



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:01 PM UTC

PDB ID : 1F4A / pdb_00001f4a
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (NCS CONSTRAINED MONOMER-ORTHORHOMBIC)
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 2000-06-07
Resolution : 2.80 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

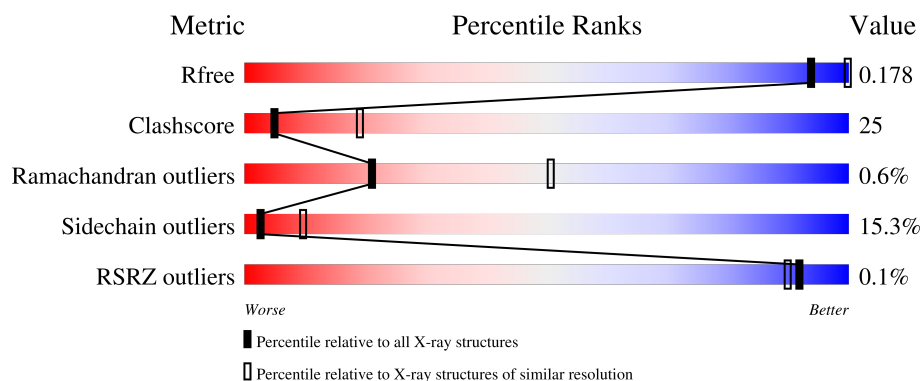
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1021	50% 36% 11% .
1	B	1021	51% 36% 11% .
1	C	1021	50% 37% 11% .
1	D	1021	50% 36% 11% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34424 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 BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	B	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	C	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			
1	D	1021	Total	C	N	O	S	84	7	0
			8238	5209	1466	1525	38			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		

- Molecule 3 is water.

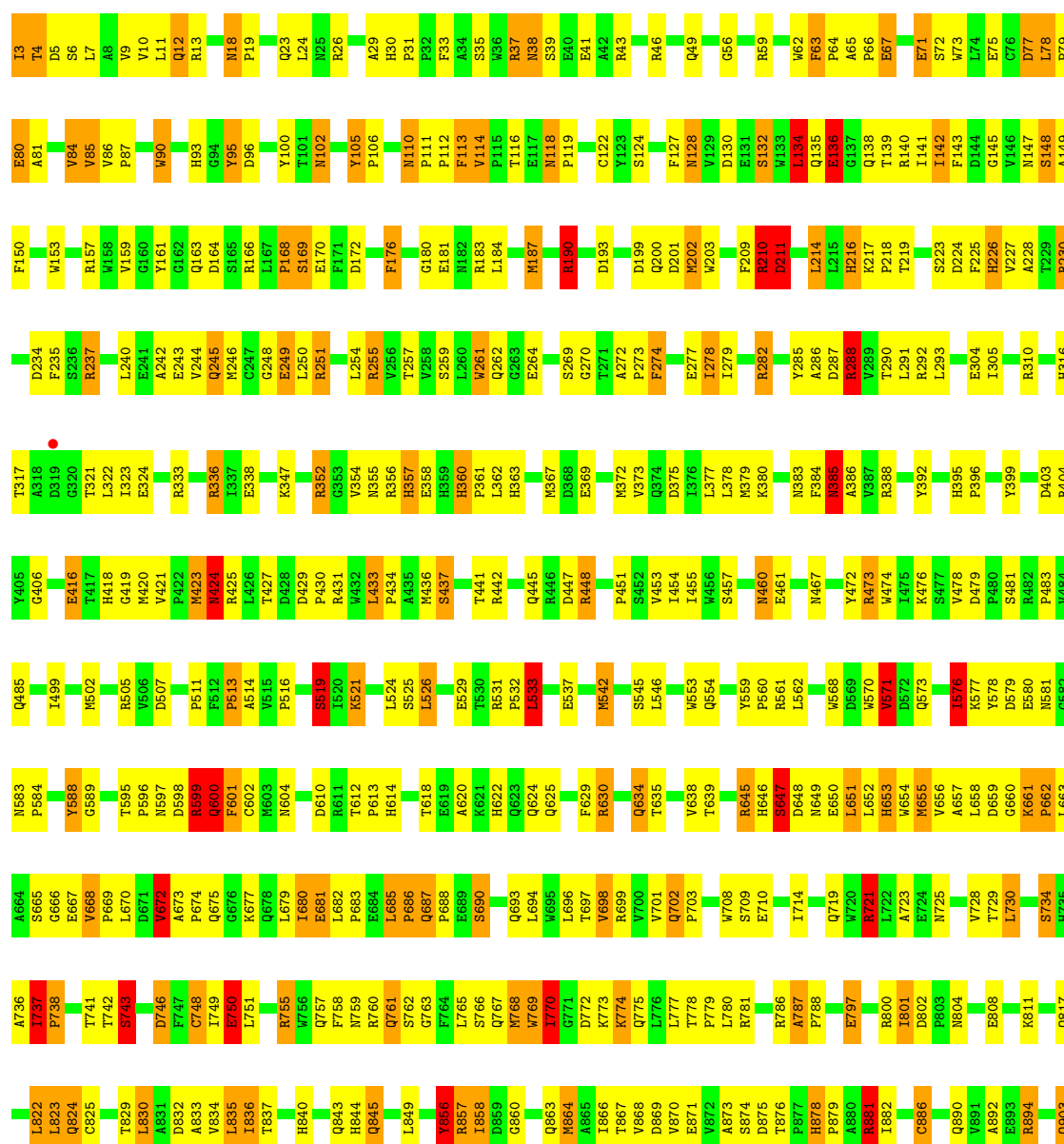
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	365	Total	O	0	0
			365	365		
3	B	366	Total	O	0	0
			366	366		
3	C	367	Total	O	0	0
			367	367		
3	D	366	Total	O	0	0
			366	366		

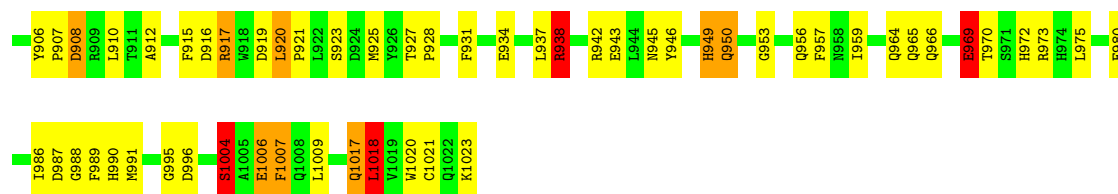
3 Residue-property plots

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: BETA-GALACTOSIDASE

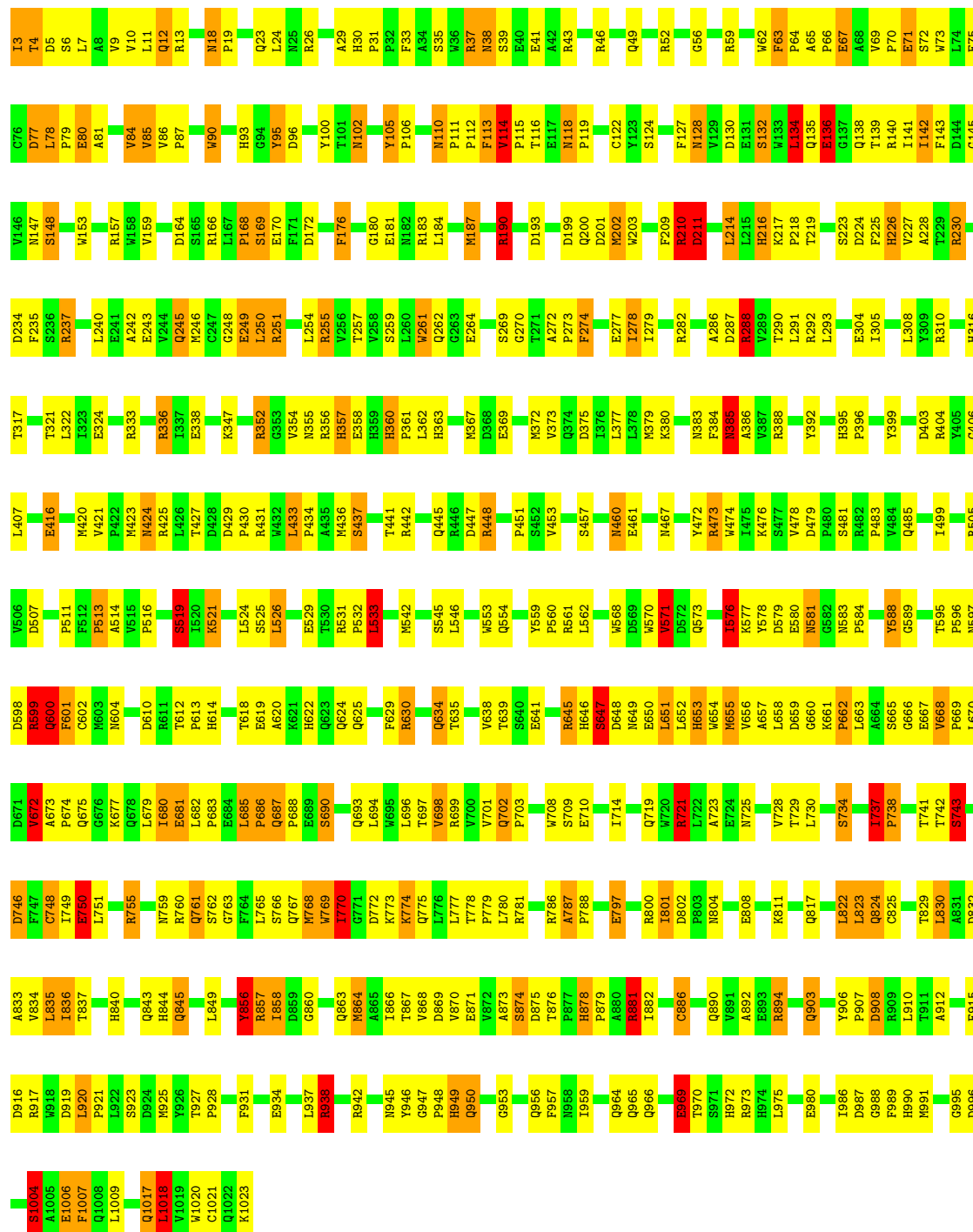
Chain A: 



