-5.71	1.28	1.38
1	W	1081	LYS	CE-NZ	5.71	1.63	1.49
1	V	1150	GLN	C-O	-5.71	1.12	1.23
1	U	1199	SER	C-O	-5.71	1.12	1.23
1	V	1120	PHE	CE1-CZ	5.71	1.48	1.37
1	P	1064	SER	CB-OG	5.70	1.49	1.42
1	V	1058	TYR	CD2-CE2	5.70	1.48	1.39
1	W	1276	ALA	CA-CB	-5.70	1.40	1.52
1	P	1043	GLU	CD-OE2	5.69	1.31	1.25
1	R	1096	VAL	CB-CG2	5.69	1.64	1.52
1	Q	1042	GLY	N-CA	5.68	1.54	1.46
1	U	1071	SER	CA-CB	5.67	1.61	1.52
1	P	1086	GLY	N-CA	5.67	1.54	1.46
1	P	1191	PHE	CE1-CZ	5.66	1.48	1.37
1	V	1313	TYR	CE2-CZ	5.66	1.46	1.38
1	V	1081	LYS	CG-CD	5.65	1.71	1.52
2	X	1022	TRP	N-CA	5.65	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	1289	TYR	CE1-CZ	5.65	1.45	1.38
1	V	1164	GLY	CA-C	-5.64	1.42	1.51
1	V	1273	PRO	C-O	5.64	1.34	1.23
1	R	1211	TYR	CD1-CE1	5.63	1.47	1.39
1	R	1171	ASP	CB-CG	5.62	1.63	1.51
1	Q	1115	TYR	CE2-CZ	5.62	1.45	1.38
1	W	1308	LYS	C-O	-5.62	1.12	1.23
1	U	1157	SER	CA-CB	5.62	1.61	1.52
2	X	1032	PRO	CB-CG	5.62	1.78	1.50
1	W	1161	PHE	CA-CB	5.61	1.66	1.53
1	Q	1103	TRP	CD2-CE2	5.61	1.48	1.41
1	Q	1238	TYR	CG-CD1	-5.60	1.31	1.39
1	U	1158	GLY	N-CA	5.60	1.54	1.46
1	P	1263	ALA	CA-CB	-5.59	1.40	1.52
1	Q	1145	PHE	CE1-CZ	5.59	1.48	1.37
1	W	1186	TYR	N-CA	-5.58	1.35	1.46
1	R	1058	TYR	CD1-CE1	5.57	1.47	1.39
1	P	1191	PHE	CD2-CE2	5.57	1.50	1.39
1	P	1103	TRP	CZ3-CH2	5.57	1.49	1.40
1	Q	1085	VAL	CB-CG1	-5.56	1.41	1.52
1	Q	1035	TYR	CG-CD2	-5.56	1.31	1.39
1	U	1132	ARG	CG-CD	5.56	1.65	1.51
1	W	1241	THR	N-CA	-5.56	1.35	1.46
1	V	1156	PRO	C-N	5.56	1.46	1.34
1	U	1313	TYR	CD1-CE1	-5.54	1.31	1.39
2	X	1037	VAL	CA-CB	5.54	1.66	1.54
2	S	1013	PRO	CA-C	5.54	1.64	1.52
1	P	1032	ASP	CA-CB	-5.54	1.41	1.53
2	X	1003	LYS	CA-C	5.53	1.67	1.52
1	W	1338	VAL	CB-CG2	-5.53	1.41	1.52
1	Q	1004	TYR	CE2-CZ	5.52	1.45	1.38
1	P	1072	TRP	CB-CG	5.52	1.60	1.50
1	R	1120	PHE	CE2-CZ	5.52	1.47	1.37
1	R	1346	PHE	CG-CD1	5.51	1.47	1.38
1	V	1278	LEU	C-O	5.51	1.33	1.23
1	W	1018	ASP	CB-CG	-5.50	1.40	1.51
1	R	1070	ASN	C-O	5.49	1.33	1.23
1	U	1131	TYR	CG-CD2	5.49	1.46	1.39
1	U	1046	VAL	CA-CB	5.48	1.66	1.54
1	Q	1161	PHE	CA-C	5.48	1.67	1.52
1	R	1141	ASP	CB-CG	-5.48	1.40	1.51
1	Q	1158	GLY	C-O	5.48	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	1156	PRO	C-N	5.47	1.46	1.34
1	W	1273	PRO	C-O	5.47	1.34	1.23
1	R	1128	PHE	CE2-CZ	5.47	1.47	1.37
1	W	1306	PHE	CE1-CZ	5.46	1.47	1.37
1	R	1103	TRP	CE3-CZ3	5.45	1.47	1.38
1	Q	1150	GLN	C-O	-5.45	1.13	1.23
1	U	1082	PHE	CB-CG	5.44	1.60	1.51
1	V	1157	SER	CA-C	5.43	1.67	1.52
1	P	1134	THR	CB-CG2	5.42	1.70	1.52
1	V	1082	PHE	CB-CG	5.42	1.60	1.51
1	Q	1191	PHE	CD1-CE1	5.42	1.50	1.39
1	R	1131	TYR	CG-CD1	5.41	1.46	1.39
1	W	1306	PHE	CG-CD2	5.41	1.46	1.38
1	R	1211	TYR	CE2-CZ	5.41	1.45	1.38
1	Q	1291	ASP	CB-CG	5.41	1.63	1.51
1	U	1098	TYR	CD2-CE2	5.40	1.47	1.39
1	U	1221	TYR	C-O	5.40	1.33	1.23
1	V	1329	ASP	C-O	-5.40	1.13	1.23
1	Q	1128	PHE	CE2-CZ	5.40	1.47	1.37
1	P	1067	ASN	CB-CG	-5.39	1.38	1.51
1	P	1017	VAL	CB-CG1	5.39	1.64	1.52
1	P	1131	TYR	CE2-CZ	5.39	1.45	1.38
1	R	1086	GLY	N-CA	5.39	1.54	1.46
1	V	1128	PHE	CG-CD2	-5.39	1.30	1.38
1	R	1016	LYS	CB-CG	-5.39	1.38	1.52
1	R	1025	ASP	CB-CG	-5.39	1.40	1.51
1	V	1301	GLY	C-O	5.38	1.32	1.23
2	S	1004	LYS	CA-C	5.38	1.67	1.52
1	U	1233	TYR	CE1-CZ	5.38	1.45	1.38
1	Q	1057	GLU	CD-OE1	-5.38	1.19	1.25
1	Q	1138	GLY	N-CA	5.38	1.54	1.46
1	P	1160	GLY	CA-C	5.37	1.60	1.51
1	V	1220	THR	CA-CB	-5.37	1.39	1.53
1	P	1262	VAL	C-O	5.36	1.33	1.23
1	U	1163	SER	CA-CB	5.36	1.60	1.52
1	W	1335	ASP	CB-CG	-5.36	1.40	1.51
1	R	1115	TYR	CZ-OH	5.35	1.47	1.37
1	R	1186	TYR	CG-CD1	5.35	1.46	1.39
1	U	1073	THR	C-O	5.35	1.33	1.23
1	V	1035	TYR	CD2-CE2	-5.35	1.31	1.39
1	V	1194	GLY	CA-C	-5.34	1.43	1.51
1	W	1120	PHE	CE2-CZ	5.34	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	1188	TYR	CE1-CZ	5.34	1.45	1.38
1	P	1163	SER	CB-OG	5.33	1.49	1.42
1	W	1120	PHE	CG-CD1	5.33	1.46	1.38
1	W	1158	GLY	N-CA	5.33	1.54	1.46
1	R	1014	TYR	CE1-CZ	5.32	1.45	1.38
1	W	1264	GLN	CG-CD	5.32	1.63	1.51
1	U	1263	ALA	CA-CB	-5.32	1.41	1.52
1	P	1081	LYS	CG-CD	5.32	1.70	1.52
1	Q	1058	TYR	CE2-CZ	5.32	1.45	1.38
1	R	1346	PHE	CE1-CZ	5.32	1.47	1.37
1	V	1289	TYR	CD1-CE1	5.32	1.47	1.39
1	W	1042	GLY	N-CA	5.31	1.54	1.46
1	P	1072	TRP	CE3-CZ3	-5.31	1.29	1.38
1	V	1152	LYS	C-O	-5.30	1.13	1.23
1	P	1169	GLY	CA-C	5.29	1.60	1.51
1	R	1074	ARG	CD-NE	-5.29	1.37	1.46
1	U	1082	PHE	CE2-CZ	5.29	1.47	1.37
1	V	1019	GLY	N-CA	-5.29	1.38	1.46
1	W	1023	PHE	C-O	5.29	1.33	1.23
1	R	1171	ASP	CG-OD1	5.28	1.37	1.25
1	R	1211	TYR	CG-CD2	5.28	1.46	1.39
1	R	1127	GLY	N-CA	5.28	1.53	1.46
1	W	1201	LYS	CB-CG	5.28	1.66	1.52
1	W	1218	ALA	CA-CB	-5.28	1.41	1.52
1	Q	1241	THR	CB-CG2	5.27	1.69	1.52
1	W	1082	PHE	CE2-CZ	5.27	1.47	1.37
1	U	1222	THR	N-CA	-5.27	1.35	1.46
1	P	1022	TYR	CB-CG	-5.26	1.43	1.51
1	V	1112	GLY	C-O	5.26	1.32	1.23
1	W	1214	ASN	CA-CB	5.26	1.66	1.53
1	V	1161	PHE	CA-CB	5.26	1.65	1.53
1	Q	1120	PHE	CD2-CE2	5.26	1.49	1.39
1	P	1171	ASP	C-O	5.26	1.33	1.23
1	V	1304	TYR	CZ-OH	-5.26	1.28	1.37
1	P	1025	ASP	CB-CG	-5.25	1.40	1.51
1	W	1254	ASN	CG-ND2	5.25	1.46	1.32
1	W	1324	ASN	CG-OD1	-5.25	1.12	1.24
1	R	1058	TYR	CD2-CE2	5.25	1.47	1.39
1	V	1168	ASN	CB-CG	-5.25	1.39	1.51
1	Q	1098	TYR	CG-CD1	-5.24	1.32	1.39
1	Q	1214	ASN	CB-CG	5.24	1.63	1.51
1	R	1263	ALA	CA-CB	-5.24	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1338	VAL	CB-CG1	5.23	1.63	1.52
1	Q	1279	GLN	CB-CG	-5.23	1.38	1.52
1	P	1025	ASP	C-O	5.22	1.33	1.23
1	V	1334	THR	CA-CB	5.22	1.67	1.53
1	W	1242	TYR	CE1-CZ	5.22	1.45	1.38
1	U	1041	LYS	CD-CE	5.21	1.64	1.51
1	Q	1071	SER	N-CA	5.21	1.56	1.46
1	Q	1344	TYR	CE1-CZ	5.21	1.45	1.38
1	V	1086	GLY	N-CA	5.21	1.53	1.46
1	V	1188	TYR	CE1-CZ	5.21	1.45	1.38
1	V	1317	LYS	CE-NZ	5.21	1.62	1.49
1	U	1122	GLN	N-CA	-5.20	1.35	1.46
1	Q	1218	ALA	C-O	5.19	1.33	1.23
1	V	1092	ARG	CZ-NH1	5.19	1.39	1.33
1	P	1085	VAL	CA-CB	-5.18	1.43	1.54
1	R	1201	LYS	CB-CG	5.18	1.66	1.52
1	V	1279	GLN	CB-CG	-5.18	1.38	1.52
1	V	1201	LYS	CD-CE	5.18	1.64	1.51
1	W	1298	VAL	CB-CG1	5.18	1.63	1.52
1	P	1314	VAL	CB-CG1	-5.18	1.42	1.52
1	U	1191	PHE	CD2-CE2	5.18	1.49	1.39
1	W	1103	TRP	CZ3-CH2	5.18	1.48	1.40
1	V	1041	LYS	CD-CE	5.17	1.64	1.51
1	W	1086	GLY	N-CA	5.17	1.53	1.46
1	U	1166	THR	N-CA	-5.17	1.36	1.46
1	P	1210	ALA	C-O	5.16	1.33	1.23
1	R	1287	ARG	CG-CD	5.16	1.64	1.51
1	V	1073	THR	C-O	5.16	1.33	1.23
2	X	1007	ARG	N-CA	5.15	1.56	1.46
1	P	1317	LYS	CD-CE	5.14	1.64	1.51
1	W	1330	ALA	CA-CB	-5.14	1.41	1.52
1	V	1018	ASP	CB-CG	-5.13	1.41	1.51
1	W	1071	SER	N-CA	5.13	1.56	1.46
1	P	1023	PHE	CE2-CZ	-5.13	1.27	1.37
1	Q	1004	TYR	CD2-CE2	5.13	1.47	1.39
1	R	1032	ASP	N-CA	-5.13	1.36	1.46
1	V	1211	TYR	CG-CD2	5.12	1.45	1.39
1	R	1081	LYS	CG-CD	5.11	1.69	1.52
1	V	1316	TYR	CE1-CZ	-5.11	1.31	1.38
1	R	1211	TYR	CD2-CE2	5.10	1.47	1.39
1	Q	1068	GLU	CD-OE1	5.10	1.31	1.25
1	V	1043	GLU	CB-CG	-5.10	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1015	GLY	N-CA	-5.10	1.38	1.46
1	U	1141	ASP	CB-CG	-5.09	1.41	1.51
1	Q	1157	SER	CA-C	5.09	1.66	1.52
1	V	1311	SER	CA-CB	-5.09	1.45	1.52
1	R	1013	LEU	CG-CD2	5.09	1.70	1.51
1	W	1069	ASN	CG-ND2	5.09	1.45	1.32
1	P	1084	ASP	CB-CG	5.08	1.62	1.51
1	V	1344	TYR	CE1-CZ	5.08	1.45	1.38
1	R	1321	LEU	C-O	5.08	1.32	1.23
1	U	1306	PHE	CG-CD2	5.07	1.46	1.38
1	U	1254	ASN	CG-ND2	5.07	1.45	1.32
1	W	1094	TYR	CG-CD1	5.07	1.45	1.39
1	P	1159	GLU	CG-CD	-5.06	1.44	1.51
1	W	1023	PHE	CG-CD1	-5.06	1.31	1.38
1	Q	1221	TYR	CE1-CZ	5.06	1.45	1.38
1	V	1158	GLY	C-O	5.05	1.31	1.23
1	W	1058	TYR	CB-CG	-5.05	1.44	1.51
2	X	1005	SER	N-CA	5.05	1.56	1.46
1	P	1241	THR	N-CA	-5.05	1.36	1.46
2	S	1020	ALA	CA-CB	5.05	1.63	1.52
1	P	1159	GLU	CD-OE2	-5.04	1.20	1.25
1	U	1324	ASN	CB-CG	-5.04	1.39	1.51
1	W	1120	PHE	CE1-CZ	5.04	1.47	1.37
1	W	1150	GLN	CD-OE1	5.04	1.35	1.24
1	R	1188	TYR	CE1-CZ	5.03	1.45	1.38
1	R	1004	TYR	CE1-CZ	5.03	1.45	1.38
1	R	1150	GLN	CB-CG	-5.02	1.39	1.52
1	W	1305	TYR	CD2-CE2	-5.02	1.31	1.39
1	P	1289	TYR	CE1-CZ	5.02	1.45	1.38
1	Q	1214	ASN	CA-CB	5.02	1.66	1.53
1	R	1163	SER	CA-CB	5.02	1.60	1.52
1	U	1032	ASP	CA-CB	-5.02	1.43	1.53
1	W	1152	LYS	C-O	-5.02	1.13	1.23
1	Q	1137	PHE	CE2-CZ	5.01	1.46	1.37
1	W	1014	TYR	CD2-CE2	5.01	1.46	1.39
1	R	1155	ASN	CA-C	-5.01	1.40	1.52
1	R	1186	TYR	N-CA	-5.01	1.36	1.46
2	X	1012	SER	N-CA	5.00	1.56	1.46
1	W	1094	TYR	CE2-CZ	5.00	1.45	1.38