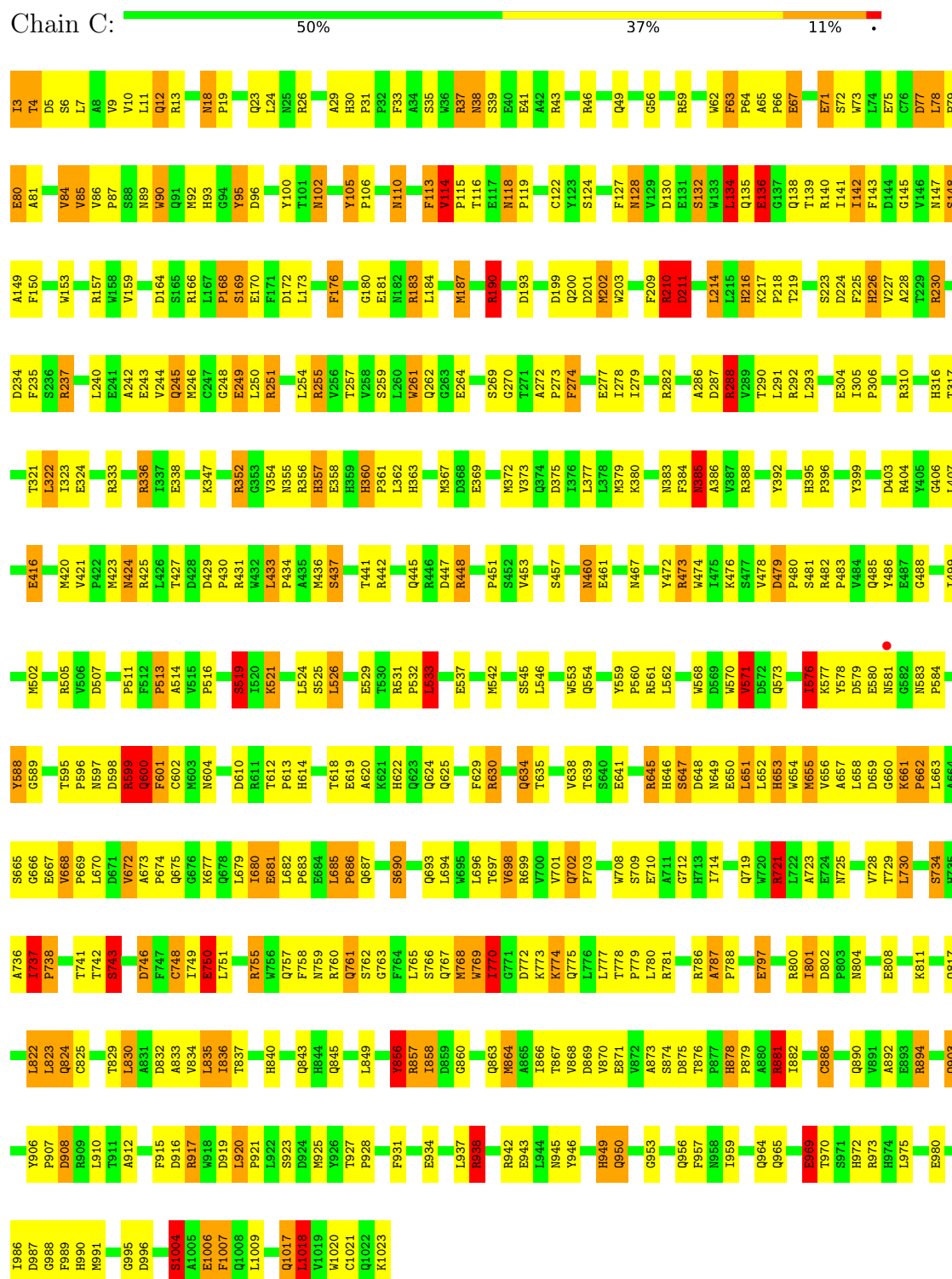


● Molecule 1: BETA-GALACTOSIDASE

Chain B: 51% 36% 11%



• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	153.40Å 173.40Å 204.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 25.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	88.0 (25.00-2.80) 80.3 (25.00-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.80Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.167 , 0.198 0.149 , 0.178	Depositor DCC
R_{free} test set	1590 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 117.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	34424	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2179e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.34	17/8515 (0.2%)	1.82	169/11615 (1.5%)
1	B	1.34	17/8515 (0.2%)	1.82	167/11615 (1.4%)
1	C	1.34	17/8515 (0.2%)	1.82	166/11615 (1.4%)
1	D	1.34	18/8515 (0.2%)	1.82	167/11615 (1.4%)
All	All	1.34	69/34060 (0.2%)	1.82	669/46460 (1.4%)

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	ASP	C-N	-9.15	1.25	1.34
1	D	479	ASP	C-N	-9.14	1.25	1.34
1	A	479	ASP	C-N	-9.14	1.25	1.34
1	C	479	ASP	C-N	-9.05	1.25	1.34
1	D	249	GLU	CA-C	-8.01	1.42	1.52
1	A	249	GLU	CA-C	-7.96	1.43	1.52
1	B	249	GLU	CA-C	-7.95	1.43	1.52
1	C	249	GLU	CA-C	-7.93	1.43	1.52
1	D	521	LYS	C-O	-7.85	1.15	1.24
1	A	521	LYS	C-O	-7.80	1.15	1.24
1	C	521	LYS	C-O	-7.80	1.15	1.24
1	B	521	LYS	C-O	-7.80	1.15	1.24
1	B	668	VAL	C-N	-6.21	1.26	1.33
1	A	668	VAL	C-N	-6.17	1.26	1.33
1	C	668	VAL	C-N	-6.17	1.26	1.33
1	C	835	LEU	N-CA	-6.17	1.39	1.46
1	D	668	VAL	C-N	-6.14	1.26	1.33
1	A	835	LEU	N-CA	-6.10	1.39	1.46
1	D	835	LEU	N-CA	-6.10	1.39	1.46
1	B	835	LEU	N-CA	-6.09	1.39	1.46
1	A	118	ASN	N-CA	-5.95	1.41	1.46
1	D	118	ASN	N-CA	-5.91	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	118	ASN	N-CA	-5.90	1.41	1.46
1	C	118	ASN	N-CA	-5.89	1.41	1.46
1	C	261	TRP	CA-C	-5.89	1.45	1.52
1	A	261	TRP	CA-C	-5.89	1.45	1.52
1	B	261	TRP	CA-C	-5.87	1.45	1.52
1	D	261	TRP	CA-C	-5.83	1.45	1.52
1	C	681	GLU	CA-C	-5.77	1.45	1.52
1	A	681	GLU	CA-C	-5.74	1.45	1.52
1	D	681	GLU	CA-C	-5.74	1.45	1.52
1	B	681	GLU	CA-C	-5.74	1.45	1.52
1	D	723	ALA	CA-C	-5.72	1.45	1.52
1	A	723	ALA	CA-C	-5.70	1.45	1.52
1	A	75	GLU	CD-OE2	5.67	1.36	1.25
1	C	75	GLU	CD-OE2	5.67	1.36	1.25
1	B	723	ALA	CA-C	-5.67	1.45	1.52
1	D	75	GLU	CD-OE2	5.66	1.36	1.25
1	B	75	GLU	CD-OE2	5.64	1.36	1.25
1	C	723	ALA	CA-C	-5.63	1.45	1.52
1	C	113	PHE	CA-C	-5.56	1.45	1.52
1	B	113	PHE	CA-C	-5.56	1.45	1.52
1	A	113	PHE	CA-C	-5.55	1.45	1.52
1	D	113	PHE	CA-C	-5.54	1.45	1.52
1	D	521	LYS	C-N	-5.51	1.26	1.34
1	B	521	LYS	C-N	-5.50	1.26	1.34
1	A	521	LYS	C-N	-5.49	1.26	1.34
1	C	521	LYS	C-N	-5.46	1.26	1.34
1	D	662	PRO	CA-C	-5.29	1.46	1.52
1	C	261	TRP	C-N	-5.27	1.26	1.33
1	B	261	TRP	C-N	-5.26	1.26	1.33
1	A	662	PRO	CA-C	-5.24	1.46	1.52
1	C	662	PRO	CA-C	-5.24	1.46	1.52
1	D	261	TRP	C-N	-5.24	1.26	1.33
1	B	662	PRO	CA-C	-5.23	1.46	1.52
1	A	261	TRP	C-N	-5.20	1.27	1.33
1	C	78	LEU	CA-C	-5.11	1.48	1.52
1	C	250	LEU	N-CA	-5.10	1.39	1.46
1	B	738	PRO	N-CA	-5.09	1.41	1.47
1	B	78	LEU	CA-C	-5.09	1.48	1.52
1	D	738	PRO	N-CA	-5.09	1.41	1.47
1	A	250	LEU	N-CA	-5.08	1.39	1.46
1	B	250	LEU	N-CA	-5.08	1.39	1.46
1	D	78	LEU	CA-C	-5.07	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	LEU	CA-C	-5.06	1.48	1.52
1	D	250	LEU	N-CA	-5.05	1.40	1.46
1	C	738	PRO	N-CA	-5.04	1.41	1.47
1	A	738	PRO	N-CA	-5.03	1.41	1.47
1	D	749	ILE	N-CA	-5.01	1.40	1.46

All (669) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	114	VAL	N-CA-CB	-14.09	102.11	111.83
1	C	114	VAL	N-CA-CB	-14.08	102.11	111.83
1	D	114	VAL	N-CA-CB	-14.08	102.12	111.83
1	A	114	VAL	N-CA-CB	-14.06	102.12	111.83
1	D	385	ASN	CB-CA-C	-12.05	89.51	109.03
1	A	385	ASN	CB-CA-C	-12.04	89.52	109.03
1	B	385	ASN	CB-CA-C	-12.04	89.53	109.03
1	C	385	ASN	CB-CA-C	-12.03	89.54	109.03
1	C	423	MET	CA-C-N	11.12	136.29	120.28
1	C	423	MET	C-N-CA	11.12	136.29	120.28
1	A	423	MET	CA-C-N	11.09	136.24	120.28
1	A	423	MET	C-N-CA	11.09	136.24	120.28
1	B	423	MET	CA-C-N	11.06	136.21	120.28
1	B	423	MET	C-N-CA	11.06	136.21	120.28
1	D	423	MET	CA-C-N	11.06	136.21	120.28
1	D	423	MET	C-N-CA	11.06	136.21	120.28
1	A	385	ASN	N-CA-CB	-10.51	96.62	110.59
1	B	385	ASN	N-CA-CB	-10.50	96.62	110.59
1	C	385	ASN	N-CA-CB	-10.50	96.63	110.59
1	D	385	ASN	N-CA-CB	-10.50	96.63	110.59
1	C	249	GLU	N-CA-CB	10.37	127.27	110.16
1	A	249	GLU	N-CA-CB	10.35	127.24	110.16
1	B	249	GLU	N-CA-CB	10.35	127.23	110.16
1	D	249	GLU	N-CA-CB	10.33	127.20	110.16
1	C	424	ASN	CB-CA-C	-9.97	92.18	110.63
1	B	424	ASN	CB-CA-C	-9.97	92.19	110.63
1	A	424	ASN	CB-CA-C	-9.96	92.20	110.63
1	D	424	ASN	CB-CA-C	-9.96	92.20	110.63
1	D	248	GLY	CA-C-N	-9.52	108.77	122.19
1	D	248	GLY	C-N-CA	-9.52	108.77	122.19
1	A	248	GLY	CA-C-N	-9.50	108.79	122.19
1	A	248	GLY	C-N-CA	-9.50	108.79	122.19
1	B	248	GLY	CA-C-N	-9.49	108.80	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	248	GLY	C-N-CA	-9.49	108.80	122.19
1	C	248	GLY	CA-C-N	-9.48	108.82	122.19
1	C	248	GLY	C-N-CA	-9.48	108.82	122.19
1	A	224	ASP	CA-CB-CG	8.90	121.50	112.60
1	C	224	ASP	CA-CB-CG	8.89	121.49	112.60
1	B	224	ASP	CA-CB-CG	8.87	121.47	112.60
1	D	224	ASP	CA-CB-CG	8.88	121.47	112.60
1	D	363	HIS	CA-CB-CG	-8.78	105.02	113.80
1	C	363	HIS	CA-CB-CG	-8.75	105.05	113.80
1	A	363	HIS	CA-CB-CG	-8.74	105.06	113.80
1	B	363	HIS	CA-CB-CG	-8.72	105.08	113.80
1	D	931	PHE	CB-CA-C	8.65	118.22	110.44
1	C	931	PHE	CB-CA-C	8.63	118.21	110.44
1	A	931	PHE	CB-CA-C	8.63	118.21	110.44
1	B	931	PHE	CB-CA-C	8.57	118.15	110.44
1	D	903[A]	GLN	N-CA-C	8.08	121.45	110.55
1	D	903[B]	GLN	N-CA-C	8.08	121.45	110.55
1	C	903[A]	GLN	N-CA-C	8.07	121.45	110.55
1	C	903[B]	GLN	N-CA-C	8.07	121.45	110.55
1	A	903[A]	GLN	N-CA-C	8.07	121.44	110.55
1	A	903[B]	GLN	N-CA-C	8.07	121.44	110.55
1	B	903[A]	GLN	N-CA-C	8.06	121.43	110.55
1	B	903[B]	GLN	N-CA-C	8.06	121.43	110.55
1	A	787	ALA	CA-C-N	7.92	129.74	119.84
1	A	787	ALA	C-N-CA	7.92	129.74	119.84
1	C	787	ALA	CA-C-N	7.91	129.73	119.84
1	C	787	ALA	C-N-CA	7.91	129.73	119.84
1	D	787	ALA	CA-C-N	7.91	129.73	119.84
1	D	787	ALA	C-N-CA	7.91	129.73	119.84
1	B	787	ALA	CA-C-N	7.91	129.72	119.84
1	B	787	ALA	C-N-CA	7.91	129.72	119.84
1	A	1004	SER	N-CA-CB	7.87	121.55	109.97
1	C	1004	SER	N-CA-CB	7.87	121.54	109.97
1	C	777	LEU	N-CA-C	-7.87	104.16	114.31
1	D	1004	SER	N-CA-CB	7.87	121.53	109.97
1	D	672	VAL	CB-CA-C	-7.86	98.86	110.33
1	C	672	VAL	CB-CA-C	-7.85	98.86	110.33
1	D	777	LEU	N-CA-C	-7.85	104.19	114.31
1	B	1004	SER	N-CA-CB	7.84	121.50	109.97
1	A	672	VAL	CB-CA-C	-7.83	98.89	110.33
1	A	777	LEU	N-CA-C	-7.83	104.20	114.31
1	B	777	LEU	N-CA-C	-7.83	104.20	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	672	VAL	CB-CA-C	-7.81	98.92	110.33
1	B	113	PHE	CA-CB-CG	-7.68	106.12	113.80
1	C	113	PHE	CA-CB-CG	-7.67	106.13	113.80
1	A	113	PHE	CA-CB-CG	-7.65	106.15	113.80
1	D	113	PHE	CA-CB-CG	-7.64	106.16	113.80
1	A	274	PHE	CA-CB-CG	-7.60	106.20	113.80
1	D	274	PHE	CA-CB-CG	-7.60	106.20	113.80
1	B	274	PHE	CA-CB-CG	-7.59	106.21	113.80
1	C	274	PHE	CA-CB-CG	-7.59	106.21	113.80
1	A	18	ASN	CA-C-N	7.59	127.26	119.82
1	A	18	ASN	C-N-CA	7.59	127.26	119.82
1	C	18	ASN	CA-C-N	7.59	127.25	119.82
1	C	18	ASN	C-N-CA	7.59	127.25	119.82
1	B	18	ASN	CA-C-N	7.58	127.25	119.82
1	B	18	ASN	C-N-CA	7.58	127.25	119.82
1	C	571	VAL	CB-CA-C	-7.57	98.77	110.95
1	C	4	THR	N-CA-C	-7.56	103.94	113.02
1	D	18	ASN	CA-C-N	7.56	127.23	119.82
1	D	18	ASN	C-N-CA	7.56	127.23	119.82
1	B	4	THR	N-CA-C	-7.56	103.95	113.02
1	A	571	VAL	CB-CA-C	-7.55	98.80	110.95
1	D	571	VAL	CB-CA-C	-7.54	98.81	110.95
1	D	4	THR	N-CA-C	-7.53	103.98	113.02
1	B	571	VAL	CB-CA-C	-7.53	98.83	110.95
1	A	4	THR	N-CA-C	-7.53	103.99	113.02
1	B	424	ASN	N-CA-CB	-7.45	98.74	110.22
1	D	424	ASN	N-CA-CB	-7.45	98.75	110.22
1	A	424	ASN	N-CA-CB	-7.45	98.75	110.22
1	C	424	ASN	N-CA-CB	-7.44	98.77	110.22
1	B	211	ASP	N-CA-C	7.41	119.88	110.33
1	D	211	ASP	N-CA-C	7.41	119.88	110.33
1	C	211	ASP	N-CA-C	7.39	119.86	110.33
1	A	211	ASP	N-CA-C	7.38	119.85	110.33
1	D	433	LEU	CA-C-O	7.33	125.38	118.63
1	C	134	LEU	N-CA-CB	7.33	121.97	110.46
1	A	134	LEU	N-CA-CB	7.33	121.97	110.46
1	C	433	LEU	CA-C-O	7.33	125.37	118.63
1	D	134	LEU	N-CA-CB	7.33	121.97	110.46
1	B	433	LEU	CA-C-O	7.33	125.37	118.63
1	B	134	LEU	N-CA-CB	7.32	121.96	110.46
1	D	226	HIS	CB-CA-C	-7.32	94.08	109.38
1	C	226	HIS	CB-CA-C	-7.32	94.08	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	HIS	CB-CA-C	-7.31	94.10	109.38
1	A	433	LEU	CA-C-O	7.31	125.35	118.63
1	A	226	HIS	CB-CA-C	-7.31	94.11	109.38
1	A	142	ILE	CB-CA-C	-7.30	99.66	110.33
1	B	142	ILE	CB-CA-C	-7.30	99.67	110.33
1	C	142	ILE	CB-CA-C	-7.30	99.67	110.33
1	D	142	ILE	CB-CA-C	-7.28	99.70	110.33
1	B	938	ARG	N-CA-CB	7.21	122.09	110.77
1	A	938	ARG	N-CA-CB	7.20	122.08	110.77
1	D	938	ARG	N-CA-CB	7.20	122.07	110.77
1	C	938	ARG	N-CA-CB	7.19	122.06	110.77
1	A	553	TRP	CA-CB-CG	-7.03	100.25	113.60
1	B	553	TRP	CA-CB-CG	-7.02	100.25	113.60
1	C	553	TRP	CA-CB-CG	-7.02	100.25	113.60
1	B	614	HIS	N-CA-C	-7.01	100.96	110.36
1	D	553	TRP	CA-CB-CG	-7.01	100.28	113.60
1	C	614	HIS	N-CA-C	-7.00	100.97	110.36
1	A	614	HIS	N-CA-C	-6.99	101.00	110.36
1	D	614	HIS	N-CA-C	-6.97	101.02	110.36
1	C	600	GLN	N-CA-CB	6.93	122.10	110.32
1	B	600	GLN	N-CA-CB	6.93	122.10	110.32
1	A	600	GLN	N-CA-CB	6.91	122.07	110.32
1	C	823	LEU	N-CA-C	-6.90	104.99	113.41
1	B	823	LEU	N-CA-C	-6.90	104.99	113.41
1	D	600	GLN	N-CA-CB	6.88	122.02	110.32
1	A	823	LEU	N-CA-C	-6.88	105.02	113.41
1	D	823	LEU	N-CA-C	-6.88	105.02	113.41
1	B	980	GLU	N-CA-CB	6.86	120.16	109.94
1	A	863	GLN	CA-C-N	-6.86	113.54	123.00
1	A	863	GLN	C-N-CA	-6.86	113.54	123.00
1	D	863	GLN	CA-C-N	-6.85	113.54	123.00
1	D	863	GLN	C-N-CA	-6.85	113.54	123.00
1	C	863	GLN	CA-C-N	-6.85	113.55	123.00
1	C	863	GLN	C-N-CA	-6.85	113.55	123.00
1	C	980	GLU	N-CA-CB	6.83	120.12	109.94
1	A	980	GLU	N-CA-CB	6.83	120.12	109.94
1	B	863	GLN	CA-C-N	-6.83	113.58	123.00
1	B	863	GLN	C-N-CA	-6.83	113.58	123.00
1	D	980	GLU	N-CA-CB	6.82	120.11	109.94
1	B	209	PHE	CA-CB-CG	-6.78	107.02	113.80
1	C	209	PHE	CA-CB-CG	-6.78	107.02	113.80
1	A	181	GLU	N-CA-C	6.77	119.73	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	PHE	CA-CB-CG	-6.77	107.03	113.80
1	D	209	PHE	CA-CB-CG	-6.76	107.04	113.80
1	B	804	ASN	CA-CB-CG	-6.75	105.85	112.60
1	A	804	ASN	CA-CB-CG	-6.75	105.85	112.60
1	C	181	GLU	N-CA-C	6.74	119.68	108.96
1	C	804	ASN	CA-CB-CG	-6.74	105.86	112.60
1	D	181	GLU	N-CA-C	6.74	119.67	108.96
1	A	613	PRO	CB-CA-C	-6.73	102.16	110.98
1	D	613	PRO	CB-CA-C	-6.73	102.16	110.98
1	D	804	ASN	CA-CB-CG	-6.72	105.88	112.60
1	B	181	GLU	N-CA-C	6.72	119.64	108.96