All (586) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	1246	ARG	NE-CZ-NH1	13.43	127.02	120.30
1	P	1025	ASP	CB-CG-OD1	-12.61	106.95	118.30
1	P	1124	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	P	1124	ARG	NE-CZ-NH2	-11.36	114.62	120.30
1	W	1030	ASP	CB-CG-OD1	11.16	128.35	118.30
1	R	1132	ARG	NE-CZ-NH1	-10.91	114.85	120.30
1	P	1187	ASP	N-CA-C	10.63	139.71	111.00
1	R	1068	GLU	OE1-CD-OE2	-10.20	111.06	123.30
1	P	1105	ASP	CB-CG-OD1	-10.11	109.20	118.30
1	V	1323	ASP	CB-CG-OD1	-10.10	109.21	118.30
1	R	1187	ASP	N-CA-C	10.07	138.20	111.00
1	R	1025	ASP	CB-CG-OD1	-10.04	109.26	118.30
1	R	1246	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	P	1169	GLY	N-CA-C	-9.72	88.79	113.10
1	W	1074	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	V	1187	ASP	N-CA-C	9.67	137.10	111.00
1	P	1157	SER	N-CA-C	9.61	136.95	111.00
1	Q	1323	ASP	CB-CG-OD1	-9.60	109.66	118.30
1	Q	1187	ASP	N-CA-C	9.58	136.85	111.00
1	V	1018	ASP	CB-CG-OD1	-9.57	109.69	118.30
1	U	1030	ASP	CB-CG-OD1	9.49	126.84	118.30
1	W	1030	ASP	CB-CG-OD2	-9.49	109.76	118.30
1	P	1171	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	U	1187	ASP	N-CA-C	9.40	136.37	111.00
1	W	1299	ASP	CB-CG-OD2	9.38	126.75	118.30
1	W	1132	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	P	1323	ASP	CB-CG-OD1	-9.37	109.87	118.30
1	W	1169	GLY	N-CA-C	-9.31	89.82	113.10
1	R	1018	ASP	CB-CG-OD1	-9.29	109.94	118.30
1	Q	1157	SER	N-CA-C	9.29	136.07	111.00
1	W	1139	LEU	CA-CB-CG	9.29	136.66	115.30
1	Q	1141	ASP	CB-CG-OD2	-9.27	109.96	118.30
1	P	1139	LEU	CA-CB-CG	9.23	136.52	115.30
1	V	1149	TYR	CB-CG-CD1	9.22	126.53	121.00
1	P	1165	VAL	CB-CA-C	-9.21	93.90	111.40
1	R	1105	ASP	CB-CG-OD1	-9.20	110.03	118.30
1	Q	1141	ASP	CB-CG-OD1	9.16	126.54	118.30
1	U	1152	LYS	CD-CE-NZ	-9.13	90.70	111.70
1	W	1171	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	P	1323	ASP	CB-CG-OD2	9.08	126.47	118.30
1	V	1105	ASP	CB-CG-OD1	-9.03	110.17	118.30
1	U	1105	ASP	CB-CG-OD1	-9.00	110.20	118.30
1	Q	1156	PRO	C-N-CA	8.98	144.16	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1278	LEU	CA-CB-CG	8.94	135.86	115.30
1	V	1157	SER	N-CA-C	8.88	134.98	111.00
1	W	1165	VAL	CB-CA-C	-8.88	94.53	111.40
1	R	1124	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	U	1315	ASP	CB-CG-OD2	8.86	126.27	118.30
2	S	1025	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	U	1278	LEU	CA-CB-CG	8.83	135.62	115.30
1	V	1048	ASP	CB-CG-OD2	8.80	126.22	118.30
1	V	1335	ASP	CB-CG-OD1	-8.79	110.39	118.30
1	U	1157	SER	N-CA-C	8.77	134.69	111.00
1	U	1165	VAL	CB-CA-C	-8.72	94.83	111.40
1	R	1156	PRO	C-N-CA	8.70	143.44	121.70
1	U	1132	ARG	NE-CZ-NH1	-8.70	115.95	120.30
1	V	1124	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	Q	1018	ASP	CB-CG-OD1	-8.57	110.59	118.30
1	W	1187	ASP	N-CA-C	8.54	134.05	111.00
1	W	1157	SER	N-CA-C	8.52	134.00	111.00
1	U	1170	ARG	N-CA-C	8.48	133.91	111.00
1	R	1124	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	R	1157	SER	N-CA-C	8.46	133.83	111.00
1	Q	1228	ASP	CB-CG-OD1	8.45	125.90	118.30
1	P	1287	ARG	CG-CD-NE	8.40	129.43	111.80
1	V	1164	GLY	N-CA-C	-8.37	92.18	113.10
1	P	1025	ASP	CB-CG-OD2	8.36	125.82	118.30
1	V	1048	ASP	CB-CG-OD1	-8.29	110.84	118.30
1	Q	1025	ASP	CB-CG-OD1	-8.27	110.86	118.30
1	U	1287	ARG	CG-CD-NE	8.27	129.16	111.80
1	Q	1124	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	U	1169	GLY	N-CA-C	-8.24	92.49	113.10
1	R	1169	GLY	N-CA-C	-8.24	92.50	113.10
1	U	1019	GLY	N-CA-C	-8.21	92.57	113.10
1	V	1156	PRO	C-N-CA	8.18	142.15	121.70
1	P	1156	PRO	C-N-CA	8.16	142.10	121.70
1	V	1152	LYS	CD-CE-NZ	-8.11	93.04	111.70
1	W	1166	THR	CA-CB-CG2	8.11	123.75	112.40
1	W	1287	ARG	CG-CD-NE	8.08	128.76	111.80
1	Q	1170	ARG	N-CA-C	8.06	132.75	111.00
1	Q	1048	ASP	CB-CG-OD2	8.02	125.52	118.30
1	P	1149	TYR	CB-CG-CD1	7.97	125.78	121.00
1	U	1165	VAL	N-CA-C	7.95	132.46	111.00
1	U	1322	ASP	CB-CG-OD2	7.93	125.44	118.30
1	Q	1019	GLY	N-CA-C	-7.89	93.38	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	1070	ASN	N-CA-C	7.88	132.28	111.00
1	W	1156	PRO	C-N-CA	7.88	141.39	121.70
1	P	1020	LEU	CB-CG-CD1	-7.87	97.62	111.00
1	V	1132	ARG	NE-CZ-NH1	-7.85	116.37	120.30
1	Q	1139	LEU	CA-CB-CG	7.81	133.26	115.30
1	V	1092	ARG	NE-CZ-NH1	7.81	124.20	120.30
1	Q	1132	ARG	NE-CZ-NH1	-7.79	116.41	120.30
1	U	1289	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	V	1025	ASP	CB-CG-OD1	-7.78	111.29	118.30
1	R	1074	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	P	1246	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	R	1170	ARG	N-CA-C	7.74	131.88	111.00
1	Q	1124	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	W	1335	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	W	1170	ARG	N-CA-C	7.71	131.82	111.00
1	W	1250	LEU	CB-CG-CD1	-7.71	97.90	111.00
1	V	1141	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	W	1071	SER	N-CA-C	7.67	131.72	111.00
1	P	1170	ARG	N-CA-C	7.65	131.65	111.00
1	P	1335	ASP	CB-CG-OD1	-7.65	111.42	118.30
1	P	1299	ASP	CB-CG-OD2	7.60	125.14	118.30
1	V	1217	ARG	CB-CG-CD	-7.60	91.84	111.60
1	V	1068	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	U	1113	ASP	CB-CG-OD1	7.56	125.10	118.30
1	R	1139	LEU	CB-CG-CD1	7.55	123.83	111.00
1	R	1225	LEU	CB-CG-CD2	7.49	123.74	111.00
1	U	1139	LEU	CA-CB-CG	7.47	132.49	115.30
1	W	1149	TYR	CB-CG-CD1	7.44	125.46	121.00
1	R	1164	GLY	N-CA-C	-7.42	94.54	113.10
1	V	1028	ASP	CB-CG-OD2	7.41	124.97	118.30
1	W	1164	GLY	N-CA-C	-7.40	94.60	113.10
1	U	1156	PRO	C-N-CA	7.36	140.10	121.70
1	U	1192	GLY	N-CA-C	-7.36	94.71	113.10
1	Q	1278	LEU	CA-CB-CG	7.35	132.21	115.30
1	U	1171	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	W	1278	LEU	CA-CB-CG	7.34	132.17	115.30
1	P	1070	ASN	N-CA-C	7.33	130.80	111.00
1	P	1081	LYS	N-CA-C	-7.32	91.23	111.00
1	U	1124	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	V	1149	TYR	OH-CZ-CE2	-7.32	100.35	120.10
1	W	1025	ASP	CB-CG-OD1	-7.31	111.72	118.30
1	Q	1074	ARG	NE-CZ-NH2	-7.31	116.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	1225	LEU	CB-CG-CD2	7.30	123.42	111.00
1	V	1149	TYR	CB-CG-CD2	-7.25	116.65	121.00
1	U	1157	SER	CB-CA-C	-7.24	96.35	110.10
1	P	1315	ASP	CB-CG-OD1	-7.24	111.79	118.30
1	P	1289	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	W	1070	ASN	N-CA-C	7.23	130.53	111.00
1	V	1328	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	P	1132	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	U	1030	ASP	CB-CG-OD2	-7.18	111.83	118.30
1	V	1314	VAL	CB-CA-C	-7.14	97.83	111.40
1	V	1019	GLY	N-CA-C	-7.14	95.25	113.10
1	R	1017	VAL	CB-CA-C	-7.13	97.85	111.40
1	U	1013	LEU	CB-CG-CD1	7.13	123.12	111.00
1	R	1161	PHE	CB-CG-CD1	7.13	125.79	120.80
1	R	1068	GLU	CA-CB-CG	7.12	129.06	113.40
1	R	1069	ASN	O-C-N	7.11	134.07	122.70
1	Q	1216	ASP	CB-CG-OD2	7.09	124.68	118.30
1	V	1287	ARG	CG-CD-NE	7.08	126.67	111.80
1	P	1275	LEU	CB-CG-CD1	7.06	123.01	111.00
1	U	1164	GLY	N-CA-C	-7.06	95.44	113.10
1	P	1017	VAL	CB-CA-C	-7.01	98.08	111.40
1	P	1143	LEU	CB-CA-C	-7.00	96.90	110.20
1	R	1278	LEU	CA-CB-CG	6.99	131.38	115.30
1	R	1081	LYS	N-CA-C	-6.96	92.22	111.00
1	Q	1068	GLU	OE1-CD-OE2	-6.95	114.96	123.30
1	Q	1068	GLU	CA-CB-CG	6.95	128.68	113.40
1	P	1071	SER	N-CA-C	6.94	129.75	111.00
1	V	1139	LEU	CA-CB-CG	6.94	131.26	115.30
1	W	1028	ASP	CB-CG-OD2	6.93	124.54	118.30
1	Q	1289	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	R	1149	TYR	CB-CG-CD1	6.92	125.15	121.00
1	R	1287	ARG	CG-CD-NE	6.91	126.31	111.80
1	R	1335	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	P	1217	ARG	CB-CG-CD	-6.89	93.68	111.60
1	W	1069	ASN	O-C-N	6.89	133.73	122.70
1	V	1313	TYR	CB-CG-CD1	-6.86	116.89	121.00
1	P	1165	VAL	N-CA-C	6.86	129.51	111.00
1	P	1166	THR	CA-CB-CG2	6.86	122.00	112.40
1	R	1323	ASP	CB-CG-OD1	-6.86	112.13	118.30
2	X	1007	ARG	N-CA-C	6.86	129.51	111.00
1	R	1171	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	Q	1135	ASP	CB-CG-OD2	6.84	124.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	1157	SER	CB-CA-C	-6.83	97.13	110.10
1	Q	1165	VAL	CB-CA-C	-6.81	98.46	111.40
1	R	1299	ASP	CB-CG-OD2	6.79	124.42	118.30
1	U	1141	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	W	1165	VAL	N-CA-C	6.79	129.34	111.00
1	R	1170	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	V	1068	GLU	CA-CB-CG	6.79	128.33	113.40
1	W	1048	ASP	CB-CG-OD2	6.79	124.41	118.30
1	V	1161	PHE	CD1-CG-CD2	-6.78	109.48	118.30
1	U	1070	ASN	N-CA-C	6.77	129.29	111.00
1	Q	1149	TYR	CB-CG-CD1	6.77	125.06	121.00
1	P	1011	LEU	CB-CA-C	-6.76	97.36	110.20
1	U	1068	GLU	CA-CB-CG	6.76	128.28	113.40
1	W	1019	GLY	N-CA-C	-6.75	96.22	113.10
1	Q	1287	ARG	CG-CD-NE	6.75	125.98	111.80
1	R	1289	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	Q	1211	TYR	CB-CA-C	6.73	123.87	110.40
1	R	1070	ASN	N-CA-C	6.72	129.14	111.00
1	P	1289	TYR	CB-CG-CD1	6.71	125.03	121.00
1	V	1165	VAL	CB-CA-C	-6.70	98.67	111.40
1	R	1041	LYS	N-CA-C	-6.70	92.92	111.00
1	U	1149	TYR	CB-CG-CD1	6.68	125.01	121.00
1	W	1113	ASP	CB-CG-OD1	6.67	124.31	118.30
1	R	1071	SER	N-CA-C	6.66	128.99	111.00
1	U	1141	ASP	N-CA-CB	-6.66	98.61	110.60
1	P	1152	LYS	CD-CE-NZ	-6.66	96.39	111.70
1	R	1007	ASP	CB-CG-OD1	6.63	124.26	118.30
1	Q	1289	TYR	CB-CG-CD1	6.62	124.97	121.00
1	R	1019	GLY	N-CA-C	-6.62	96.56	113.10
1	V	1170	ARG	N-CA-C	6.61	128.84	111.00
1	P	1217	ARG	CG-CD-NE	6.60	125.67	111.80
1	V	1017	VAL	CB-CA-C	-6.59	98.87	111.40
1	P	1194	GLY	N-CA-C	-6.58	96.64	113.10
1	P	1192	GLY	N-CA-C	-6.58	96.66	113.10
1	P	1161	PHE	CB-CG-CD2	6.57	125.40	120.80
1	V	1212	ILE	N-CA-C	6.56	128.71	111.00
1	P	1161	PHE	N-CA-C	-6.55	93.32	111.00
1	P	1325	GLN	CB-CA-C	6.54	123.48	110.40
1	V	1323	ASP	CB-CG-OD2	6.53	124.17	118.30
1	Q	1017	VAL	CB-CA-C	-6.53	99.00	111.40
1	Q	1028	ASP	CB-CG-OD2	6.52	124.17	118.30
1	V	1141	ASP	CB-CG-OD1	6.52	124.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	1081	LYS	N-CA-C	-6.52	93.40	111.00
1	R	1155	ASN	N-CA-CB	6.52	122.33	110.60
1	Q	1193	ILE	N-CA-C	-6.51	93.42	111.00
1	R	1285	LEU	C-N-CA	-6.51	108.63	122.30
1	U	1289	TYR	CB-CG-CD1	6.49	124.89	121.00
1	P	1212	ILE	N-CA-C	6.47	128.48	111.00
1	R	1340	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	R	1226	LYS	CD-CE-NZ	-6.47	96.82	111.70
1	U	1287	ARG	CD-NE-CZ	6.47	132.65	123.60
1	P	1028	ASP	CB-CG-OD2	6.45	124.11	118.30
1	Q	1217	ARG	CB-CG-CD	-6.43	94.88	111.60
1	Q	1090	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	P	1050	LEU	CA-CB-CG	6.42	130.06	115.30
1	W	1092	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	V	1149	TYR	CE1-CZ-OH	6.41	137.41	120.10
1	R	1069	ASN	N-CA-C	6.39	128.26	111.00
1	W	1069	ASN	CA-C-N	-6.39	103.13	117.20
1	R	1165	VAL	CB-CA-C	-6.38	99.27	111.40
1	U	1071	SER	N-CA-C	6.38	128.22	111.00
1	W	1290	ASP	CB-CG-OD2	-6.38	112.56	118.30
2	X	1030	ARG	N-CA-C	6.35	128.16	111.00
1	Q	1081	LYS	N-CA-C	-6.35	93.85	111.00
1	R	1323	ASP	N-CA-CB	-6.35	99.17	110.60
1	V	1104	THR	CA-CB-CG2	-6.35	103.51	112.40
1	V	1071	SER	N-CA-C	6.35	128.14	111.00
1	Q	1299	ASP	CB-CG-OD2	6.33	124.00	118.30
1	R	1152	LYS	CD-CE-NZ	-6.33	97.14	111.70
1	U	1325	GLN	N-CA-CB	6.33	121.99	110.60
1	Q	1193	ILE	CB-CA-C	-6.32	98.95	111.60
1	U	1199	SER	N-CA-CB	-6.32	101.01	110.50
1	Q	1217	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	P	1157	SER	CB-CA-C	-6.32	98.10	110.10
1	Q	1070	ASN	N-CA-C	6.28	127.97	111.00
1	U	1124	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	V	1092	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	R	1044	THR	N-CA-C	-6.27	94.08	111.00
1	P	1030	ASP	CB-CG-OD1	6.27	123.94	118.30
1	R	1228	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	U	1143	LEU	CB-CA-C	-6.26	98.30	110.20
2	X	1028	LYS	C-N-CA	6.26	137.35	121.70
1	U	1134	THR	N-CA-C	6.25	127.89	111.00
1	W	1291	ASP	CB-CA-C	6.25	122.91	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1149	TYR	OH-CZ-CE2	-6.24	103.25	120.10
1	V	1161	PHE	N-CA-C	-6.24	94.15	111.00
1	P	1161	PHE	CD1-CG-CD2	-6.24	110.19	118.30
1	R	1322	ASP	CB-CG-OD1	-6.22	112.70	118.30
1	V	1212	ILE	CB-CA-C	-6.22	99.15	111.60
1	V	1025	ASP	CB-CG-OD2	6.22	123.90	118.30
1	W	1161	PHE	CB-CG-CD1	6.22	125.16	120.80
1	R	1165	VAL	N-CA-C	6.21	127.77	111.00
1	R	1011	LEU	CB-CA-C	-6.19	98.44	110.20
1	V	1121	MET	CG-SD-CE	6.18	110.10	100.20
1	Q	1169	GLY	N-CA-C	-6.18	97.64	113.10
1	W	1289	TYR	CB-CG-CD2	-6.17	117.30	121.00
2	S	1036	CYS	CA-CB-SG	6.17	125.11	114.00
1	U	1017	VAL	CB-CA-C	-6.17	99.67	111.40
1	U	1291	ASP	CB-CA-C	6.17	122.74	110.40
1	Q	1164	GLY	N-CA-C	-6.17	97.68	113.10
1	R	1071	SER	CB-CA-C	-6.16	98.39	110.10
1	Q	1101	THR	CA-CB-CG2	-6.15	103.79	112.40
1	W	1289	TYR	CB-CG-CD1	6.15	124.69	121.00
1	Q	1069	ASN	O-C-N	6.14	132.52	122.70
1	W	1013	LEU	CB-CG-CD1	6.12	121.41	111.00
1	R	1166	THR	CA-CB-CG2	6.11	120.95	112.40
1	Q	1168	ASN	C-N-CA	-6.10	109.49	122.30
1	W	1323	ASP	CB-CG-OD1	-6.10	112.81	118.30
1	W	1149	TYR	OH-CZ-CE2	-6.10	103.64	120.10
1	R	1030	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	Q	1071	SER	N-CA-C	6.09	127.44	111.00
1	V	1069	ASN	N-CA-C	6.09	127.44	111.00
1	V	1141	ASP	N-CA-CB	-6.08	99.66	110.60
1	V	1113	ASP	CB-CG-OD1	6.08	123.77	118.30
1	Q	1020	LEU	CB-CG-CD1	-6.08	100.67	111.00
1	W	1216	ASP	CB-CG-OD2	6.08	123.77	118.30
1	P	1161	PHE	CB-CA-C	6.07	122.54	110.40
1	W	1134	THR	OG1-CB-CG2	6.07	123.96	110.00
1	Q	1287	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	R	1289	TYR	CB-CG-CD1	6.06	124.64	121.00
1	V	1013	LEU	CB-CG-CD1	6.06	121.30	111.00
1	W	1069	ASN	N-CA-C	6.05	127.34	111.00
1	U	1323	ASP	CB-CA-C	-6.05	98.31	110.40
1	U	1164	GLY	O-C-N	6.04	132.36	122.70
1	R	1025	ASP	CB-CG-OD2	6.02	123.72	118.30
1	V	1202	ARG	NE-CZ-NH1	-6.02	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	1161	PHE	CD1-CG-CD2	-5.99	110.51	118.30
1	P	1340	LEU	CB-CG-CD2	5.99	121.18	111.00
1	Q	1315	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	V	1194	GLY	N-CA-C	-5.99	98.12	113.10
1	P	1211	TYR	CB-CA-C	5.99	122.38	110.40
1	Q	1048	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	P	1171	ASP	CB-CG-OD1	5.98	123.69	118.30
1	U	1069	ASN	N-CA-C	5.98	127.14	111.00
1	R	1212	ILE	N-CA-C	5.96	127.11	111.00
1	W	1124	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	W	1199	SER	N-CA-CB	-5.95	101.57	110.50
1	R	1252	TRP	CB-CA-C	5.95	122.30	110.40
1	Q	1250	LEU	CA-CB-CG	5.94	128.96	115.30
1	V	1289	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	R	1217	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	W	1328	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	U	1252	TRP	CB-CA-C	5.92	122.24	110.40
1	R	1211	TYR	CB-CA-C	5.92	122.23	110.40
1	W	1074	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	U	1161	PHE	N-CA-C	-5.91	95.03	111.00
1	V	1322	ASP	CB-CG-OD2	5.91	123.62	118.30
1	W	1296	LYS	CD-CE-NZ	-5.91	98.11	111.70
1	W	1252	TRP	CB-CA-C	5.91	122.21	110.40
1	Q	1011	LEU	CB-CA-C	-5.89	99.01	110.20
1	U	1228	ASP	CB-CG-OD1	5.89	123.60	118.30
1	R	1103	TRP	CA-CB-CG	5.88	124.88	113.70
1	P	1325	GLN	N-CA-CB	5.87	121.16	110.60
1	Q	1291	ASP	CB-CA-C	5.87	122.13	110.40
1	R	1325	GLN	N-CA-CB	5.87	121.16	110.60
1	U	1181	GLY	N-CA-C	5.87	127.77	113.10
1	R	1217	ARG	CB-CG-CD	-5.86	96.36	111.60
1	Q	1161	PHE	CD1-CG-CD2	-5.86	110.68	118.30
1	P	1048	ASP	CB-CG-OD2	5.86	123.58	118.30
1	Q	1141	ASP	N-CA-CB	-5.86	100.05	110.60
1	W	1011	LEU	CB-CA-C	-5.86	99.07	110.20
1	R	1157	SER	CB-CA-C	-5.85	98.98	110.10
1	V	1140	VAL	N-CA-C	-5.85	95.20	111.00
1	V	1089	ASP	CB-CG-OD1	5.84	123.56	118.30
1	W	1147	VAL	N-CA-C	-5.84	95.23	111.00
1	W	1314	VAL	CG1-CB-CG2	5.84	120.24	110.90
1	Q	1164	GLY	O-C-N	5.83	132.03	122.70
1	W	1104	THR	CA-CB-CG2	-5.83	104.23	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	W	1099	ASP	CB-CG-OD1	5.83	123.55	118.30
1	Q	1214	ASN	N-CA-C	-5.83	95.27	111.00
1	R	1134	THR	OG1-CB-CG2	5.83	123.40	110.00
1	Q	1115	TYR	CB-CG-CD1	-5.83	117.50	121.00
1	V	1089	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	Q	1289	TYR	OH-CZ-CE2	-5.82	104.39	120.10
1	V	1103	TRP	CA-CB-CG	5.81	124.74	113.70
1	P	1141	ASP	N-CA-CB	-5.81	100.14	110.60
1	U	1011	LEU	CB-CA-C	-5.80	99.17	110.20
1	W	1226	LYS	CD-CE-NZ	-5.80	98.37	111.70
1	V	1157	SER	CB-CA-C	-5.79	99.09	110.10
1	P	1069	ASN	N-CA-C	5.79	126.64	111.00
1	V	1211	TYR	CB-CA-C	5.79	121.99	110.40
1	R	1155	ASN	CB-CA-C	-5.79	98.81	110.40
1	Q	1271	LEU	N-CA-C	-5.78	95.38	111.00
1	P	1044	THR	N-CA-C	-5.78	95.40	111.00
1	V	1278	LEU	CA-CB-CG	5.78	128.58	115.30
1	P	1193	ILE	CG1-CB-CG2	-5.77	98.71	111.40
1	R	1013	LEU	CB-CG-CD1	5.76	120.80	111.00
1	W	1161	PHE	CD1-CG-CD2	-5.76	110.81	118.30
1	U	1299	ASP	CB-CG-OD2	5.76	123.49	118.30
1	P	1327	THR	CA-CB-CG2	-5.76	104.34	112.40
1	R	1216	ASP	CB-CG-OD2	5.75	123.48	118.30
1	P	1084	ASP	N-CA-C	-5.75	95.48	111.00
1	V	1168	ASN	C-N-CA	-5.75	110.23	122.30
1	W	1325	GLN	N-CA-C	-5.75	95.48	111.00
1	V	1169	GLY	N-CA-C	-5.74	98.75	113.10
1	V	1009	ASN	N-CA-C	5.74	126.49	111.00
1	P	1216	ASP	CB-CG-OD2	5.72	123.45	118.30
1	R	1285	LEU	CB-CG-CD1	-5.72	101.27	111.00
1	R	1139	LEU	CA-CB-CG	5.72	128.46	115.30
1	W	1164	GLY	O-C-N	5.72	131.85	122.70
1	U	1156	PRO	CA-C-O	-5.72	106.48	120.20
1	R	1018	ASP	N-CA-CB	-5.71	100.31	110.60
1	V	1071	SER	CB-CA-C	-5.71	99.25	110.10
1	Q	1335	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	P	1181	GLY	N-CA-C	5.70	127.35	113.10
1	W	1287	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	R	1313	TYR	CB-CG-CD1	-5.69	117.59	121.00
2	S	1009	CYS	N-CA-C	5.69	126.36	111.00
1	U	1050	LEU	CB-CG-CD1	-5.69	101.33	111.00
1	P	1321	LEU	CA-CB-CG	5.68	128.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	1212	ILE	CB-CA-C	-5.68	100.25	111.60
1	Q	1165	VAL	N-CA-C	5.67	126.32	111.00
1	U	1193	ILE	CG1-CB-CG2	-5.67	98.93	111.40
1	U	1161	PHE	CD1-CG-CD2	-5.67	110.93	118.30
1	V	1161	PHE	CB-CG-CD2	5.66	124.77	120.80
1	P	1048	ASP	CB-CG-OD1	-5.65	113.22	118.30
1	W	1193	ILE	CB-CA-C	-5.65	100.30	111.60
1	Q	1069	ASN	N-CA-C	5.65	126.25	111.00
1	Q	1115	TYR	CB-CG-CD2	5.65	124.39	121.00
1	W	1016	LYS	CD-CE-NZ	5.65	124.69	111.70
1	V	1202	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	W	1161	PHE	N-CA-C	-5.64	95.77	111.00
1	R	1164	GLY	O-C-N	5.64	131.72	122.70
1	Q	1044	THR	N-CA-C	-5.63	95.79	111.00
1	Q	1323	ASP	N-CA-CB	-5.63	100.46	110.60
1	W	1228	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	V	1228	ASP	CB-CG-OD1	5.63	123.37	118.30
1	U	1230	ASN	CB-CA-C	-5.62	99.16	110.40
1	U	1193	ILE	N-CA-C	-5.62	95.83	111.00
1	Q	1156	PRO	O-C-N	5.62	131.69	122.70
1	R	1127	GLY	N-CA-C	5.61	127.13	113.10
1	Q	1030	ASP	CB-CG-OD1	5.61	123.35	118.30
1	R	1143	LEU	CB-CA-C	-5.61	99.54	110.20
1	U	1300	VAL	CG1-CB-CG2	5.60	119.87	110.90
1	U	1068	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	Q	1289	TYR	N-CA-CB	5.59	120.67	110.60
1	R	1074	ARG	CG-CD-NE	-5.59	100.06	111.80
1	P	1164	GLY	O-C-N	5.58	131.63	122.70
1	W	1140	VAL	C-N-CA	-5.57	107.77	121.70
1	U	1217	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	W	1155	ASN	C-N-CD	5.56	140.08	128.40
1	W	1187	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	Q	1013	LEU	CB-CG-CD1	5.55	120.44	111.00
1	U	1081	LYS	N-CA-C	-5.55	96.01	111.00
1	P	1275	LEU	N-CA-C	-5.55	96.02	111.00
1	Q	1118	ASP	CB-CG-OD1	5.55	123.29	118.30
1	W	1134	THR	N-CA-C	5.55	125.97	111.00
1	P	1068	GLU	CA-CB-CG	5.54	125.59	113.40
1	P	1105	ASP	OD1-CG-OD2	5.53	133.81	123.30
1	U	1071	SER	CB-CA-C	-5.53	99.59	110.10
1	P	1072	TRP	N-CA-CB	-5.53	100.65	110.60
1	W	1153	ASN	N-CA-CB	5.53	120.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	U	1161	PHE	CB-CG-CD1	5.52	124.67	120.80
1	Q	1217	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	U	1323	ASP	CB-CG-OD2	5.52	123.27	118.30
1	V	1323	ASP	CB-CA-C	-5.51	99.37	110.40
1	V	1184	ILE	CA-CB-CG1	-5.50	100.55	111.00
1	P	1156	PRO	O-C-N	5.50	131.50	122.70
1	U	1212	ILE	CB-CA-C	-5.50	100.60	111.60
1	V	1124	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	W	1081	LYS	N-CA-C	-5.49	96.18	111.00
1	P	1153	ASN	N-CA-CB	5.48	120.47	110.60
1	R	1168	ASN	N-CA-C	5.48	125.80	111.00
1	P	1287	ARG	CD-NE-CZ	5.48	131.27	123.60
1	V	1132	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	W	1007	ASP	CB-CG-OD1	5.46	123.21	118.30
1	R	1118	ASP	CB-CG-OD1	5.44	123.20	118.30
1	V	1104	THR	N-CA-C	5.44	125.69	111.00
1	U	1009	ASN	N-CA-C	5.44	125.68	111.00
1	U	1044	THR	N-CA-C	-5.44	96.32	111.00
1	P	1221	TYR	N-CA-C	-5.43	96.33	111.00
1	R	1030	ASP	CB-CG-OD1	5.43	123.19	118.30
1	Q	1166	THR	CA-CB-CG2	5.42	119.99	112.40
1	P	1315	ASP	CB-CG-OD2	5.42	123.18	118.30
1	Q	1212	ILE	CB-CA-C	-5.41	100.77	111.60
1	U	1041	LYS	N-CA-C	-5.41	96.38	111.00
1	V	1171	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	P	1199	SER	N-CA-CB	-5.41	102.39	110.50
1	Q	1287	ARG	CD-NE-CZ	5.40	131.16	123.60
1	P	1314	VAL	CB-CA-C	-5.39	101.15	111.40
1	Q	1041	LYS	N-CA-C	-5.39	96.44	111.00
1	R	1009	ASN	N-CA-C	5.39	125.54	111.00
1	U	1153	ASN	N-CA-CB	5.38	120.28	110.60
1	P	1225	LEU	CB-CG-CD2	5.38	120.14	111.00
1	P	1295	LEU	CA-CB-CG	5.37	127.65	115.30
1	W	1017	VAL	CB-CA-C	-5.36	101.22	111.40
1	W	1157	SER	CB-CA-C	-5.36	99.92	110.10
1	U	1303	THR	CA-CB-CG2	-5.36	104.90	112.40
1	Q	1037	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	P	1291	ASP	CB-CA-C	5.35	121.10	110.40
2	X	1015	GLU	N-CA-C	5.35	125.44	111.00
1	U	1221	TYR	N-CA-C	-5.34	96.57	111.00
1	U	1287	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	V	1074	ARG	CG-CD-NE	-5.34	100.58	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1011	LEU	CB-CG-CD2	5.34	120.07	111.00
1	P	1338	VAL	C-N-CA	-5.33	108.36	121.70
1	V	1275	LEU	CB-CG-CD1	5.33	120.07	111.00
1	U	1275	LEU	CB-CG-CD1	5.33	120.06	111.00
1	Q	1022	TYR	CB-CG-CD2	-5.33	117.81	121.00
1	Q	1325	GLN	N-CA-CB	5.32	120.18	110.60
1	V	1315	ASP	CB-CG-OD2	5.32	123.09	118.30
1	P	1030	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	R	1069	ASN	CA-C-N	-5.31	105.52	117.20
1	W	1328	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	V	1285	LEU	C-N-CA	-5.30	111.16	122.30
1	R	1090	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	V	1193	ILE	CG1-CB-CG2	-5.30	99.74	111.40
1	U	1166	THR	N-CA-CB	-5.29	100.24	110.30
1	U	1228	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	P	1103	TRP	CA-CB-CG	5.29	123.75	113.70
1	P	1078	ALA	N-CA-C	-5.29	96.72	111.00
1	P	1250	LEU	CB-CG-CD1	-5.29	102.01	111.00
1	R	1140	VAL	N-CA-C	-5.29	96.73	111.00
2	X	1038	LYS	N-CA-C	5.28	125.27	111.00
1	W	1009	ASN	N-CA-C	5.28	125.25	111.00
1	Q	1009	ASN	N-CA-C	5.28	125.24	111.00
1	W	1063	ASN	N-CA-CB	-5.27	101.11	110.60
1	V	1241	THR	N-CA-CB	-5.27	100.29	110.30
1	U	1197	ILE	CG1-CB-CG2	-5.27	99.81	111.40
1	Q	1228	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	W	1217	ARG	CB-CG-CD	-5.26	97.91	111.60
1	V	1167	ASN	CB-CA-C	-5.26	99.87	110.40
1	Q	1323	ASP	CB-CG-OD2	5.26	123.03	118.30
1	U	1310	MET	CB-CA-C	-5.25	99.89	110.40
1	P	1211	TYR	CA-C-N	5.25	128.76	117.20
1	V	1211	TYR	CA-C-N	5.25	128.75	117.20
1	R	1193	ILE	N-CA-C	-5.25	96.83	111.00
1	U	1096	VAL	CB-CA-C	-5.24	101.44	111.40
1	W	1331	GLY	N-CA-C	-5.24	100.00	113.10
1	R	1153	ASN	N-CA-CB	5.24	120.03	110.60
1	R	1181	GLY	N-CA-C	5.24	126.19	113.10
1	Q	1103	TRP	CA-CB-CG	5.24	123.65	113.70
1	W	1096	VAL	CB-CA-C	-5.23	101.47	111.40
1	P	1068	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	R	1197	ILE	CG1-CB-CG2	-5.22	99.92	111.40
1	U	1033	GLN	CB-CA-C	-5.22	99.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	1335	ASP	OD1-CG-OD2	5.21	133.21	123.30
1	R	1028	ASP	CB-CG-OD1	-5.21	113.61	118.30
1	R	1113	ASP	CB-CG-OD1	5.21	122.99	118.30
1	P	1335	ASP	CB-CA-C	-5.20	99.99	110.40
2	X	1013	PRO	N-CA-C	5.20	125.63	112.10
1	P	1312	THR	CA-CB-CG2	-5.20	105.12	112.40
1	W	1314	VAL	CB-CA-C	-5.20	101.52	111.40
1	Q	1314	VAL	CB-CA-C	-5.20	101.53	111.40
1	V	1252	TRP	CB-CA-C	5.19	120.78	110.40
1	W	1041	LYS	N-CA-C	-5.19	96.98	111.00
1	R	1016	LYS	CB-CG-CD	-5.19	98.11	111.60
1	R	1075	VAL	CG1-CB-CG2	5.19	119.20	110.90
1	R	1291	ASP	CB-CA-C	5.19	120.78	110.40
1	Q	1252	TRP	CB-CA-C	5.18	120.76	110.40
1	V	1217	ARG	CG-CD-NE	5.18	122.67	111.80
1	Q	1147	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	U	1184	ILE	CG1-CB-CG2	-5.17	100.03	111.40
1	U	1193	ILE	CB-CA-C	-5.17	101.27	111.60
1	V	1118	ASP	CB-CG-OD1	5.16	122.94	118.30
1	P	1230	ASN	CB-CA-C	-5.15	100.09	110.40
1	P	1156	PRO	CA-C-O	-5.15	107.83	120.20
1	Q	1161	PHE	N-CA-C	-5.15	97.10	111.00
1	Q	1187	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	U	1212	ILE	CG1-CB-CG2	-5.15	100.08	111.40
1	V	1315	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	Q	1012	ASP	CB-CG-OD2	5.13	122.92	118.30
1	R	1141	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	W	1103	TRP	CA-CB-CG	5.13	123.45	113.70
1	Q	1096	VAL	CB-CA-C	-5.13	101.65	111.40
1	Q	1071	SER	CB-CA-C	-5.13	100.36	110.10
1	R	1057	GLU	CG-CD-OE2	5.13	128.56	118.30
1	V	1312	THR	CA-CB-CG2	-5.13	105.22	112.40
1	P	1140	VAL	N-CA-C	-5.12	97.16	111.00
1	V	1298	VAL	CA-CB-CG1	-5.12	103.21	110.90
1	R	1036	MET	CG-SD-CE	-5.12	92.01	100.20
1	R	1078	ALA	N-CA-C	-5.12	97.18	111.00
1	U	1328	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	W	1105	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	W	1323	ASP	N-CA-CB	-5.11	101.41	110.60
1	P	1214	ASN	C-N-CA	-5.11	111.58	122.30
1	R	1048	ASP	CB-CG-OD2	5.11	122.89	118.30
1	P	1067	ASN	N-CA-CB	-5.10	101.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	1300	VAL	CG1-CB-CG2	5.10	119.06	110.90
1	R	1081	LYS	CA-CB-CG	5.10	124.63	113.40
2	X	1016	SER	N-CA-C	5.10	124.76	111.00
2	S	1004	LYS	N-CA-C	5.09	124.75	111.00
2	X	1045	CYS	CA-CB-SG	5.09	123.17	114.00
1	R	1272	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	W	1011	LEU	CB-CG-CD2	5.08	119.64	111.00
1	Q	1289	TYR	CE1-CZ-OH	5.08	133.81	120.10
1	Q	1211	TYR	CA-C-N	5.07	128.35	117.20
1	W	1298	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	Q	1225	LEU	CB-CG-CD2	5.06	119.61	111.00
1	P	1164	GLY	N-CA-C	-5.06	100.46	113.10
1	Q	1312	THR	CA-CB-CG2	-5.06	105.32	112.40
1	R	1275	LEU	CA-CB-CG	5.06	126.93	115.30
1	R	1032	ASP	CB-CG-OD1	-5.05	113.75	118.30
1	R	1134	THR	N-CA-C	5.05	124.64	111.00
1	P	1184	ILE	CA-CB-CG1	-5.05	101.41	111.00
1	U	1289	TYR	OH-CZ-CE2	-5.05	106.47	120.10
1	U	1299	ASP	OD1-CG-OD2	-5.05	113.71	123.30
1	W	1193	ILE	N-CA-C	-5.05	97.37	111.00
1	R	1241	THR	N-CA-CB	-5.04	100.73	110.30
1	W	1121	MET	CG-SD-CE	5.04	108.26	100.20
1	U	1007	ASP	CB-CG-OD1	5.04	122.83	118.30
1	P	1092	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	W	1140	VAL	N-CA-C	-5.03	97.43	111.00
1	W	1071	SER	CB-CA-C	-5.02	100.56	110.10
1	Q	1230	ASN	CB-CA-C	-5.02	100.36	110.40
1	Q	1016	LYS	CB-CG-CD	-5.02	98.55	111.60
1	Q	1018	ASP	N-CA-CB	-5.02	101.56	110.60
1	U	1211	TYR	CB-CA-C	5.02	120.44	110.40
1	U	1295	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	W	1149	TYR	CE1-CZ-OH	5.02	133.65	120.10
1	V	1099	ASP	CB-CG-OD2	5.01	122.81	118.30
1	Q	1069	ASN	CA-C-N	-5.01	106.18	117.20
2	S	1022	TRP	CB-CA-C	5.01	120.42	110.40
1	Q	1105	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	W	1168	ASN	N-CA-C	5.00	124.51	111.00
1	U	1340	LEU	CB-CG-CD1	-5.00	102.50	111.00
1	W	1027	LYS	CB-CA-C	5.00	120.40	110.40

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Q	1070	ASN	CA
1	R	1070	ASN	CA
1	U	1170	ARG	CA
1	V	1070	ASN	CA

All (65) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	1030	ASP	Peptide
1	P	1067	ASN	Peptide
1	P	1068	GLU	Peptide
1	P	1069	ASN	Peptide
1	P	1140	VAL	Peptide
1	P	1156	PRO	Peptide
1	P	1161	PHE	Peptide
1	P	1165	VAL	Peptide
1	P	1168	ASN	Peptide
1	P	1210	ALA	Peptide
1	P	1286	GLY	Peptide
1	P	1322	ASP	Peptide
1	Q	1067	ASN	Peptide
1	Q	1068	GLU	Peptide
1	Q	1069	ASN	Peptide
1	Q	1140	VAL	Peptide
1	Q	1161	PHE	Peptide
1	Q	1165	VAL	Peptide
1	Q	1168	ASN	Peptide
1	Q	1210	ALA	Peptide
1	Q	1286	GLY	Peptide
1	R	1067	ASN	Peptide
1	R	1068	GLU	Peptide
1	R	1069	ASN	Peptide
1	R	1140	VAL	Peptide
1	R	1165	VAL	Peptide
1	R	1168	ASN	Peptide
1	R	1210	ALA	Peptide
1	R	1286	GLY	Peptide
2	S	1007	ARG	Peptide
2	S	1017	LYS	Peptide
1	U	1067	ASN	Peptide
1	U	1068	GLU	Peptide
1	U	1069	ASN	Peptide
1	U	1140	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	U	1156	PRO	Peptide
1	U	1161	PHE	Peptide
1	U	1165	VAL	Peptide
1	U	1168	ASN	Peptide
1	U	1209	ALA	Peptide
1	U	1210	ALA	Peptide
1	U	1286	GLY	Peptide
1	V	1067	ASN	Peptide
1	V	1068	GLU	Peptide
1	V	1069	ASN	Peptide
1	V	1140	VAL	Peptide
1	V	1165	VAL	Peptide
1	V	1168	ASN	Peptide
1	V	1210	ALA	Peptide
1	V	1286	GLY	Peptide
1	W	1067	ASN	Peptide
1	W	1068	GLU	Peptide
1	W	1069	ASN	Peptide
1	W	1140	VAL	Peptide
1	W	1156	PRO	Peptide
1	W	1161	PHE	Peptide
1	W	1165	VAL	Peptide
1	W	1168	ASN	Peptide
1	W	1210	ALA	Peptide
1	W	1286	GLY	Peptide
2	X	1006	VAL	Peptide
2	X	1022	TRP	Peptide
2	X	1032	PRO	Peptide
2	X	1038	LYS	Peptide
2	X	1043	PHE	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	P	2636	0	2404	321	0
1	Q	2636	0	2404	331	0
1	R	2636	0	2404	325	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	2636	0	2404	308	0
1	V	2636	0	2404	331	0
1	W	2636	0	2404	348	0
2	S	359	0	376	77	0
2	X	359	0	376	76	0
All	All	16534	0	15176	2040	0

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 64.