1	C	159	VAL	N-CA-C	6.72	118.05	111.67
1	B	613	PRO	CB-CA-C	-6.71	102.18	110.98
1	D	159	VAL	N-CA-C	6.71	118.05	111.67
1	A	159	VAL	N-CA-C	6.71	118.04	111.67
1	C	613	PRO	CB-CA-C	-6.70	102.20	110.98
1	B	159	VAL	N-CA-C	6.70	118.03	111.67
1	A	856	TYR	CA-C-N	-6.69	113.36	122.86
1	A	856	TYR	C-N-CA	-6.69	113.36	122.86
1	B	856	TYR	CA-C-N	-6.67	113.38	122.86
1	B	856	TYR	C-N-CA	-6.67	113.38	122.86
1	C	856	TYR	CA-C-N	-6.67	113.39	122.86
1	C	856	TYR	C-N-CA	-6.67	113.39	122.86
1	D	856	TYR	CA-C-N	-6.66	113.40	122.86
1	D	856	TYR	C-N-CA	-6.66	113.40	122.86
1	A	352	ARG	CA-C-N	-6.64	116.26	122.17
1	A	352	ARG	C-N-CA	-6.64	116.26	122.17
1	C	352	ARG	CA-C-N	-6.62	116.28	122.17
1	C	352	ARG	C-N-CA	-6.62	116.28	122.17
1	C	1007	PHE	CA-CB-CG	-6.62	107.19	113.80
1	B	352	ARG	CA-C-N	-6.60	116.29	122.17
1	B	352	ARG	C-N-CA	-6.60	116.29	122.17
1	C	949	HIS	CA-CB-CG	-6.60	107.20	113.80
1	D	1007	PHE	CA-CB-CG	-6.60	107.20	113.80
1	A	949	HIS	CA-CB-CG	-6.60	107.20	113.80
1	B	949	HIS	CA-CB-CG	-6.59	107.20	113.80
1	D	949	HIS	CA-CB-CG	-6.59	107.20	113.80
1	A	1007	PHE	CA-CB-CG	-6.59	107.21	113.80
1	B	725	ASN	CA-CB-CG	-6.57	106.03	112.60
1	B	1007	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	725	ASN	CA-CB-CG	-6.56	106.04	112.60
1	B	770	ILE	CA-C-N	-6.56	113.01	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	ILE	C-N-CA	-6.56	113.01	120.42
1	D	770	ILE	CA-C-N	-6.56	113.01	120.42
1	D	770	ILE	C-N-CA	-6.56	113.01	120.42
1	D	352	ARG	CA-C-N	-6.56	116.33	122.17
1	D	352	ARG	C-N-CA	-6.56	116.33	122.17
1	C	725	ASN	CA-CB-CG	-6.52	106.08	112.60
1	D	725	ASN	CA-CB-CG	-6.52	106.08	112.60
1	A	770	ILE	CA-C-N	-6.52	113.05	120.42
1	A	770	ILE	C-N-CA	-6.52	113.05	120.42
1	C	770	ILE	CA-C-N	-6.52	113.05	120.42
1	C	770	ILE	C-N-CA	-6.52	113.05	120.42
1	A	802	ASP	CA-C-N	6.51	126.20	119.82
1	A	802	ASP	C-N-CA	6.51	126.20	119.82
1	B	424	ASN	N-CA-C	6.48	119.16	111.71
1	D	424	ASN	N-CA-C	6.48	119.16	111.71
1	A	424	ASN	N-CA-C	6.46	119.13	111.71
1	C	802	ASP	CA-C-N	6.44	126.13	119.82
1	C	802	ASP	C-N-CA	6.44	126.13	119.82
1	B	802	ASP	CA-C-N	6.43	126.12	119.82
1	B	802	ASP	C-N-CA	6.43	126.12	119.82
1	D	802	ASP	CA-C-N	6.43	126.12	119.82
1	D	802	ASP	C-N-CA	6.43	126.12	119.82
1	C	424	ASN	N-CA-C	6.42	119.09	111.71
1	C	521	LYS	N-CA-C	-6.40	104.30	111.28
1	A	105	TYR	CA-C-N	6.40	126.15	119.05
1	A	105	TYR	C-N-CA	6.40	126.15	119.05
1	C	105	TYR	CA-C-N	6.39	126.15	119.05
1	C	105	TYR	C-N-CA	6.39	126.15	119.05
1	D	105	TYR	CA-C-N	6.37	126.12	119.05
1	D	105	TYR	C-N-CA	6.37	126.12	119.05
1	B	521	LYS	N-CA-C	-6.36	104.34	111.28
1	B	105	TYR	CA-C-N	6.36	126.11	119.05
1	B	105	TYR	C-N-CA	6.36	126.11	119.05
1	A	521	LYS	N-CA-C	-6.36	104.35	111.28
1	B	383	ASN	N-CA-C	6.36	122.74	113.40
1	A	383	ASN	N-CA-C	6.35	122.74	113.40
1	D	383	ASN	N-CA-C	6.33	122.71	113.40
1	C	383	ASN	N-CA-C	6.33	122.70	113.40
1	D	521	LYS	N-CA-C	-6.32	104.39	111.28
1	C	629	PHE	CA-CB-CG	-6.26	107.54	113.80
1	B	881	ARG	CD-NE-CZ	6.25	133.14	124.40
1	C	881	ARG	CD-NE-CZ	6.24	133.13	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	881	ARG	CD-NE-CZ	6.24	133.13	124.40
1	A	629	PHE	CA-CB-CG	-6.23	107.57	113.80
1	A	881	ARG	CD-NE-CZ	6.23	133.12	124.40
1	B	629	PHE	CA-CB-CG	-6.22	107.58	113.80
1	C	288	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	D	629	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	288	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	B	288	ARG	CD-NE-CZ	-6.20	115.72	124.40
1	D	288	ARG	CD-NE-CZ	-6.18	115.74	124.40
1	D	142	ILE	N-CA-C	6.17	117.01	108.12
1	A	142	ILE	N-CA-C	6.17	117.00	108.12
1	C	142	ILE	N-CA-C	6.17	117.00	108.12
1	B	588	TYR	N-CA-C	6.17	116.58	108.07
1	A	588	TYR	N-CA-C	6.16	116.57	108.07
1	B	142	ILE	N-CA-C	6.15	116.98	108.12
1	D	588	TYR	N-CA-C	6.14	116.54	108.07
1	C	588	TYR	N-CA-C	6.13	116.54	108.07
1	A	360	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	750	GLU	N-CA-CB	6.11	122.06	111.00
1	D	360	HIS	CA-CB-CG	-6.11	107.69	113.80
1	C	360	HIS	CA-CB-CG	-6.11	107.69	113.80
1	C	750	GLU	N-CA-CB	6.11	122.05	111.00
1	B	750	GLU	N-CA-CB	6.09	122.03	111.00
1	C	723	ALA	O-C-N	6.09	129.49	123.46
1	B	360	HIS	CA-CB-CG	-6.09	107.71	113.80
1	A	750	GLU	N-CA-CB	6.08	122.01	111.00
1	B	723	ALA	O-C-N	6.08	129.47	123.46
1	A	878	HIS	CA-C-N	6.07	125.98	119.85
1	A	878	HIS	C-N-CA	6.07	125.98	119.85
1	A	723	ALA	O-C-N	6.06	129.46	123.46
1	B	878	HIS	CA-C-N	6.06	125.97	119.85
1	B	878	HIS	C-N-CA	6.06	125.97	119.85
1	D	723	ALA	O-C-N	6.06	129.46	123.46
1	C	118	ASN	CA-C-O	6.05	127.24	120.34
1	B	118	ASN	CA-C-O	6.05	127.24	120.34
1	D	878	HIS	CA-C-N	6.04	125.95	119.85
1	D	878	HIS	C-N-CA	6.04	125.95	119.85
1	C	938	ARG	CG-CD-NE	-6.03	98.73	112.00
1	C	139	THR	CA-C-N	-6.03	113.12	122.59
1	C	139	THR	C-N-CA	-6.03	113.12	122.59
1	C	878	HIS	CA-C-N	6.02	125.94	119.85
1	C	878	HIS	C-N-CA	6.02	125.94	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	ASN	CA-C-O	6.02	127.20	120.34
1	B	938	ARG	CG-CD-NE	-6.02	98.76	112.00
1	A	110	ASN	CA-CB-CG	-6.02	106.58	112.60
1	B	139	THR	CA-C-N	-6.01	113.15	122.59
1	B	139	THR	C-N-CA	-6.01	113.15	122.59
1	D	118	ASN	CA-C-O	6.01	127.19	120.34
1	A	938	ARG	CG-CD-NE	-6.01	98.78	112.00
1	A	139	THR	CA-C-N	-6.01	113.16	122.59
1	A	139	THR	C-N-CA	-6.01	113.16	122.59
1	B	110	ASN	CA-CB-CG	-6.01	106.59	112.60
1	D	139	THR	CA-C-N	-6.01	113.16	122.59
1	D	139	THR	C-N-CA	-6.01	113.16	122.59
1	D	110	ASN	CA-CB-CG	-6.00	106.59	112.60
1	D	938	ARG	CG-CD-NE	-6.00	98.80	112.00
1	B	210	ARG	N-CA-CB	6.00	120.69	111.22
1	A	210	ARG	N-CA-CB	5.99	120.69	111.22
1	C	110	ASN	CA-CB-CG	-5.99	106.61	112.60
1	D	210	ARG	N-CA-CB	5.99	120.68	111.22
1	A	128	ASN	CA-C-N	-5.99	115.77	123.19
1	A	128	ASN	C-N-CA	-5.99	115.77	123.19
1	D	95	TYR	N-CA-C	5.98	118.29	111.11
1	C	210	ARG	N-CA-CB	5.98	120.67	111.22
1	A	483	PRO	CA-C-N	-5.97	115.40	123.10
1	A	483	PRO	C-N-CA	-5.97	115.40	123.10
1	A	95	TYR	N-CA-C	5.97	118.27	111.11
1	B	483	PRO	CA-C-N	-5.97	115.40	123.10
1	B	483	PRO	C-N-CA	-5.97	115.40	123.10
1	B	176	PHE	CA-CB-CG	-5.96	107.84	113.80
1	B	128	ASN	CA-C-N	-5.96	115.80	123.19
1	B	128	ASN	C-N-CA	-5.96	115.80	123.19
1	C	483	PRO	CA-C-N	-5.96	115.42	123.10
1	C	483	PRO	C-N-CA	-5.96	115.42	123.10
1	D	128	ASN	CA-C-N	-5.96	115.80	123.19
1	D	128	ASN	C-N-CA	-5.96	115.80	123.19
1	C	95	TYR	N-CA-C	5.95	118.25	111.11
1	C	128	ASN	CA-C-N	-5.95	115.81	123.19
1	C	128	ASN	C-N-CA	-5.95	115.81	123.19
1	B	95	TYR	N-CA-C	5.94	118.24	111.11
1	A	864	MET	N-CA-CB	5.93	119.88	110.57
1	B	601	PHE	CA-CB-CG	-5.93	107.87	113.80
1	D	483	PRO	CA-C-N	-5.93	115.45	123.10
1	D	483	PRO	C-N-CA	-5.93	115.45	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	PHE	CA-CB-CG	-5.93	107.87	113.80
1	C	864	MET	N-CA-CB	5.92	119.87	110.57
1	A	601	PHE	CA-CB-CG	-5.92	107.88	113.80
1	D	601	PHE	CA-CB-CG	-5.92	107.88	113.80
1	A	176	PHE	CA-CB-CG	-5.92	107.89	113.80
1	C	176	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	864	MET	N-CA-CB	5.91	119.85	110.57
1	D	864	MET	N-CA-CB	5.91	119.85	110.57
1	C	601	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	598	ASP	N-CA-C	5.90	119.45	112.72
1	B	448	ARG	N-CA-C	5.89	119.57	112.38
1	B	598	ASP	N-CA-C	5.88	119.42	112.72
1	D	448	ARG	N-CA-C	5.88	119.55	112.38
1	A	448	ARG	N-CA-C	5.87	119.55	112.38
1	C	63	PHE	CA-C-N	5.87	125.98	119.87
1	C	63	PHE	C-N-CA	5.87	125.98	119.87
1	C	598	ASP	N-CA-C	5.87	119.41	112.72
1	D	63	PHE	CA-C-N	5.87	125.97	119.87
1	D	63	PHE	C-N-CA	5.87	125.97	119.87
1	C	448	ARG	N-CA-C	5.87	119.54	112.38
1	D	598	ASP	N-CA-C	5.87	119.41	112.72
1	C	680	ILE	N-CA-C	5.86	116.44	107.77
1	B	680	ILE	N-CA-C	5.86	116.44	107.77
1	D	680	ILE	N-CA-C	5.86	116.44	107.77
1	A	680	ILE	N-CA-C	5.85	116.43	107.77
1	A	63	PHE	CA-C-N	5.85	125.95	119.87
1	A	63	PHE	C-N-CA	5.85	125.95	119.87
1	A	702	GLN	CA-C-O	5.84	124.44	119.71
1	C	384	PHE	CA-C-N	5.84	132.41	122.36
1	C	384	PHE	C-N-CA	5.84	132.41	122.36
1	B	702	GLN	CA-C-O	5.84	124.44	119.71
1	D	829	THR	N-CA-CB	5.84	119.72	110.55
1	A	384	PHE	CA-C-N	5.83	132.39	122.36
1	A	384	PHE	C-N-CA	5.83	132.39	122.36
1	D	384	PHE	CA-C-N	5.83	132.39	122.36
1	D	384	PHE	C-N-CA	5.83	132.39	122.36
1	D	702	GLN	CA-C-O	5.83	124.43	119.71
1	B	384	PHE	CA-C-N	5.83	132.38	122.36
1	B	384	PHE	C-N-CA	5.83	132.38	122.36
1	B	63	PHE	CA-C-N	5.82	125.92	119.87
1	B	63	PHE	C-N-CA	5.82	125.92	119.87
1	D	599	ARG	CB-CA-C	-5.82	109.85	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	829	THR	N-CA-CB	5.81	119.68	110.55
1	A	829	THR	N-CA-CB	5.81	119.67	110.55
1	A	599	ARG	CB-CA-C	-5.80	109.86	116.54
1	B	829	THR	N-CA-CB	5.80	119.66	110.55
1	C	702	GLN	CA-C-O	5.78	124.39	119.71
1	C	721	ARG	N-CA-CB	5.77	119.69	110.16
1	D	721	ARG	N-CA-CB	5.77	119.68	110.16
1	A	721	ARG	N-CA-CB	5.76	119.67	110.16
1	C	599	ARG	CB-CA-C	-5.76	109.92	116.54
1	B	721	ARG	N-CA-CB	5.75	119.66	110.16
1	B	599	ARG	CB-CA-C	-5.75	109.92	116.54
1	D	226	HIS	ND1-CE1-NE2	5.75	114.14	108.40
1	C	519	SER	N-CA-C	-5.74	101.92	110.23
1	A	226	HIS	ND1-CE1-NE2	5.73	114.13	108.40
1	B	226	HIS	ND1-CE1-NE2	5.73	114.13	108.40
1	C	226	HIS	ND1-CE1-NE2	5.73	114.13	108.40
1	D	424	ASN	CA-CB-CG	-5.72	106.88	112.60
1	B	424	ASN	CA-CB-CG	-5.71	106.89	112.60
1	C	424	ASN	CA-CB-CG	-5.71	106.89	112.60
1	D	460	ASN	CA-CB-CG	5.71	118.31	112.60
1	A	424	ASN	CA-CB-CG	-5.71	106.89	112.60
1	D	519	SER	N-CA-C	-5.71	101.95	110.23
1	A	519	SER	N-CA-C	-5.71	101.96	110.23
1	B	172	ASP	CA-CB-CG	-5.70	106.90	112.60
1	B	519	SER	N-CA-C	-5.69	101.98	110.23
1	A	460	ASN	CA-CB-CG	5.69	118.29	112.60
1	A	245	GLN	CB-CG-CD	-5.68	102.94	112.60
1	C	245	GLN	CB-CG-CD	-5.68	102.95	112.60
1	C	460	ASN	CA-CB-CG	5.67	118.27	112.60
1	C	172	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	142	ILE	N-CA-CB	-5.67	103.25	111.52
1	B	142	ILE	N-CA-CB	-5.66	103.26	111.52
1	C	93	HIS	CA-CB-CG	-5.66	108.14	113.80
1	D	245	GLN	CB-CG-CD	-5.66	102.98	112.60
1	B	245	GLN	CB-CG-CD	-5.66	102.99	112.60
1	A	93	HIS	CA-CB-CG	-5.65	108.15	113.80
1	A	172	ASP	CA-CB-CG	-5.65	106.95	112.60
1	B	93	HIS	CA-CB-CG	-5.65	108.15	113.80
1	D	172	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	142	ILE	N-CA-CB	-5.65	103.27	111.52
1	B	460	ASN	CA-CB-CG	5.64	118.24	112.60
1	C	142	ILE	N-CA-CB	-5.63	103.29	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	HIS	CA-CB-CG	-5.63	108.17	113.80
1	C	521	LYS	O-C-N	-5.60	116.18	122.12
1	B	576	ILE	N-CA-C	5.60	116.64	108.58
1	A	576	ILE	N-CA-C	5.59	116.63	108.58
1	D	128	ASN	N-CA-C	5.58	118.34	109.24
1	B	128	ASN	N-CA-C	5.58	118.33	109.24
1	C	576	ILE	N-CA-C	5.58	116.61	108.58
1	D	521	LYS	O-C-N	-5.58	116.21	122.12
1	C	128	ASN	N-CA-C	5.58	118.33	109.24
1	A	651	LEU	CB-CA-C	-5.57	98.31	109.35
1	C	920	LEU	CA-C-N	5.57	125.33	119.76
1	C	920	LEU	C-N-CA	5.57	125.33	119.76
1	A	128	ASN	N-CA-C	5.57	118.32	109.24
1	B	651	LEU	CB-CA-C	-5.57	98.32	109.35
1	D	651	LEU	CB-CA-C	-5.57	98.32	109.35
1	A	521	LYS	O-C-N	-5.57	116.22	122.12
1	B	168	PRO	CB-CA-C	-5.57	103.81	111.21
1	D	168	PRO	CB-CA-C	-5.57	103.81	111.21
1	D	576	ILE	N-CA-C	5.57	116.59	108.58
1	B	920	LEU	CA-C-N	5.56	125.32	119.76
1	B	920	LEU	C-N-CA	5.56	125.32	119.76
1	A	168	PRO	CB-CA-C	-5.56	103.82	111.21
1	B	521	LYS	O-C-N	-5.56	116.23	122.12
1	C	651	LEU	CB-CA-C	-5.55	98.36	109.35
1	B	863	GLN	CB-CA-C	-5.55	99.56	109.71
1	D	863	GLN	CB-CA-C	-5.55	99.56	109.71
1	C	168	PRO	CB-CA-C	-5.54	103.83	111.21
1	A	920	LEU	CA-C-N	5.54	125.30	119.76
1	A	920	LEU	C-N-CA	5.54	125.30	119.76
1	A	863	GLN	CB-CA-C	-5.54	99.57	109.71
1	C	863	GLN	CB-CA-C	-5.54	99.58	109.71
1	C	226	HIS	ND1-CG-CD2	5.51	111.61	106.10
1	D	226	HIS	ND1-CG-CD2	5.50	111.60	106.10
1	A	136	GLU	CB-CA-C	-5.50	98.45	111.65
1	B	226	HIS	ND1-CG-CD2	5.50	111.60	106.10
1	C	136	GLU	CB-CA-C	-5.50	98.45	111.65
1	B	136	GLU	CB-CA-C	-5.50	98.45	111.65
1	D	136	GLU	CB-CA-C	-5.49	98.47	111.65
1	A	56	GLY	N-CA-C	5.49	117.45	110.20
1	A	226	HIS	ND1-CG-CD2	5.49	111.59	106.10
1	B	249	GLU	O-C-N	5.49	129.48	123.22
1	D	920	LEU	CA-C-N	5.48	125.24	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	920	LEU	C-N-CA	5.48	125.24	119.76
1	C	336	ARG	CB-CA-C	-5.48	98.27	109.94
1	D	56	GLY	N-CA-C	5.48	117.43	110.20
1	B	56	GLY	N-CA-C	5.48	117.43	110.20
1	C	56	GLY	N-CA-C	5.48	117.43	110.20
1	D	336	ARG	CB-CA-C	-5.46	98.30	109.94
1	A	336	ARG	CB-CA-C	-5.46	98.30	109.94
1	B	336	ARG	CB-CA-C	-5.46	98.31	109.94
1	D	702	GLN	CA-CB-CG	-5.44	103.21	114.10
1	D	743	SER	CA-C-N	-5.44	110.98	121.58
1	D	743	SER	C-N-CA	-5.44	110.98	121.58
1	A	249	GLU	O-C-N	5.43	129.41	123.22
1	A	743	SER	CA-C-N	-5.43	111.00	121.58
1	A	743	SER	C-N-CA	-5.43	111.00	121.58
1	C	249	GLU	O-C-N	5.43	129.41	123.22
1	B	702	GLN	CA-CB-CG	-5.42	103.25	114.10
1	B	743	SER	CA-C-N	-5.42	111.01	121.58
1	B	743	SER	C-N-CA	-5.42	111.01	121.58
1	A	702	GLN	CA-CB-CG	-5.41	103.27	114.10
1	B	416	GLU	N-CA-CB	5.41	119.59	110.77
1	C	743	SER	CA-C-N	-5.41	111.02	121.58
1	C	743	SER	C-N-CA	-5.41	111.02	121.58
1	D	249	GLU	O-C-N	5.41	129.39	123.22
1	B	748	CYS	N-CA-CB	5.41	120.25	110.83
1	B	190	ARG	CB-CA-C	5.41	119.45	110.90
1	C	702	GLN	CA-CB-CG	-5.41	103.28	114.10
1	D	190	ARG	CB-CA-C	5.40	119.43	110.90
1	A	190	ARG	CB-CA-C	5.39	119.42	110.90
1	A	416	GLU	N-CA-CB	5.39	119.56	110.77
1	A	513	PRO	CB-CA-C	-5.39	104.50	111.46
1	C	513	PRO	CB-CA-C	-5.39	104.51	111.46
1	C	190	ARG	CB-CA-C	5.39	119.41	110.90
1	C	416	GLU	N-CA-CB	5.39	119.55	110.77
1	D	513	PRO	CB-CA-C	-5.39	104.51	111.46
1	D	748	CYS	N-CA-CB	5.39	120.20	110.83
1	A	748	CYS	N-CA-CB	5.39	120.20	110.83
1	B	886	CYS	CA-C-N	-5.39	115.51	123.05
1	B	886	CYS	C-N-CA	-5.39	115.51	123.05
1	D	886	CYS	CA-C-N	-5.39	115.51	123.05
1	D	886	CYS	C-N-CA	-5.39	115.51	123.05
1	C	969	GLU	N-CA-CB	5.38	118.46	110.49
1	D	969	GLU	N-CA-CB	5.38	118.46	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	416	GLU	N-CA-CB	5.38	119.54	110.77
1	C	423	MET	N-CA-C	5.38	117.14	111.28
1	C	748	CYS	N-CA-CB	5.38	120.19	110.83
1	A	969	GLU	N-CA-CB	5.38	118.45	110.49
1	A	886	CYS	CA-C-N	-5.38	115.52	123.05
1	A	886	CYS	C-N-CA	-5.38	115.52	123.05
1	B	969	GLU	N-CA-CB	5.38	118.45	110.49
1	A	423	MET	N-CA-C	5.37	117.13	111.28
1	B	386	ALA	N-CA-CB	-5.37	102.70	111.66
1	D	423	MET	N-CA-C	5.36	117.13	111.28
1	D	386	ALA	N-CA-CB	-5.36	102.71	111.66
1	B	423	MET	N-CA-C	5.36	117.12	111.28
1	C	386	ALA	N-CA-CB	-5.36	102.71	111.66
1	B	513	PRO	CB-CA-C	-5.35	104.55	111.46
1	C	886	CYS	CA-C-N	-5.35	115.56	123.05