All (2040) 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:V:1081:LYS:CD	1:V:1081:LYS:CE	1.77	1.62
1:R:1161:PHE:CB	1:R:1161:PHE:CG	1.84	1.61
1:R:1134:THR:CB	1:R:1134:THR:CG2	1.77	1.60
1:V:1134:THR:CB	1:V:1134:THR:CG2	1.76	1.60
1:W:1081:LYS:CD	1:W:1081:LYS:CE	1.75	1.59
1:R:1081:LYS:CD	1:R:1081:LYS:CE	1.81	1.59
1:Q:1334:THR:CA	1:Q:1334:THR:CB	1.75	1.58
1:U:1161:PHE:CB	1:U:1161:PHE:CG	1.86	1.57
1:W:1161:PHE:CB	1:W:1161:PHE:CG	1.86	1.55
1:P:1161:PHE:CB	1:P:1161:PHE:CG	1.86	1.55
1:Q:1161:PHE:CB	1:Q:1161:PHE:CG	1.83	1.54
1:W:1134:THR:CB	1:W:1134:THR:CG2	1.80	1.54
1:P:1157:SER:N	1:P:1157:SER:CA	1.71	1.53
1:V:1161:PHE:CG	1:V:1161:PHE:CB	1.87	1.53
1:U:1157:SER:N	1:U:1157:SER:CA	1.72	1.52
1:W:1041:LYS:NZ	1:W:1041:LYS:CE	1.69	1.52
2:X:1032:PRO:CB	2:X:1032:PRO:CG	1.78	1.50
1:Q:1157:SER:N	1:Q:1157:SER:CA	1.73	1.50
1:W:1157:SER:N	1:W:1157:SER:CA	1.73	1.49
1:R:1157:SER:N	1:R:1157:SER:CA	1.72	1.48
2:X:1045:CYS:SG	2:X:1045:CYS:CB	2.03	1.46
1:V:1157:SER:N	1:V:1157:SER:CA	1.72	1.46
2:S:1019:CYS:SG	2:S:1019:CYS:CB	2.04	1.46
2:S:1026:MET:HG3	2:S:1034:VAL:CG1	1.54	1.37
1:R:1184:ILE:HD13	1:R:1184:ILE:O	1.29	1.31
1:U:1184:ILE:O	1:U:1184:ILE:HD13	1.16	1.29
1:U:1237:GLN:OE1	1:U:1239:THR:HG22	1.33	1.26
2:S:1026:MET:CG	2:S:1034:VAL:HG12	1.64	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1162:THR:O	1:P:1165:VAL:HG21	1.35	1.25
2:S:1016:SER:OG	2:S:1019:CYS:HB3	1.12	1.25
1:Q:1047:THR:HG23	1:Q:1048:ASP:N	1.29	1.24
1:Q:1047:THR:CG2	1:Q:1048:ASP:N	1.90	1.21
1:Q:1184:ILE:O	1:Q:1184:ILE:HD13	1.40	1.20
1:U:1211:TYR:HD2	1:U:1250:LEU:HD23	1.03	1.19
1:Q:1162:THR:O	1:Q:1165:VAL:HG21	1.41	1.19
1:W:1237:GLN:OE1	1:W:1239:THR:HG22	1.42	1.19
1:P:1162:THR:O	1:P:1165:VAL:CG2	1.90	1.18
1:Q:1208:THR:O	1:Q:1210:ALA:N	1.76	1.18
1:V:1184:ILE:O	1:V:1184:ILE:HD13	1.40	1.17
1:U:1162:THR:O	1:U:1165:VAL:HG21	1.43	1.17
1:P:1184:ILE:O	1:P:1184:ILE:HD13	1.44	1.16
1:Q:1237:GLN:OE1	1:Q:1239:THR:HG22	1.43	1.16
1:V:1047:THR:HG23	1:V:1048:ASP:N	1.49	1.15
1:W:1184:ILE:O	1:W:1184:ILE:HD13	1.47	1.15
1:P:1287:ARG:HD3	1:U:1287:ARG:HD3	1.28	1.15
1:R:1165:VAL:HG12	1:R:1166:THR:H	1.09	1.14
2:S:1027:LYS:O	2:S:1028:LYS:HB2	1.44	1.14
1:W:1069:ASN:OD1	1:W:1070:ASN:CA	1.96	1.14
1:W:1162:THR:O	1:W:1165:VAL:CG2	1.95	1.14
1:V:1184:ILE:CD1	1:V:1184:ILE:H	1.62	1.12
2:X:1007:ARG:NH1	2:X:1007:ARG:HB2	1.64	1.12
1:Q:1047:THR:CG2	1:Q:1048:ASP:H	1.54	1.12
1:U:1165:VAL:HG12	1:U:1166:THR:H	1.13	1.11
1:P:1047:THR:CG2	1:P:1050:LEU:H	1.64	1.10
1:U:1208:THR:O	1:U:1210:ALA:N	1.84	1.10
2:X:1023:GLN:O	2:X:1026:MET:HB3	1.49	1.10
1:R:1237:GLN:OE1	1:R:1239:THR:HG22	1.51	1.10
1:W:1211:TYR:HD2	1:W:1250:LEU:HD23	1.01	1.09
1:U:1157:SER:O	1:U:1161:PHE:HD1	1.35	1.09
1:V:1162:THR:O	1:V:1165:VAL:HG21	1.51	1.09
1:V:1324:ASN:ND2	1:V:1326:PHE:HB3	1.69	1.08
1:Q:1324:ASN:ND2	1:Q:1326:PHE:HB3	1.67	1.08
1:Q:1162:THR:O	1:Q:1165:VAL:CG2	2.02	1.07
1:R:1049:GLN:HG3	1:R:1082:PHE:O	1.55	1.07
1:V:1047:THR:CG2	1:V:1048:ASP:N	2.13	1.07
1:Q:1159:GLU:OE1	1:Q:1159:GLU:HA	1.55	1.07
1:V:1162:THR:O	1:V:1165:VAL:CG2	2.00	1.07
1:W:1211:TYR:CD2	1:W:1250:LEU:HD23	1.89	1.07
1:V:1069:ASN:OD1	1:V:1070:ASN:CA	2.00	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1222:THR:HB	1:V:1239:THR:HB	1.34	1.07
1:V:1237:GLN:OE1	1:V:1239:THR:HG22	1.54	1.06
2:S:1020:ALA:O	2:S:1023:GLN:HG3	1.56	1.06
1:W:1165:VAL:HG12	1:W:1166:THR:H	1.18	1.06
1:R:1184:ILE:CD1	1:R:1184:ILE:H	1.69	1.05
1:R:1069:ASN:OD1	1:R:1070:ASN:CA	2.03	1.05
1:R:1184:ILE:O	1:R:1184:ILE:CD1	2.04	1.05
1:P:1047:THR:HG22	1:P:1050:LEU:H	1.14	1.05
1:U:1237:GLN:OE1	1:U:1239:THR:CG2	2.04	1.05
1:Q:1184:ILE:H	1:Q:1184:ILE:CD1	1.70	1.04
1:U:1184:ILE:HD13	1:U:1184:ILE:C	1.75	1.04
1:V:1159:GLU:HA	1:V:1159:GLU:OE1	1.54	1.04
1:R:1047:THR:HG23	1:R:1048:ASP:H	1.16	1.04
2:S:1011:THR:HG22	2:S:1041:SER:HA	1.38	1.04
1:U:1211:TYR:CD2	1:U:1250:LEU:HD23	1.91	1.04
1:W:1047:THR:HG22	1:W:1050:LEU:H	1.23	1.04
1:W:1047:THR:HG23	1:W:1048:ASP:N	1.58	1.04
1:W:1049:GLN:HG3	1:W:1082:PHE:O	1.58	1.04
1:P:1237:GLN:OE1	1:P:1239:THR:HG22	1.58	1.03
1:R:1211:TYR:HD2	1:R:1250:LEU:HD23	1.17	1.03
1:U:1162:THR:O	1:U:1165:VAL:CG2	2.04	1.03
1:U:1047:THR:HG22	1:U:1050:LEU:H	1.18	1.03
1:R:1324:ASN:ND2	1:R:1326:PHE:HB3	1.73	1.03
1:V:1047:THR:HG23	1:V:1048:ASP:H	0.89	1.03
1:R:1162:THR:O	1:R:1165:VAL:CG2	2.07	1.02
1:U:1184:ILE:O	1:U:1184:ILE:CD1	2.07	1.02
1:V:1184:ILE:HD13	1:V:1184:ILE:H	1.23	1.02
2:X:1025:ARG:HH11	2:X:1025:ARG:CG	1.70	1.02
2:S:1016:SER:OG	2:S:1019:CYS:CB	2.06	1.02
1:P:1184:ILE:O	1:P:1184:ILE:CD1	2.07	1.01
2:X:1025:ARG:HH11	2:X:1025:ARG:HG3	1.22	1.01
1:Q:1222:THR:HB	1:Q:1239:THR:HB	1.41	1.01
1:V:1184:ILE:O	1:V:1184:ILE:CD1	2.09	1.01
1:P:1047:THR:HG23	1:P:1048:ASP:N	1.69	1.01
1:R:1165:VAL:HG12	1:R:1166:THR:N	1.72	1.01
1:Q:1237:GLN:OE1	1:Q:1239:THR:CG2	2.09	1.00
1:W:1047:THR:HG23	1:W:1048:ASP:H	1.08	1.00
1:P:1184:ILE:HD13	1:P:1184:ILE:H	1.24	1.00
1:Q:1156:PRO:HD3	1:Q:1166:THR:O	1.62	0.99
1:U:1222:THR:HB	1:U:1239:THR:HB	1.40	0.99
1:P:1211:TYR:HD2	1:P:1250:LEU:HD23	1.22	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1162:THR:O	1:R:1165:VAL:HG21	1.63	0.99
1:P:1184:ILE:CD1	1:P:1184:ILE:H	1.76	0.99
1:Q:1184:ILE:HD13	1:Q:1184:ILE:H	1.23	0.98
1:R:1168:ASN:C	1:R:1170:ARG:N	2.08	0.98
1:V:1211:TYR:HD2	1:V:1250:LEU:HD23	1.25	0.98
1:W:1211:TYR:HD1	1:W:1211:TYR:H	1.04	0.98
1:U:1060:ILE:HG23	1:U:1071:SER:HB3	1.43	0.98
1:R:1184:ILE:HD13	1:R:1184:ILE:H	1.28	0.98
1:P:1208:THR:O	1:P:1210:ALA:N	1.96	0.98
1:U:1324:ASN:ND2	1:U:1326:PHE:HB3	1.78	0.98
1:W:1020:LEU:HD13	1:W:1033:GLN:HB2	1.46	0.98
1:Q:1211:TYR:HD2	1:Q:1250:LEU:HD23	1.25	0.97
1:P:1139:LEU:O	1:P:1140:VAL:HG12	1.64	0.97
2:X:1004:LYS:HB2	2:X:1004:LYS:NZ	1.79	0.97
1:Q:1238:TYR:OH	1:Q:1257:GLN:HG2	1.65	0.97
1:R:1211:TYR:CD2	1:R:1250:LEU:HD23	2.00	0.97
1:P:1324:ASN:HD21	1:P:1327:THR:HG23	1.29	0.96
1:P:1168:ASN:C	1:P:1170:ARG:N	2.14	0.96
2:S:1016:SER:HG	2:S:1019:CYS:HB3	1.21	0.96
1:W:1162:THR:O	1:W:1165:VAL:HG21	1.62	0.96
1:P:1047:THR:HG23	1:P:1048:ASP:H	1.30	0.96
1:R:1047:THR:HG23	1:R:1048:ASP:N	1.66	0.96
1:Q:1211:TYR:HD1	1:Q:1211:TYR:H	1.05	0.96
1:P:1159:GLU:OE1	1:P:1159:GLU:HA	1.66	0.95
2:X:1039:LYS:HB3	2:X:1044:GLU:OE2	1.64	0.95
1:R:1047:THR:HG22	1:R:1050:LEU:H	1.30	0.95
1:U:1049:GLN:HG3	1:U:1082:PHE:O	1.66	0.95
1:V:1011:LEU:HD11	1:W:1346:PHE:CD2	2.02	0.95
1:R:1184:ILE:HD13	1:R:1184:ILE:C	1.85	0.95
1:U:1047:THR:HG23	1:U:1048:ASP:H	1.30	0.94
1:P:1049:GLN:HG3	1:P:1082:PHE:O	1.66	0.94
1:W:1047:THR:CG2	1:W:1048:ASP:N	2.29	0.94
1:R:1308:LYS:O	1:R:1308:LYS:HD3	1.66	0.94
1:V:1159:GLU:OE1	1:V:1159:GLU:CA	2.14	0.94
1:W:1208:THR:O	1:W:1210:ALA:N	2.00	0.94
1:Q:1136:PHE:O	1:Q:1139:LEU:HD13	1.68	0.94
1:U:1165:VAL:HG12	1:U:1166:THR:N	1.75	0.94
1:U:1184:ILE:CD1	1:U:1184:ILE:H	1.81	0.94
2:X:1021:GLN:O	2:X:1025:ARG:N	2.01	0.94
1:P:1346:PHE:CD2	1:R:1011:LEU:HD11	2.02	0.94
2:S:1021:GLN:HA	2:S:1024:ARG:O	1.67	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1184:ILE:H	1:U:1184:ILE:HD12	1.31	0.94
1:P:1324:ASN:O	1:P:1326:PHE:N	2.00	0.94
1:W:1184:ILE:CD1	1:W:1184:ILE:H	1.80	0.93
2:S:1007:ARG:HD2	2:S:1037:VAL:HG21	1.47	0.93
1:Q:1184:ILE:O	1:Q:1184:ILE:CD1	2.16	0.93
1:U:1020:LEU:HD13	1:U:1033:GLN:HB2	1.51	0.92
1:V:1207:ASN:ND2	1:V:1215:GLY:O	2.01	0.92
1:R:1157:SER:O	1:R:1161:PHE:HD1	1.52	0.92
1:V:1047:THR:HG22	1:V:1050:LEU:H	1.33	0.92
1:P:1184:ILE:HD13	1:P:1184:ILE:N	1.82	0.92
1:U:1047:THR:HG23	1:U:1048:ASP:N	1.84	0.92
1:Q:1157:SER:O	1:Q:1161:PHE:HD1	1.52	0.92
1:W:1184:ILE:O	1:W:1184:ILE:CD1	2.17	0.91
2:X:1021:GLN:HB3	2:X:1025:ARG:HG3	1.50	0.91
1:V:1083:GLN:OE1	1:V:1084:ASP:N	2.03	0.91
1:P:1165:VAL:HG12	1:P:1166:THR:H	1.32	0.91
1:R:1168:ASN:O	1:R:1169:GLY:C	2.09	0.91
1:U:1157:SER:O	1:U:1161:PHE:CD1	2.21	0.91
1:V:1324:ASN:HD22	1:V:1326:PHE:HB3	1.32	0.91
2:X:1026:MET:SD	2:X:1033:SER:HA	2.11	0.91
1:U:1157:SER:N	1:U:1157:SER:HA	1.86	0.91
1:V:1184:ILE:HD13	1:V:1184:ILE:N	1.79	0.91
1:Q:1157:SER:N	1:Q:1157:SER:HA	1.83	0.91
1:W:1184:ILE:HD13	1:W:1184:ILE:H	1.34	0.91
1:W:1069:ASN:OD1	1:W:1070:ASN:HA	1.71	0.90
1:W:1165:VAL:HG12	1:W:1166:THR:N	1.84	0.90
1:V:1211:TYR:HD1	1:V:1211:TYR:H	1.20	0.90
1:V:1049:GLN:HG3	1:V:1082:PHE:O	1.71	0.90
1:W:1168:ASN:C	1:W:1170:ARG:N	2.13	0.90
1:Q:1037:ARG:HG2	1:Q:1059:GLN:HG3	1.52	0.90
1:U:1117:SER:O	1:U:1246:ARG:NH2	2.05	0.90
1:V:1060:ILE:HG23	1:V:1071:SER:HB3	1.51	0.89
2:X:1021:GLN:HB3	2:X:1025:ARG:NH1	1.88	0.89
2:S:1026:MET:HG3	2:S:1034:VAL:HG12	0.91	0.89
1:V:1211:TYR:CD2	1:V:1250:LEU:HD23	2.07	0.89
1:W:1324:ASN:ND2	1:W:1326:PHE:HB3	1.88	0.89
1:P:1184:ILE:CD1	1:P:1184:ILE:N	2.35	0.89
1:V:1047:THR:CG2	1:V:1050:LEU:H	1.85	0.89
1:Q:1049:GLN:HG3	1:Q:1082:PHE:O	1.73	0.88
1:Q:1168:ASN:C	1:Q:1170:ARG:N	2.25	0.88
1:R:1211:TYR:H	1:R:1211:TYR:HD1	1.16	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1237:GLN:OE1	1:R:1239:THR:CG2	2.21	0.88
1:P:1165:VAL:HG12	1:P:1166:THR:N	1.88	0.88
1:Q:1060:ILE:HG23	1:Q:1071:SER:HB3	1.54	0.88
1:V:1264:GLN:HG2	1:V:1274:SER:HB2	1.54	0.88
2:X:1023:GLN:O	2:X:1026:MET:CB	2.21	0.88
1:W:1037:ARG:HG2	1:W:1059:GLN:HG3	1.54	0.88
1:R:1020:LEU:HD13	1:R:1033:GLN:HB2	1.52	0.88
1:R:1287:ARG:HD3	1:V:1287:ARG:HD3	1.55	0.88
1:W:1222:THR:HB	1:W:1239:THR:HB	1.53	0.88
1:P:1211:TYR:CD2	1:P:1250:LEU:HD23	2.08	0.88
2:S:1037:VAL:HG12	2:S:1039:LYS:NZ	1.87	0.88
1:P:1157:SER:N	1:P:1157:SER:HA	1.84	0.88
1:Q:1159:GLU:OE1	1:Q:1159:GLU:CA	2.22	0.88
1:V:1157:SER:N	1:V:1157:SER:HA	1.89	0.88
1:R:1047:THR:CG2	1:R:1048:ASP:N	2.34	0.87
1:Q:1207:ASN:ND2	1:Q:1215:GLY:O	2.05	0.87
1:Q:1317:LYS:HE3	1:Q:1337:ILE:HD12	1.56	0.87
1:R:1157:SER:N	1:R:1157:SER:HA	1.88	0.87
1:U:1047:THR:CG2	1:U:1050:LEU:H	1.87	0.87
1:V:1218:ALA:HB1	1:V:1244:ALA:HB2	1.53	0.87
2:X:1004:LYS:HB2	2:X:1004:LYS:HZ3	1.34	0.87
1:W:1069:ASN:OD1	1:W:1070:ASN:N	2.06	0.86
1:V:1159:GLU:C	1:V:1159:GLU:CD	2.33	0.86
1:W:1157:SER:N	1:W:1157:SER:HA	1.87	0.86
1:V:1324:ASN:O	1:V:1326:PHE:N	2.09	0.86
1:R:1184:ILE:CD1	1:R:1184:ILE:N	2.33	0.86
1:P:1222:THR:HB	1:P:1239:THR:HB	1.58	0.86
1:U:1072:TRP:CD1	1:V:1066:GLU:HG2	2.11	0.86
2:X:1021:GLN:O	2:X:1024:ARG:N	2.08	0.85
1:U:1011:LEU:HD11	1:V:1346:PHE:CD2	2.11	0.85
1:P:1324:ASN:ND2	1:P:1326:PHE:HB3	1.91	0.85
1:R:1168:ASN:HA	1:R:1170:ARG:H	1.41	0.85
1:R:1208:THR:O	1:R:1210:ALA:N	2.07	0.85
1:U:1036:MET:HE1	1:U:1038:LEU:HD22	1.56	0.85
1:P:1036:MET:HE1	1:P:1038:LEU:HD22	1.58	0.85
2:X:1007:ARG:HB2	2:X:1007:ARG:CZ	2.04	0.85
1:Q:1287:ARG:HD3	1:W:1287:ARG:HD3	1.58	0.85
1:R:1047:THR:CG2	1:R:1050:LEU:H	1.88	0.85
1:U:1036:MET:HE1	1:U:1038:LEU:CD2	2.06	0.85
1:W:1159:GLU:OE1	1:W:1159:GLU:HA	1.76	0.85
2:X:1006:VAL:HG22	2:X:1007:ARG:HH12	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1041:SER:HB2	2:X:1044:GLU:HB2	1.58	0.85
1:V:1184:ILE:CD1	1:V:1184:ILE:N	2.25	0.85
1:Q:1011:LEU:HD11	1:R:1346:PHE:CD2	2.12	0.84
1:U:1168:ASN:C	1:U:1170:ARG:N	2.24	0.84
1:U:1324:ASN:O	1:U:1326:PHE:N	2.10	0.84
1:W:1324:ASN:HD22	1:W:1326:PHE:HB3	1.40	0.84
1:Q:1047:THR:HG22	1:Q:1048:ASP:N	1.91	0.84
1:Q:1184:ILE:HD13	1:Q:1184:ILE:N	1.88	0.84
1:Q:1222:THR:CB	1:Q:1239:THR:HB	2.07	0.84
1:Q:1211:TYR:CD2	1:Q:1250:LEU:HD23	2.13	0.84
1:V:1160:GLY:O	1:V:1161:PHE:O	1.95	0.84
1:V:1237:GLN:OE1	1:V:1239:THR:CG2	2.26	0.84
1:U:1211:TYR:H	1:U:1211:TYR:HD1	1.23	0.83
1:V:1168:ASN:HA	1:V:1170:ARG:H	1.42	0.83
2:X:1006:VAL:CG2	2:X:1007:ARG:HH12	1.89	0.83
2:S:1014:ALA:CB	2:S:1017:LYS:HD3	2.08	0.83
1:Q:1020:LEU:HD13	1:Q:1033:GLN:HB2	1.58	0.83
1:W:1159:GLU:CD	1:W:1159:GLU:C	2.37	0.83
1:Q:1184:ILE:CD1	1:Q:1184:ILE:N	2.35	0.83
1:V:1184:ILE:H	1:V:1184:ILE:HD12	1.44	0.83
1:R:1324:ASN:HD22	1:R:1326:PHE:HB3	1.39	0.83
1:P:1047:THR:CG2	1:P:1048:ASP:N	2.36	0.82
2:X:1007:ARG:HB2	2:X:1007:ARG:HH11	1.41	0.82
1:U:1222:THR:CB	1:U:1239:THR:HB	2.09	0.82
1:U:1159:GLU:OE1	1:U:1159:GLU:HA	1.79	0.82
1:V:1045:GLN:HG3	1:V:1045:GLN:O	1.79	0.82
1:W:1036:MET:HE1	1:W:1038:LEU:HD22	1.59	0.82
1:R:1135:ASP:HB3	1:R:1141:ASP:HA	1.62	0.82
1:V:1168:ASN:C	1:V:1170:ARG:N	2.33	0.82
2:S:1026:MET:CG	2:S:1034:VAL:CG1	2.41	0.82
1:U:1020:LEU:HD13	1:U:1033:GLN:CB	2.09	0.81
1:V:1155:ASN:HB3	1:V:1157:SER:H	1.45	0.81
1:W:1069:ASN:OD1	1:W:1070:ASN:CB	2.28	0.81
1:P:1165:VAL:HA	1:P:1166:THR:HG22	1.62	0.81
1:R:1207:ASN:ND2	1:R:1215:GLY:O	2.13	0.81
1:U:1047:THR:CG2	1:U:1048:ASP:N	2.43	0.81
1:R:1162:THR:O	1:R:1165:VAL:HG23	1.80	0.81
2:S:1011:THR:HG22	2:S:1041:SER:CA	2.11	0.81
1:P:1324:ASN:C	1:P:1326:PHE:N	2.31	0.81
1:R:1083:GLN:OE1	1:R:1084:ASP:N	2.13	0.81
1:W:1155:ASN:HB3	1:W:1157:SER:H	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1025:ARG:HG3	2:X:1025:ARG:NH1	1.96	0.81
1:P:1159:GLU:OE1	1:P:1159:GLU:CA	2.22	0.81
1:V:1156:PRO:O	1:V:1161:PHE:CD1	2.34	0.81
1:R:1184:ILE:HD13	1:R:1184:ILE:N	1.88	0.81
1:P:1211:TYR:H	1:P:1211:TYR:HD1	1.25	0.81
1:P:1237:GLN:OE1	1:P:1239:THR:CG2	2.28	0.81
1:V:1156:PRO:O	1:V:1161:PHE:CG	2.34	0.81
1:W:1036:MET:HE1	1:W:1038:LEU:HB3	1.61	0.81
1:P:1047:THR:HG22	1:P:1050:LEU:N	1.94	0.80
2:S:1014:ALA:HB1	2:S:1017:LYS:HD3	1.63	0.80
1:Q:1154:GLY:O	1:Q:1165:VAL:HG12	1.80	0.80
1:V:1083:GLN:CD	1:V:1084:ASP:H	1.83	0.80
1:V:1157:SER:O	1:V:1161:PHE:HD1	1.63	0.80
1:R:1160:GLY:O	1:R:1161:PHE:O	1.99	0.80
1:R:1069:ASN:OD1	1:R:1070:ASN:HA	1.82	0.80
1:W:1117:SER:O	1:W:1246:ARG:NH2	2.13	0.80
1:P:1287:ARG:CD	1:U:1287:ARG:HD3	2.11	0.80
1:Q:1069:ASN:OD1	1:Q:1070:ASN:CA	2.29	0.80
1:R:1020:LEU:HD13	1:R:1033:GLN:CB	2.12	0.80
1:V:1036:MET:HG2	1:V:1037:ARG:N	1.96	0.80
1:Q:1157:SER:O	1:Q:1161:PHE:CD1	2.34	0.80
1:W:1308:LYS:O	1:W:1308:LYS:HD3	1.81	0.80
1:W:1157:SER:O	1:W:1161:PHE:HD1	1.65	0.79
1:U:1324:ASN:HD22	1:U:1326:PHE:HB3	1.44	0.79
1:Q:1047:THR:HG22	1:Q:1050:LEU:H	1.47	0.79
1:W:1036:MET:CE	1:W:1038:LEU:HB3	2.12	0.79
1:W:1160:GLY:O	1:W:1161:PHE:O	2.01	0.79
2:S:1025:ARG:N	2:S:1027:LYS:O	2.14	0.79
1:V:1069:ASN:OD1	1:V:1070:ASN:CB	2.29	0.79
1:Q:1324:ASN:HD22	1:Q:1326:PHE:HB3	1.42	0.79
1:R:1159:GLU:C	1:R:1159:GLU:CD	2.41	0.79
1:W:1047:THR:CG2	1:W:1050:LEU:H	1.96	0.79
1:P:1128:PHE:CD2	1:P:1150:GLN:HB3	2.18	0.79
1:R:1155:ASN:O	1:R:1165:VAL:HG11	1.82	0.79
2:X:1027:LYS:O	2:X:1028:LYS:HG2	1.82	0.79
1:R:1168:ASN:HA	1:R:1170:ARG:N	1.98	0.78
2:X:1026:MET:O	2:X:1030:ARG:HA	1.82	0.78
1:R:1190:GLY:O	1:R:1191:PHE:HB2	1.80	0.78
1:Q:1047:THR:CG2	1:Q:1050:LEU:H	1.97	0.78
1:R:1156:PRO:O	1:R:1161:PHE:CG	2.35	0.78
1:U:1030:ASP:O	1:W:1163:SER:HB3	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1116:GLY:H	1:U:1119:ASN:HD22	1.30	0.78
1:U:1190:GLY:O	1:U:1191:PHE:HB2	1.81	0.78
1:U:1264:GLN:HG2	1:U:1274:SER:HB2	1.66	0.78
1:R:1083:GLN:CD	1:R:1084:ASP:N	2.37	0.78
1:V:1163:SER:HB3	1:W:1030:ASP:O	1.83	0.78
1:W:1036:MET:HE1	1:W:1038:LEU:CD2	2.14	0.78
1:U:1303:THR:HB	1:U:1313:TYR:HB3	1.66	0.78
1:P:1238:TYR:OH	1:P:1257:GLN:HG2	1.84	0.78
1:R:1218:ALA:HB1	1:R:1244:ALA:HB2	1.66	0.78
1:R:1324:ASN:ND2	1:R:1327:THR:H	1.81	0.78
1:U:1036:MET:CE	1:U:1038:LEU:HD22	2.12	0.78
1:P:1160:GLY:O	1:P:1161:PHE:O	2.01	0.77
1:V:1317:LYS:HE3	1:V:1337:ILE:HD12	1.66	0.77
1:W:1154:GLY:O	1:W:1165:VAL:HG12	1.85	0.77
1:W:1159:GLU:OE1	1:W:1159:GLU:CA	2.32	0.77
1:P:1020:LEU:HD13	1:P:1033:GLN:CB	2.15	0.77
1:U:1058:TYR:HD1	1:U:1073:THR:HA	1.49	0.77
1:U:1159:GLU:C	1:U:1159:GLU:CD	2.43	0.77
1:R:1069:ASN:OD1	1:R:1070:ASN:N	2.16	0.77
1:U:1066:GLU:HG2	1:W:1072:TRP:CD1	2.18	0.77
1:W:1002:GLU:HG3	1:W:1002:GLU:O	1.84	0.77
1:Q:1165:VAL:HA	1:Q:1166:THR:HG22	1.67	0.77
1:R:1264:GLN:HG2	1:R:1274:SER:HB2	1.66	0.77
1:V:1083:GLN:CD	1:V:1084:ASP:N	2.38	0.77
1:W:1136:PHE:HB3	1:W:1140:VAL:CG1	2.14	0.77
1:P:1037:ARG:HG2	1:P:1059:GLN:HG3	1.64	0.77
1:Q:1117:SER:O	1:Q:1246:ARG:NH2	2.18	0.77
1:R:1184:ILE:H	1:R:1184:ILE:HD12	1.50	0.77
1:W:1184:ILE:CD1	1:W:1184:ILE:N	2.45	0.77
1:P:1036:MET:CE	1:P:1038:LEU:HB3	2.15	0.77
1:V:1156:PRO:HD3	1:V:1166:THR:O	1.85	0.77
1:R:1168:ASN:CA	1:R:1170:ARG:H	1.96	0.77
1:P:1208:THR:C	1:P:1210:ALA:H	1.86	0.76
1:P:1324:ASN:ND2	1:P:1327:THR:HG23	1.98	0.76
1:W:1324:ASN:O	1:W:1326:PHE:N	2.17	0.76
1:P:1154:GLY:C	1:P:1165:VAL:CG1	2.54	0.76
1:R:1317:LYS:HE3	1:R:1337:ILE:HD12	1.66	0.76
1:U:1168:ASN:HA	1:U:1170:ARG:N	2.00	0.76
1:W:1002:GLU:OE1	1:W:1005:ASN:HB2	1.85	0.76
1:R:1157:SER:O	1:R:1161:PHE:CD1	2.36	0.76
1:U:1126:ASN:OD1	1:V:1064:SER:HA	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1116:GLY:H	1:P:1119:ASN:HD22	1.34	0.76
1:P:1154:GLY:O	1:P:1165:VAL:HG12	1.85	0.76
1:R:1134:THR:CG2	1:R:1134:THR:HB	2.10	0.76
1:W:1190:GLY:O	1:W:1191:PHE:HB2	1.86	0.76
1:W:1324:ASN:C	1:W:1326:PHE:N	2.33	0.76
1:P:1098:TYR:CE2	1:P:1102:SER:HB3	2.21	0.76
2:S:1037:VAL:HG12	2:S:1039:LYS:HZ2	1.46	0.76
1:U:1060:ILE:HG23	1:U:1071:SER:CB	2.16	0.76
1:P:1011:LEU:HD11	1:Q:1346:PHE:CD2	2.21	0.76
1:V:1116:GLY:O	1:V:1123:GLN:HB3	1.86	0.76
1:W:1068:GLU:O	1:W:1069:ASN:HB3	1.86	0.76
1:U:1324:ASN:C	1:U:1326:PHE:N	2.36	0.76
1:U:1159:GLU:OE1	1:U:1159:GLU:CA	2.33	0.76
2:X:1018:LYS:HB3	2:X:1021:GLN:CD	2.06	0.76
1:W:1154:GLY:O	1:W:1165:VAL:CG1	2.34	0.75
1:V:1184:ILE:HD13	1:V:1184:ILE:C	1.92	0.75
1:W:1020:LEU:HD13	1:W:1033:GLN:CB	2.16	0.75
1:P:1324:ASN:C	1:P:1326:PHE:H	1.87	0.75
1:Q:1060:ILE:HG23	1:Q:1071:SER:CB	2.15	0.75
2:X:1036:CYS:O	2:X:1037:VAL:HG12	1.86	0.75
1:W:1101:THR:HA	1:W:1237:GLN:HG3	1.68	0.75
1:P:1133:ASN:HD22	1:P:1145:PHE:HE1	1.32	0.75
1:Q:1184:ILE:HD13	1:Q:1184:ILE:C	2.00	0.75
1:W:1255:LYS:HB3	1:W:1283:LYS:HB2	1.69	0.75
2:X:1025:ARG:CG	2:X:1025:ARG:NH1	2.42	0.75
1:U:1324:ASN:ND2	1:U:1327:THR:H	1.84	0.75
1:P:1168:ASN:O	1:P:1169:GLY:C	2.24	0.75
1:P:1159:GLU:C	1:P:1159:GLU:CD	2.44	0.74
1:P:1036:MET:HE1	1:P:1038:LEU:HB3	1.67	0.74
1:P:1045:GLN:HG3	1:P:1045:GLN:O	1.86	0.74
1:V:1260:GLU:HG2	1:V:1278:LEU:HD13	1.69	0.74
1:W:1303:THR:HB	1:W:1313:TYR:HB3	1.69	0.74
1:Q:1020:LEU:HD13	1:Q:1033:GLN:CB	2.16	0.74
1:R:1156:PRO:O	1:R:1161:PHE:CD1	2.40	0.74
2:S:1027:LYS:O	2:S:1028:LYS:CB	2.27	0.74
1:W:1156:PRO:O	1:W:1161:PHE:CG	2.40	0.74
1:Q:1058:TYR:HD1	1:Q:1073:THR:HA	1.51	0.74
1:U:1218:ALA:HB1	1:U:1244:ALA:HB2	1.69	0.74
1:V:1135:ASP:HB3	1:V:1141:ASP:HA	1.70	0.74
1:R:1136:PHE:HB3	1:R:1140:VAL:CG1	2.17	0.74
1:U:1045:GLN:O	1:U:1045:GLN:HG3	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1312:THR:HG22	1:U:1341:GLY:O	1.87	0.74
1:V:1069:ASN:OD1	1:V:1070:ASN:N	2.20	0.74
1:R:1083:GLN:CD	1:R:1084:ASP:H	1.91	0.74
1:V:1036:MET:HE1	1:V:1038:LEU:HB3	1.68	0.74
1:R:1002:GLU:HG3	1:R:1002:GLU:O	1.88	0.74
1:W:1045:GLN:HG3	1:W:1045:GLN:O	1.88	0.74
1:V:1324:ASN:ND2	1:V:1327:THR:H	1.85	0.74
1:Q:1164:GLY:C	1:Q:1165:VAL:HG22	2.06	0.74
1:W:1060:ILE:HA	1:W:1071:SER:HB2	1.70	0.74
1:P:1317:LYS:HE3	1:P:1337:ILE:HD12	1.67	0.73
1:Q:1163:SER:HB3	1:R:1030:ASP:O	1.87	0.73
1:W:1324:ASN:C	1:W:1326:PHE:H	1.90	0.73
1:Q:1060:ILE:HA	1:Q:1071:SER:HB2	1.71	0.73
1:R:1212:ILE:O	1:R:1252:TRP:N	2.21	0.73
1:R:1266:GLN:HG3	1:R:1266:GLN:O	1.86	0.73
1:Q:1024:SER:HB2	1:Q:1337:ILE:HG23	1.69	0.73
1:P:1096:VAL:HG22	1:P:1148:GLN:HG2	1.70	0.73
1:P:1156:PRO:HD3	1:P:1166:THR:O	1.88	0.73
1:Q:1002:GLU:OE1	1:Q:1005:ASN:HB2	1.87	0.73
2:S:1039:LYS:O	2:S:1041:SER:N	2.20	0.73
1:W:1168:ASN:CA	1:W:1170:ARG:H	2.01	0.73
1:W:1237:GLN:OE1	1:W:1239:THR:CG2	2.30	0.73
2:S:1007:ARG:HA	2:S:1035:THR:OG1	1.89	0.73
1:W:1134:THR:CG2	1:W:1134:THR:CA	2.66	0.73
1:Q:1308:LYS:O	1:Q:1308:LYS:HD3	1.88	0.73
1:R:1188:TYR:CD1	1:R:1188:TYR:N	2.57	0.73
1:U:1184:ILE:HD12	1:U:1184:ILE:N	2.02	0.73
1:W:1156:PRO:O	1:W:1161:PHE:CD1	2.42	0.73
1:V:1222:THR:CB	1:V:1239:THR:HB	2.16	0.72
1:P:1324:ASN:ND2	1:P:1327:THR:H	1.87	0.72
1:Q:1202:ARG:NE	1:Q:1215:GLY:HA3	2.04	0.72
1:R:1168:ASN:C	1:R:1170:ARG:H	1.91	0.72
1:U:1155:ASN:O	1:U:1165:VAL:HG11	1.88	0.72
1:W:1168:ASN:HA	1:W:1170:ARG:H	1.54	0.72
1:R:1069:ASN:OD1	1:R:1070:ASN:CB	2.37	0.72
1:U:1024:SER:HB2	1:U:1337:ILE:HG23	1.71	0.72
1:Q:1168:ASN:CA	1:Q:1170:ARG:H	2.03	0.72
1:R:1154:GLY:C	1:R:1165:VAL:CG1	2.58	0.72
1:U:1135:ASP:HB3	1:U:1141:ASP:HA	1.69	0.72
2:X:1021:GLN:C	2:X:1025:ARG:H	1.93	0.72
1:P:1184:ILE:HD13	1:P:1184:ILE:C	1.94	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1324:ASN:O	1:P:1325:GLN:C	2.26	0.72
1:U:1118:ASP:OD1	1:V:1065:ALA:HB1	1.90	0.72
1:V:1289:TYR:O	1:V:1290:ASP:HB2	1.88	0.72
1:R:1037:ARG:HG2	1:R:1059:GLN:HG3	1.70	0.72
1:R:1222:THR:HB	1:R:1239:THR:HB	1.72	0.72
1:V:1058:TYR:HD1	1:V:1073:THR:HA	1.55	0.72
1:R:1155:ASN:C	1:R:1165:VAL:HG11	2.09	0.72
1:Q:1289:TYR:O	1:Q:1290:ASP:HB2	1.89	0.72
1:W:1154:GLY:C	1:W:1165:VAL:CG1	2.58	0.72
1:R:1117:SER:O	1:R:1246:ARG:NH2	2.22	0.72
1:P:1202:ARG:NE	1:P:1215:GLY:HA3	2.05	0.71
1:W:1168:ASN:O	1:W:1169:GLY:C	2.26	0.71
1:P:1289:TYR:O	1:P:1290:ASP:HB2	1.90	0.71
1:W:1036:MET:CE	1:W:1038:LEU:HD22	2.19	0.71
1:P:1308:LYS:O	1:P:1308:LYS:HD3	1.90	0.71
1:R:1037:ARG:NH1	1:R:1074:ARG:CZ	2.54	0.71
1:W:1281:LYS:HD2	1:W:1283:LYS:HE3	1.71	0.71
1:P:1069:ASN:OD1	1:P:1070:ASN:CA	2.38	0.71
1:Q:1156:PRO:O	1:Q:1161:PHE:CD1	2.43	0.71
1:R:1155:ASN:N	1:R:1165:VAL:HG11	2.05	0.71
1:U:1017:VAL:HG12	1:U:1018:ASP:N	2.03	0.71
1:V:1168:ASN:CA	1:V:1170:ARG:H	2.03	0.71
1:W:1157:SER:O	1:W:1161:PHE:CD1	2.43	0.71
1:P:1154:GLY:O	1:P:1165:VAL:CG1	2.38	0.71
1:W:1187:ASP:O	1:W:1188:TYR:C	2.29	0.71
2:X:1021:GLN:CB	2:X:1025:ARG:HG3	2.20	0.71
1:P:1154:GLY:C	1:P:1165:VAL:HG11	2.11	0.71
1:R:1136:PHE:O	1:R:1139:LEU:HD13	1.90	0.71
1:U:1128:PHE:CD2	1:U:1150:GLN:HB3	2.25	0.71
1:W:1184:ILE:HD13	1:W:1184:ILE:N	1.98	0.71
1:V:1047:THR:CG2	1:V:1048:ASP:H	1.79	0.71
1:R:1188:TYR:N	1:R:1188:TYR:HD1	1.89	0.71
2:S:1028:LYS:N	2:S:1029:VAL:O	2.23	0.71
1:W:1184:ILE:HD13	1:W:1184:ILE:C	2.04	0.71
1:R:1165:VAL:HA	1:R:1166:THR:HG22	1.73	0.71
1:U:1308:LYS:O	1:U:1308:LYS:HD3	1.90	0.71
1:V:1165:VAL:HA	1:V:1166:THR:HG22	1.72	0.71
1:U:1026:ASN:ND2	1:U:1333:ASN:OD1	2.21	0.70
1:Q:1128:PHE:CD2	1:Q:1150:GLN:HB3	2.26	0.70
1:U:1069:ASN:OD1	1:U:1070:ASN:CA	2.39	0.70
1:W:1207:ASN:ND2	1:W:1215:GLY:O	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1096:VAL:HG22	1:W:1148:GLN:HG2	1.73	0.70
1:W:1156:PRO:HD3	1:W:1166:THR:O	1.91	0.70
1:R:1139:LEU:O	1:R:1139:LEU:HD22	1.91	0.70
1:U:1098:TYR:CE2	1:U:1102:SER:HB3	2.25	0.70
1:W:1202:ARG:NE	1:W:1215:GLY:HA3	2.06	0.70
1:U:1346:PHE:CD2	1:W:1011:LEU:HD11	2.26	0.70
1:V:1020:LEU:HD13	1:V:1033:GLN:CB	2.22	0.70
1:W:1222:THR:CB	1:W:1239:THR:HB	2.22	0.70
1:Q:1155:ASN:HB3	1:Q:1157:SER:H	1.55	0.70
1:Q:1264:GLN:HG2	1:Q:1274:SER:HB2	1.72	0.70
1:R:1058:TYR:HD1	1:R:1073:THR:HA	1.56	0.70
1:U:1047:THR:HG22	1:U:1050:LEU:N	2.00	0.70
1:R:1289:TYR:O	1:R:1290:ASP:HB2	1.90	0.70
1:U:1190:GLY:O	1:U:1191:PHE:CB	2.39	0.70
1:V:1036:MET:HE1	1:V:1038:LEU:HD22	1.74	0.70
1:V:1164:GLY:C	1:V:1165:VAL:HG22	2.11	0.70
2:X:1023:GLN:HB2	2:X:1035:THR:HA	1.73	0.70
1:Q:1083:GLN:CD	1:Q:1084:ASP:N	2.46	0.70
1:Q:1208:THR:C	1:Q:1210:ALA:H	1.94	0.70
1:Q:1217:ARG:HD3	1:Q:1219:GLU:OE2	1.91	0.70
1:R:1161:PHE:O	1:R:1162:THR:HG23	1.92	0.70
1:U:1156:PRO:HD3	1:U:1166:THR:O	1.92	0.70
1:U:1309:ASN:ND2	1:W:1009:ASN:HB2	2.06	0.70
1:R:1154:GLY:O	1:R:1165:VAL:CG1	2.39	0.70
1:Q:1324:ASN:ND2	1:Q:1327:THR:H	1.89	0.69
1:R:1116:GLY:H	1:R:1119:ASN:HD22	1.37	0.69
1:U:1324:ASN:O	1:U:1325:GLN:C	2.31	0.69
1:V:1208:THR:O	1:V:1210:ALA:N	2.25	0.69