1	C	886	CYS	C-N-CA	-5.35	115.56	123.05
1	A	386	ALA	N-CA-CB	-5.35	102.73	111.66
1	C	653[A]	HIS	CA-C-N	-5.34	113.47	123.03
1	C	653[A]	HIS	C-N-CA	-5.34	113.47	123.03
1	C	653[B]	HIS	CA-C-N	-5.34	113.47	123.03
1	C	653[B]	HIS	C-N-CA	-5.34	113.47	123.03
1	A	421	VAL	CB-CA-C	-5.33	104.78	110.16
1	C	980	GLU	N-CA-C	5.33	117.50	111.11
1	A	980	GLU	N-CA-C	5.32	117.50	111.11
1	D	421	VAL	CB-CA-C	-5.32	104.78	110.16
1	C	421	VAL	CB-CA-C	-5.32	104.79	110.16
1	B	980	GLU	N-CA-C	5.32	117.49	111.11
1	B	421	VAL	CB-CA-C	-5.31	104.80	110.16
1	C	264	GLU	CA-C-O	5.31	124.89	119.05
1	C	781	ARG	N-CA-C	5.31	117.26	109.24
1	D	980	GLU	N-CA-C	5.31	117.48	111.11
1	A	653[A]	HIS	CA-C-N	-5.31	113.53	123.03
1	A	653[A]	HIS	C-N-CA	-5.31	113.53	123.03
1	A	653[B]	HIS	CA-C-N	-5.31	113.53	123.03
1	A	653[B]	HIS	C-N-CA	-5.31	113.53	123.03
1	D	653[A]	HIS	CA-C-N	-5.30	113.54	123.03
1	D	653[A]	HIS	C-N-CA	-5.30	113.54	123.03
1	D	653[B]	HIS	CA-C-N	-5.30	113.54	123.03
1	D	653[B]	HIS	C-N-CA	-5.30	113.54	123.03
1	C	634	GLN	CA-C-O	5.30	125.93	119.78
1	A	634	GLN	CA-C-O	5.30	125.93	119.78
1	B	634	GLN	CA-C-O	5.30	125.92	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASN	CA-CB-CG	5.29	117.89	112.60
1	D	264	GLU	CA-C-O	5.29	124.87	119.05
1	D	781	ARG	N-CA-C	5.29	117.22	109.24
1	B	653[A]	HIS	CA-C-N	-5.28	113.57	123.03
1	B	653[A]	HIS	C-N-CA	-5.28	113.57	123.03
1	B	653[B]	HIS	CA-C-N	-5.28	113.57	123.03
1	B	653[B]	HIS	C-N-CA	-5.28	113.57	123.03
1	D	102	ASN	CA-CB-CG	5.28	117.88	112.60
1	B	685	LEU	CA-C-O	5.28	123.99	119.66
1	A	781	ARG	N-CA-C	5.28	117.21	109.24
1	C	927	THR	CA-C-O	5.28	124.45	119.59
1	C	102	ASN	CA-CB-CG	5.27	117.87	112.60
1	B	102	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	264	GLU	CA-C-O	5.27	124.85	119.05
1	A	685	LEU	CA-C-O	5.27	123.98	119.66
1	D	685	LEU	CA-C-O	5.26	123.98	119.66
1	B	1018	LEU	CB-CA-C	-5.26	99.01	109.79
1	A	1018	LEU	CB-CA-C	-5.25	99.02	109.79
1	D	404	ARG	N-CA-C	5.25	118.15	111.69
1	B	264	GLU	CA-C-O	5.25	124.83	119.05
1	B	781	ARG	N-CA-C	5.25	117.17	109.24
1	D	634	GLN	CA-C-O	5.25	125.87	119.78
1	C	404	ARG	N-CA-C	5.25	118.14	111.69
1	D	1018	LEU	CB-CA-C	-5.23	99.06	109.79
1	A	927	THR	CA-C-O	5.23	124.40	119.59
1	A	404	ARG	N-CA-C	5.23	118.12	111.69
1	C	210	ARG	N-CA-C	-5.23	101.76	109.18
1	C	1018	LEU	CB-CA-C	-5.22	99.08	109.79
1	A	210	ARG	N-CA-C	-5.22	101.77	109.18
1	B	404	ARG	N-CA-C	5.22	118.11	111.69
1	C	685	LEU	CA-C-O	5.22	123.94	119.66
1	B	908	ASP	N-CA-C	-5.22	106.77	112.72
1	B	927	THR	CA-C-O	5.22	124.39	119.59
1	D	261	TRP	CB-CA-C	-5.22	99.82	109.37
1	D	908	ASP	N-CA-C	-5.21	106.78	112.72
1	B	261	TRP	CB-CA-C	-5.21	99.84	109.37
1	A	908	ASP	N-CA-C	-5.20	106.79	112.72
1	B	210	ARG	N-CA-C	-5.20	101.80	109.18
1	A	261	TRP	CB-CA-C	-5.19	99.87	109.37
1	C	183	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	D	927	THR	CA-C-O	5.19	124.37	119.59
1	C	261	TRP	CB-CA-C	-5.19	99.87	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	ARG	N-CA-C	-5.18	101.82	109.18
1	C	216	HIS	CA-CB-CG	-5.18	108.62	113.80
1	B	216	HIS	CA-CB-CG	-5.18	108.62	113.80
1	C	908	ASP	N-CA-C	-5.17	106.83	112.72
1	D	714	ILE	CB-CA-C	-5.16	103.91	110.98
1	B	183	ARG	CD-NE-CZ	-5.16	117.18	124.40
1	A	216	HIS	CA-CB-CG	-5.15	108.65	113.80
1	D	183	ARG	CD-NE-CZ	-5.15	117.19	124.40
1	C	526	LEU	N-CA-C	-5.15	102.69	109.84
1	A	714	ILE	CB-CA-C	-5.14	103.93	110.98
1	C	714	ILE	CB-CA-C	-5.14	103.93	110.98
1	B	714	ILE	CB-CA-C	-5.14	103.94	110.98
1	A	769	TRP	CB-CA-C	-5.13	98.65	109.38
1	B	526	LEU	N-CA-C	-5.13	102.70	109.84
1	D	769	TRP	CB-CA-C	-5.13	98.65	109.38
1	A	526	LEU	N-CA-C	-5.13	102.71	109.84
1	C	769	TRP	CB-CA-C	-5.13	98.66	109.38
1	C	875	ASP	N-CA-C	5.13	118.67	112.93
1	D	526	LEU	N-CA-C	-5.13	102.72	109.84
1	D	216	HIS	CA-CB-CG	-5.12	108.68	113.80
1	A	183	ARG	CD-NE-CZ	-5.12	117.23	124.40
1	A	875	ASP	N-CA-C	5.11	118.66	112.93
1	B	769	TRP	CB-CA-C	-5.11	98.70	109.38
1	C	132	SER	N-CA-C	5.10	116.84	111.28
1	D	875	ASP	N-CA-C	5.09	118.63	112.93
1	C	193	ASP	CA-CB-CG	-5.09	107.51	112.60
1	D	288	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	B	875	ASP	N-CA-C	5.08	118.62	112.93
1	C	190	ARG	N-CA-CB	5.08	117.43	110.07
1	A	453	VAL	CA-C-N	-5.08	116.50	122.14
1	A	453	VAL	C-N-CA	-5.08	116.50	122.14
1	B	132	SER	N-CA-C	5.08	116.81	111.28
1	A	132	SER	N-CA-C	5.07	116.81	111.28
1	C	729	THR	N-CA-CB	5.07	118.51	110.55
1	C	453	VAL	CA-C-N	-5.07	116.51	122.14
1	C	453	VAL	C-N-CA	-5.07	116.51	122.14
1	B	190	ARG	N-CA-CB	5.07	117.42	110.07
1	D	453	VAL	CA-C-N	-5.07	116.52	122.14
1	D	453	VAL	C-N-CA	-5.07	116.52	122.14
1	D	729	THR	N-CA-CB	5.06	118.50	110.55
1	B	729	THR	N-CA-CB	5.06	118.49	110.55
1	B	533	LEU	CB-CA-C	5.05	118.55	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	447	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	193	ASP	CA-CB-CG	-5.05	107.55	112.60
1	D	132	SER	N-CA-C	5.05	116.78	111.28
1	B	193	ASP	CA-CB-CG	-5.04	107.56	112.60
1	B	453	VAL	CA-C-N	-5.04	116.54	122.14
1	B	453	VAL	C-N-CA	-5.04	116.54	122.14
1	A	533	LEU	CB-CA-C	5.04	118.52	110.16
1	D	533	LEU	CB-CA-C	5.04	118.52	110.16
1	B	639	THR	CA-CB-CG2	-5.04	101.94	110.50
1	C	686	PRO	CB-CA-C	-5.04	104.62	111.12
1	A	447	ASP	CA-CB-CG	-5.03	107.57	112.60
1	D	737	ILE	N-CA-CB	5.03	118.26	111.21
1	B	737	ILE	N-CA-CB	5.03	118.25	111.21
1	A	288	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	737	ILE	N-CA-CB	5.03	118.25	111.21
1	C	639	THR	CA-CB-CG2	-5.03	101.95	110.50
1	A	190	ARG	N-CA-CB	5.03	117.36	110.07
1	A	729	THR	N-CA-CB	5.03	118.44	110.55
1	C	533	LEU	CB-CA-C	5.03	118.50	110.16
1	D	193	ASP	CA-CB-CG	-5.03	107.57	112.60
1	B	787	ALA	O-C-N	5.03	125.72	121.20
1	C	323	ILE	N-CA-C	-5.03	105.94	110.82
1	B	710	GLU	CB-CA-C	-5.02	100.00	110.40
1	D	323	ILE	N-CA-C	-5.02	105.95	110.82
1	A	323	ILE	N-CA-C	-5.02	105.95	110.82
1	B	288	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	C	737	ILE	N-CA-CB	5.02	118.24	111.21
1	D	278	ILE	CA-C-N	-5.02	116.17	121.84
1	D	278	ILE	C-N-CA	-5.02	116.17	121.84
1	A	710	GLU	CB-CA-C	-5.02	100.01	110.40
1	C	288	ARG	NE-CZ-NH1	-5.02	116.48	121.50
1	A	639	THR	CA-C-N	-5.02	115.12	122.19
1	A	639	THR	C-N-CA	-5.02	115.12	122.19
1	A	639	THR	CA-CB-CG2	-5.02	101.97	110.50
1	B	686	PRO	CB-CA-C	-5.02	104.65	111.12
1	D	190	ARG	N-CA-CB	5.02	117.34	110.07
1	D	710	GLU	CB-CA-C	-5.02	100.02	110.40
1	A	686	PRO	CB-CA-C	-5.01	104.65	111.12
1	B	639	THR	CA-C-N	-5.01	115.12	122.19
1	B	639	THR	C-N-CA	-5.01	115.12	122.19
1	C	322	LEU	CB-CA-C	-5.01	102.07	110.29
1	C	710	GLU	CB-CA-C	-5.01	100.03	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	639	THR	CA-CB-CG2	-5.01	101.98	110.50
1	D	686	PRO	CB-CA-C	-5.01	104.66	111.12
1	B	447	ASP	CA-CB-CG	-5.00	107.59	112.60
1	D	297	ASN	CA-CB-CG	-5.00	107.59	112.60
1	A	542	MET	N-CA-C	5.00	116.42	108.67
1	A	787	ALA	O-C-N	5.00	125.70	121.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8238	0	7824	423	0
1	B	8238	0	7824	397	0
1	C	8238	0	7824	400	0
1	D	8238	0	7824	402	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	365	0	0	10	0
3	B	366	0	0	10	0
3	C	367	0	0	10	0
3	D	366	0	0	10	0
All	All	34424	0	31296	1597	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 25.