1:W:1190:GLY:O	1:W:1191:PHE:CB	2.40	0.69
1:Q:1154:GLY:C	1:Q:1165:VAL:CG1	2.61	0.69
1:R:1202:ARG:NE	1:R:1215:GLY:HA3	2.07	0.69
1:V:1168:ASN:HA	1:V:1170:ARG:N	2.05	0.69
1:P:1157:SER:O	1:P:1161:PHE:HD1	1.75	0.69
1:R:1168:ASN:CA	1:R:1170:ARG:N	2.55	0.69
1:U:1136:PHE:HB3	1:U:1140:VAL:CG1	2.21	0.69
1:V:1303:THR:HB	1:V:1313:TYR:HB3	1.73	0.69
1:Q:1098:TYR:CE2	1:Q:1102:SER:HB3	2.27	0.69
1:W:1134:THR:CG2	1:W:1134:THR:HB	2.16	0.69
1:Q:1168:ASN:HA	1:Q:1170:ARG:N	2.08	0.69
1:U:1002:GLU:HG3	1:U:1002:GLU:O	1.93	0.69
1:V:1098:TYR:CE2	1:V:1102:SER:HB3	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1202:ARG:HE	1:V:1215:GLY:HA3	1.57	0.69
1:W:1211:TYR:N	1:W:1211:TYR:CD1	2.59	0.69
1:P:1303:THR:HB	1:P:1313:TYR:HB3	1.74	0.69
1:R:1159:GLU:OE1	1:R:1159:GLU:HA	1.92	0.69
2:S:1029:VAL:HG21	1:W:1288:GLY:H	1.58	0.69
1:V:1002:GLU:O	1:V:1002:GLU:HG3	1.91	0.69
1:V:1136:PHE:HB3	1:V:1140:VAL:CG1	2.22	0.69
1:V:1344:TYR:C	1:V:1344:TYR:CD2	2.66	0.69
1:P:1184:ILE:CD1	1:P:1184:ILE:C	2.55	0.69
1:Q:1069:ASN:OD1	1:Q:1070:ASN:CB	2.40	0.69
1:R:1002:GLU:OE1	1:R:1005:ASN:CB	2.41	0.69
1:R:1190:GLY:O	1:R:1191:PHE:CB	2.37	0.69
1:V:1002:GLU:OE1	1:V:1005:ASN:HB3	1.92	0.69
2:S:1021:GLN:O	2:S:1026:MET:HB2	1.92	0.69
1:P:1184:ILE:HD11	1:P:1195:GLY:H	1.58	0.69
1:V:1264:GLN:HG2	1:V:1274:SER:CB	2.23	0.69
1:W:1168:ASN:HA	1:W:1170:ARG:N	2.07	0.68
1:P:1058:TYR:HD1	1:P:1073:THR:HA	1.56	0.68
1:P:1160:GLY:C	1:P:1161:PHE:O	2.29	0.68
1:U:1096:VAL:O	1:U:1098:TYR:N	2.26	0.68
1:U:1207:ASN:ND2	1:U:1215:GLY:O	2.19	0.68
1:Q:1286:GLY:O	1:Q:1288:GLY:O	2.10	0.68
1:V:1135:ASP:O	1:V:1136:PHE:C	2.31	0.68
1:W:1128:PHE:CD2	1:W:1150:GLN:HB3	2.29	0.68
1:P:1136:PHE:HB3	1:P:1140:VAL:CG1	2.22	0.68
1:V:1160:GLY:C	1:V:1161:PHE:O	2.29	0.68
1:P:1036:MET:HE1	1:P:1038:LEU:CD2	2.24	0.68
1:P:1155:ASN:HB3	1:P:1157:SER:H	1.58	0.68
1:P:1196:ALA:O	1:P:1222:THR:HG22	1.94	0.68
2:X:1021:GLN:HB3	2:X:1025:ARG:HH11	1.57	0.68
1:P:1036:MET:CE	1:P:1038:LEU:HD22	2.23	0.68
1:Q:1168:ASN:HA	1:Q:1170:ARG:H	1.59	0.68
1:W:1154:GLY:C	1:W:1165:VAL:HG11	2.14	0.68
1:P:1020:LEU:HD13	1:P:1033:GLN:HB2	1.75	0.68
1:R:1324:ASN:HD21	1:R:1327:THR:HG23	1.58	0.68
1:U:1202:ARG:NE	1:U:1215:GLY:HA3	2.08	0.68
1:V:1117:SER:O	1:V:1246:ARG:NH2	2.25	0.68
1:V:1165:VAL:HG12	1:V:1166:THR:H	1.59	0.68
1:W:1264:GLN:HG2	1:W:1274:SER:HB2	1.73	0.68
2:X:1013:PRO:O	2:X:1015:GLU:N	2.26	0.68
1:V:1202:ARG:NE	1:V:1215:GLY:HA3	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1164:GLY:C	1:V:1165:VAL:CG2	2.59	0.68
1:W:1133:ASN:O	1:W:1144:ASN:HB2	1.92	0.68
1:Q:1047:THR:HG23	1:Q:1048:ASP:H	0.63	0.68
1:U:1116:GLY:N	1:U:1119:ASN:HD22	1.91	0.68
1:W:1133:ASN:HD21	1:W:1137:PHE:H	1.40	0.68
1:Q:1085:VAL:O	1:Q:1131:TYR:OH	2.12	0.67
1:U:1168:ASN:CA	1:U:1170:ARG:N	2.57	0.67
1:R:1264:GLN:HG2	1:R:1274:SER:CB	2.23	0.67
1:Q:1135:ASP:O	1:Q:1138:GLY:N	2.19	0.67
1:V:1096:VAL:HG22	1:V:1148:GLN:HG2	1.74	0.67
1:V:1154:GLY:C	1:V:1165:VAL:HG11	2.13	0.67
1:W:1116:GLY:O	1:W:1123:GLN:HB3	1.95	0.67
1:P:1002:GLU:HG3	1:P:1002:GLU:O	1.93	0.67
1:V:1069:ASN:OD1	1:V:1070:ASN:HA	1.94	0.67
1:Q:1208:THR:O	1:Q:1209:ALA:C	2.33	0.67
1:V:1133:ASN:O	1:V:1144:ASN:HB2	1.95	0.67
2:X:1010:THR:OG1	2:X:1015:GLU:OE1	2.11	0.67
1:Q:1002:GLU:OE1	1:Q:1005:ASN:CB	2.43	0.67
1:V:1020:LEU:HD13	1:V:1033:GLN:HB2	1.76	0.67
1:R:1116:GLY:O	1:R:1123:GLN:HB3	1.94	0.67
1:R:1238:TYR:OH	1:R:1257:GLN:HG2	1.94	0.67
1:U:1136:PHE:O	1:U:1139:LEU:HD13	1.94	0.67
1:U:1238:TYR:OH	1:U:1257:GLN:HG2	1.94	0.67
1:R:1184:ILE:CD1	1:R:1184:ILE:C	2.49	0.67
1:U:1163:SER:HB3	1:V:1030:ASP:O	1.93	0.67
1:P:1117:SER:O	1:P:1246:ARG:NH2	2.28	0.66
1:R:1310:MET:HG3	1:R:1311:SER:N	2.10	0.66
1:V:1324:ASN:HD22	1:V:1326:PHE:CB	2.06	0.66
1:Q:1047:THR:CG2	1:Q:1049:GLN:N	2.59	0.66
1:Q:1083:GLN:OE1	1:Q:1084:ASP:N	2.28	0.66
1:Q:1159:GLU:CD	1:Q:1159:GLU:C	2.53	0.66
1:V:1324:ASN:C	1:V:1326:PHE:N	2.46	0.66
1:U:1068:GLU:O	1:U:1069:ASN:HB3	1.95	0.66
1:W:1128:PHE:HD2	1:W:1150:GLN:HB3	1.60	0.66
1:Q:1190:GLY:O	1:Q:1191:PHE:CD1	2.48	0.66
1:U:1168:ASN:HA	1:U:1170:ARG:H	1.60	0.66
1:W:1049:GLN:OE1	1:W:1083:GLN:HG2	1.94	0.66
1:Q:1324:ASN:HD21	1:Q:1327:THR:HG23	1.61	0.66
1:U:1139:LEU:O	1:U:1139:LEU:HD22	1.94	0.66
1:V:1232:ILE:CG2	1:V:1234:LEU:HD22	2.25	0.66
1:R:1134:THR:HG23	1:R:1135:ASP:OD2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1210:ALA:O	1:R:1211:TYR:C	2.34	0.66
1:U:1264:GLN:HG2	1:U:1274:SER:CB	2.26	0.66
1:U:1324:ASN:C	1:U:1326:PHE:H	1.96	0.66
1:V:1191:PHE:HA	1:V:1226:LYS:O	1.95	0.66
1:Q:1133:ASN:O	1:Q:1144:ASN:HB2	1.96	0.66
1:P:1065:ALA:C	1:P:1067:ASN:H	1.98	0.66
1:P:1101:THR:HA	1:P:1237:GLN:HG3	1.78	0.66
1:P:1306:PHE:CD2	1:P:1311:SER:HA	2.31	0.66
1:Q:1153:ASN:O	1:Q:1171:ASP:HB3	1.96	0.66
1:W:1060:ILE:HA	1:W:1071:SER:CB	2.26	0.66
2:X:1025:ARG:HH11	2:X:1025:ARG:HG2	1.59	0.66
1:Q:1168:ASN:CA	1:Q:1170:ARG:N	2.59	0.66
1:P:1130:THR:HG23	1:P:1148:GLN:HB3	1.76	0.65
1:R:1101:THR:HA	1:R:1237:GLN:HG3	1.78	0.65
2:S:1007:ARG:HB2	2:S:1007:ARG:HH11	1.62	0.65
1:U:1289:TYR:O	1:U:1290:ASP:HB2	1.94	0.65
1:Q:1133:ASN:HD21	1:Q:1136:PHE:HA	1.60	0.65
1:R:1047:THR:HG23	1:R:1049:GLN:H	1.61	0.65
1:W:1168:ASN:CA	1:W:1170:ARG:N	2.58	0.65
2:X:1027:LYS:HA	2:X:1030:ARG:HA	1.77	0.65
1:Q:1165:VAL:HG12	1:Q:1166:THR:H	1.61	0.65
1:W:1083:GLN:CD	1:W:1084:ASP:N	2.50	0.65
1:W:1136:PHE:O	1:W:1139:LEU:HD13	1.95	0.65
1:W:1184:ILE:HD11	1:W:1195:GLY:H	1.60	0.65
1:Q:1211:TYR:CD1	1:Q:1211:TYR:N	2.63	0.65
1:W:1168:ASN:C	1:W:1170:ARG:H	1.95	0.65
1:U:1155:ASN:C	1:U:1165:VAL:HG11	2.16	0.65
1:U:1155:ASN:CB	1:U:1157:SER:H	2.09	0.65
1:U:1155:ASN:HB3	1:U:1157:SER:H	1.60	0.65
1:V:1068:GLU:O	1:V:1069:ASN:HB3	1.95	0.65
2:S:1038:LYS:O	2:S:1039:LYS:HB2	1.96	0.65
1:U:1165:VAL:CG1	1:U:1166:THR:H	1.99	0.65
1:V:1165:VAL:HG12	1:V:1166:THR:N	2.11	0.65
1:W:1211:TYR:HD1	1:W:1211:TYR:N	1.85	0.65
1:P:1217:ARG:HD3	1:P:1219:GLU:OE2	1.96	0.65
1:U:1168:ASN:CA	1:U:1170:ARG:H	2.09	0.65
1:U:1133:ASN:O	1:U:1144:ASN:HB2	1.97	0.65
1:Q:1009:ASN:HB2	1:R:1309:ASN:ND2	2.12	0.65
2:S:1037:VAL:O	2:S:1038:LYS:O	2.14	0.65
1:P:1133:ASN:O	1:P:1144:ASN:HB2	1.98	0.64
1:R:1045:GLN:O	1:R:1045:GLN:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1154:GLY:O	1:U:1165:VAL:CG1	2.46	0.64
2:X:1021:GLN:N	2:X:1021:GLN:HE21	1.94	0.64
1:V:1097:VAL:CG1	1:V:1097:VAL:O	2.45	0.64
1:W:1238:TYR:OH	1:W:1257:GLN:HG2	1.97	0.64
1:W:1248:GLY:HA3	1:W:1330:ALA:HB1	1.79	0.64
1:P:1135:ASP:O	1:P:1136:PHE:C	2.36	0.64
1:P:1136:PHE:O	1:P:1139:LEU:HD13	1.97	0.64
1:Q:1264:GLN:HG2	1:Q:1274:SER:CB	2.27	0.64
1:R:1134:THR:CG2	1:R:1134:THR:CA	2.73	0.64
2:S:1017:LYS:NZ	2:S:1017:LYS:CB	2.60	0.64
1:V:1157:SER:O	1:V:1161:PHE:CD1	2.50	0.64
1:V:1217:ARG:HD3	1:V:1219:GLU:OE2	1.97	0.64
1:W:1344:TYR:C	1:W:1344:TYR:CD2	2.71	0.64
1:P:1344:TYR:C	1:P:1344:TYR:CD2	2.71	0.64
1:W:1202:ARG:CZ	1:W:1215:GLY:HA3	2.27	0.64
1:P:1047:THR:CG2	1:P:1050:LEU:N	2.49	0.64
1:U:1096:VAL:C	1:U:1098:TYR:H	2.00	0.64
1:U:1247:VAL:O	1:U:1250:LEU:HB2	1.98	0.64
2:S:1037:VAL:HG12	2:S:1039:LYS:HZ3	1.62	0.64
1:U:1060:ILE:HA	1:U:1071:SER:CB	2.27	0.64
1:U:1096:VAL:C	1:U:1098:TYR:N	2.50	0.64
1:W:1162:THR:O	1:W:1165:VAL:HG23	1.92	0.64
1:R:1303:THR:HB	1:R:1313:TYR:HB3	1.79	0.64
1:W:1160:GLY:C	1:W:1161:PHE:O	2.32	0.64
1:R:1202:ARG:CZ	1:R:1215:GLY:HA3	2.26	0.64
1:V:1134:THR:CG2	1:V:1134:THR:CA	2.71	0.64
1:V:1134:THR:CG2	1:V:1134:THR:HB	2.14	0.64
1:W:1060:ILE:HG23	1:W:1071:SER:HB3	1.79	0.64
1:P:1136:PHE:HB3	1:P:1140:VAL:HG13	1.79	0.64
1:R:1060:ILE:HG23	1:R:1071:SER:HB3	1.80	0.64
1:R:1247:VAL:O	1:R:1250:LEU:HB2	1.96	0.64
1:R:1324:ASN:O	1:R:1325:GLN:C	2.34	0.64
1:W:1065:ALA:C	1:W:1067:ASN:H	2.01	0.64
1:Q:1312:THR:HG22	1:Q:1341:GLY:O	1.98	0.63
1:U:1154:GLY:C	1:U:1165:VAL:CG1	2.66	0.63
1:V:1161:PHE:O	1:V:1162:THR:HG23	1.98	0.63
1:R:1324:ASN:C	1:R:1326:PHE:N	2.50	0.63
1:U:1058:TYR:CD1	1:U:1073:THR:HA	2.33	0.63
1:U:1069:ASN:OD1	1:U:1070:ASN:HA	1.98	0.63
1:V:1116:GLY:H	1:V:1119:ASN:HD22	1.46	0.63
1:P:1069:ASN:OD1	1:P:1070:ASN:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1071:SER:O	1:P:1071:SER:OG	2.15	0.63
1:P:1123:GLN:OE1	1:P:1124:ARG:HB2	1.98	0.63
1:P:1294:ILE:O	1:P:1332:ILE:HD13	1.98	0.63
1:R:1049:GLN:OE1	1:R:1083:GLN:HG2	1.97	0.63
1:U:1147:VAL:O	1:U:1147:VAL:CG1	2.43	0.63
1:U:1154:GLY:C	1:U:1165:VAL:HG11	2.19	0.63
2:X:1042:ARG:NH1	2:X:1043:PHE:N	2.47	0.63
1:P:1310:MET:HG3	1:P:1311:SER:N	2.12	0.63
1:P:1202:ARG:CZ	1:P:1215:GLY:HA3	2.29	0.63
1:Q:1294:ILE:O	1:Q:1332:ILE:HD13	1.98	0.63
1:R:1279:GLN:HG3	1:R:1280:SER:N	2.13	0.63
1:P:1020:LEU:HD13	1:P:1033:GLN:HB3	1.79	0.63
1:P:1222:THR:CB	1:P:1239:THR:HB	2.28	0.63
1:R:1107:LEU:O	1:R:1108:PRO:C	2.32	0.63
1:U:1210:ALA:O	1:U:1211:TYR:C	2.36	0.63
1:V:1190:GLY:O	1:V:1191:PHE:CD1	2.50	0.63
1:V:1190:GLY:O	1:V:1191:PHE:HB2	1.99	0.63
1:P:1196:ALA:O	1:P:1222:THR:CG2	2.46	0.63
1:V:1060:ILE:HG23	1:V:1071:SER:CB	2.24	0.63
1:W:1155:ASN:N	1:W:1165:VAL:HG11	2.12	0.63
1:P:1260:GLU:HG2	1:P:1278:LEU:HB3	1.79	0.63
2:S:1012:SER:HA	2:S:1038:LYS:NZ	2.14	0.63
1:Q:1046:VAL:HG11	1:R:1306:PHE:HB3	1.81	0.63
1:Q:1303:THR:HB	1:Q:1313:TYR:HB3	1.81	0.63
1:U:1009:ASN:HB2	1:V:1309:ASN:ND2	2.14	0.63
1:P:1186:TYR:O	1:P:1192:GLY:HA2	1.99	0.62
1:R:1002:GLU:OE1	1:R:1005:ASN:HB3	1.99	0.62
1:R:1187:ASP:O	1:R:1188:TYR:C	2.37	0.62
1:Q:1118:ASP:OD1	1:R:1065:ALA:HB1	1.98	0.62
1:Q:1156:PRO:O	1:Q:1161:PHE:CG	2.52	0.62
1:U:1135:ASP:O	1:U:1136:PHE:C	2.37	0.62
1:U:1101:THR:HA	1:U:1237:GLN:HG3	1.81	0.62
1:V:1024:SER:HB2	1:V:1337:ILE:HG23	1.82	0.62
1:V:1324:ASN:C	1:V:1326:PHE:H	2.00	0.62
1:P:1135:ASP:HB3	1:P:1141:ASP:HA	1.80	0.62
1:Q:1139:LEU:O	1:Q:1139:LEU:HD22	1.99	0.62
1:Q:1191:PHE:HA	1:Q:1226:LYS:O	1.99	0.62
1:V:1154:GLY:C	1:V:1165:VAL:CG1	2.68	0.62
1:W:1202:ARG:NH2	1:W:1215:GLY:HA3	2.13	0.62
1:P:1264:GLN:HG2	1:P:1274:SER:HB2	1.81	0.62
1:P:1155:ASN:N	1:P:1165:VAL:HG11	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1184:ILE:H	1:Q:1184:ILE:HD12	1.59	0.62
1:Q:1196:ALA:O	1:Q:1222:THR:HG22	1.99	0.62
1:R:1071:SER:O	1:R:1071:SER:OG	2.11	0.62
1:R:1102:SER:O	1:R:1104:THR:N	2.32	0.62
1:V:1083:GLN:CG	1:V:1084:ASP:H	2.12	0.62
1:Q:1184:ILE:CD1	1:Q:1184:ILE:C	2.62	0.62
1:Q:1218:ALA:HB1	1:Q:1244:ALA:HB2	1.81	0.62
1:R:1211:TYR:HD1	1:R:1211:TYR:N	1.95	0.62
1:P:1134:THR:HG23	1:P:1135:ASP:OD2	1.99	0.62
1:Q:1101:THR:HA	1:Q:1237:GLN:HG3	1.82	0.62
1:V:1128:PHE:CD2	1:V:1150:GLN:HB3	2.35	0.62
1:W:1218:ALA:HB1	1:W:1244:ALA:HB2	1.81	0.62
2:X:1006:VAL:HG22	2:X:1007:ARG:NH1	2.14	0.62
1:R:1136:PHE:HB3	1:R:1140:VAL:HG13	1.80	0.62
1:R:1154:GLY:C	1:R:1165:VAL:HG11	2.19	0.62
1:R:1306:PHE:CD2	1:R:1311:SER:HA	2.35	0.62
1:U:1107:LEU:HD21	1:U:1262:VAL:CG2	2.30	0.62
1:W:1135:ASP:HB3	1:W:1141:ASP:HA	1.81	0.62
1:Q:1135:ASP:HB3	1:Q:1141:ASP:HA	1.82	0.62
1:R:1135:ASP:O	1:R:1138:GLY:N	2.29	0.62
1:U:1184:ILE:HD11	1:U:1195:GLY:H	1.63	0.62
1:W:1294:ILE:O	1:W:1332:ILE:HD13	1.99	0.62
1:P:1324:ASN:HD22	1:P:1326:PHE:HB3	1.64	0.61
1:Q:1002:GLU:HG3	1:Q:1002:GLU:O	2.00	0.61
1:Q:1047:THR:CG2	1:Q:1049:GLN:H	2.14	0.61
1:R:1133:ASN:HD21	1:R:1136:PHE:HA	1.65	0.61
1:U:1136:PHE:HB3	1:U:1140:VAL:HG13	1.82	0.61
1:P:1139:LEU:O	1:P:1140:VAL:CG1	2.44	0.61
1:P:1309:ASN:ND2	1:R:1009:ASN:HB2	2.14	0.61
1:R:1159:GLU:OE1	1:R:1159:GLU:CA	2.48	0.61
1:U:1128:PHE:HD2	1:U:1150:GLN:HB3	1.64	0.61
1:U:1147:VAL:O	1:U:1147:VAL:HG12	2.00	0.61
1:W:1299:ASP:OD1	1:W:1300:VAL:N	2.33	0.61
1:W:1313:TYR:CZ	1:W:1341:GLY:HA3	2.35	0.61
1:P:1036:MET:HG2	1:P:1037:ARG:N	2.15	0.61
1:R:1050:LEU:HD21	1:R:1080:LEU:HG	1.82	0.61
1:R:1324:ASN:HD22	1:R:1326:PHE:CB	2.13	0.61
1:V:1131:TYR:HB3	1:V:1147:VAL:HG12	1.83	0.61
1:V:1255:LYS:HB3	1:V:1283:LYS:HB2	1.82	0.61
1:W:1152:LYS:HE3	1:W:1203:THR:HG22	1.81	0.61
1:P:1064:SER:HA	1:R:1126:ASN:OD1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:1135:ASP:O	1:U:1138:GLY:N	2.30	0.61
1:W:1247:VAL:O	1:W:1250:LEU:HB2	2.00	0.61
1:P:1184:ILE:O	1:P:1184:ILE:CG1	2.49	0.61
1:P:1289:TYR:CD1	1:P:1326:PHE:HD1	2.17	0.61
1:U:1134:THR:HG23	1:U:1135:ASP:OD2	2.00	0.61
1:V:1051:THR:HG23	1:V:1081:LYS:HB3	1.81	0.61
1:W:1051:THR:HG23	1:W:1081:LYS:HB3	1.83	0.61
1:P:1096:VAL:C	1:P:1098:TYR:N	2.54	0.61
1:P:1272:ARG:HG2	1:P:1272:ARG:O	2.01	0.61
1:R:1049:GLN:OE1	1:R:1083:GLN:CG	2.49	0.61
1:U:1309:ASN:ND2	1:W:1009:ASN:CB	2.64	0.61
1:Q:1133:ASN:ND2	1:Q:1136:PHE:HA	2.16	0.61
1:U:1126:ASN:OD1	1:V:1064:SER:CA	2.49	0.61
1:P:1072:TRP:CD1	1:Q:1066:GLU:HG2	2.36	0.60
1:P:1128:PHE:HD2	1:P:1150:GLN:HB3	1.64	0.60
1:Q:1324:ASN:O	1:Q:1325:GLN:C	2.38	0.60
1:R:1095:GLY:HA2	1:R:1148:GLN:OE1	2.01	0.60
1:V:1231:ASN:O	1:V:1265:TYR:HA	2.02	0.60
1:P:1030:ASP:O	1:R:1163:SER:HB3	2.00	0.60
1:U:1294:ILE:O	1:U:1332:ILE:HD13	2.01	0.60
1:V:1195:GLY:HA2	1:V:1222:THR:O	2.01	0.60
1:W:1257:GLN:OE1	1:W:1283:LYS:NZ	2.33	0.60
1:Q:1334:THR:CA	1:Q:1334:THR:CG2	2.76	0.60
1:R:1211:TYR:N	1:R:1211:TYR:CD1	2.66	0.60
1:U:1036:MET:HG2	1:U:1037:ARG:N	2.15	0.60
1:W:1068:GLU:O	1:W:1069:ASN:CB	2.47	0.60
1:W:1165:VAL:HA	1:W:1166:THR:HG22	1.83	0.60
1:P:1060:ILE:HA	1:P:1071:SER:HB2	1.83	0.60
1:V:1049:GLN:OE1	1:V:1083:GLN:HG2	2.02	0.60
1:V:1190:GLY:O	1:V:1191:PHE:CB	2.48	0.60
1:W:1264:GLN:HG2	1:W:1274:SER:CB	2.31	0.60
1:Q:1324:ASN:O	1:Q:1326:PHE:N	2.34	0.60
1:U:1154:GLY:O	1:U:1165:VAL:HG12	2.02	0.60
1:V:1126:ASN:OD1	1:W:1064:SER:HA	2.01	0.60
1:P:1060:ILE:HG23	1:P:1071:SER:HB3	1.84	0.60
1:P:1187:ASP:O	1:P:1188:TYR:C	2.40	0.60
1:Q:1079:GLY:HA3	1:Q:1088:PHE:O	2.01	0.60
1:R:1083:GLN:CG	1:R:1084:ASP:H	2.14	0.60
1:U:1060:ILE:CG2	1:U:1071:SER:HB3	2.27	0.60
1:W:1184:ILE:H	1:W:1184:ILE:HD12	1.66	0.60
1:P:1264:GLN:HG2	1:P:1274:SER:CB	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1324:ASN:HD22	1:Q:1327:THR:H	1.48	0.60
1:R:1128:PHE:CD2	1:R:1150:GLN:HB3	2.37	0.60
1:U:1248:GLY:HA3	1:U:1330:ALA:HB1	1.83	0.60
1:W:1324:ASN:O	1:W:1325:GLN:C	2.38	0.60
2:X:1026:MET:O	2:X:1030:ARG:C	2.40	0.60
1:Q:1047:THR:HG23	1:Q:1049:GLN:H	1.66	0.60
1:Q:1289:TYR:O	1:Q:1290:ASP:CB	2.48	0.60
1:R:1196:ALA:HB3	1:R:1222:THR:HG23	1.84	0.60
1:U:1023:PHE:O	1:U:1338:VAL:N	2.32	0.60
1:P:1168:ASN:CA	1:P:1170:ARG:N	2.65	0.60
1:Q:1139:LEU:O	1:Q:1140:VAL:HG12	2.02	0.60
1:R:1155:ASN:HB3	1:R:1157:SER:H	1.67	0.60
1:W:1184:ILE:CD1	1:W:1184:ILE:C	2.63	0.60
1:R:1065:ALA:C	1:R:1067:ASN:H	2.05	0.59
1:R:1133:ASN:O	1:R:1144:ASN:CB	2.50	0.59
1:Q:1045:GLN:HG3	1:Q:1045:GLN:O	2.02	0.59
1:Q:1202:ARG:CZ	1:Q:1215:GLY:HA3	2.32	0.59
1:R:1147:VAL:O	1:R:1147:VAL:CG1	2.48	0.59
1:V:1036:MET:CE	1:V:1038:LEU:HB3	2.33	0.59
1:V:1050:LEU:HD21	1:V:1080:LEU:HG	1.83	0.59
1:V:1168:ASN:O	1:V:1169:GLY:C	2.40	0.59
1:R:1043:GLU:HA	1:R:1052:GLY:O	2.03	0.59
1:U:1196:ALA:HB3	1:U:1222:THR:HG23	1.83	0.59
1:P:1324:ASN:HD22	1:P:1327:THR:H	1.49	0.59
1:U:1097:VAL:O	1:U:1097:VAL:CG1	2.47	0.59
1:U:1160:GLY:O	1:U:1161:PHE:O	2.21	0.59
1:U:1344:TYR:C	1:U:1344:TYR:CD2	2.75	0.59
1:V:1147:VAL:O	1:V:1147:VAL:CG1	2.50	0.59
1:W:1208:THR:C	1:W:1210:ALA:H	2.03	0.59
1:Q:1107:LEU:N	1:Q:1107:LEU:HD23	2.18	0.59
1:Q:1210:ALA:O	1:Q:1211:TYR:C	2.40	0.59
1:P:1020:LEU:HD22	1:P:1021:HIS:N	2.17	0.59
1:U:1053:TYR:OH	1:U:1089:ASP:OD2	2.19	0.59
1:V:1260:GLU:CG	1:V:1278:LEU:HD13	2.33	0.59
1:Q:1060:ILE:HA	1:Q:1071:SER:CB	2.32	0.59
1:Q:1324:ASN:C	1:Q:1326:PHE:N	2.55	0.59
1:R:1162:THR:C	1:R:1165:VAL:CG2	2.71	0.59
1:U:1266:GLN:HG3	1:U:1266:GLN:O	2.01	0.59
1:W:1002:GLU:OE1	1:W:1005:ASN:CB	2.50	0.59
1:Q:1145:PHE:HA	1:Q:1183:SER:O	2.03	0.59
1:Q:1154:GLY:C	1:Q:1165:VAL:HG11	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1272:ARG:O	1:V:1272:ARG:HG2	2.01	0.59
2:X:1012:SER:HB2	2:X:1013:PRO:HD3	1.85	0.59
1:Q:1017:VAL:HG12	1:Q:1018:ASP:N	2.16	0.59
1:Q:1096:VAL:C	1:Q:1098:TYR:N	2.56	0.59
1:Q:1154:GLY:O	1:Q:1165:VAL:CG1	2.51	0.59
1:V:1211:TYR:HB3	1:V:1287:ARG:NH1	2.18	0.59
1:W:1230:ASN:C	1:W:1231:ASN:ND2	2.56	0.59
1:W:1324:ASN:ND2	1:W:1327:THR:H	2.01	0.59
1:R:1164:GLY:C	1:R:1165:VAL:CG2	2.71	0.59
2:S:1007:ARG:HG3	2:S:1037:VAL:HB	1.85	0.59
1:V:1102:SER:O	1:V:1103:TRP:C	2.41	0.59
1:P:1168:ASN:CA	1:P:1170:ARG:H	2.16	0.58
1:P:1168:ASN:HA	1:P:1170:ARG:N	2.18	0.58
1:R:1299:ASP:OD1	1:R:1300:VAL:N	2.36	0.58
2:S:1018:LYS:O	2:S:1020:ALA:N	2.28	0.58
1:U:1292:GLU:HG2	1:U:1326:PHE:CD2	2.38	0.58
1:V:1187:ASP:O	1:V:1188:TYR:C	2.40	0.58
1:U:1324:ASN:HD22	1:U:1326:PHE:CB	2.16	0.58
1:R:1116:GLY:N	1:R:1119:ASN:HD22	2.01	0.58
1:R:1208:THR:C	1:R:1210:ALA:H	2.06	0.58
2:S:1018:LYS:HB2	2:S:1018:LYS:NZ	2.17	0.58
1:W:1134:THR:HG23	1:W:1135:ASP:OD2	2.03	0.58
1:W:1136:PHE:HB3	1:W:1140:VAL:HG13	1.85	0.58
1:P:1139:LEU:C	1:P:1140:VAL:HG12	2.24	0.58
1:V:1002:GLU:OE1	1:V:1005:ASN:CB	2.51	0.58
1:V:1155:ASN:N	1:V:1165:VAL:HG11	2.18	0.58
1:W:1272:ARG:HG2	1:W:1272:ARG:O	2.04	0.58
1:U:1023:PHE:CD2	1:U:1023:PHE:N	2.72	0.58
1:W:1096:VAL:O	1:W:1098:TYR:N	2.36	0.58
1:P:1155:ASN:CB	1:P:1157:SER:H	2.16	0.58
1:Q:1083:GLN:CD	1:Q:1084:ASP:H	2.06	0.58
2:S:1012:SER:H	2:S:1040:THR:HA	1.68	0.58
1:U:1036:MET:HE1	1:U:1038:LEU:HB3	1.86	0.58
1:W:1324:ASN:HA	1:W:1328:ARG:NH2	2.19	0.58
2:X:1042:ARG:NH1	2:X:1043:PHE:H	2.01	0.58
1:P:1211:TYR:N	1:P:1211:TYR:CD1	2.72	0.58
1:P:1116:GLY:O	1:P:1123:GLN:HB3	2.03	0.58
1:P:1315:ASP:O	1:P:1339:ALA:N	2.35	0.58
1:Q:1072:TRP:CD1	1:R:1066:GLU:HG2	2.39	0.58
1:W:1135:ASP:HB3	1:W:1142:GLY:H	1.69	0.58
1:W:1202:ARG:HE	1:W:1215:GLY:HA3	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1049:GLN:OE1	1:P:1083:GLN:CG	2.52	0.58
1:Q:1336:ASN:ND2	1:Q:1336:ASN:H	2.00	0.58
1:W:1071:SER:OG	1:W:1071:SER:O	2.19	0.58
1:W:1312:THR:HG23	1:W:1342:LEU:HD13	1.85	0.58
2:X:1026:MET:SD	2:X:1033:SER:CA	2.91	0.58
1:R:1222:THR:CB	1:R:1239:THR:HB	2.33	0.58
1:R:1324:ASN:O	1:R:1326:PHE:N	2.36	0.58
1:V:1247:VAL:O	1:V:1250:LEU:HB2	2.04	0.58
1:U:1306:PHE:CD2	1:U:1311:SER:HA	2.39	0.57
1:U:1310:MET:HG3	1:U:1311:SER:N	2.16	0.57
1:V:1017:VAL:HG12	1:V:1018:ASP:N	2.18	0.57
2:X:1018:LYS:HD3	2:X:1021:GLN:OE1	2.04	0.57
1:P:1077:PHE:CE2	1:P:1093:ASN:OD1	2.57	0.57
1:Q:1156:PRO:O	1:Q:1161:PHE:CE1	2.57	0.57
1:Q:1344:TYR:C	1:Q:1344:TYR:CD2	2.76	0.57
1:U:1017:VAL:CG1	1:U:1018:ASP:N	2.67	0.57
1:V:1162:THR:O	1:V:1165:VAL:HG23	1.99	0.57
1:W:1036:MET:HE1	1:W:1038:LEU:CB	2.34	0.57
1:R:1168:ASN:O	1:R:1170:ARG:N	2.30	0.57
1:V:1107:LEU:N	1:V:1107:LEU:HD23	2.19	0.57
1:V:1324:ASN:O	1:V:1325:GLN:C	2.42	0.57
1:W:1156:PRO:O	1:W:1161:PHE:CD2	2.57	0.57
1:Q:1027:LYS:HA	1:Q:1030:ASP:HB2	1.86	0.57
1:Q:1037:ARG:NH1	1:Q:1074:ARG:NH2	2.53	0.57
1:R:1162:THR:H	1:R:1165:VAL:HG21	1.70	0.57
1:R:1294:ILE:O	1:R:1332:ILE:HD13	2.04	0.57
1:U:1164:GLY:C	1:U:1165:VAL:HG22	2.24	0.57
1:V:1136:PHE:O	1:V:1139:LEU:HD13	2.03	0.57
1:P:1287:ARG:HD3	1:U:1287:ARG:CD	2.18	0.57
1:V:1047:THR:HG22	1:V:1048:ASP:N	2.13	0.57
1:V:1097:VAL:O	1:V:1097:VAL:HG13	2.05	0.57
1:P:1163:SER:OG	1:P:1164:GLY:N	2.36	0.57
1:Q:1168:ASN:O	1:Q:1169:GLY:C	2.42	0.57
1:Q:1163:SER:OG	1:Q:1164:GLY:N	2.38	0.57
1:V:1047:THR:HG22	1:V:1050:LEU:N	2.12	0.57
1:W:1092:ARG:HH11	1:W:1126:ASN:ND2	2.02	0.57
1:P:1144:ASN:O	1:P:1185:THR:N	2.37	0.57
1:P:1160:GLY:O	1:P:1161:PHE:C	2.41	0.57
1:P:1211:TYR:HD1	1:P:1211:TYR:N	2.00	0.57
1:Q:1162:THR:O	1:Q:1163:SER:C	2.43	0.57
1:R:1154:GLY:O	1:R:1165:VAL:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:1026:MET:HE1	2:S:1033:SER:HA	1.86	0.57
1:U:1309:ASN:HD21	1:W:1009:ASN:CB	2.18	0.57
1:V:1144:ASN:C	1:V:1144:ASN:HD22	2.08	0.57
1:V:1144:ASN:N	1:V:1144:ASN:ND2	2.51	0.57
1:V:1279:GLN:HG3	1:V:1280:SER:N	2.19	0.57
1:W:1135:ASP:O	1:W:1136:PHE:C	2.42	0.57
1:Q:1165:VAL:HG12	1:Q:1166:THR:N	2.19	0.56
1:R:1037:ARG:NE	1:R:1059:GLN:HE21	2.02	0.56
1:R:1058:TYR:CD1	1:R:1073:THR:HA	2.39	0.56
1:R:1196:ALA:O	1:R:1222:THR:HG22	2.05	0.56
1:U:1202:ARG:HE	1:U:1215:GLY:HA3	1.68	0.56
1:U:1208:THR:O	1:U:1209:ALA:C	2.39	0.56
1:P:1171:ASP:N	1:P:1171:ASP:OD2	2.38	0.56
1:U:1168:ASN:O	1:U:1169:GLY:C	2.39	0.56
1:U:1211:TYR:HB2	1:U:1250:LEU:O	2.04	0.56
1:P:1083:GLN:CD	1:P:1084:ASP:N	2.59	0.56
1:P:1097:VAL:O	1:P:1101:THR:HG23	2.05	0.56
1:P:1134:THR:HG23	1:P:1135:ASP:N	2.21	0.56
1:R:1088:PHE:HA	1:R:1130:THR:O	2.05	0.56
1:V:1145:PHE:HA	1:V:1183:SER:O	2.05	0.56
1:V:1211:TYR:CD1	1:V:1211:TYR:N	2.73	0.56
1:W:1058:TYR:HD1	1:W:1073:THR:HA	1.70	0.56
1:W:1083:GLN:CG	1:W:1084:ASP:H	2.18	0.56
1:W:1147:VAL:O	1:W:1147:VAL:HG12	2.05	0.56
1:P:1139:LEU:O	1:P:1139:LEU:HD22	2.06	0.56
1:R:1102:SER:C	1:R:1104:THR:N	2.58	0.56
1:U:1208:THR:C	1:U:1210:ALA:H	2.02	0.56
1:U:1313:TYR:CZ	1:U:1341:GLY:HA3	2.40	0.56
1:V:1026:ASN:HB2	1:V:1335:ASP:OD2	2.05	0.56
1:P:1202:ARG:HE	1:P:1215:GLY:HA3	1.71	0.56
1:P:1232:ILE:CG2	1:P:1234:LEU:HD22	2.35	0.56
1:Q:1107:LEU:HD21	1:Q:1262:VAL:CG2	2.36	0.56
1:R:1162:THR:C	1:R:1165:VAL:HG21	2.25	0.56
2:S:1028:LYS:H	2:S:1029:VAL:C	2.08	0.56
1:U:1160:GLY:C	1:U:1161:PHE:O	2.44	0.56
1:P:1191:PHE:HA	1:P:1226:LYS:O	2.05	0.56
1:Q:1037:ARG:CG	1:Q:1059:GLN:HG3	2.32	0.56
1:R:1208:THR:O	1:R:1208:THR:OG1	2.14	0.56
1:V:1036:MET:CE	1:V:1038:LEU:HD22	2.35	0.56
1:V:1260:GLU:HG2	1:V:1278:LEU:CD1	2.36	0.56
1:W:1049:GLN:OE1	1:W:1083:GLN:CG	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1168:ASN:OD1	1:W:1168:ASN:N	2.38	0.56
1:W:1208:THR:O	1:W:1209:ALA:C	2.40	0.56
1:P:1316:TYR:CD1	1:P:1338:VAL:HG22	2.41	0.56
1:Q:1036:MET:HE1	1:Q:1038:LEU:HB3	1.87	0.56
1:W:1107:LEU:O	1:W:1108:PRO:C	2.39	0.56
1:P:1324:ASN:HA	1:P:1328:ARG:NH2	2.21	0.56
1:R:1002:GLU:OE1	1:R:1005:ASN:HB2	2.06	0.56
1:U:1085:VAL:O	1:U:1131:TYR:OH	2.22	0.56
1:U:1168:ASN:N	1:U:1168:ASN:OD1	2.37	0.56
2:X:1023:GLN:CB	2:X:1035:THR:HA	2.35	0.56
1:R:1287:ARG:HD3	1:V:1287:ARG:CD	2.33	0.56
2:S:1010:THR:HG23	2:S:1036:CYS:SG	2.46	0.56
1:V:1154:GLY:O	1:V:1165:VAL:HG12	2.05	0.56
1:P:1082:PHE:O	1:P:1083:GLN:HB3	2.06	0.56
2:S:1018:LYS:HB2	2:S:1018:LYS:HZ2	1.70	0.56
1:U:1184:ILE:HD13	1:U:1184:ILE:N	2.21	0.56
1:W:1083:GLN:OE1	1:W:1084:ASP:N	2.39	0.56
1:Q:1036:MET:HE1	1:Q:1038:LEU:HD22	1.88	0.55
1:R:1230:ASN:O	1:R:1232:ILE:N	2.39	0.55
2:S:1032:PRO:HD3	1:W:1291:ASP:OD2	2.05	0.55
1:V:1045:GLN:O	1:V:1045:GLN:CG	2.53	0.55
1:W:1083:GLN:CD	1:W:1084:ASP:H	2.08	0.55
1:W:1133:ASN:HD21	1:W:1137:PHE:N	2.04	0.55
1:P:1184:ILE:H	1:P:1184:ILE:HD12	1.65	0.55
1:R:1135:ASP:HA	1:R:1143:LEU:O	2.06	0.55
1:R:1308:LYS:O	1:R:1308:LYS:CD	2.48	0.55
1:P:1037:ARG:NE	1:P:1059:GLN:HE21	2.03	0.55
1:R:1160:GLY:C	1:R:1161:PHE:O	2.43	0.55
1:U:1272:ARG:HG2	1:U:1272:ARG:O	2.07	0.55
1:W:1161:PHE:O	1:W:1162:THR:HG23	2.06	0.55
1:W:1230:ASN:C	1:W:1231:ASN:HD22	2.09	0.55
1:P:1255:LYS:HB3	1:P:1283:LYS:HB2	1.89	0.55
1:U:1190:GLY:O	1:U:1191:PHE:CD1	2.60	0.55
1:V:1009:ASN:HB2	1:W:1309:ASN:ND2	2.21	0.55
1:V:1190:GLY:O	1:V:1191:PHE:HD1	1.90	0.55
1:W:1099:ASP:OD1	1:W:1132:ARG:NH2	2.39	0.55
1:Q:1093:ASN:O	1:Q:1124:ARG:HA	2.06	0.55
1:U:1187:ASP:O	1:U:1188:TYR:C	2.45	0.55
1:V:1289:TYR:CD1	1:V:1326:PHE:HD1	2.25	0.55
1:W:1065:ALA:C	1:W:1067:ASN:N	2.60	0.55
2:X:1019:CYS:O	2:X:1023:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1144:ASN:C	1:Q:1144:ASN:HD22	2.10	0.55
1:Q:1190:GLY:O	1:Q:1191:PHE:CB	2.54	0.55
1:Q:1255:LYS:NZ	1:Q:1257:GLN:HE21	2.05	0.55
1:R:1083:GLN:CG	1:R:1084:ASP:N	2.69	0.55
2:S:1010:THR:OG1	2:S:1038:LYS:HA	2.07	0.55
1:P:1116:GLY:N	1:P:1119:ASN:HD22	2.01	0.55