All (1597) 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:B:746:ASP:HA	1:B:760:ARG:HG3	1.34	1.10
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.34	1.09
1:B:427:THR:HA	1:B:436:MET:HE1	1.09	1.08
1:D:427:THR:HA	1:D:436:MET:HE1	1.09	1.07
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.34	1.06
1:A:427:THR:HA	1:A:436:MET:HE1	1.09	1.05
1:B:693:GLN:HG2	1:B:721:ARG:HD3	1.39	1.05
1:D:693:GLN:HG2	1:D:721:ARG:HD3	1.39	1.04
1:C:427:THR:HA	1:C:436:MET:HE1	1.09	1.04
1:A:693:GLN:HG2	1:A:721:ARG:HD3	1.39	1.03
1:C:693:GLN:HG2	1:C:721:ARG:HD3	1.39	1.01
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.44	0.99
1:C:597:ASN:HD22	1:C:599:ARG:H	1.11	0.98
1:D:597:ASN:HD22	1:D:599:ARG:H	1.11	0.98
1:C:597:ASN:ND2	1:C:599:ARG:H	1.65	0.95
1:B:38:ASN:ND2	1:B:41:GLU:H	1.66	0.94
1:A:38:ASN:ND2	1:A:41:GLU:H	1.66	0.94
1:A:597:ASN:ND2	1:A:599:ARG:H	1.65	0.94
1:D:597:ASN:ND2	1:D:599:ARG:H	1.65	0.94
1:A:255:ARG:HG2	1:A:255:ARG:HH11	1.34	0.93
1:B:427:THR:HA	1:B:436:MET:CE	1.99	0.93
1:B:255:ARG:HG2	1:B:255:ARG:HH11	1.34	0.93
1:C:38:ASN:ND2	1:C:41:GLU:H	1.66	0.93
1:B:597:ASN:ND2	1:B:599:ARG:H	1.65	0.92
1:C:255:ARG:HG2	1:C:255:ARG:HH11	1.34	0.92
1:D:38:ASN:ND2	1:D:41:GLU:H	1.66	0.92
1:C:427:THR:HA	1:C:436:MET:CE	1.99	0.92
1:A:427:THR:HA	1:A:436:MET:CE	1.99	0.92
1:B:597:ASN:HD22	1:B:599:ARG:H	1.11	0.92
1:D:427:THR:HA	1:D:436:MET:CE	1.99	0.91
1:A:597:ASN:HD22	1:A:599:ARG:H	1.11	0.91
1:D:255:ARG:HG2	1:D:255:ARG:HH11	1.34	0.89
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.58	0.86
1:A:734:SER:HB3	1:A:860:GLY:HA3	1.57	0.86
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.57	0.86
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.58	0.85
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.58	0.85
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.58	0.85
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.57	0.85
1:D:856:TYR:HB3	1:D:864:MET:CE	2.07	0.85
1:A:856:TYR:HB3	1:A:864:MET:CE	2.07	0.84
1:C:856:TYR:HB3	1:C:864:MET:CE	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.57	0.84
1:B:856:TYR:HB3	1:B:864:MET:CE	2.07	0.83
1:D:734:SER:CB	1:D:860:GLY:HA3	2.08	0.83
1:D:654:TRP:NE1	1:D:666:GLY:HA3	1.94	0.83
1:B:734:SER:CB	1:B:860:GLY:HA3	2.08	0.82
1:A:734:SER:CB	1:A:860:GLY:HA3	2.09	0.82
1:C:654:TRP:NE1	1:C:666:GLY:HA3	1.94	0.82
1:C:949:HIS:CD2	1:C:1020:TRP:HE1	1.98	0.82
1:B:654:TRP:NE1	1:B:666:GLY:HA3	1.94	0.82
1:C:734:SER:CB	1:C:860:GLY:HA3	2.09	0.82
1:D:949:HIS:CD2	1:D:1020:TRP:HE1	1.98	0.82
1:A:654:TRP:NE1	1:A:666:GLY:HA3	1.94	0.81
1:B:830:LEU:CD2	1:B:835:LEU:HB2	2.11	0.81
1:A:830:LEU:CD2	1:A:835:LEU:HB2	2.11	0.81
1:C:830:LEU:CD2	1:C:835:LEU:HB2	2.11	0.81
1:B:949:HIS:CD2	1:B:1020:TRP:HE1	1.98	0.81
1:A:949:HIS:CD2	1:A:1020:TRP:HE1	1.98	0.80
1:D:830:LEU:CD2	1:D:835:LEU:HB2	2.11	0.80
1:C:134:LEU:HD12	1:C:134:LEU:N	1.97	0.80
1:A:360:HIS:ND1	1:A:361:PRO:HD2	1.97	0.80
1:C:360:HIS:ND1	1:C:361:PRO:HD2	1.97	0.80
1:A:134:LEU:N	1:A:134:LEU:HD12	1.97	0.79
1:D:360:HIS:ND1	1:D:361:PRO:HD2	1.97	0.79
1:B:77:ASP:O	1:B:78:LEU:HD23	1.83	0.79
1:C:77:ASP:O	1:C:78:LEU:HD23	1.83	0.79
1:B:134:LEU:N	1:B:134:LEU:HD12	1.97	0.78
1:D:77:ASP:O	1:D:78:LEU:HD23	1.83	0.78
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.65	0.78
1:A:77:ASP:O	1:A:78:LEU:HD23	1.83	0.78
1:B:360:HIS:ND1	1:B:361:PRO:HD2	1.97	0.77
1:A:928:PRO:HB2	1:A:973:ARG:NH1	1.99	0.77
1:B:9:VAL:O	1:B:12:GLN:HB3	1.85	0.77
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.65	0.77
1:C:928:PRO:HB2	1:C:973:ARG:NH1	1.99	0.77
1:D:134:LEU:N	1:D:134:LEU:HD12	1.97	0.77
1:A:11:LEU:HD21	1:A:187:MET:CE	2.15	0.77
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.66	0.77
1:B:928:PRO:HB2	1:B:973:ARG:NH1	1.99	0.77
1:C:1004:SER:HB2	1:C:1006:GLU:OE2	1.85	0.77
1:A:1004:SER:HB2	1:A:1006:GLU:OE2	1.85	0.77
1:D:928:PRO:HB2	1:D:973:ARG:NH1	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:O	1:D:12:GLN:HB3	1.85	0.76
1:B:11:LEU:HD21	1:B:187:MET:CE	2.15	0.76
1:D:11:LEU:HD21	1:D:187:MET:CE	2.15	0.76
1:A:9:VAL:O	1:A:12:GLN:HB3	1.85	0.76
1:C:9:VAL:O	1:C:12:GLN:HB3	1.85	0.76
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.14	0.76
1:C:11:LEU:HD21	1:C:187:MET:CE	2.15	0.76
1:D:746:ASP:CA	1:D:760:ARG:HG3	2.14	0.76
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.76
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.68	0.76
1:D:1004:SER:HB2	1:D:1006:GLU:OE2	1.85	0.76
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.75
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.68	0.75
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.14	0.75
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.68	0.75
1:A:949:HIS:HD2	1:A:1020:TRP:HE1	1.35	0.75
1:B:1004:SER:HB2	1:B:1006:GLU:OE2	1.85	0.75
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.68	0.75
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.68	0.74
1:C:38:ASN:HD22	1:C:41:GLU:H	1.35	0.74
1:A:38:ASN:HD22	1:A:41:GLU:H	1.35	0.74
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.69	0.74
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.74
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.14	0.74
1:B:436:MET:HE3	1:B:467:ASN:HD22	1.53	0.74
1:D:579:ASP:OD1	1:D:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.53	0.73
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.70	0.73
1:C:778:THR:HG23	1:C:779:PRO:HD2	1.70	0.73
1:D:436:MET:HE3	1:D:467:ASN:HD22	1.53	0.73
1:B:237:ARG:HH11	1:B:237:ARG:HB3	1.54	0.73
1:B:579:ASP:OD1	1:B:583:ASN:HB2	1.89	0.73
1:C:559:TYR:HB2	1:C:562:LEU:HD12	1.71	0.73
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.89	0.73
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.02	0.73
1:A:579:ASP:OD1	1:A:583:ASN:HB2	1.89	0.72
1:A:778:THR:HG23	1:A:779:PRO:HD2	1.70	0.72
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.54	0.72
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.54	0.72
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.72
1:D:436:MET:CE	1:D:467:ASN:HD22	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.71	0.72
1:C:949:HIS:HD2	1:C:1020:TRP:HE1	1.35	0.72
1:B:3:ILE:HG13	1:B:4:THR:N	2.04	0.72
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.71	0.72
1:B:949:HIS:HD2	1:B:1020:TRP:HE1	1.35	0.72
1:D:559:TYR:HB2	1:D:562:LEU:HD12	1.71	0.72
1:A:559:TYR:HB2	1:A:562:LEU:HD12	1.71	0.72
1:D:3:ILE:HG13	1:D:4:THR:N	2.04	0.72
1:D:380:LYS:HE2	3:D:4077:HOH:O	1.90	0.72
1:A:652:LEU:HD11	1:A:698:VAL:HB	1.71	0.72
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.55	0.72
1:B:237:ARG:HH11	1:B:237:ARG:CB	2.02	0.72
1:D:949:HIS:HD2	1:D:1020:TRP:HE1	1.35	0.72
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.72	0.71
1:A:436:MET:CE	1:A:467:ASN:HD22	2.03	0.71
1:B:928:PRO:HB2	1:B:973:ARG:HH11	1.55	0.71
1:C:655:MET:HG3	1:C:656:VAL:N	2.03	0.71
1:C:928:PRO:HB2	1:C:973:ARG:HH11	1.55	0.71
1:A:3:ILE:HG13	1:A:4:THR:N	2.04	0.71
1:A:436:MET:HE3	1:A:467:ASN:HD22	1.53	0.71
1:B:38:ASN:HD22	1:B:41:GLU:H	1.35	0.71
1:A:928:PRO:HB2	1:A:973:ARG:HH11	1.55	0.71
1:C:436:MET:CE	1:C:467:ASN:HD22	2.03	0.71
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.02	0.71
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.02	0.71
1:B:559:TYR:HB2	1:B:562:LEU:HD12	1.71	0.71
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.71	0.71
1:C:3:ILE:HG13	1:C:4:THR:N	2.04	0.71
1:C:367:MET:HB3	1:C:372:MET:HE2	1.73	0.71
1:B:380:LYS:HE2	3:B:4134:HOH:O	1.90	0.71
1:B:436:MET:CE	1:B:467:ASN:HD22	2.03	0.71
1:C:380:LYS:HE2	3:C:4174:HOH:O	1.90	0.71
1:C:436:MET:HE3	1:C:467:ASN:HD22	1.53	0.71
1:C:650:GLU:HB3	1:C:670:LEU:HD12	1.73	0.71
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.73	0.70
1:D:367:MET:HB3	1:D:372:MET:HE2	1.73	0.70
1:A:367:MET:HB3	1:A:372:MET:HE2	1.73	0.70
1:C:836:ILE:HD13	1:C:836:ILE:N	2.07	0.69
1:D:38:ASN:HD22	1:D:41:GLU:H	1.35	0.69
1:A:655:MET:HG3	1:A:656:VAL:N	2.03	0.69
1:B:367:MET:HB3	1:B:372:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LYS:HE2	3:A:4077:HOH:O	1.90	0.69
1:A:836:ILE:HD13	1:A:836:ILE:N	2.07	0.69
1:B:650:GLU:HB3	1:B:670:LEU:HD12	1.73	0.69
1:B:655:MET:HG3	1:B:656:VAL:N	2.03	0.69
1:C:63:PHE:HB3	1:C:64:PRO:HD2	1.75	0.69
1:D:836:ILE:HD13	1:D:836:ILE:N	2.07	0.69
1:B:836:ILE:HD13	1:B:836:ILE:N	2.07	0.69
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.73	0.68
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.75	0.68
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.92	0.68
1:C:255:ARG:HG2	1:C:255:ARG:NH1	2.07	0.68
1:D:11:LEU:HD21	1:D:187:MET:HE3	1.76	0.68
1:A:287:ASP:CG	1:D:425:ARG:HH22	2.00	0.68
1:B:835:LEU:C	1:B:836:ILE:HD13	2.19	0.68
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.91	0.68
1:D:1020:TRP:HD1	1:D:1021:CYS:N	1.91	0.68
1:A:835:LEU:C	1:A:836:ILE:HD13	2.19	0.68
1:B:35:SER:OG	1:B:37:ARG:NH1	2.27	0.68
1:C:923:SER:HB3	3:C:4345:HOH:O	1.94	0.68
1:D:35:SER:OG	1:D:37:ARG:NH1	2.27	0.68
1:C:35:SER:OG	1:C:37:ARG:NH1	2.27	0.68
1:A:923:SER:HB3	3:A:4380:HOH:O	1.94	0.67
1:D:923:SER:HB3	3:D:4380:HOH:O	1.94	0.67
1:A:11:LEU:HD21	1:A:187:MET:HE3	1.76	0.67