1:Q:1082:PHE:O	1:Q:1083:GLN:HB3	2.07	0.55
1:V:1133:ASN:HD22	1:V:1145:PHE:HE1	1.53	0.55
1:Q:1155:ASN:N	1:Q:1165:VAL:HG11	2.22	0.55
1:Q:1187:ASP:O	1:Q:1188:TYR:C	2.46	0.55
1:Q:1313:TYR:CZ	1:Q:1341:GLY:HA3	2.41	0.55
1:R:1060:ILE:HA	1:R:1071:SER:HB2	1.88	0.55
1:R:1196:ALA:HB3	1:R:1222:THR:CG2	2.37	0.55
1:U:1155:ASN:N	1:U:1165:VAL:HG11	2.21	0.55
1:V:1277:TYR:C	1:V:1278:LEU:HD22	2.28	0.55
1:W:1324:ASN:HA	1:W:1328:ARG:HH22	1.72	0.55
1:P:1005:ASN:C	1:P:1005:ASN:OD1	2.45	0.55
1:Q:1310:MET:HG3	1:Q:1311:SER:N	2.22	0.55
1:Q:1324:ASN:HD22	1:Q:1326:PHE:CB	2.15	0.55
1:V:1005:ASN:OD1	1:V:1005:ASN:O	2.25	0.55
1:V:1296:LYS:HG2	1:V:1320:LEU:HB2	1.89	0.55
1:W:1133:ASN:ND2	1:W:1136:PHE:HA	2.22	0.55
1:P:1118:ASP:OD1	1:Q:1065:ALA:HB1	2.07	0.55
1:R:1235:ALA:O	1:R:1261:ALA:HA	2.07	0.55
1:U:1102:SER:O	1:U:1103:TRP:C	2.46	0.54
1:P:1157:SER:O	1:P:1161:PHE:CD1	2.57	0.54
1:Q:1026:ASN:O	1:Q:1028:ASP:N	2.33	0.54
1:Q:1202:ARG:HE	1:Q:1215:GLY:HA3	1.69	0.54
1:U:1255:LYS:HB3	1:U:1283:LYS:HB2	1.88	0.54
1:W:1165:VAL:CG1	1:W:1166:THR:H	2.03	0.54
1:P:1283:LYS:O	1:P:1284:ASN:C	2.45	0.54
1:Q:1275:LEU:HD22	1:Q:1276:ALA:N	2.22	0.54
1:Q:1296:LYS:HG2	1:Q:1320:LEU:HB2	1.89	0.54
1:Q:1334:THR:CB	1:Q:1334:THR:HA	2.18	0.54
1:R:1119:ASN:HB2	1:R:1246:ARG:NH2	2.23	0.54
2:X:1018:LYS:HA	2:X:1018:LYS:HE3	1.90	0.54
1:P:1049:GLN:OE1	1:P:1083:GLN:HG3	2.07	0.54
1:P:1066:GLU:HG2	1:R:1072:TRP:CD1	2.42	0.54
1:Q:1190:GLY:O	1:Q:1191:PHE:HB2	2.07	0.54
1:P:1107:LEU:HD21	1:P:1262:VAL:CG2	2.37	0.54
1:P:1134:THR:CG2	1:P:1135:ASP:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1164:GLY:C	1:Q:1165:VAL:CG2	2.62	0.54
1:Q:1255:LYS:HB3	1:Q:1283:LYS:HB2	1.90	0.54
1:R:1009:ASN:HA	1:R:1044:THR:HA	1.89	0.54
1:U:1153:ASN:O	1:U:1171:ASP:HB3	2.08	0.54
1:V:1168:ASN:CA	1:V:1170:ARG:N	2.67	0.54
1:W:1047:THR:HG22	1:W:1050:LEU:N	2.07	0.54
1:W:1310:MET:HG3	1:W:1311:SER:N	2.23	0.54
1:U:1144:ASN:N	1:U:1144:ASN:ND2	2.54	0.54
1:V:1133:ASN:O	1:V:1144:ASN:CB	2.55	0.54
1:Q:1058:TYR:CD1	1:Q:1073:THR:HA	2.37	0.54
1:Q:1069:ASN:OD1	1:Q:1070:ASN:HB3	2.07	0.54
1:Q:1306:PHE:CD2	1:Q:1311:SER:HA	2.43	0.54
2:X:1006:VAL:HG23	2:X:1007:ARG:HH12	1.73	0.54
1:Q:1083:GLN:OE1	1:Q:1083:GLN:C	2.46	0.54
2:S:1038:LYS:O	2:S:1039:LYS:CB	2.56	0.54
1:V:1036:MET:HE1	1:V:1038:LEU:CD2	2.38	0.54
1:V:1162:THR:O	1:V:1163:SER:C	2.46	0.54
1:W:1098:TYR:CE2	1:W:1102:SER:HB3	2.42	0.54
1:P:1058:TYR:CD1	1:P:1073:THR:HA	2.40	0.54
1:V:1058:TYR:CD1	1:V:1073:THR:HA	2.38	0.54
1:V:1184:ILE:HD11	1:V:1195:GLY:H	1.72	0.54
1:W:1045:GLN:O	1:W:1045:GLN:CG	2.56	0.54
2:X:1023:GLN:C	2:X:1026:MET:CB	2.76	0.54
1:P:1131:TYR:O	1:P:1146:ALA:HA	2.08	0.53
1:P:1147:VAL:O	1:P:1147:VAL:CG1	2.53	0.53
1:R:1210:ALA:O	1:R:1212:ILE:N	2.41	0.53
2:S:1009:CYS:SG	2:S:1044:GLU:HB2	2.47	0.53
1:U:1107:LEU:O	1:U:1108:PRO:C	2.45	0.53
1:V:1288:GLY:O	1:V:1290:ASP:N	2.41	0.53
2:X:1026:MET:O	2:X:1030:ARG:CA	2.56	0.53
1:U:1096:VAL:O	1:U:1097:VAL:C	2.43	0.53
1:U:1107:LEU:CD2	1:U:1262:VAL:CG2	2.86	0.53
1:Q:1096:VAL:O	1:Q:1098:TYR:N	2.41	0.53
1:Q:1271:LEU:HG	1:Q:1272:ARG:N	2.24	0.53
2:S:1011:THR:CG2	2:S:1041:SER:HA	2.27	0.53
1:U:1060:ILE:HA	1:U:1071:SER:HB2	1.89	0.53
1:U:1289:TYR:CD1	1:U:1326:PHE:HD1	2.26	0.53
1:U:1303:THR:HA	1:U:1313:TYR:HA	1.90	0.53
1:V:1171:ASP:OD2	1:V:1171:ASP:N	2.41	0.53
1:W:1196:ALA:O	1:W:1222:THR:HG22	2.08	0.53
1:P:1060:ILE:HG23	1:P:1071:SER:CB	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1184:ILE:N	1:P:1184:ILE:HD12	2.23	0.53
1:Q:1128:PHE:HD2	1:Q:1150:GLN:HB3	1.73	0.53
2:S:1015:GLU:OE2	2:S:1016:SER:N	2.41	0.53
1:W:1336:ASN:H	1:W:1336:ASN:ND2	2.06	0.53
1:Q:1312:THR:HG23	1:Q:1342:LEU:HD13	1.90	0.53
1:U:1202:ARG:CZ	1:U:1215:GLY:HA3	2.39	0.53
1:U:1289:TYR:O	1:U:1290:ASP:CB	2.57	0.53
1:V:1306:PHE:CD2	1:V:1311:SER:HA	2.44	0.53
1:P:1037:ARG:CG	1:P:1059:GLN:HG3	2.36	0.53
1:P:1299:ASP:OD1	1:P:1300:VAL:N	2.41	0.53
1:Q:1168:ASN:OD1	1:Q:1168:ASN:N	2.41	0.53
1:U:1284:ASN:N	1:U:1291:ASP:OD1	2.41	0.53
1:V:1107:LEU:O	1:V:1108:PRO:C	2.43	0.53
1:W:1056:TRP:HA	1:W:1075:VAL:O	2.09	0.53
1:W:1135:ASP:O	1:W:1138:GLY:N	2.38	0.53
2:S:1007:ARG:CD	2:S:1037:VAL:HG21	2.31	0.53
1:U:1065:ALA:HB1	1:W:1118:ASP:OD1	2.08	0.53
1:V:1134:THR:HG23	1:V:1135:ASP:OD2	2.08	0.53
1:W:1093:ASN:O	1:W:1124:ARG:HA	2.09	0.53
1:P:1096:VAL:O	1:P:1098:TYR:N	2.42	0.53
1:Q:1097:VAL:O	1:Q:1097:VAL:CG1	2.57	0.53
1:R:1133:ASN:O	1:R:1144:ASN:HB3	2.09	0.53
1:R:1160:GLY:O	1:R:1161:PHE:C	2.46	0.53
1:R:1289:TYR:CD1	1:R:1326:PHE:HD1	2.26	0.53
2:S:1017:LYS:NZ	2:S:1017:LYS:HB3	2.22	0.53
1:U:1133:ASN:O	1:U:1144:ASN:CB	2.57	0.53
1:U:1157:SER:C	1:U:1161:PHE:HD1	2.10	0.53
1:U:1230:ASN:C	1:U:1231:ASN:ND2	2.61	0.53
1:W:1035:TYR:HE2	1:W:1037:ARG:HE	1.57	0.53
1:R:1047:THR:HG22	1:R:1050:LEU:N	2.12	0.53
1:R:1130:THR:HG23	1:R:1148:GLN:HB3	1.91	0.53
1:R:1287:ARG:HH11	1:R:1287:ARG:HG3	1.72	0.53
2:X:1041:SER:CB	2:X:1044:GLU:HB2	2.36	0.53
1:P:1208:THR:C	1:P:1210:ALA:N	2.49	0.53
1:P:1310:MET:HE2	1:R:1080:LEU:HD13	1.91	0.53
1:Q:1001:ALA:N	1:Q:1346:PHE:OXT	2.41	0.53
1:Q:1018:ASP:CG	1:Q:1343:VAL:HG22	2.30	0.53
1:U:1036:MET:CE	1:U:1038:LEU:HB3	2.39	0.53
1:V:1211:TYR:HD1	1:V:1211:TYR:N	1.99	0.53
1:Q:1319:ASN:ND2	1:Q:1334:THR:C	2.63	0.52
2:S:1029:VAL:HG21	1:W:1288:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1135:ASP:HA	1:V:1143:LEU:O	2.10	0.52
1:W:1043:GLU:HA	1:W:1052:GLY:O	2.08	0.52
1:W:1144:ASN:HD22	1:W:1144:ASN:C	2.11	0.52
1:R:1005:ASN:C	1:R:1005:ASN:OD1	2.47	0.52
1:R:1147:VAL:O	1:R:1147:VAL:HG12	2.09	0.52
1:U:1088:PHE:HA	1:U:1130:THR:O	2.08	0.52
1:U:1133:ASN:HD22	1:U:1145:PHE:HE1	1.58	0.52
1:V:1135:ASP:HB3	1:V:1140:VAL:O	2.09	0.52
1:W:1208:THR:C	1:W:1210:ALA:N	2.63	0.52
1:P:1266:GLN:HB2	1:P:1272:ARG:NH1	2.25	0.52
1:Q:1334:THR:CB	1:Q:1334:THR:C	2.71	0.52
1:R:1184:ILE:HD11	1:R:1195:GLY:H	1.73	0.52
1:R:1190:GLY:O	1:R:1191:PHE:CD1	2.62	0.52
1:V:1135:ASP:O	1:V:1138:GLY:N	2.38	0.52
1:P:1046:VAL:HG11	1:Q:1306:PHE:HB3	1.92	0.52
1:P:1203:THR:OG1	1:P:1206:GLN:HG2	2.09	0.52
1:R:1133:ASN:O	1:R:1144:ASN:HB2	2.09	0.52
1:V:1027:LYS:HA	1:V:1030:ASP:HB2	1.90	0.52
1:V:1083:GLN:OE1	1:V:1083:GLN:C	2.47	0.52
1:V:1090:TYR:OH	1:W:1032:ASP:OD1	2.19	0.52
1:V:1324:ASN:HD21	1:V:1327:THR:HG23	1.74	0.52
1:P:1164:GLY:C	1:P:1165:VAL:HG22	2.29	0.52
1:P:1309:ASN:ND2	1:R:1009:ASN:CB	2.72	0.52
1:Q:1069:ASN:OD1	1:Q:1070:ASN:N	2.41	0.52
1:Q:1144:ASN:O	1:Q:1184:ILE:HA	2.09	0.52
2:S:1029:VAL:HG12	2:S:1030:ARG:H	1.74	0.52
2:S:1038:LYS:O	2:S:1039:LYS:HD3	2.10	0.52
1:V:1155:ASN:HB3	1:V:1157:SER:N	2.21	0.52
1:V:1208:THR:O	1:V:1209:ALA:C	2.46	0.52
1:V:1312:THR:HG23	1:V:1342:LEU:HD13	1.90	0.52
1:W:1289:TYR:O	1:W:1290:ASP:HB2	2.08	0.52
1:P:1045:GLN:O	1:P:1045:GLN:CG	2.55	0.52
1:P:1168:ASN:C	1:P:1170:ARG:H	2.04	0.52
1:P:1286:GLY:O	1:P:1288:GLY:O	2.28	0.52
1:Q:1136:PHE:HB3	1:Q:1140:VAL:CG1	2.40	0.52
1:R:1033:GLN:O	1:R:1034:THR:C	2.47	0.52
1:U:1037:ARG:HG2	1:U:1059:GLN:HG3	1.91	0.52
1:U:1144:ASN:C	1:U:1144:ASN:HD22	2.12	0.52
1:V:1210:ALA:O	1:V:1212:ILE:N	2.43	0.52
1:W:1231:ASN:O	1:W:1265:TYR:HA	2.10	0.52
1:P:1202:ARG:NH2	1:P:1215:GLY:HA3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1047:THR:HG23	1:Q:1049:GLN:N	2.25	0.52
1:R:1036:MET:HE1	1:R:1038:LEU:HB3	1.91	0.52
1:R:1248:GLY:HA3	1:R:1330:ALA:HB1	1.92	0.52
2:S:1014:ALA:O	2:S:1017:LYS:HG3	2.09	0.52
1:W:1017:VAL:HG12	1:W:1018:ASP:N	2.24	0.52
1:Q:1196:ALA:O	1:Q:1222:THR:CG2	2.57	0.52
1:Q:1212:ILE:HG12	1:Q:1250:LEU:O	2.10	0.52
1:Q:1230:ASN:O	1:Q:1232:ILE:N	2.43	0.52
1:U:1020:LEU:HD22	1:U:1021:HIS:N	2.25	0.52
1:U:1083:GLN:CD	1:U:1084:ASP:N	2.63	0.52
1:V:1060:ILE:HA	1:V:1071:SER:CB	2.40	0.52
1:P:1096:VAL:CG2	1:P:1148:GLN:HG2	2.39	0.52
1:Q:1051:THR:HG23	1:Q:1081:LYS:HB3	1.90	0.52
1:V:1313:TYR:CZ	1:V:1341:GLY:HA3	2.45	0.52
1:W:1308:LYS:O	1:W:1308:LYS:CD	2.54	0.52
1:Q:1042:GLY:O	1:Q:1053:TYR:HA	2.09	0.52
1:Q:1082:PHE:O	1:Q:1083:GLN:CB	2.58	0.52
1:Q:1289:TYR:CD1	1:Q:1326:PHE:HD1	2.28	0.52
1:R:1186:TYR:O	1:R:1192:GLY:HA2	2.09	0.52
1:R:1316:TYR:CD1	1:R:1338:VAL:HG22	2.44	0.52
1:R:1344:TYR:C	1:R:1344:TYR:CD2	2.83	0.52
1:V:1167:ASN:HD21	1:V:1170:ARG:HH11	1.58	0.52
1:W:1060:ILE:HG23	1:W:1071:SER:CB	2.40	0.52
1:W:1144:ASN:O	1:W:1184:ILE:HA	2.10	0.52
1:Q:1036:MET:HG2	1:Q:1037:ARG:N	2.25	0.51
1:U:1231:ASN:O	1:U:1265:TYR:HA	2.10	0.51
1:W:1317:LYS:HE3	1:W:1337:ILE:HD12	1.91	0.51
1:Q:1096:VAL:C	1:Q:1098:TYR:H	2.12	0.51
1:Q:1299:ASP:OD1	1:Q:1300:VAL:N	2.43	0.51
1:U:1102:SER:O	1:U:1104:THR:N	2.44	0.51
1:Q:1211:TYR:HB3	1:Q:1287:ARG:NH1	2.26	0.51
1:R:1096:VAL:C	1:R:1098:TYR:N	2.62	0.51
1:R:1133:ASN:ND2	1:R:1136:PHE:HA	2.25	0.51
1:R:1155:ASN:C	1:R:1165:VAL:CG1	2.79	0.51
1:R:1191:PHE:HA	1:R:1226:LYS:O	2.10	0.51
1:R:1208:THR:O	1:R:1209:ALA:C	2.47	0.51
1:R:1324:ASN:HD22	1:R:1327:THR:H	1.55	0.51
1:U:1097:VAL:O	1:U:1097:VAL:HG13	2.09	0.51
1:V:1095:GLY:HA2	1:V:1148:GLN:OE1	2.10	0.51
1:W:1082:PHE:O	1:W:1083:GLN:HB3	2.09	0.51
1:W:1083:GLN:CG	1:W:1084:ASP:N	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1156:PRO:O	1:P:1161:PHE:CG	2.64	0.51
1:Q:1095:GLY:HA2	1:Q:1148:GLN:OE1	2.10	0.51
1:Q:1118:ASP:CG	1:R:1065:ALA:HB1	2.31	0.51
1:R:1140:VAL:HG22	1:R:1141:ASP:N	2.26	0.51
1:R:1214:ASN:H	1:R:1254:ASN:HD21	1.58	0.51
1:U:1156:PRO:O	1:U:1161:PHE:CG	2.64	0.51
1:V:1184:ILE:O	1:V:1184:ILE:CG1	2.54	0.51
1:W:1214:ASN:H	1:W:1254:ASN:HD21	1.58	0.51
1:P:1147:VAL:O	1:P:1147:VAL:HG12	2.10	0.51
1:Q:1152:LYS:HE3	1:Q:1203:THR:HG22	1.93	0.51
1:R:1060:ILE:HA	1:R:1071:SER:CB	2.40	0.51
1:Q:1190:GLY:O	1:Q:1191:PHE:HD1	1.92	0.51
2:S:1012:SER:O	2:S:1013:PRO:O	2.28	0.51
2:S:1023:GLN:NE2	2:S:1024:ARG:HG2	2.26	0.51
1:W:1196:ALA:HB3	1:W:1222:THR:HG23	1.93	0.51
2:X:1021:GLN:HE21	2:X:1021:GLN:H	1.56	0.51
2:X:1038:LYS:HE2	2:X:1038:LYS:N	2.25	0.51
1:P:1133:ASN:O	1:P:1144:ASN:CB	2.58	0.51
1:Q:1137:PHE:HB2	1:Q:1139:LEU:HD12	1.92	0.51
1:R:1171:ASP:OD2	1:R:1171:ASP:N	2.44	0.51
1:V:1046:VAL:HG11	1:W:1306:PHE:HB3	1.93	0.51
1:W:1085:VAL:O	1:W:1131:TYR:OH	2.26	0.51
1:W:1260:GLU:HG2	1:W:1278:LEU:HD13	1.92	0.51
2:X:1018:LYS:O	2:X:1021:GLN:NE2	2.43	0.51
1:U:1116:GLY:O	1:U:1123:GLN:HB3	2.11	0.51
1:W:1210:ALA:O	1:W:1211:TYR:C	2.48	0.51
1:W:1260:GLU:HG2	1:W:1278:LEU:CD1	2.41	0.51
1:P:1306:PHE:HB3	1:R:1046:VAL:HG11	1.93	0.51
1:P:1325:GLN:O	1:P:1329:ASP:CG	2.49	0.51
1:R:1162:THR:O	1:R:1163:SER:C	2.48	0.51
1:U:1162:THR:C	1:U:1165:VAL:HG21	2.28	0.51
1:U:1191:PHE:HA	1:U:1226:LYS:O	2.11	0.51
1:V:1101:THR:HA	1:V:1237:GLN:HG3	1.92	0.51
1:V:1165:VAL:CA	1:V:1166:THR:HG22	2.37	0.51
1:W:1095:GLY:HA2	1:W:1148:GLN:OE1	2.11	0.51
1:W:1102:SER:O	1:W:1104:THR:N	2.44	0.51
1:Q:1083:GLN:CG	1:Q:1084:ASP:H	2.23	0.51
1:Q:1165:VAL:CA	1:Q:1166:THR:HG22	2.40	0.51
1:U:1049:GLN:HB2	1:U:1083:GLN:HG2	1.93	0.51
1:W:1286:GLY:O	1:W:1288:GLY:O	2.28	0.51
1:V:1020:LEU:HD22	1:V:1021:HIS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1292:GLU:HG2	1:V:1326:PHE:CD2	2.46	0.50
1:W:1079:GLY:HA3	1:W:1088:PHE:O	2.12	0.50
1:P:1074:ARG:HG2	1:P:1124:ARG:NH2	2.26	0.50
1:Q:1009:ASN:CB	1:R:1309:ASN:ND2	2.74	0.50
1:R:1023:PHE:N	1:R:1023:PHE:CD2	2.78	0.50
1:R:1271:LEU:HG	1:R:1272:ARG:N	2.25	0.50
1:U:1043:GLU:HA	1:U:1052:GLY:O	2.12	0.50
1:U:1102:SER:C	1:U:1104:THR:N	2.63	0.50
1:U:1256:ALA:HA	1:U:1281:LYS:O	2.10	0.50
1:W:1133:ASN:HD21	1:W:1136:PHE:HA	1.77	0.50
1:W:1292:GLU:HG2	1:W:1326:PHE:CD2	2.47	0.50
1:U:1098:TYR:CZ	1:U:1102:SER:HB3	2.46	0.50
1:U:1152:LYS:HE3	1:U:1203:THR:HG22	1.93	0.50
1:U:1219:GLU:O	1:U:1242:TYR:N	2.33	0.50
1:V:1197:ILE:HD12	1:V:1197:ILE:N	2.26	0.50
1:W:1191:PHE:H	1:W:1227:TYR:HA	1.76	0.50
1:P:1255:LYS:NZ	1:P:1257:GLN:HE21	2.09	0.50
1:Q:1009:ASN:HA	1:Q:1044:THR:HA	1.94	0.50
1:Q:1065:ALA:C	1:Q:1067:ASN:H	2.14	0.50
1:R:1135:ASP:O	1:R:1136:PHE:C	2.49	0.50
1:U:1068:GLU:O	1:U:1069:ASN:CB	2.57	0.50
1:U:1212:ILE:O	1:U:1252:TRP:N	2.44	0.50
1:U:1337:ILE:HG22	1:U:1338:VAL:N	2.26	0.50
1:V:1096:VAL:C	1:V:1098:TYR:N	2.64	0.50
1:V:1160:GLY:O	1:V:1161:PHE:C	2.49	0.50
1:W:1005:ASN:C	1:W:1005:ASN:OD1	2.50	0.50
1:W:1096:VAL:C	1:W:1098:TYR:N	2.63	0.50
1:W:1134:THR:HG23	1:W:1135:ASP:N	2.25	0.50
1:W:1171:ASP:OD2	1:W:1171:ASP:N	2.44	0.50
1:P:1002:GLU:OE1	1:P:1005:ASN:CB	2.60	0.50
1:Q:1184:ILE:HD11	1:Q:1195:GLY:H	1.77	0.50
1:Q:1296:LYS:HG2	1:Q:1320:LEU:CB	2.42	0.50
1:R:1065:ALA:C	1:R:1067:ASN:N	2.65	0.50
1:U:1049:GLN:CG	1:U:1082:PHE:O	2.49	0.50
1:P:1001:ALA:N	1:P:1346:PHE:OXT	2.44	0.50
1:P:1289:TYR:O	1:P:1290:ASP:CB	2.57	0.50
1:Q:1107:LEU:O	1:Q:1108:PRO:C	2.45	0.50
1:R:1047:THR:HG23	1:R:1049:GLN:N	2.26	0.50
1:R:1083:GLN:OE1	1:R:1083:GLN:C	2.49	0.50
1:R:1097:VAL:O	1:R:1097:VAL:CG1	2.60	0.50
2:S:1021:GLN:CA	2:S:1024:ARG:O	2.50	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1042:GLY:O	1:V:1053:TYR:HA	2.11	0.50
2:X:1028:LYS:H	2:X:1029:VAL:C	2.14	0.50
1:P:1049:GLN:OE1	1:P:1083:GLN:HG2	2.12	0.50
1:W:1327:THR:O	1:W:1328:ARG:C	2.50	0.50
1:P:1211:TYR:O	1:P:1212:ILE:HG23	2.12	0.50
1:V:1198:SER:HG	1:V:1220:THR:HG1	1.52	0.50
2:X:1042:ARG:HH11	2:X:1043:PHE:N	2.08	0.50
1:P:1208:THR:O	1:P:1209:ALA:C	2.50	0.50
1:P:1266:GLN:O	1:P:1266:GLN:HG3	2.09	0.50
1:Q:1133:ASN:HD22	1:Q:1145:PHE:HE1	1.59	0.50
2:S:1007:ARG:HB2	2:S:1007:ARG:NH1	2.25	0.50
1:V:1020:LEU:HD13	1:V:1033:GLN:HB3	1.93	0.50
1:P:1005:ASN:OD1	1:P:1005:ASN:O	2.30	0.49
1:P:1157:SER:C	1:P:1161:PHE:HD1	2.15	0.49
1:Q:1036:MET:CE	1:Q:1038:LEU:HB3	2.42	0.49
1:Q:1135:ASP:O	1:Q:1136:PHE:C	2.50	0.49
1:Q:1160:GLY:C	1:Q:1161:PHE:O	2.51	0.49
1:U:1197:ILE:HD12	1:U:1197:ILE:N	2.27	0.49
1:W:1069:ASN:CG	1:W:1070:ASN:N	2.65	0.49
1:W:1191:PHE:HA	1:W:1226:LYS:O	2.12	0.49
1:P:1038:LEU:HD23	1:P:1038:LEU:H	1.76	0.49
1:Q:1116:GLY:O	1:Q:1123:GLN:HB3	2.12	0.49
1:Q:1130:THR:HG23	1:Q:1148:GLN:HB3	1.92	0.49
1:Q:1260:GLU:HG2	1:Q:1278:LEU:HB3	1.95	0.49
1:R:1303:THR:HA	1:R:1313:TYR:HA	1.94	0.49
1:V:1082:PHE:O	1:V:1083:GLN:HB3	2.11	0.49
1:V:1191:PHE:CA	1:V:1226:LYS:O	2.60	0.49
1:V:1312:THR:HG22	1:V:1341:GLY:O	2.12	0.49
1:P:1009:ASN:HB2	1:Q:1309:ASN:ND2	2.27	0.49
1:P:1028:ASP:OD2	1:R:1161:PHE:CD2	2.65	0.49
1:Q:1197:ILE:HD12	1:Q:1197:ILE:N	2.27	0.49
1:R:1096:VAL:HG22	1:R:1148:GLN:HG2	1.94	0.49
2:S:1037:VAL:CG1	2:S:1039:LYS:HZ2	2.19	0.49
1:U:1169:GLY:C	1:U:1170:ARG:HG3	2.32	0.49
1:U:1210:ALA:O	1:U:1212:ILE:N	2.45	0.49
1:U:1231:ASN:ND2	1:U:1231:ASN:N	2.61	0.49
1:W:1023:PHE:O	1:W:1338:VAL:N	2.38	0.49
1:W:1210:ALA:O	1:W:1212:ILE:N	2.46	0.49
1:V:1184:ILE:N	1:V:1184:ILE:HD12	2.12	0.49
1:W:1188:TYR:N	1:W:1188:TYR:CD1	2.81	0.49
1:P:1255:LYS:HZ3	1:P:1257:GLN:HE21	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1037:ARG:NH1	1:R:1074:ARG:NH2	2.60	0.49
1:R:1165:VAL:CG1	1:R:1166:THR:H	2.01	0.49
1:V:1211:TYR:O	1:V:1212:ILE:HG23	2.12	0.49
1:W:1306:PHE:CD2	1:W:1311:SER:HA	2.47	0.49
1:P:1065:ALA:HB1	1:R:1170:ARG:HD3	1.94	0.49
2:S:1007:ARG:HG3	2:S:1037:VAL:CG2	2.43	0.49
1:U:1012:ASP:OD2	1:U:1012:ASP:C	2.51	0.49
1:U:1306:PHE:HB3	1:W:1046:VAL:HG11	1.94	0.49
1:W:1012:ASP:C	1:W:1012:ASP:OD2	2.47	0.49
1:U:1037:ARG:NE	1:U:1059:GLN:HE21	2.10	0.49
1:Q:1102:SER:O	1:Q:1103:TRP:C	2.51	0.49
1:U:1324:ASN:HD21	1:U:1327:THR:HG23	1.78	0.49
1:V:1003:VAL:HG23	1:V:1011:LEU:HB3	1.95	0.49
1:V:1005:ASN:OD1	1:V:1005:ASN:C	2.51	0.49
1:U:1159:GLU:OE1	1:U:1160:GLY:N	2.46	0.49
1:W:1037:ARG:NH1	1:W:1074:ARG:CZ	2.76	0.49
1:P:1065:ALA:C	1:P:1067:ASN:N	2.67	0.49
1:P:1162:THR:O	1:P:1165:VAL:HG23	2.00	0.49
1:Q:1107:LEU:HD21	1:Q:1262:VAL:HG21	1.94	0.49
1:U:1130:THR:HG23	1:U:1148:GLN:HB3	1.95	0.49
1:U:1162:THR:O	1:U:1165:VAL:HG23	2.08	0.49
1:W:1196:ALA:O	1:W:1222:THR:CG2	2.61	0.49
1:Q:1065:ALA:C	1:Q:1067:ASN:N	2.65	0.48
1:Q:1098:TYR:CZ	1:Q:1102:SER:HB3	2.47	0.48
1:Q:1118:ASP:HB3	1:Q:1170:ARG:HB3	1.94	0.48
1:Q:1167:ASN:HD21	1:Q:1170:ARG:HH11	1.62	0.48
1:P:1096:VAL:C	1:P:1098:TYR:H	2.15	0.48
1:P:1107:LEU:CD2	1:P:1262:VAL:CG2	2.92	0.48
1:R:1272:ARG:HG2	1:R:1272:ARG:O	2.13	0.48
2:S:1019:CYS:SG	2:S:1019:CYS:O	2.71	0.48
1:V:1093:ASN:O	1:V:1124:ARG:HA	2.13	0.48
1:V:1210:ALA:O	1:V:1211:TYR:C	2.52	0.48
1:W:1037:ARG:NE	1:W:1059:GLN:HE21	2.11	0.48
1:W:1131:TYR:O	1:W:1146:ALA:HA	2.13	0.48
1:P:1135:ASP:O	1:P:1138:GLY:N	2.41	0.48
1:Q:1168:ASN:C	1:Q:1170:ARG:H	2.06	0.48
1:V:1300:VAL:O	1:V:1316:TYR:HB3	2.14	0.48
1:P:1190:GLY:O	1:P:1191:PHE:CD1	2.66	0.48
1:Q:1107:LEU:CD2	1:Q:1262:VAL:CG2	2.91	0.48
1:Q:1198:SER:HG	1:Q:1220:THR:HG1	1.62	0.48
1:Q:1255:LYS:HZ2	1:Q:1257:GLN:HE21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1299:ASP:OD1	1:R:1299:ASP:C	2.51	0.48
1:V:1036:MET:CG	1:V:1037:ARG:N	2.73	0.48
1:W:1324:ASN:CA	1:W:1328:ARG:NH2	2.77	0.48
1:W:1325:GLN:O	1:W:1329:ASP:CG	2.51	0.48
1:P:1036:MET:HE1	1:P:1038:LEU:CB	2.40	0.48
1:P:1096:VAL:O	1:P:1097:VAL:C	2.52	0.48
1:P:1168:ASN:HA	1:P:1170:ARG:H	1.77	0.48
1:R:1036:MET:HG2	1:R:1037:ARG:N	2.28	0.48
1:U:1009:ASN:CB	1:V:1309:ASN:ND2	2.75	0.48
1:U:1165:VAL:HA	1:U:1166:THR:HG22	1.95	0.48
1:V:1196:ALA:HB3	1:V:1222:THR:HG23	1.94	0.48
1:W:1083:GLN:HG3	1:W:1084:ASP:H	1.78	0.48
1:W:1096:VAL:O	1:W:1097:VAL:C	2.50	0.48
1:Q:1147:VAL:O	1:Q:1147:VAL:HG12	2.13	0.48
1:R:1165:VAL:CG1	1:R:1166:THR:N	2.51	0.48
1:U:1036:MET:HE3	1:U:1038:LEU:HD22	1.96	0.48
1:U:1095:GLY:HA3	1:U:1121:MET:O	2.14	0.48
1:U:1161:PHE:O	1:U:1162:THR:HG23	2.12	0.48
1:V:1306:PHE:HD2	1:V:1311:SER:HA	1.78	0.48
2:X:1041:SER:HB3	2:X:1044:GLU:H	1.78	0.48
1:P:1163:SER:O	1:P:1165:VAL:HG23	2.14	0.48
1:P:1304:TYR:HE2	1:P:1306:PHE:CD1	2.31	0.48
1:Q:1156:PRO:O	1:Q:1161:PHE:CD2	2.66	0.48
1:R:1036:MET:HE1	1:R:1038:LEU:HD22	1.95	0.48
1:V:1159:GLU:CD	1:V:1160:GLY:N	2.67	0.48
1:W:1145:PHE:HA	1:W:1183:SER:O	2.14	0.48
1:W:1152:LYS:HE3	1:W:1203:THR:CG2	2.44	0.48
2:X:1027:LYS:O	2:X:1028:LYS:CG	2.58	0.48
1:P:1057:GLU:H	1:P:1075:VAL:HG12	1.78	0.48
1:Q:1096:VAL:HG13	1:Q:1148:GLN:HG2	1.94	0.48
1:Q:1222:THR:HB	1:Q:1239:THR:CB	2.29	0.48
1:R:1144:ASN:N	1:R:1144:ASN:ND2	2.57	0.48
1:U:1069:ASN:OD1	1:U:1070:ASN:CB	2.61	0.48
1:V:1043:GLU:HA	1:V:1052:GLY:O	2.14	0.48
1:W:1102:SER:O	1:W:1103:TRP:C	2.51	0.48
1:W:1317:LYS:HG2	1:W:1319:ASN:HB2	1.96	0.48
1:P:1082:PHE:O	1:P:1083:GLN:CB	2.62	0.48
1:R:1036:MET:CE	1:R:1038:LEU:HB3	2.44	0.48
1:U:1161:PHE:HB3	1:V:1027:LYS:O	2.14	0.48
1:W:1024:SER:HB2	1:W:1337:ILE:HG23	1.95	0.48
2:X:1023:GLN:C	2:X:1026:MET:HB2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1303:THR:HA	1:P:1313:TYR:HA	1.95	0.48
1:Q:1017:VAL:CG1	1:Q:1018:ASP:N	2.76	0.48
2:S:1010:THR:CG2	2:S:1036:CYS:SG	3.02	0.48
2:S:1026:MET:HG3	2:S:1034:VAL:HG13	1.76	0.48
1:U:1319:ASN:ND2	1:U:1334:THR:C	2.67	0.48
1:V:1060:ILE:HA	1:V:1071:SER:HB2	1.96	0.48
1:V:1303:THR:HA	1:V:1313:TYR:HA	1.95	0.48
2:X:1023:GLN:HB2	2:X:1035:THR:CA	2.44	0.48
1:P:1123:GLN:OE1	1:P:1124:ARG:CB	2.62	0.47
1:P:1162:THR:O	1:P:1163:SER:C	2.52	0.47
1:P:1271:LEU:HG	1:P:1272:ARG:N	2.28	0.47
1:Q:1272:ARG:O	1:Q:1272:ARG:HG2	2.13	0.47
1:V:1266:GLN:OE1	1:V:1272:ARG:HD2	2.13	0.47
1:W:1212:ILE:CG1	1:W:1250:LEU:O	2.62	0.47
1:U:1162:THR:C	1:U:1165:VAL:CG2	2.82	0.47
1:U:1260:GLU:HG2	1:U:1278:LEU:HB3	1.96	0.47
1:V:1131:TYR:O	1:V:1146:ALA:HA	2.13	0.47
1:V:1152:LYS:HE3	1:V:1203:THR:HG22	1.96	0.47
1:V:1189:GLU:C	1:V:1190:GLY:O	2.52	0.47
1:V:1202:ARG:CZ	1:V:1215:GLY:HA3	2.44	0.47
1:W:1299:ASP:OD1	1:W:1299:ASP:C	2.51	0.47
1:P:1324:ASN:HA	1:P:1328:ARG:HH22	1.79	0.47
1:R:1098:TYR:CE2	1:R:1102:SER:HB3	2.49	0.47
1:R:1256:ALA:HA	1:R:1281:LYS:O	2.14	0.47
1:U:1191:PHE:H	1:U:1227:TYR:HA	1.80	0.47
1:W:1102:SER:C	1:W:1104:THR:N	2.66	0.47
1:W:1195:GLY:HA2	1:W:1222:THR:O	2.15	0.47
1:P:1023:PHE:CD2	1:P:1023:PHE:N	2.82	0.47
1:P:1095:GLY:HA2	1:P:1148:GLN:OE1	2.14	0.47
1:Q:1202:ARG:NH2	1:Q:1215:GLY:HA3	2.29	0.47
1:R:1140:VAL:CG2	1:R:1141:ASP:N	2.77	0.47
1:U:1184:ILE:CD1	1:U:1195:GLY:H	2.26	0.47
1:V:1047:THR:HG21	1:V:1050:LEU:H	1.74	0.47
1:V:1157:SER:HB3	1:V:1158:GLY:H	1.39	0.47
1:V:1310:MET:HG3	1:V:1311:SER:N	2.28	0.47
1:W:1184:ILE:HD11	1:W:1195:GLY:N	2.29	0.47
1:Q:1281:LYS:HD2	1:Q:1283:LYS:HE3	1.96	0.47
1:R:1060:ILE:HG23	1:R:1071:SER:CB	2.44	0.47
1:R:1184:ILE:N	1:R:1184:ILE:HD12	2.17	0.47
1:R:1219:GLU:O	1:R:1241:THR:HA	2.14	0.47
1:V:1011:LEU:HD23	1:V:1011:LEU:HA	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1202:ARG:HH21	1:W:1215:GLY:HA3	1.80	0.47
1:W:1212:ILE:HG13	1:W:1250:LEU:O	2.13	0.47
1:P:1002:GLU:OE1	1:P:1005:ASN:HB2	2.14	0.47
1:P:1047:THR:HG23	1:P:1049:GLN:N	2.29	0.47
1:Q:1266:GLN:O	1:Q:1266:GLN:HG3	2.07	0.47
1:R:1156:PRO:O	1:R:1161:PHE:CD2	2.68	0.47
1:U:1045:GLN:O	1:U:1045:GLN:CG	2.60	0.47
1:V:1065:ALA:C	1:V:1067:ASN:N	2.67	0.47
1:V:1154:GLY:O	1:V:1165:VAL:CG1	2.62	0.47
1:V:1302:ALA:N	1:V:1314:VAL:O	2.42	0.47
1:W:1260:GLU:CG	1:W:1278:LEU:HD13	2.44	0.47
1:P:1210:ALA:O	1:P:1211:TYR:C	2.52	0.47
1:P:1214:ASN:H	1:P:1254:ASN:HD21	1.62	0.47
1:P:1313:TYR:CZ	1:P:1341:GLY:HA3	2.49	0.47
1:R:1065:ALA:O	1:R:1067:ASN:N	2.48	0.47
2:S:1007:ARG:HD2	2:S:1037:VAL:CG2	2.32	0.47
1:U:1096:VAL:HG13	1:U:1148:GLN:HG2	1.95	0.47
1:V:1137:PHE:HB2	1:V:1139:LEU:CD1	2.44	0.47
1:V:1162:THR:C	1:V:1165:VAL:CG2	2.79	0.47
1:V:1308:LYS:O	1:V:1308:LYS:HD3	2.15	0.47
1:W:1097:VAL:O	1:W:1101:THR:HG23	2.15	0.47
1:W:1303:THR:HA	1:W:1313:TYR:HA	1.97	0.47
1:R:1108:PRO:HB3	1:R:1303:THR:HG22	1.96	0.47
1:R:1284:ASN:N	1:R:1291:ASP:OD1	2.45	0.47
1:U:1103:TRP:O	1:U:1233:TYR:OH	2.26	0.47
1:U:1135:ASP:O	1:U:1137:PHE:N	2.48	0.47
1:U:1171:ASP:OD2	1:U:1171:ASP:N	2.48	0.47
1:U:1275:LEU:HD22	1:U:1276:ALA:H	1.77	0.47
1:W:1033:GLN:O	1:W:1034:THR:C	2.53	0.47
1:W:1130:THR:OG1	1:W:1148:GLN:NE2	2.48	0.47
1:P:1047:THR:HG21	1:P:1050:LEU:H	1.68	0.47
1:Q:1157:SER:C	1:Q:1161:PHE:HD1	2.15	0.47
1:Q:1208:THR:O	1:Q:1208:THR:OG1	2.31	0.47
1:R:1099:ASP:OD1	1:R:1099:ASP:N	2.48	0.47
1:R:1102:SER:O	1:R:1103:TRP:C	2.52	0.47
1:U:1064:SER:HB2	1:U:1068:GLU:OE2	2.15	0.47
1:V:1098:TYR:CZ	1:V:1102:SER:HB3	2.50	0.47
1:V:1159:GLU:OE1	1:V:1159:GLU:C	2.51	0.47
1:P:1001:ALA:N	1:P:1013:LEU:O	2.48	0.47
1:P:1037:ARG:NH1	1:P:1074:ARG:NH2	2.63	0.47
1:P:1061:GLN:HB3	1:P:1063:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1058:TYR:CE1	1:Q:1072:TRP:C	2.88	0.47
1:R:1024:SER:HB2	1:R:1337:ILE:HG23	1.97	0.47
1:R:1094:TYR:HA	1:R:1124:ARG:H	1.80	0.47
1:R:1164:GLY:C	1:R:1165:VAL:HG23	2.33	0.47
1:U:1275:LEU:HD22	1:U:1276:ALA:N	2.30	0.47
1:V:1079:GLY:HA3	1:V:1088:PHE:O	2.15	0.47
1:V:1083:GLN:CG	1:V:1084:ASP:N	2.72	0.47
1:P:1188:TYR:N	1:P:1188:TYR:CD1	2.83	0.46
1:Q:1083:GLN:CG	1:Q:1084:ASP:N	2.77	0.46
1:Q:1212:ILE:O	1:Q:1252:TRP:N	2.46	0.46
1:R:1168:ASN:OD1	1:R:1168:ASN:N	2.49	0.46
1:U:1159:GLU:OE1	1:U:1159:GLU:C	2.54	0.46
1:U:1317:LYS:HE3	1:U:1337:ILE:HD12	1.97	0.46
1:V:1068:GLU:O	1:V:1069:ASN:CB	2.55	0.46
1:V:1208:THR:C	1:V:1210:ALA:H	2.17	0.46
1:W:1231:ASN:ND2	1:W:1231:ASN:N	2.62	0.46
1:Q:1011:LEU:HD23	1:Q:1011:LEU:HA	1.57	0.46
1:Q:1047:THR:HG21	1:Q:1050:LEU:H	1.77	0.46
1:Q:1077:PHE:CE2	1:Q:1093:ASN:OD1	2.68	0.46
1:W:1312:THR:HG22	1:W:1341:GLY:O	2.15	0.46
1:Q:1248:GLY:HA3	1:Q:1330:ALA:HB1	1.97	0.46
1:R:1005:ASN:OD1	1:R:1005:ASN:O	2.32	0.46
1:R:1049:GLN:CG	1:R:1082:PHE:O	2.44	0.46
1:R:1202:ARG:NH2	1:R:1215:GLY:HA3	2.30	0.46
1:U:1065:ALA:C	1:U:1067:ASN:N	2.69	0.46
1:V:1017:VAL:CG1	1:V:1018:ASP:N	2.79	0.46
1:V:1220:THR:HA	1:V:1241:THR:HA	1.97	0.46
1:W:1156:PRO:HA	1:W:1165:VAL:HB	1.97	0.46
1:W:1324:ASN:HD21	1:W:1327:THR:HG23	1.81	0.46
1:P:1208:THR:O	1:P:1208:THR:OG1	2.27	0.46
1:Q:1157:SER:HB3	1:Q:1158:GLY:H	1.32	0.46
1:R:1211:TYR:HB2	1:R:1250:LEU:O	2.16	0.46
2:S:1012:SER:HA	2:S:1038:LYS:HZ1	1.78	0.46
1:U:1002:GLU:OE1	1:U:1005:ASN:HB2	2.15	0.46
1:V:1056:TRP:CZ2	1:V:1058:TYR:HB2	2.50	0.46
1:V:1096:VAL:O	1:V:1098:TYR:N	2.48	0.46
1:V:1343:VAL:HG12	1:V:1344:TYR:N	2.30	0.46
1:W:1011:LEU:HD23	1:W:1011:LEU:HA	1.79	0.46
1:W:1144:ASN:N	1:W:1144:ASN:ND2	2.62	0.46
1:W:1155:ASN:CB	1:W:1157:SER:H	2.23	0.46
1:W:1162:THR:H	1:W:1165:VAL:HG21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1095:GLY:HA3	1:P:1121:MET:O	2.15	0.46
1:P:1103:TRP:CD2	1:P:1226:LYS:HD3	2.51	0.46
1:P:1212:ILE:HG13	1:P:1250:LEU:O	2.16	0.46
1:Q:1079:GLY:CA	1:Q:1088:PHE:O	2.64	0.46
1:Q:1126:ASN:OD1	1:R:1064:SER:HA	2.16	0.46
1:Q:1171:ASP:OD2	1:Q:1171:ASP:N	2.49	0.46
2:S:1038:LYS:CE	2:S:1039:LYS:H	2.28	0.46
1:U:1066:GLU:HG2	1:W:1072:TRP:HD1	1.77	0.46
1:U:1193:ILE:HG23	1:U:1193:ILE:HD12	1.63	0.46
1:V:1156:PRO:O	1:V:1161:PHE:CD2	2.68	0.46
1:P:1193:ILE:HG23	1:P:1193:ILE:HD12	1.53	0.46
1:R:1292:GLU:HG2	1:R:1326:PHE:CD2	2.49	0.46
1:V:1077:PHE:HB3	1:V:1091:GLY:HA3	1.96	0.46
1:V:1102:SER:C	1:V:1104:THR:N	2.69	0.46
1:V:1168:ASN:C	1:V:1170:ARG:H	2.07	0.46
1:W:1134:THR:CG2	1:W:1135:ASP:N	2.79	0.46
1:W:1157:SER:HB3	1:W:1158:GLY:H	1.33	0.46
1:P:1026:ASN:C	1:P:1028:ASP:H	2.19	0.46
1:P:1060:ILE:HA	1:P:1071:SER:CB	2.46	0.46
1:P:1231:ASN:O	1:P:1265:TYR:HA	2.16	0.46
1:R:1093:ASN:O	1:R:1124:ARG:HA	2.16	0.46
1:U:1271:LEU:HG	1:U:1272:ARG:N	2.30	0.46
1:W:1184:ILE:CD1	1:W:1195:GLY:H	2.28	0.46
1:Q:1107:LEU:CD2	1:Q:1262:VAL:HG21	2.45	0.46
1:Q:1134:THR:HG23	1:Q:1135:ASP:N	2.31	0.46
1:R:1232:ILE:CG2	1:R:1234:LEU:HD22	2.46	0.46
1:U:1107:LEU:CD2	1:U:1262:VAL:HG21	2.45	0.46
1:U:1281:LYS:HD2	1:U:1283:LYS:HE3	1.97	0.46
1:W:1082:PHE:O	1:W:1083:GLN:CB	2.64	0.46
1:W:1116:GLY:N	1:W:1119:ASN:HD22	2.13	0.46
1:P:1042:GLY:O	1:P:1053:TYR:HA	2.15	0.46
1:P:1085:VAL:O	1:P:1131:TYR:OH	2.31	0.46
1:Q:1018:ASP:OD2	1:Q:1018:ASP:C	2.53	0.46
1:Q:1162:THR:C	1:Q:1165:VAL:HG21	2.29	0.46
1:U:1309:ASN:HD21	1:W:1009:ASN:CG	2.19	0.46
1:V:1139:LEU:O	1:V:1140:VAL:HG12	2.16	0.46
1:W:1027:LYS:HE3	1:W:1027:LYS:HB3	1.33	0.46
1:W:1147:VAL:O	1:W:1147:VAL:CG1	2.57	0.46
1:W:1324:ASN:HD22	1:W:1326:PHE:CB	2.19	0.46
1:P:1052:GLY:O	1:P:1053:TYR:HB3	2.16	0.46
1:P:1256:ALA:HA	1:P:1281:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1082:PHE:HB2	1:R:1085:VAL:HB	1.97	0.46
1:W:1058:TYR:CD1	1:W:1073:THR:HA	2.51	0.46
1:P:1212:ILE:O	1:P:1252:TRP:N	2.49	0.45
1:P:1312:THR:HG23	1:P:1342:LEU:HD13	1.98	0.45
1:Q:1131:TYR:O	1:Q:1146:ALA:HA	2.16	0.45
1:Q:1231:ASN:O	1:Q:1265:TYR:HA	2.16	0.45
1:Q:1281:LYS:HD2	1:Q:1283:LYS:CE	2.46	0.45
1:V:1035:TYR:HE2	1:V:1037:ARG:HE	1.65	0.45
1:V:1168:ASN:OD1	1:V:1168:ASN:N	2.50	0.45
1:W:1057:GLU:O	1:W:1074:ARG:HB2	2.16	0.45
1:P:1310:MET:HG3	1:P:1311:SER:H	1.82	0.45
1:Q:1005:ASN:C	1:Q:1005:ASN:OD1	2.54	0.45
1:R:1266:GLN:HB2	1:R:1272:ARG:NH1	2.32	0.45
1:R:1324:ASN:HA	1:R:1328:ARG:HH22	1.80	0.45
2:S:1012:SER:HA	2:S:1038:LYS:HZ2	1.79	0.45
1:V:1147:VAL:HG12	1:V:1147:VAL:O	2.16	0.45
1:W:1070:ASN:C	1:W:1070:ASN:HD22	2.20	0.45
1:W:1116:GLY:H	1:W:1119:ASN:HD22	1.63	0.45
1:P:1337:ILE:HG22	1:P:1338:VAL:N	2.31	0.45
1:Q:1088:PHE:HE1	1:Q:1129:ALA:HB1	1.81	0.45
1:R:1266:GLN:OE1	1:R:1272:ARG:HD2	2.15	0.45
2:S:1027:LYS:HG2	2:S:1030:ARG:HA	1.99	0.45
1:U:1001:ALA:N	1:U:1013:LEU:O	2.50	0.45
1:U:1139:LEU:O	1:U:1140:VAL:HG12	2.17	0.45
1:U:1159:GLU:CD	1:U:1160:GLY:N	2.70	0.45
1:W:1133:ASN:O	1:W:1144:ASN:CB	2.63	0.45
1:W:1212:ILE:HD11	1:W:1250:LEU:HD13	1.98	0.45
2:X:1007:ARG:CZ	2:X:1007:ARG:CB	2.88	0.45
1:Q:1037:ARG:NH1	1:Q:1074:ARG:CZ	2.79	0.45
1:W:1056:TRP:CZ2	1:W:1058:TYR:HB2	2.51	0.45
1:Q:1097:VAL:O	1:Q:1101:THR:HG23	2.17	0.45
1:V:1082:PHE:O	1:V:1083:GLN:CB	2.65	0.45
1:V:1139:LEU:O	1:V:1139:LEU:HD22	2.16	0.45
1:V:1196:ALA:O	1:V:1222:THR:HG23	2.17	0.45
2:X:1030:ARG:HE	2:X:1030:ARG:HB3	1.50	0.45
2:S:1010:THR:OG1	2:S:1038:LYS:HB2	2.15	0.45
1:V:1228:ASP:O	1:V:1229:ALA:HB2	2.17	0.45
1:W:1202:ARG:NE	1:W:1215:GLY:CA	2.79	0.45
1:P:1011:LEU:HD23	1:P:1011:LEU:HA	1.79	0.45
1:P:1098:TYR:CD2	1:P:1102:SER:HB3	2.51	0.45
1:Q:1016:LYS:HB3	1:Q:1345:GLN:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1230:ASN:C	1:Q:1231:ASN:HD22	2.20	0.45
1:R:1018:ASP:CG	1:R:1343:VAL:HG22	2.37	0.45
1:R:1096:VAL:O	1:R:1097:VAL:C	2.52	0.45
2:S:1017:LYS:NZ	2:S:1017:LYS:HB2	2.30	0.45
1:U:1049:GLN:OE1	1:U:1083:GLN:CG	2.65	0.45
1:U:1325:GLN:O	1:U:1329:ASP:CG	2.55	0.45
1:V:1148:GLN:O	1:V:1181:GLY:N	2.50	0.45
1:W:1288:GLY:O	1:W:1290:ASP:N	2.49	0.45
2:X:1023:GLN:HA	2:X:1034:VAL:O	2.16	0.45
1:Q:1050:LEU:HD21	1:Q:1080:LEU:HG	1.98	0.45
1:Q:1242:TYR:N	1:Q:1242:TYR:CD1	2.85	0.45
1:Q:1283:LYS:O	1:Q:1284:ASN:C	2.55	0.45
2:S:1001:ALA:HB2	2:S:1037:VAL:HG21	1.99	0.45
1:U:1022:TYR:HA	1:U:1338:VAL:O	2.15	0.45
1:W:1036:MET:HG2	1:W:1037:ARG:N	2.32	0.45
2:X:1024:ARG:O	2:X:1027:LYS:O	2.35	0.45
2:X:1027:LYS:HG3	2:X:1030:ARG:HH11	1.82	0.45
1:P:1292:GLU:HG2	1:P:1326:PHE:CD2	2.51	0.45
1:U:1156:PRO:O	1:U:1161:PHE:CD1	2.70	0.45
1:W:1097:VAL:O	1:W:1097:VAL:CG1	2.62	0.45
1:W:1319:ASN:ND2	1:W:1334:THR:C	2.71	0.45
1:P:1157:SER:HB3	1:P:1158:GLY:H	1.37	0.45
1:P:1168:ASN:OD1	1:P:1168:ASN:N	2.49	0.45
1:R:1137:PHE:HB2	1:R:1139:LEU:HD12	1.99	0.45
1:V:1059:GLN:OE1	1:V:1061:GLN:OE1	2.35	0.45
1:V:1212:ILE:O	1:V:1252:TRP:O	2.35	0.45
1:V:1281:LYS:HD2	1:V:1283:LYS:HE3	1.99	0.45
1:W:1095:GLY:HA3	1:W:1121:MET:O	2.18	0.45
1:W:1114:THR:OG1	1:W:1260:GLU:OE1	2.35	0.45
1:W:1277:TYR:OH	1:W:1296:LYS:HE3	2.17	0.45
1:P:1133:ASN:HD21	1:P:1136:PHE:HA	1.81	0.44
1:V:1192:GLY:N	1:V:1226:LYS:O	2.49	0.44
1:V:1271:LEU:HG	1:V:1272:ARG:N	2.31	0.44
2:X:1021:GLN:O	2:X:1024:ARG:CA	2.64	0.44
1:P:1018:ASP:C	1:P:1018:ASP:OD2	2.56	0.44
1:P:1097:VAL:O	1:P:1097:VAL:CG1	2.61	0.44
1:U:1050:LEU:HD21	1:U:1080:LEU:HG	1.98	0.44
1:U:1107:LEU:HD12	1:U:1111:GLY:N	2.32	0.44
1:V:1049:GLN:OE1	1:V:1083:GLN:CG	2.63	0.44
1:W:1219:GLU:O	1:W:1241:THR:HA	2.17	0.44
1:Q:1283:LYS:HA	1:Q:1283:LYS:HD3	1.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1035:TYR:HE2	1:R:1037:ARG:HE	1.65	0.44
1:R:1042:GLY:O	1:R:1053:TYR:HA	2.18	0.44
1:R:1144:ASN:ND2	1:R:1144:ASN:H	2.15	0.44
1:U:1027:LYS:HA	1:U:1030:ASP:HB2	1.98	0.44
1:U:1186:TYR:CE2	1:U:1188:TYR:CD1	3.05	0.44
1:V:1170:ARG:HD2	1:W:1067:ASN:ND2	2.32	0.44
1:W:1157:SER:C	1:W:1161:PHE:HD1	2.19	0.44
1:P:1231:ASN:ND2	1:P:1231:ASN:N	2.65	0.44
1:Q:1134:THR:HG23	1:Q:1135:ASP:OD2	2.17	0.44
1:R:1036:MET:HE1	1:R:1038:LEU:N	2.33	0.44
1:R:1049:GLN:OE1	1:R:1083:GLN:HG3	2.17	0.44
1:R:1192:GLY:N	1:R:1226:LYS:O	2.47	0.44
1:R:1220:THR:HA	1:R:1241:THR:HA	1.99	0.44
1:U:1107:LEU:HD21	1:U:1262:VAL:HG21	1.98	0.44
1:V:1069:ASN:OD1	1:V:1070:ASN:HB3	2.16	0.44
1:V:1159:GLU:C	1:V:1159:GLU:OE2	2.54	0.44
1:V:1165:VAL:CG1	1:V:1166:THR:H	2.29	0.44
1:W:1017:VAL:CG1	1:W:1018:ASP:N	2.80	0.44
1:P:1036:MET:CG	1:P:1037:ARG:N	2.81	0.44
1:P:1144:ASN:C	1:P:1144:ASN:HD22	2.19	0.44
1:P:1195:GLY:HA2	1:P:1222:THR:O	2.17	0.44
1:R:1139:LEU:O	1:R:1139:LEU:CD2	2.65	0.44
1:V:1272:ARG:O	1:V:1272:ARG:CG	2.66	0.44
1:V:1325:GLN:O	1:V:1329:ASP:CG	2.56	0.44
1:W:1212:ILE:O	1:W:1252:TRP:N	2.51	0.44
1:P:1077:PHE:HB3	1:P:1091:GLY:HA3	1.99	0.44
1:P:1196:ALA:O	1:P:1222:THR:HG23	2.18	0.44
1:Q:1271:LEU:HG	1:Q:1272:ARG:H	1.82	0.44
1:Q:1328:ARG:O	1:Q:1329:ASP:C	2.50	0.44
1:R:1219:GLU:HB2	1:R:1242:TYR:HB2	1.99	0.44
1:R:1312:THR:HG22	1:R:1341:GLY:O	2.18	0.44
1:U:1072:TRP:HD1	1:V:1066:GLU:HG2	1.77	0.44
1:U:1095:GLY:HA2	1:U:1148:GLN:OE1	2.18	0.44
1:U:1264:GLN:CG	1:U:1274:SER:HB2	2.42	0.44
1:V:1013:LEU:HD22	1:V:1013:LEU:HA	1.74	0.44
1:V:1196:ALA:O	1:V:1222:THR:CG2	2.65	0.44
1:P:1312:THR:HG22	1:P:1342:LEU:HA	2.00	0.44
1:Q:1026:ASN:HB2	1:Q:1335:ASP:OD2	2.18	0.44
1:Q:1303:THR:HA	1:Q:1313:TYR:HA	1.99	0.44
1:R:1264:GLN:CG	1:R:1274:SER:HB2	2.42	0.44
2:S:1030:ARG:HG3	1:W:1290:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1108:PRO:HG3	1:V:1303:THR:HG22	2.00	0.44
1:W:1156:PRO:O	1:W:1161:PHE:CE1	2.71	0.44
1:P:1009:ASN:HA	1:P:1044:THR:HA	2.00	0.44
1:R:1219:GLU:O	1:R:1242:TYR:N	2.45	0.44
2:S:1038:LYS:HE2	2:S:1039:LYS:H	1.83	0.44
1:U:1005:ASN:C	1:U:1005:ASN:OD1	2.56	0.44
1:U:1220:THR:HA	1:U:1241:THR:HA	2.00	0.44
1:U:1309:ASN:HD22	1:W:1009:ASN:HB2	1.82	0.44
1:V:1023:PHE:CD2	1:V:1023:PHE:N	2.85	0.44
1:W:1213:GLY:O	1:W:1215:GLY:N	2.51	0.44
1:P:1053:TYR:OH	1:P:1089:ASP:OD2	2.31	0.44
1:P:1064:SER:CA	1:R:1126:ASN:OD1	2.66	0.44
1:P:1098:TYR:CZ	1:P:1102:SER:HB3	2.51	0.44
1:P:1309:ASN:HD21	1:R:1009:ASN:CB	2.29	0.44
1:Q:1325:GLN:O	1:Q:1329:ASP:CG	2.56	0.44
1:R:1152:LYS:HE3	1:R:1203:THR:HG22	2.00	0.44
1:R:1155:ASN:CA	1:R:1165:VAL:HG11	2.48	0.44
1:R:1277:TYR:C	1:R:1278:LEU:HD22	2.38	0.44
1:U:1156:PRO:O	1:U:1161:PHE:CD2	2.71	0.44
1:P:1121:MET:CE	1:P:1148:GLN:HG3	2.48	0.43
1:R:1162:THR:N	1:R:1165:VAL:HG21	2.30	0.43
1:R:1189:GLU:C	1:R:1190:GLY:O	2.56	0.43
1:U:1165:VAL:CG1	1:U:1166:THR:N	2.50	0.43
1:W:1155:ASN:C	1:W:1157:SER:H	2.22	0.43
1:W:1163:SER:OG	1:W:1164:GLY:N	2.51	0.43
1:W:1168:ASN:O	1:W:1170:ARG:N	2.49	0.43
1:P:1096:VAL:HG22	1:P:1148:GLN:CG	2.45	0.43
1:Q:1102:SER:C	1:Q:1104:THR:N	2.70	0.43
1:R:1312:THR:HG23	1:R:1342:LEU:HD13	2.00	0.43
2:S:1042:ARG:O	2:S:1044:GLU:N	2.32	0.43
1:U:1055:GLN:HG2	1:U:1056:TRP:N	2.33	0.43
1:U:1064:SER:HA	1:W:1126:ASN:OD1	2.18	0.43
1:V:1116:GLY:N	1:V:1119:ASN:HD22	2.13	0.43
1:V:1163:SER:CB	1:W:1030:ASP:O	2.58	0.43
1:V:1298:VAL:CG1	1:V:1299:ASP:N	2.79	0.43
1:W:1160:GLY:O	1:W:1161:PHE:C	2.57	0.43
1:W:1192:GLY:N	1:W:1226:LYS:O	2.50	0.43
1:W:1203:THR:OG1	1:W:1206:GLN:HG2	2.18	0.43
1:W:1294:ILE:O	1:W:1332:ILE:CD1	2.64	0.43
1:P:1099:ASP:OD1	1:P:1132:ARG:NH2	2.51	0.43
1:P:1165:VAL:CA	1:P:1166:THR:HG22	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1190:GLY:O	1:P:1191:PHE:CB	2.66	0.43
1:Q:1308:LYS:O	1:Q:1308:LYS:CD	2.63	0.43
1:Q:1310:MET:SD	1:Q:1344:TYR:HB2	2.58	0.43
1:R:1325:GLN:O	1:R:1329:ASP:CG	2.56	0.43
1:U:1049:GLN:OE1	1:U:1083:GLN:HG3	2.17	0.43
1:U:1069:ASN:HD21	1:V:1069:ASN:HD22	1.64	0.43
1:U:1083:GLN:CG	1:U:1084:ASP:H	2.31	0.43
1:V:1162:THR:C	1:V:1165:VAL:HG21	2.32	0.43
1:V:1208:THR:C	1:V:1210:ALA:N	2.71	0.43
1:W:1155:ASN:O	1:W:1165:VAL:HG11	2.18	0.43
1:P:1290:ASP:HB3	1:P:1291:ASP:H	1.27	0.43
1:Q:1009:ASN:CB	1:R:1309:ASN:HD21	2.32	0.43
1:Q:1230:ASN:C	1:Q:1231:ASN:ND2	2.71	0.43
1:R:1132:ARG:HH11	1:R:1132:ARG:HD2	1.51	0.43
1:V:1009:ASN:CB	1:W:1309:ASN:ND2	2.80	0.43
1:W:1139:LEU:O	1:W:1139:LEU:HD22	2.18	0.43
1:W:1190:GLY:O	1:W:1191:PHE:CD1	2.72	0.43
1:W:1310:MET:HG3	1:W:1311:SER:H	1.83	0.43
1:P:1009:ASN:CB	1:Q:1309:ASN:ND2	2.82	0.43
1:Q:1275:LEU:HD22	1:Q:1276:ALA:H	1.83	0.43
1:R:1069:ASN:CG	1:R:1070:ASN:N	2.71	0.43
1:R:1128:PHE:HD2	1:R:1150:GLN:HB3	1.82	0.43
1:R:1196:ALA:O	1:R:1222:THR:CG2	2.67	0.43
1:V:1130:THR:HG21	1:V:1132:ARG:NH1	2.32	0.43
1:W:1009:ASN:HA	1:W:1044:THR:HA	2.01	0.43
1:W:1155:ASN:C	1:W:1165:VAL:HG11	2.39	0.43
1:P:1156:PRO:O	1:P:1161:PHE:CD2	2.72	0.43
1:P:1306:PHE:CE2	1:P:1311:SER:HA	2.54	0.43
1:Q:1090:TYR:CG	1:Q:1091:GLY:N	2.85	0.43
1:R:1277:TYR:O	1:R:1278:LEU:HD22	2.18	0.43
1:R:1324:ASN:C	1:R:1326:PHE:H	2.22	0.43
2:S:1007:ARG:HG3	2:S:1037:VAL:CB	2.48	0.43
1:U:1184:ILE:HD13	1:U:1184:ILE:H	1.70	0.43
1:U:1190:GLY:O	1:U:1191:PHE:HD1	2.02	0.43
1:V:1211:TYR:HA	1:V:1287:ARG:HH12	1.83	0.43
1:P:1050:LEU:HD21	1:P:1080:LEU:HG	1.99	0.43
1:P:1059:GLN:OE1	1:P:1061:GLN:OE1	2.36	0.43
1:P:1156:PRO:O	1:P:1161:PHE:CD1	2.72	0.43
1:P:1197:ILE:HD12	1:P:1197:ILE:N	2.34	0.43
1:Q:1077:PHE:HB2	1:Q:1090:TYR:O	2.19	0.43
1:R:1026:ASN:HD22	1:R:1333:ASN:CG	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1083:GLN:HG3	1:R:1084:ASP:H	1.83	0.43
1:R:1193:ILE:HD12	1:R:1193:ILE:HG23	1.78	0.43
1:R:1231:ASN:O	1:R:1265:TYR:HA	2.18	0.43
2:S:1014:ALA:HB2	2:S:1017:LYS:HD3	1.97	0.43
1:U:1036:MET:HE1	1:U:1038:LEU:HD23	1.95	0.43
1:U:1281:LYS:HD2	1:U:1283:LYS:CE	2.48	0.43
1:W:1077:PHE:HB3	1:W:1091:GLY:HA3	2.00	0.43
1:Q:1290:ASP:HB3	1:Q:1291:ASP:H	1.39	0.43
1:R:1070:ASN:HD22	1:R:1071:SER:N	2.17	0.43
1:R:1107:LEU:HD21	1:R:1262:VAL:CG2	2.49	0.43
1:U:1088:PHE:HE1	1:U:1129:ALA:HB1	1.83	0.43
1:U:1131:TYR:HB3	1:U:1147:VAL:HG12	2.01	0.43
1:U:1139:LEU:O	1:U:1139:LEU:CD2	2.66	0.43
1:U:1217:ARG:HD3	1:U:1219:GLU:OE2	2.19	0.43
1:U:1312:THR:HG23	1:U:1342:LEU:HD13	2.00	0.43
1:V:1290:ASP:HB3	1:V:1291:ASP:H	1.16	0.43
1:W:1289:TYR:CD1	1:W:1326:PHE:HD1	2.37	0.43
2:X:1006:VAL:O	2:X:1034:VAL:HG21	2.19	0.43
1:P:1003:VAL:HG23	1:P:1011:LEU:HB3	2.00	0.43
1:P:1102:SER:O	1:P:1104:THR:N	2.52	0.43
1:P:1218:ALA:HB1	1:P:1244:ALA:HB2	2.00	0.43
1:Q:1238:TYR:HH	1:Q:1257:GLN:HG2	1.79	0.43
1:Q:1287:ARG:HD3	1:W:1287:ARG:CD	2.38	0.43
1:R:1096:VAL:C	1:R:1098:TYR:H	2.23	0.43
1:R:1310:MET:HG3	1:R:1311:SER:H	1.81	0.43
1:U:1002:GLU:OE1	1:U:1005:ASN:CB	2.67	0.43
1:U:1145:PHE:HA	1:U:1183:SER:O	2.18	0.43
1:U:1230:ASN:C	1:U:1231:ASN:HD22	2.22	0.43
1:U:1290:ASP:HB3	1:U:1291:ASP:H	1.50	0.43
1:U:1313:TYR:HE1	1:U:1343:VAL:HG23	1.84	0.43
1:V:1213:GLY:O	1:V:1215:GLY:N	2.52	0.43
1:W:1037:ARG:NH1	1:W:1074:ARG:NH2	2.66	0.43
1:W:1280:SER:N	1:W:1295:LEU:O	2.45	0.43
2:X:1023:GLN:HB2	2:X:1035:THR:CB	2.49	0.43
2:X:1023:GLN:C	2:X:1026:MET:HB3	2.31	0.43
2:X:1025:ARG:NH1	2:X:1025:ARG:HG2	2.27	0.43
1:P:1196:ALA:HB3	1:P:1222:THR:HG23	2.01	0.43
1:Q:1108:PRO:HG3	1:Q:1303:THR:HG22	2.01	0.43
1:U:1003:VAL:HG22	1:U:1013:LEU:H	1.84	0.43
1:W:1188:TYR:N	1:W:1188:TYR:HD1	2.17	0.43
1:W:1256:ALA:HA	1:W:1281:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:1327:THR:O	1:W:1330:ALA:N	2.52	0.43
1:R:1037:ARG:HH11	1:R:1074:ARG:CZ	2.31	0.42
1:U:1061:GLN:HB3	1:U:1063:ASN:OD1	2.19	0.42
1:V:1014:TYR:CD1	1:V:1039:GLY:O	2.72	0.42
1:V:1170:ARG:HD3	1:W:1065:ALA:HB1	2.01	0.42
1:V:1298:VAL:HG12	1:V:1299:ASP:N	2.34	0.42
1:V:1324:ASN:HA	1:V:1328:ARG:HH22	1.84	0.42
1:Q:1036:MET:HE1	1:Q:1038:LEU:CD2	2.49	0.42
1:Q:1197:ILE:HG23	1:Q:1221:TYR:CD2	2.55	0.42
1:Q:1253:ALA:O	1:Q:1254:ASN:C	2.57	0.42
1:R:1021:HIS:O	1:R:1339:ALA:HA	2.19	0.42
1:R:1327:THR:O	1:R:1330:ALA:N	2.52	0.42
2:S:1016:SER:HG	2:S:1019:CYS:CB	2.10	0.42
1:V:1065:ALA:C	1:V:1067:ASN:H	2.22	0.42
1:V:1126:ASN:OD1	1:W:1064:SER:CA	2.66	0.42
1:P:1168:ASN:O	1:P:1170:ARG:N	2.49	0.42
1:Q:1316:TYR:CD1	1:Q:1338:VAL:HG22	2.54	0.42
1:R:1011:LEU:HD23	1:R:1011:LEU:HA	1.83	0.42
1:R:1051:THR:HG23	1:R:1081:LYS:HB3	2.01	0.42
1:R:1324:ASN:HA	1:R:1328:ARG:NH2	2.34	0.42
1:V:1319:ASN:ND2	1:V:1334:THR:O	2.53	0.42
1:W:1135:ASP:CB	1:W:1140:VAL:O	2.67	0.42
1:W:1186:TYR:CE2	1:W:1188:TYR:CD1	3.07	0.42
1:P:1012:ASP:C	1:P:1012:ASP:OD2	2.57	0.42
1:Q:1193:ILE:HG23	1:Q:1193:ILE:HD12	1.76	0.42
1:Q:1307:ASN:OD1	1:Q:1309:ASN:HB2	2.20	0.42
1:R:1092:ARG:HH11	1:R:1126:ASN:ND2	2.16	0.42
1:R:1121:MET:CE	1:R:1148:GLN:HG3	2.49	0.42
1:W:1003:VAL:HG23	1:W:1011:LEU:HB3	2.00	0.42
1:P:1102:SER:C	1:P:1104:THR:N	2.73	0.42
1:P:1191:PHE:H	1:P:1227:TYR:HA	1.85	0.42
1:R:1296:LYS:O	1:R:1297:TYR:HB3	2.19	0.42
1:U:1253:ALA:O	1:U:1254:ASN:C	2.58	0.42
1:U:1324:ASN:HA	1:U:1328:ARG:NH2	2.34	0.42
1:W:1090:TYR:CG	1:W:1091:GLY:N	2.87	0.42
1:P:1018:ASP:CG	1:P:1343:VAL:HG22	2.39	0.42
1:Q:1102:SER:O	1:Q:1104:THR:N	2.52	0.42
1:Q:1191:PHE:CA	1:Q:1226:LYS:O	2.66	0.42
1:Q:1196:ALA:HB3	1:Q:1222:THR:HG23	2.01	0.42
1:R:1131:TYR:O	1:R:1146:ALA:HA	2.20	0.42
1:U:1304:TYR:HE2	1:U:1306:PHE:CD1	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1027:LYS:HB2	1:V:1027:LYS:HE3	1.94	0.42
1:P:1227:TYR:N	1:P:1234:LEU:O	2.52	0.42
1:P:1248:GLY:HA3	1:P:1330:ALA:HB1	2.00	0.42
1:V:1265:TYR:O	1:V:1273:PRO:HD2	2.19	0.42
1:W:1162:THR:O	1:W:1163:SER:C	2.58	0.42
1:W:1162:THR:O	1:W:1165:VAL:HG22	2.06	0.42
2:X:1008:TRP:O	2:X:1009:CYS:O	2.37	0.42
1:Q:1186:TYR:CE2	1:Q:1188:TYR:CD1	3.08	0.42
1:Q:1289:TYR:CE1	1:Q:1329:ASP:OD2	2.73	0.42
1:R:1298:VAL:CG1	1:R:1299:ASP:N	2.82	0.42
2:S:1017:LYS:HB3	2:S:1017:LYS:HZ2	1.85	0.42
1:U:1240:GLN:HG3	1:U:1240:GLN:O	2.20	0.42
1:V:1037:ARG:CD	1:V:1059:GLN:HG3	2.49	0.42
1:V:1136:PHE:HB3	1:V:1140:VAL:HG13	2.01	0.42
1:V:1193:ILE:HG23	1:V:1193:ILE:HD12	1.79	0.42
1:V:1289:TYR:O	1:V:1290:ASP:CB	2.58	0.42
1:W:1193:ILE:HG23	1:W:1193:ILE:HD12	1.76	0.42
1:P:1190:GLY:O	1:P:1191:PHE:HB2	2.20	0.42
1:Q:1047:THR:HG22	1:Q:1050:LEU:N	2.25	0.42
1:Q:1113:ASP:O	1:Q:1295:LEU:HD22	2.20	0.42
1:Q:1134:THR:O	1:Q:1144:ASN:HB3	2.19	0.42
1:R:1156:PRO:HD3	1:R:1166:THR:O	2.20	0.42
1:R:1162:THR:CA	1:R:1165:VAL:HG21	2.50	0.42
1:V:1206:GLN:HE21	1:V:1206:GLN:HB3	1.76	0.42
1:P:1161:PHE:CD2	1:Q:1028:ASP:OD2	2.73	0.42
1:P:1307:ASN:OD1	1:P:1309:ASN:HB2	2.20	0.42
1:Q:1002:GLU:OE1	1:Q:1005:ASN:HB3	2.18	0.42
1:Q:1160:GLY:O	1:Q:1161:PHE:O	2.38	0.42
1:Q:1192:GLY:N	1:Q:1226:LYS:O	2.50	0.42
1:Q:1292:GLU:HG2	1:Q:1326:PHE:CD2	2.55	0.42
1:R:1327:THR:O	1:R:1328:ARG:C	2.58	0.42
1:V:1344:TYR:CD2	1:V:1344:TYR:O	2.73	0.42
1:W:1097:VAL:HG21	1:W:1220:THR:OG1	2.20	0.42
1:P:1135:ASP:HB3	1:P:1140:VAL:O	2.20	0.41
1:P:1190:GLY:O	1:P:1191:PHE:HD1	2.03	0.41
1:Q:1161:PHE:HB3	1:R:1027:LYS:O	2.20	0.41
1:Q:1213:GLY:O	1:Q:1215:GLY:N	2.53	0.41
1:R:1130:THR:OG1	1:R:1148:GLN:NE2	2.51	0.41
2:X:1023:GLN:HA	2:X:1035:THR:HA	2.02	0.41
1:P:1056:TRP:HA	1:P:1075:VAL:O	2.20	0.41
1:P:1155:ASN:O	1:P:1165:VAL:HG11	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1001:ALA:N	1:Q:1013:LEU:O	2.53	0.41
1:Q:1211:TYR:HD1	1:Q:1211:TYR:N	1.89	0.41
1:Q:1232:ILE:CG2	1:Q:1234:LEU:HD22	2.50	0.41
1:Q:1237:GLN:OE1	1:Q:1239:THR:HG23	2.11	0.41
1:Q:1324:ASN:HD22	1:Q:1327:THR:N	2.17	0.41
1:R:1195:GLY:HA2	1:R:1222:THR:O	2.20	0.41
1:U:1083:GLN:CD	1:U:1084:ASP:H	2.23	0.41
1:V:1118:ASP:OD1	1:W:1065:ALA:HB1	2.19	0.41
1:W:1137:PHE:HB2	1:W:1139:LEU:CD1	2.50	0.41
1:W:1230:ASN:O	1:W:1232:ILE:N	2.53	0.41
1:R:1302:ALA:N	1:R:1314:VAL:O	2.54	0.41
1:V:1033:GLN:O	1:V:1034:THR:C	2.59	0.41
1:W:1001:ALA:N	1:W:1346:PHE:OXT	2.53	0.41
1:W:1087:SER:O	1:W:1131:TYR:HA	2.21	0.41
1:W:1088:PHE:HA	1:W:1130:THR:O	2.20	0.41
2:X:1011:THR:HB	2:X:1012:SER:H	1.49	0.41
1:P:1152:LYS:HE3	1:P:1203:THR:HG22	2.03	0.41
1:P:1165:VAL:CG1	1:P:1166:THR:H	2.13	0.41
1:Q:1061:GLN:HB3	1:Q:1063:ASN:OD1	2.19	0.41
1:Q:1195:GLY:HA2	1:Q:1222:THR:O	2.21	0.41
1:R:1096:VAL:O	1:R:1098:TYR:N	2.53	0.41
1:U:1077:PHE:CE2	1:U:1093:ASN:OD1	2.73	0.41
1:U:1131:TYR:O	1:U:1146:ALA:HA	2.21	0.41
1:U:1202:ARG:NH2	1:U:1215:GLY:HA3	2.34	0.41
1:V:1203:THR:OG1	1:V:1206:GLN:HG2	2.19	0.41
1:V:1276:ALA:HB3	1:V:1299:ASP:HB3	2.03	0.41
1:V:1277:TYR:O	1:V:1278:LEU:HD22	2.20	0.41
1:W:1184:ILE:CD1	1:W:1195:GLY:O	2.69	0.41
2:X:1018:LYS:O	2:X:1021:GLN:HG2	2.19	0.41
1:P:1020:LEU:CD2	1:P:1021:HIS:N	2.82	0.41
1:P:1232:ILE:HG22	1:P:1234:LEU:HD22	2.02	0.41
1:Q:1168:ASN:HB3	1:Q:1171:ASP:OD2	2.20	0.41
1:Q:1228:ASP:O	1:Q:1229:ALA:HB2	2.20	0.41
1:U:1227:TYR:CD2	1:U:1227:TYR:C	2.94	0.41
1:U:1316:TYR:CD1	1:U:1338:VAL:HG22	2.54	0.41
1:V:1135:ASP:O	1:V:1137:PHE:N	2.53	0.41
1:V:1211:TYR:HB3	1:V:1287:ARG:HH12	1.85	0.41
1:W:1134:THR:CG2	1:W:1134:THR:C	2.88	0.41
1:P:1144:ASN:O	1:P:1184:ILE:HA	2.20	0.41
1:P:1319:ASN:ND2	1:P:1334:THR:C	2.74	0.41
1:Q:1023:PHE:CD2	1:Q:1023:PHE:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1036:MET:CE	1:Q:1038:LEU:HD22	2.50	0.41
1:Q:1147:VAL:O	1:Q:1147:VAL:CG1	2.60	0.41
1:R:1167:ASN:OD1	1:R:1167:ASN:N	2.51	0.41
1:R:1200:SER:O	1:R:1201:LYS:C	2.57	0.41
1:V:1205:ALA:O	1:V:1208:THR:HG23	2.21	0.41
1:V:1266:GLN:HB2	1:V:1272:ARG:NH1	2.35	0.41
1:W:1094:TYR:HA	1:W:1124:ARG:H	1.86	0.41
1:W:1130:THR:HG21	1:W:1132:ARG:NH1	2.35	0.41
1:P:1026:ASN:O	1:P:1029:VAL:HG22	2.21	0.41
1:P:1186:TYR:CE2	1:P:1188:TYR:CD1	3.09	0.41
1:Q:1119:ASN:HB2	1:Q:1246:ARG:NH2	2.34	0.41
1:Q:1299:ASP:OD1	1:Q:1299:ASP:C	2.59	0.41
1:Q:1324:ASN:C	1:Q:1326:PHE:H	2.24	0.41
2:S:1012:SER:N	2:S:1040:THR:HA	2.32	0.41
1:U:1009:ASN:HA	1:U:1044:THR:HA	2.03	0.41
1:U:1083:GLN:CG	1:U:1084:ASP:N	2.84	0.41
1:U:1110:PHE:CE2	1:U:1315:ASP:HB3	2.56	0.41
1:U:1144:ASN:O	1:U:1185:THR:N	2.54	0.41
1:V:1102:SER:O	1:V:1104:THR:N	2.54	0.41
1:V:1196:ALA:N	1:V:1222:THR:O	2.51	0.41
1:V:1344:TYR:O	1:V:1344:TYR:HD2	2.03	0.41
1:W:1026:ASN:HB2	1:W:1335:ASP:OD2	2.20	0.41
1:W:1070:ASN:HD22	1:W:1071:SER:N	2.18	0.41
1:P:1247:VAL:O	1:P:1250:LEU:HB2	2.21	0.41
1:P:1336:ASN:O	1:P:1337:ILE:HG13	2.20	0.41
1:Q:1310:MET:HG3	1:Q:1311:SER:H	1.84	0.41
1:W:1055:GLN:O	1:W:1076:ALA:HA	2.20	0.41
2:X:1012:SER:CB	2:X:1013:PRO:HD3	2.48	0.41
1:Q:1049:GLN:O	1:Q:1083:GLN:HB3	2.20	0.41
1:Q:1137:PHE:HB2	1:Q:1139:LEU:CD1	2.51	0.41
1:Q:1200:SER:O	1:Q:1201:LYS:C	2.59	0.41
1:Q:1250:LEU:HD21	1:Q:1329:ASP:HB3	2.03	0.41
1:R:1319:ASN:ND2	1:R:1334:THR:O	2.54	0.41
2:S:1004:LYS:HB2	2:S:1004:LYS:NZ	2.36	0.41
1:U:1010:LYS:HE3	1:U:1010:LYS:HB2	1.81	0.41
1:U:1118:ASP:HB3	1:U:1170:ARG:HB3	2.01	0.41
1:U:1219:GLU:O	1:U:1241:THR:HA	2.20	0.41
1:V:1096:VAL:C	1:V:1098:TYR:H	2.23	0.41
1:V:1208:THR:O	1:V:1208:THR:OG1	2.34	0.41
1:V:1214:ASN:H	1:V:1254:ASN:HD21	1.69	0.41
1:Q:1191:PHE:H	1:Q:1227:TYR:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:1049:GLN:HB2	1:R:1083:GLN:HG2	2.03	0.41
1:R:1056:TRP:HA	1:R:1075:VAL:O	2.21	0.41
1:U:1037:ARG:NH1	1:U:1074:ARG:CZ	2.84	0.41
1:U:1065:ALA:C	1:U:1067:ASN:H	2.25	0.41
1:U:1133:ASN:HD21	1:U:1136:PHE:HA	1.85	0.41
1:U:1214:ASN:H	1:U:1254:ASN:HD21	1.69	0.41
1:V:1319:ASN:ND2	1:V:1334:THR:C	2.74	0.41
1:W:1211:TYR:O	1:W:1212:ILE:HG23	2.21	0.41
1:W:1222:THR:HB	1:W:1239:THR:CB	2.39	0.41
1:P:1046:VAL:HB	1:P:1050:LEU:HD13	2.04	0.40
1:P:1083:GLN:OE1	1:P:1083:GLN:C	2.60	0.40
1:Q:1134:THR:CG2	1:Q:1135:ASP:N	2.84	0.40
1:Q:1159:GLU:CD	1:Q:1160:GLY:N	2.74	0.40
1:W:1290:ASP:HB3	1:W:1291:ASP:H	1.43	0.40
1:Q:1156:PRO:O	1:Q:1161:PHE:CE2	2.74	0.40
1:R:1304:TYR:O	1:R:1311:SER:HB2	2.21	0.40
1:U:1126:ASN:OD1	1:V:1064:SER:C	2.59	0.40
1:V:1018:ASP:C	1:V:1018:ASP:OD2	2.60	0.40
1:V:1064:SER:HB2	1:V:1068:GLU:OE2	2.21	0.40
1:V:1164:GLY:O	1:V:1165:VAL:HG22	2.21	0.40
1:W:1059:GLN:OE1	1:W:1061:GLN:OE1	2.39	0.40
1:W:1312:THR:CG2	1:W:1342:LEU:HD13	2.51	0.40
2:X:1012:SER:CB	2:X:1013:PRO:CD	2.99	0.40
1:P:1139:LEU:O	1:P:1140:VAL:CB	2.69	0.40
1:P:1161:PHE:O	1:P:1162:THR:HG23	2.21	0.40
1:Q:1097:VAL:O	1:Q:1097:VAL:HG13	2.19	0.40
1:U:1056:TRP:CZ2	1:U:1058:TYR:HB2	2.57	0.40
1:V:1104:THR:HG22	1:V:1235:ALA:HB3	2.03	0.40
1:W:1119:ASN:HB2	1:W:1246:ARG:NH2	2.35	0.40
1:W:1296:LYS:HG2	1:W:1320:LEU:CB	2.51	0.40
1:P:1184:ILE:O	1:P:1184:ILE:HG12	2.20	0.40
1:R:1265:TYR:O	1:R:1273:PRO:HD2	2.21	0.40
1:U:1092:ARG:HH11	1:U:1126:ASN:ND2	2.19	0.40
1:V:1003:VAL:HG22	1:V:1013:LEU:H	1.85	0.40
1:V:1162:THR:H	1:V:1165:VAL:HG21	1.87	0.40
1:V:1186:TYR:O	1:V:1192:GLY:HA2	2.21	0.40
1:W:1014:TYR:O	1:W:1039:GLY:N	2.44	0.40
1:P:1037:ARG:CD	1:P:1059:GLN:HG3	2.52	0.40
1:R:1117:SER:HA	1:R:1123:GLN:OE1	2.21	0.40
1:R:1319:ASN:ND2	1:R:1334:THR:C	2.74	0.40
1:U:1164:GLY:C	1:U:1165:VAL:CG2	2.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:1016:LYS:HB3	1:V:1345:GLN:HB3	2.03	0.40
2:X:1017:LYS:NZ	2:X:1017:LYS:HB2	2.36	0.40
2:X:1026:MET:HG3	2:X:1034:VAL:O	2.21	0.40

There are no symmetry-related clashes.

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	P	333/346 (96%)	256 (77%)	45 (14%)	32 (10%)	0	3
1	Q	333/346 (96%)	257 (77%)	43 (13%)	33 (10%)	0	2
1	R	333/346 (96%)	262 (79%)	33 (10%)	38 (11%)	0	2
1	U	333/346 (96%)	259 (78%)	42 (13%)	32 (10%)	0	3
1	V	333/346 (96%)	259 (78%)	41 (12%)	33 (10%)	0	2
1	W	333/346 (96%)	261 (78%)	42 (13%)	30 (9%)	1	3
2	S	43/45 (96%)	8 (19%)	11 (26%)	24 (56%)	0	0
2	X	43/45 (96%)	13 (30%)	10 (23%)	20 (46%)	0	0
All	All	2084/2166 (96%)	1575 (76%)	267 (13%)	242 (12%)	0	1

All (242) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	1002	GLU
1	P	1003	VAL
1	P	1007	ASP
1	P	1071	SER
1	P	1083	GLN
1	P	1124	ARG
1	P	1140	VAL

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Mol	Chain	Res	Type
1	P	1157	SER
1	P	1163	SER
1	P	1189	GLU
1	P	1211	TYR
1	P	1284	ASN
1	Q	1003	VAL
1	Q	1007	ASP
1	Q	1070	ASN
1	Q	1071	SER
1	Q	1083	GLN
1	Q	1085	VAL
1	Q	1124	ARG
1	Q	1140	VAL
1	Q	1157	SER
1	Q	1189	GLU
1	Q	1209	ALA
1	R	1003	VAL
1	R	1070	ASN
1	R	1071	SER
1	R	1083	GLN
1	R	1085	VAL
1	R	1110	PHE
1	R	1124	ARG
1	R	1136	PHE
1	R	1140	VAL
1	R	1157	SER
1	R	1161	PHE
1	R	1163	SER
1	R	1188	TYR
1	R	1189	GLU
1	R	1309	ASN
2	S	1002	SER
2	S	1005	SER
2	S	1009	CYS
2	S	1010	THR
2	S	1012	SER
2	S	1013	PRO
2	S	1014	ALA
2	S	1019	CYS
2	S	1021	GLN
2	S	1028	LYS
2	S	1029	VAL

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Mol	Chain	Res	Type
2	S	1036	CYS
2	S	1038	LYS
2	S	1039	LYS
2	S	1040	THR
2	S	1043	PHE
2	S	1044	GLU
1	U	1003	VAL
1	U	1007	ASP
1	U	1071	SER
1	U	1083	GLN
1	U	1124	ARG
1	U	1136	PHE
1	U	1140	VAL
1	U	1163	SER
1	U	1189	GLU
1	U	1209	ALA
1	U	1290	ASP
1	V	1003	VAL
1	V	1007	ASP
1	V	1066	GLU
1	V	1071	SER
1	V	1083	GLN
1	V	1085	VAL
1	V	1110	PHE
1	V	1124	ARG
1	V	1140	VAL
1	V	1157	SER
1	V	1163	SER
1	V	1189	GLU
1	W	1002	GLU
1	W	1003	VAL
1	W	1007	ASP
1	W	1069	ASN
1	W	1071	SER
1	W	1083	GLN
1	W	1085	VAL
1	W	1124	ARG
1	W	1136	PHE
1	W	1140	VAL
1	W	1157	SER
1	W	1189	GLU
1	W	1209	ALA

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Mol	Chain	Res	Type
1	W	1211	TYR
2	X	1004	LYS
2	X	1009	CYS
2	X	1012	SER
2	X	1013	PRO
2	X	1014	ALA
2	X	1028	LYS
2	X	1032	PRO
2	X	1033	SER
1	P	1066	GLU
1	P	1069	ASN
1	P	1085	VAL
1	P	1103	TRP
1	P	1136	PHE
1	P	1161	PHE
1	P	1188	TYR
1	P	1209	ALA
1	P	1231	ASN
1	Q	1047	THR
1	Q	1066	GLU
1	Q	1110	PHE
1	Q	1136	PHE
1	Q	1159	GLU
1	Q	1163	SER
1	Q	1169	GLY
1	Q	1188	TYR
1	Q	1190	GLY
1	Q	1284	ASN
1	Q	1290	ASP
1	R	1002	GLU
1	R	1005	ASN
1	R	1007	ASP
1	R	1066	GLU
1	R	1169	GLY
1	R	1190	GLY
1	R	1209	ALA
1	R	1211	TYR
1	R	1290	ASP
1	R	1328	ARG
2	S	1004	LYS
2	S	1015	GLU
2	S	1018	LYS

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Mol	Chain	Res	Type
2	S	1020	ALA
1	U	1047	THR
1	U	1066	GLU
1	U	1085	VAL
1	U	1097	VAL
1	U	1157	SER
1	U	1188	TYR
1	V	1069	ASN
1	V	1136	PHE
1	V	1161	PHE
1	V	1169	GLY
1	V	1188	TYR
1	V	1211	TYR
1	V	1328	ARG
1	W	1097	VAL
1	W	1106	VAL
1	W	1110	PHE
1	W	1159	GLU
1	W	1161	PHE
1	W	1188	TYR
1	W	1231	ASN
1	W	1328	ARG
2	X	1006	VAL
2	X	1018	LYS
2	X	1031	GLY
2	X	1037	VAL
1	P	1110	PHE
1	P	1290	ASP
1	P	1309	ASN
1	Q	1211	TYR
1	Q	1231	ASN
1	Q	1309	ASN
1	R	1047	THR
1	R	1103	TRP
1	R	1191	PHE
1	R	1229	ALA
1	R	1289	TYR
2	S	1023	GLN
2	S	1032	PRO
2	S	1037	VAL
1	U	1002	GLU
1	U	1004	TYR

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Mol	Chain	Res	Type
1	U	1070	ASN
1	U	1161	PHE
1	U	1211	TYR
1	U	1284	ASN
1	U	1328	ARG
1	V	1191	PHE
1	V	1229	ALA
1	V	1290	ASP
1	W	1169	GLY
1	W	1284	ASN
1	W	1309	ASN
1	W	1327	THR
2	X	1015	GLU
2	X	1020	ALA
2	X	1044	GLU
1	P	1004	TYR
1	P	1047	THR
1	P	1070	ASN
1	P	1169	GLY
1	Q	1069	ASN
1	Q	1328	ARG
1	R	1284	ASN
1	U	1110	PHE
1	U	1169	GLY
1	U	1231	ASN
1	U	1309	ASN
1	V	1004	TYR
1	V	1047	THR
1	V	1159	GLU
1	V	1165	VAL
1	V	1190	GLY
1	V	1284	ASN
1	W	1027	LYS
1	W	1163	SER
1	W	1290	ASP
2	X	1022	TRP
2	X	1039	LYS
1	P	1034	THR
1	P	1097	VAL
1	Q	1161	PHE
1	Q	1191	PHE
1	Q	1230	ASN

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Mol	Chain	Res	Type
1	R	1004	TYR
1	R	1034	THR
1	R	1069	ASN
1	R	1167	ASN
1	R	1216	ASP
1	U	1106	VAL
1	U	1159	GLU
1	U	1191	PHE
1	V	1070	ASN
1	V	1289	TYR
1	V	1325	GLN
1	W	1047	THR
2	X	1036	CYS
2	X	1038	LYS
1	P	1191	PHE
1	P	1268	ASP
1	Q	1027	LYS
1	Q	1106	VAL
1	R	1231	ASN
1	U	1069	ASN
1	V	1212	ILE
1	V	1309	ASN
2	X	1035	THR
1	Q	1097	VAL
1	R	1106	VAL

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	P	266/275 (97%)	203 (76%)	63 (24%)	1 3
1	Q	266/275 (97%)	208 (78%)	58 (22%)	1 5
1	R	266/275 (97%)	195 (73%)	71 (27%)	0 2
1	U	266/275 (97%)	200 (75%)	66 (25%)	0 3
1	V	266/275 (97%)	199 (75%)	67 (25%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	W	266/275 (97%)	201 (76%)	65 (24%)	0 3
2	S	41/41 (100%)	24 (58%)	17 (42%)	0 0
2	X	41/41 (100%)	26 (63%)	15 (37%)	0 1
All	All	1678/1732 (97%)	1256 (75%)	422 (25%)	0 3

All (422) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1002	GLU
1	P	1003	VAL
1	P	1010	LYS
1	P	1013	LEU
1	P	1016	LYS
1	P	1020	LEU
1	P	1027	LYS
1	P	1028	ASP
1	P	1037	ARG
1	P	1047	THR
1	P	1049	GLN
1	P	1050	LEU
1	P	1060	ILE
1	P	1069	ASN
1	P	1070	ASN
1	P	1071	SER
1	P	1075	VAL
1	P	1080	LEU
1	P	1081	LYS
1	P	1083	GLN
1	P	1085	VAL
1	P	1096	VAL
1	P	1103	TRP
1	P	1124	ARG
1	P	1130	THR
1	P	1134	THR
1	P	1139	LEU
1	P	1140	VAL
1	P	1144	ASN
1	P	1147	VAL
1	P	1148	GLN
1	P	1153	ASN
1	P	1159	GLU

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Mol	Chain	Res	Type
1	P	1163	SER
1	P	1165	VAL
1	P	1166	THR
1	P	1168	ASN
1	P	1171	ASP
1	P	1184	ILE
1	P	1187	ASP
1	P	1188	TYR
1	P	1197	ILE
1	P	1200	SER
1	P	1201	LYS
1	P	1206	GLN
1	P	1211	TYR
1	P	1225	LEU
1	P	1234	LEU
1	P	1237	GLN
1	P	1239	THR
1	P	1262	VAL
1	P	1268	ASP
1	P	1275	LEU
1	P	1278	LEU
1	P	1281	LYS
1	P	1287	ARG
1	P	1303	THR
1	P	1308	LYS
1	P	1312	THR
1	P	1324	ASN
1	P	1340	LEU
1	P	1342	LEU
1	P	1345	GLN
1	Q	1002	GLU
1	Q	1010	LYS
1	Q	1013	LEU
1	Q	1016	LYS
1	Q	1020	LEU
1	Q	1027	LYS
1	Q	1037	ARG
1	Q	1047	THR
1	Q	1049	GLN
1	Q	1050	LEU
1	Q	1051	THR
1	Q	1060	ILE

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Mol	Chain	Res	Type
1	Q	1069	ASN
1	Q	1070	ASN
1	Q	1071	SER
1	Q	1075	VAL
1	Q	1080	LEU
1	Q	1081	LYS
1	Q	1083	GLN
1	Q	1096	VAL
1	Q	1103	TRP
1	Q	1106	VAL
1	Q	1107	LEU
1	Q	1124	ARG
1	Q	1134	THR
1	Q	1135	ASP
1	Q	1139	LEU
1	Q	1144	ASN
1	Q	1147	VAL
1	Q	1159	GLU
1	Q	1162	THR
1	Q	1163	SER
1	Q	1165	VAL
1	Q	1166	THR
1	Q	1168	ASN
1	Q	1171	ASP
1	Q	1184	ILE
1	Q	1187	ASP
1	Q	1197	ILE
1	Q	1201	LYS
1	Q	1206	GLN
1	Q	1211	TYR
1	Q	1225	LEU
1	Q	1234	LEU
1	Q	1239	THR
1	Q	1262	VAL
1	Q	1268	ASP
1	Q	1275	LEU
1	Q	1278	LEU
1	Q	1287	ARG
1	Q	1292	GLU
1	Q	1303	THR
1	Q	1308	LYS
1	Q	1312	THR

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Mol	Chain	Res	Type
1	Q	1323	ASP
1	Q	1324	ASN
1	Q	1340	LEU
1	Q	1345	GLN
1	R	1002	GLU
1	R	1003	VAL
1	R	1010	LYS
1	R	1013	LEU
1	R	1016	LYS
1	R	1020	LEU
1	R	1027	LYS
1	R	1028	ASP
1	R	1036	MET
1	R	1037	ARG
1	R	1047	THR
1	R	1049	GLN
1	R	1050	LEU
1	R	1051	THR
1	R	1060	ILE
1	R	1069	ASN
1	R	1070	ASN
1	R	1071	SER
1	R	1074	ARG
1	R	1075	VAL
1	R	1080	LEU
1	R	1081	LYS
1	R	1083	GLN
1	R	1085	VAL
1	R	1089	ASP
1	R	1096	VAL
1	R	1103	TRP
1	R	1106	VAL
1	R	1122	GLN
1	R	1124	ARG
1	R	1128	PHE
1	R	1134	THR
1	R	1135	ASP
1	R	1139	LEU
1	R	1140	VAL
1	R	1144	ASN
1	R	1159	GLU
1	R	1161	PHE

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Mol	Chain	Res	Type
1	R	1163	SER
1	R	1165	VAL
1	R	1166	THR
1	R	1168	ASN
1	R	1171	ASP
1	R	1184	ILE
1	R	1187	ASP
1	R	1188	TYR
1	R	1193	ILE
1	R	1200	SER
1	R	1201	LYS
1	R	1206	GLN
1	R	1208	THR
1	R	1211	TYR
1	R	1217	ARG
1	R	1225	LEU
1	R	1234	LEU
1	R	1237	GLN
1	R	1239	THR
1	R	1268	ASP
1	R	1272	ARG
1	R	1278	LEU
1	R	1287	ARG
1	R	1292	GLU
1	R	1300	VAL
1	R	1303	THR
1	R	1308	LYS
1	R	1312	THR
1	R	1314	VAL
1	R	1323	ASP
1	R	1324	ASN
1	R	1340	LEU
1	R	1345	GLN
2	S	1003	LYS
2	S	1004	LYS
2	S	1007	ARG
2	S	1008	TRP
2	S	1009	CYS
2	S	1015	GLU
2	S	1016	SER
2	S	1017	LYS
2	S	1018	LYS

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Mol	Chain	Res	Type
2	S	1019	CYS
2	S	1021	GLN
2	S	1022	TRP
2	S	1027	LYS
2	S	1028	LYS
2	S	1030	ARG
2	S	1042	ARG
2	S	1043	PHE
1	U	1002	GLU
1	U	1006	LYS
1	U	1010	LYS
1	U	1013	LEU
1	U	1016	LYS
1	U	1020	LEU
1	U	1027	LYS
1	U	1028	ASP
1	U	1037	ARG
1	U	1045	GLN
1	U	1047	THR
1	U	1049	GLN
1	U	1050	LEU
1	U	1051	THR
1	U	1060	ILE
1	U	1067	ASN
1	U	1069	ASN
1	U	1070	ASN
1	U	1075	VAL
1	U	1080	LEU
1	U	1081	LYS
1	U	1089	ASP
1	U	1096	VAL
1	U	1103	TRP
1	U	1122	GLN
1	U	1123	GLN
1	U	1124	ARG
1	U	1128	PHE
1	U	1134	THR
1	U	1135	ASP
1	U	1139	LEU
1	U	1144	ASN
1	U	1153	ASN
1	U	1159	GLU

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Mol	Chain	Res	Type
1	U	1163	SER
1	U	1165	VAL
1	U	1166	THR
1	U	1168	ASN
1	U	1171	ASP
1	U	1184	ILE
1	U	1187	ASP
1	U	1188	TYR
1	U	1200	SER
1	U	1201	LYS
1	U	1206	GLN
1	U	1211	TYR
1	U	1212	ILE
1	U	1217	ARG
1	U	1234	LEU
1	U	1237	GLN
1	U	1239	THR
1	U	1252	TRP
1	U	1262	VAL
1	U	1268	ASP
1	U	1272	ARG
1	U	1275	LEU
1	U	1278	LEU
1	U	1287	ARG
1	U	1290	ASP
1	U	1292	GLU
1	U	1303	THR
1	U	1308	LYS
1	U	1312	THR
1	U	1324	ASN
1	U	1340	LEU
1	U	1345	GLN
1	V	1002	GLU
1	V	1003	VAL
1	V	1005	ASN
1	V	1010	LYS
1	V	1013	LEU
1	V	1016	LYS
1	V	1020	LEU
1	V	1027	LYS
1	V	1028	ASP
1	V	1036	MET

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Mol	Chain	Res	Type
1	V	1037	ARG
1	V	1045	GLN
1	V	1047	THR
1	V	1049	GLN
1	V	1050	LEU
1	V	1060	ILE
1	V	1069	ASN
1	V	1070	ASN
1	V	1074	ARG
1	V	1075	VAL
1	V	1080	LEU
1	V	1081	LYS
1	V	1083	GLN
1	V	1085	VAL
1	V	1089	ASP
1	V	1096	VAL
1	V	1103	TRP
1	V	1106	VAL
1	V	1124	ARG
1	V	1134	THR
1	V	1135	ASP
1	V	1139	LEU
1	V	1144	ASN
1	V	1148	GLN
1	V	1153	ASN
1	V	1159	GLU
1	V	1163	SER
1	V	1165	VAL
1	V	1166	THR
1	V	1168	ASN
1	V	1171	ASP
1	V	1184	ILE
1	V	1187	ASP
1	V	1188	TYR
1	V	1197	ILE
1	V	1201	LYS
1	V	1202	ARG
1	V	1206	GLN
1	V	1208	THR
1	V	1211	TYR
1	V	1225	LEU
1	V	1226	LYS

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Mol	Chain	Res	Type
1	V	1230	ASN
1	V	1234	LEU
1	V	1237	GLN
1	V	1239	THR
1	V	1268	ASP
1	V	1275	LEU
1	V	1278	LEU
1	V	1287	ARG
1	V	1303	THR
1	V	1308	LYS
1	V	1312	THR
1	V	1314	VAL
1	V	1324	ASN
1	V	1340	LEU
1	V	1345	GLN
1	W	1010	LYS
1	W	1011	LEU
1	W	1013	LEU
1	W	1016	LYS
1	W	1020	LEU
1	W	1028	ASP
1	W	1047	THR
1	W	1049	GLN
1	W	1050	LEU
1	W	1051	THR
1	W	1060	ILE
1	W	1069	ASN
1	W	1070	ASN
1	W	1071	SER
1	W	1075	VAL
1	W	1080	LEU
1	W	1083	GLN
1	W	1096	VAL
1	W	1103	TRP
1	W	1106	VAL
1	W	1122	GLN
1	W	1124	ARG
1	W	1134	THR
1	W	1135	ASP
1	W	1139	LEU
1	W	1144	ASN
1	W	1147	VAL

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Mol	Chain	Res	Type
1	W	1148	GLN
1	W	1153	ASN
1	W	1159	GLU
1	W	1161	PHE
1	W	1163	SER
1	W	1165	VAL
1	W	1166	THR
1	W	1168	ASN
1	W	1171	ASP
1	W	1184	ILE
1	W	1187	ASP
1	W	1188	TYR
1	W	1193	ILE
1	W	1200	SER
1	W	1201	LYS
1	W	1206	GLN
1	W	1211	TYR
1	W	1217	ARG
1	W	1226	LYS
1	W	1231	ASN
1	W	1234	LEU
1	W	1237	GLN
1	W	1239	THR
1	W	1262	VAL
1	W	1268	ASP
1	W	1272	ARG
1	W	1275	LEU
1	W	1278	LEU
1	W	1287	ARG
1	W	1292	GLU
1	W	1303	THR
1	W	1308	LYS
1	W	1312	THR
1	W	1323	ASP
1	W	1324	ASN
1	W	1340	LEU
1	W	1342	LEU
1	W	1345	GLN
2	X	1002	SER
2	X	1003	LYS
2	X	1004	LYS
2	X	1006	VAL

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Mol	Chain	Res	Type
2	X	1007	ARG
2	X	1015	GLU
2	X	1017	LYS
2	X	1018	LYS
2	X	1021	GLN
2	X	1025	ARG
2	X	1027	LYS
2	X	1030	ARG
2	X	1038	LYS
2	X	1042	ARG
2	X	1044	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	1055	GLN
1	P	1059	GLN
1	P	1119	ASN
1	P	1122	GLN
1	P	1133	ASN
1	P	1144	ASN
1	P	1231	ASN
1	P	1254	ASN
1	P	1257	GLN
1	P	1309	ASN
1	P	1324	ASN
1	Q	1067	ASN
1	Q	1070	ASN
1	Q	1119	ASN
1	Q	1122	GLN
1	Q	1133	ASN
1	Q	1144	ASN
1	Q	1231	ASN
1	Q	1254	ASN
1	Q	1257	GLN
1	Q	1309	ASN
1	Q	1324	ASN
1	R	1055	GLN
1	R	1059	GLN
1	R	1070	ASN
1	R	1119	ASN
1	R	1122	GLN

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Mol	Chain	Res	Type
1	R	1133	ASN
1	R	1144	ASN
1	R	1231	ASN
1	R	1254	ASN
1	R	1309	ASN
1	R	1324	ASN
2	S	1021	GLN
2	S	1023	GLN
1	U	1033	GLN
1	U	1055	GLN
1	U	1059	GLN
1	U	1070	ASN
1	U	1119	ASN
1	U	1122	GLN
1	U	1133	ASN
1	U	1144	ASN
1	U	1231	ASN
1	U	1254	ASN
1	U	1309	ASN
1	U	1324	ASN
1	V	1070	ASN
1	V	1119	ASN
1	V	1122	GLN
1	V	1133	ASN
1	V	1144	ASN
1	V	1231	ASN
1	V	1254	ASN
1	V	1309	ASN
1	V	1324	ASN
1	W	1059	GLN
1	W	1070	ASN
1	W	1122	GLN
1	W	1133	ASN
1	W	1144	ASN
1	W	1231	ASN
1	W	1254	ASN
1	W	1309	ASN
1	W	1324	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	P	337/346 (97%)	0.22	4 (1%) 79 54	17, 29, 47, 60	0
1	Q	337/346 (97%)	0.21	4 (1%) 79 54	17, 29, 47, 59	0
1	R	337/346 (97%)	0.26	5 (1%) 73 46	17, 29, 47, 59	0
1	U	337/346 (97%)	0.27	3 (0%) 84 63	17, 29, 47, 59	0
1	V	337/346 (97%)	0.23	6 (1%) 68 40	17, 29, 47, 59	0
1	W	337/346 (97%)	0.19	2 (0%) 89 72	17, 29, 47, 59	0
2	S	45/45 (100%)	3.18	30 (66%) 0 0	71, 80, 80, 80	0
2	X	45/45 (100%)	3.52	39 (86%) 0 0	77, 80, 80, 80	0
All	All	2112/2166 (97%)	0.36	93 (4%) 34 13	17, 30, 56, 80	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	S	1043	PHE	9.0
2	S	1001	ALA	8.8
2	S	1002	SER	8.3
2	X	1037	VAL	7.6
2	S	1005	SER	7.3
2	X	1022	TRP	6.9
2	X	1045	CYS	6.0
2	X	1011	THR	5.4
2	S	1032	PRO	5.3
2	S	1004	LYS	5.1
2	X	1031	GLY	5.1
2	X	1005	SER	5.0
2	X	1040	THR	5.0
2	X	1012	SER	4.9
2	S	1020	ALA	4.8
2	X	1032	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	X	1027	LYS	4.7
2	X	1008	TRP	4.6
2	S	1008	TRP	4.6
2	X	1009	CYS	4.4
2	X	1003	LYS	4.4
2	X	1029	VAL	4.4
1	V	1188	TYR	4.4
2	X	1036	CYS	4.4
2	S	1011	THR	4.4
2	S	1014	ALA	4.1
2	S	1022	TRP	4.1
2	S	1003	LYS	4.0
2	X	1001	ALA	3.9
2	S	1045	CYS	3.8
1	P	1188	TYR	3.8
1	W	1188	TYR	3.7
2	S	1024	ARG	3.7
2	S	1013	PRO	3.7
1	R	1157	SER	3.7
2	X	1004	LYS	3.6
2	X	1019	CYS	3.6
2	S	1029	VAL	3.6
2	X	1042	ARG	3.6
2	X	1013	PRO	3.5
2	S	1035	THR	3.5
1	Q	1214	ASN	3.4
2	X	1041	SER	3.3
2	X	1010	THR	3.3
2	S	1023	GLN	3.3
2	X	1006	VAL	3.2
2	S	1036	CYS	3.2
2	X	1014	ALA	3.2
2	S	1015	GLU	3.2
2	X	1016	SER	3.2
2	S	1006	VAL	3.2
2	X	1039	LYS	3.1
1	R	1188	TYR	3.1
2	X	1035	THR	3.1
1	V	1214	ASN	3.1
1	Q	1188	TYR	3.1
2	X	1024	ARG	3.0
2	X	1033	SER	3.0

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Mol	Chain	Res	Type	RSRZ
2	S	1009	CYS	2.9
1	W	1157	SER	2.9
2	S	1040	THR	2.9
1	U	1157	SER	2.8
2	X	1002	SER	2.8
2	X	1043	PHE	2.8
2	X	1028	LYS	2.8
1	V	1211	TYR	2.7
1	V	1157	SER	2.7
1	R	1211	TYR	2.7
1	V	1215	GLY	2.6
2	S	1030	ARG	2.6
2	S	1044	GLU	2.5
2	X	1018	LYS	2.5
2	X	1007	ARG	2.4
2	X	1030	ARG	2.4
2	X	1044	GLU	2.4
2	S	1038	LYS	2.4
1	Q	1215	GLY	2.4
2	S	1010	THR	2.4
2	X	1025	ARG	2.3
1	Q	1211	TYR	2.3
1	R	1215	GLY	2.3
1	V	1007	ASP	2.2
2	S	1025	ARG	2.2
2	X	1038	LYS	2.2
2	S	1031	GLY	2.2
1	P	1211	TYR	2.1
1	U	1188	TYR	2.1
1	P	1287	ARG	2.1
1	P	1214	ASN	2.1
2	S	1028	LYS	2.1
1	R	1214	ASN	2.1
1	U	1211	TYR	2.1
2	X	1015	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.