1:D:211:ASP:OD1	1:D:211:ASP:N	2.27	0.67
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.76	0.67
1:D:255:ARG:HG2	1:D:255:ARG:NH1	2.07	0.67
1:D:965:GLN:O	1:D:969:GLU:HG3	1.94	0.67
1:B:965:GLN:O	1:B:969:GLU:HG3	1.94	0.67
1:C:59:ARG:NH2	1:C:81:ALA:O	2.28	0.67
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.77	0.67
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.91	0.67
1:C:11:LEU:HD21	1:C:187:MET:HE3	1.76	0.67
1:C:965:GLN:O	1:C:969:GLU:HG3	1.94	0.67
1:A:211:ASP:N	1:A:211:ASP:OD1	2.27	0.67
1:A:35:SER:OG	1:A:37:ARG:NH1	2.27	0.67
1:C:835:LEU:C	1:C:836:ILE:HD13	2.19	0.67
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.75	0.67
1:A:59:ARG:NH2	1:A:81:ALA:O	2.28	0.66
1:B:255:ARG:HG2	1:B:255:ARG:NH1	2.07	0.66
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:375:ASP:O	1:C:379:MET:HG3	1.95	0.66
1:D:835:LEU:C	1:D:836:ILE:HD13	2.19	0.66
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.77	0.66
1:A:965:GLN:O	1:A:969:GLU:HG3	1.94	0.66
1:A:7:LEU:N	1:A:71:GLU:OE2	2.28	0.66
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.75	0.66
1:B:824:GLN:HG3	1:B:825:CYS:N	2.11	0.66
1:B:923:SER:HB3	3:B:4305:HOH:O	1.94	0.66
1:D:655:MET:HG3	1:D:656:VAL:N	2.03	0.66
1:D:824:GLN:HG3	1:D:825:CYS:N	2.11	0.66
1:A:856:TYR:HB3	1:A:864:MET:HE1	1.77	0.66
1:B:7:LEU:N	1:B:71:GLU:OE2	2.28	0.66
1:B:11:LEU:HD21	1:B:187:MET:HE3	1.76	0.66
1:D:59:ARG:NH2	1:D:81:ALA:O	2.28	0.66
1:B:59:ARG:NH2	1:B:81:ALA:O	2.28	0.66
1:D:427:THR:CA	1:D:436:MET:HE1	2.05	0.66
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.77	0.66
1:A:375:ASP:O	1:A:379:MET:HG3	1.95	0.66
1:B:211:ASP:OD1	1:B:211:ASP:N	2.27	0.65
1:C:30:HIS:HB2	1:C:31:PRO:HD2	1.77	0.65
1:C:824:GLN:HG3	1:C:825:CYS:N	2.11	0.65
1:C:7:LEU:N	1:C:71:GLU:OE2	2.28	0.65
1:D:7:LEU:N	1:D:71:GLU:OE2	2.28	0.65
1:D:775:GLN:OE1	1:D:890:GLN:NE2	2.30	0.65
1:B:375:ASP:O	1:B:379:MET:HG3	1.95	0.65
1:C:856:TYR:HB3	1:C:864:MET:HE1	1.77	0.65
1:D:856:TYR:HB3	1:D:864:MET:HE1	1.77	0.65
1:C:210:ARG:HD3	3:C:4138:HOH:O	1.97	0.65
1:D:375:ASP:O	1:D:379:MET:HG3	1.95	0.65
1:A:824:GLN:HG3	1:A:825:CYS:N	2.10	0.65
1:B:80:GLU:CD	1:B:80:GLU:H	2.01	0.65
1:B:742:THR:HG22	1:B:743:SER:N	2.12	0.65
1:B:775:GLN:OE1	1:B:890:GLN:NE2	2.30	0.65
1:C:775:GLN:OE1	1:C:890:GLN:NE2	2.30	0.65
1:D:742:THR:HG22	1:D:743:SER:N	2.12	0.65
1:A:742:THR:HG22	1:A:743:SER:N	2.12	0.64
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.77	0.64
1:B:499:ILE:HB	1:B:533:LEU:HB2	1.80	0.64
1:B:856:TYR:HB3	1:B:864:MET:HE1	1.77	0.64
1:C:742:THR:HG22	1:C:743:SER:N	2.12	0.64
1:A:499:ILE:HB	1:A:533:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HD3	3:A:4036:HOH:O	1.97	0.64
1:A:775:GLN:OE1	1:A:890:GLN:NE2	2.30	0.64
1:A:287:ASP:OD2	1:D:425:ARG:NH2	2.31	0.64
1:D:499:ILE:HB	1:D:533:LEU:HB2	1.79	0.64
1:B:210:ARG:HD3	3:B:4098:HOH:O	1.97	0.64
1:B:797:GLU:O	1:B:801:ILE:HD12	1.98	0.64
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.77	0.64
1:A:282:ARG:HH12	1:D:419:GLY:C	2.06	0.64
1:C:499:ILE:HB	1:C:533:LEU:HB2	1.79	0.64
1:D:210:ARG:HD3	3:D:4036:HOH:O	1.97	0.64
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.81	0.63
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.81	0.63
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.81	0.63
1:B:746:ASP:HA	1:B:760:ARG:CG	2.22	0.63
1:C:746:ASP:HA	1:C:760:ARG:CG	2.22	0.63
1:C:797:GLU:O	1:C:801:ILE:HD12	1.98	0.63
1:B:649:ASN:OD1	1:B:703:PRO:HD2	1.99	0.63
1:C:533:LEU:C	1:C:533:LEU:HD12	2.24	0.63
1:B:66:PRO:HD2	1:B:67:GLU:HG2	1.81	0.63
1:A:66:PRO:HD2	1:A:67:GLU:HG2	1.81	0.63
1:A:856:TYR:CD2	1:A:864:MET:HE1	2.34	0.63
1:C:211:ASP:N	1:C:211:ASP:OD1	2.27	0.63
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.81	0.63
1:D:649:ASN:OD1	1:D:703:PRO:HD2	1.99	0.63
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.81	0.62
1:D:100:TYR:HB2	1:D:203:TRP:CD2	2.34	0.62
1:A:797:GLU:O	1:A:801:ILE:HD12	1.98	0.62
1:B:856:TYR:CD2	1:B:864:MET:HE1	2.34	0.62
1:D:746:ASP:HA	1:D:760:ARG:CG	2.22	0.62
1:A:255:ARG:HG2	1:A:255:ARG:NH1	2.07	0.62
1:A:649:ASN:OD1	1:A:703:PRO:HD2	1.99	0.62
1:C:100:TYR:HB2	1:C:203:TRP:CD2	2.34	0.62
1:A:100:TYR:HB2	1:A:203:TRP:CD2	2.34	0.62
1:B:906:TYR:HB3	1:B:907:PRO:HD2	1.81	0.62
1:B:100:TYR:HB2	1:B:203:TRP:CD2	2.34	0.62
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.99	0.62
1:D:856:TYR:CD2	1:D:864:MET:HE1	2.34	0.62
1:A:272:ALA:HB1	1:A:273:PRO:HD2	1.81	0.62
1:A:533:LEU:HD12	1:A:533:LEU:C	2.24	0.62
1:B:533:LEU:HD12	1:B:533:LEU:C	2.24	0.62
1:A:906:TYR:HB3	1:A:907:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:GLN:HG3	1:C:768:MET:N	2.15	0.62
1:C:856:TYR:CD2	1:C:864:MET:HE1	2.34	0.62
1:D:80:GLU:CD	1:D:80:GLU:H	2.01	0.62
1:A:767:GLN:HG3	1:A:768:MET:N	2.15	0.62
1:D:533:LEU:HD12	1:D:533:LEU:C	2.24	0.62
1:A:427:THR:CA	1:A:436:MET:HE1	2.05	0.62
1:C:66:PRO:HD2	1:C:67:GLU:HG2	1.81	0.62
1:C:778:THR:CG2	1:C:779:PRO:HD2	2.30	0.62
1:D:797:GLU:O	1:D:801:ILE:HD12	1.98	0.62
1:D:66:PRO:HD2	1:D:67:GLU:HG2	1.81	0.61
1:A:419:GLY:C	1:D:282:ARG:HH12	2.08	0.61
1:A:778:THR:CG2	1:A:779:PRO:HD2	2.30	0.61
1:D:906:TYR:HB3	1:D:907:PRO:HD2	1.81	0.61
1:B:822:LEU:HD12	1:B:824:GLN:N	2.16	0.61
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.81	0.61
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.81	0.61
1:C:928:PRO:O	1:C:973:ARG:NH1	2.33	0.61
1:A:651:LEU:HD12	1:A:669:PRO:HA	1.83	0.61
1:D:610:ASP:OD2	1:D:612:THR:HG23	2.01	0.61
1:A:304:GLU:C	1:A:305:ILE:HG13	2.26	0.61
1:A:928:PRO:O	1:A:973:ARG:NH1	2.34	0.61
1:C:227:VAL:HG13	1:C:240:LEU:HD11	1.83	0.61
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.30	0.61
1:C:651:LEU:HD12	1:C:669:PRO:HA	1.83	0.61
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.81	0.61
1:B:202:MET:HE3	1:B:357:HIS:CD2	2.36	0.61
1:B:928:PRO:O	1:B:973:ARG:NH1	2.34	0.61
1:D:928:PRO:O	1:D:973:ARG:NH1	2.34	0.61
1:A:202:MET:HE3	1:A:357:HIS:CD2	2.36	0.61
1:B:227:VAL:HG13	1:B:240:LEU:HD11	1.83	0.60
1:D:102:ASN:ND2	1:D:201:ASP:HB2	2.16	0.60
1:D:778:THR:CG2	1:D:779:PRO:HD2	2.30	0.60
1:A:80:GLU:H	1:A:80:GLU:CD	2.01	0.60
1:B:427:THR:CA	1:B:436:MET:HE1	2.05	0.60
1:D:822:LEU:HD12	1:D:824:GLN:N	2.16	0.60
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.16	0.60
1:A:822:LEU:HD12	1:A:824:GLN:N	2.16	0.60
1:B:822:LEU:HD11	1:B:824:GLN:O	2.01	0.60
1:C:595:THR:HG23	1:C:596:PRO:HA	1.82	0.60
1:D:822:LEU:HD11	1:D:824:GLN:O	2.01	0.60
1:A:610:ASP:OD2	1:A:612:THR:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:ND2	1:C:201:ASP:HB2	2.16	0.60
1:C:304:GLU:C	1:C:305:ILE:HG13	2.26	0.60
1:C:822:LEU:HD11	1:C:824:GLN:O	2.01	0.60
1:C:870:VAL:HG12	1:C:871:GLU:N	2.16	0.60
1:D:595:THR:HG23	1:D:596:PRO:HA	1.82	0.60
1:C:202:MET:HE3	1:C:357:HIS:CD2	2.36	0.60
1:A:595:THR:HG23	1:A:596:PRO:HA	1.82	0.60
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.16	0.60
1:B:830:LEU:HD21	1:B:835:LEU:HB2	1.84	0.60
1:B:140:ARG:NH1	1:B:170:GLU:OE1	2.31	0.60
1:B:595:THR:HG23	1:B:596:PRO:HA	1.82	0.60
1:B:734:SER:HB3	1:B:860:GLY:CA	2.30	0.60
1:C:822:LEU:HD12	1:C:824:GLN:N	2.16	0.60
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.02	0.60
1:C:511:PRO:HA	1:C:516:PRO:HB3	1.84	0.60
1:C:734:SER:HB3	1:C:860:GLY:CA	2.30	0.60
1:A:282:ARG:HD3	1:D:418:HIS:O	2.01	0.60
1:B:767:GLN:HG3	1:B:768:MET:N	2.15	0.60
1:D:651:LEU:HD12	1:D:669:PRO:HA	1.83	0.60
1:A:128:ASN:HA	1:A:180:GLY:O	2.02	0.60
1:B:610:ASP:OD2	1:B:612:THR:HG23	2.01	0.60
1:B:651:LEU:HD12	1:B:669:PRO:HA	1.83	0.60
1:C:128:ASN:HA	1:C:180:GLY:O	2.02	0.60
1:A:734:SER:HB3	1:A:860:GLY:CA	2.30	0.59
1:A:830:LEU:HD21	1:A:835:LEU:HB2	1.84	0.59
1:B:870:VAL:HG12	1:B:871:GLU:N	2.16	0.59
1:D:227:VAL:HG13	1:D:240:LEU:HD11	1.83	0.59
1:D:830:LEU:HD21	1:D:835:LEU:HB2	1.84	0.59
1:B:505:ARG:HG2	1:B:996:ASP:OD2	2.02	0.59
1:C:759:ASN:OD1	1:C:761:GLN:N	2.35	0.59
1:D:734:SER:HB3	1:D:860:GLY:CA	2.30	0.59
1:A:227:VAL:HG13	1:A:240:LEU:HD11	1.83	0.59
1:A:759:ASN:OD1	1:A:761:GLN:N	2.35	0.59
1:A:822:LEU:HD11	1:A:824:GLN:O	2.01	0.59
1:C:610:ASP:OD2	1:C:612:THR:HG23	2.01	0.59
1:D:701:VAL:HG12	1:D:702:GLN:N	2.17	0.59
1:D:767:GLN:HG3	1:D:768:MET:N	2.15	0.59
1:A:696:LEU:HD12	1:A:697:THR:N	2.18	0.59
1:D:202:MET:HE3	1:D:357:HIS:CD2	2.36	0.59
1:A:425:ARG:HH22	1:D:287:ASP:CG	2.11	0.59
1:A:870:VAL:HG12	1:A:871:GLU:N	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLU:C	1:B:305:ILE:HG13	2.26	0.59
1:B:696:LEU:HD12	1:B:697:THR:N	2.18	0.59
1:D:128:ASN:HA	1:D:180:GLY:O	2.02	0.59
1:A:505:ARG:HG2	1:A:996:ASP:OD2	2.02	0.59
1:D:696:LEU:HD12	1:D:697:THR:N	2.18	0.59
1:B:128:ASN:HA	1:B:180:GLY:O	2.02	0.59
1:D:505:ARG:HG2	1:D:996:ASP:OD2	2.02	0.59
1:D:511:PRO:HA	1:D:516:PRO:HB3	1.84	0.59
1:D:870:VAL:HG12	1:D:871:GLU:N	2.16	0.59
1:D:304:GLU:C	1:D:305:ILE:HG13	2.26	0.59
1:D:856:TYR:HD2	1:D:864:MET:HE1	1.68	0.59
1:A:701:VAL:HG12	1:A:702:GLN:N	2.17	0.58
1:B:336:ARG:NH2	1:B:338:GLU:OE1	2.36	0.58
1:C:645:ARG:HH22	1:C:650:GLU:CD	2.11	0.58
1:C:140:ARG:NH1	1:C:170:GLU:OE1	2.31	0.58
1:C:696:LEU:HD12	1:C:697:THR:N	2.17	0.58
1:C:856:TYR:HD2	1:C:864:MET:HE1	1.68	0.58
1:A:511:PRO:HA	1:A:516:PRO:HB3	1.84	0.58
1:B:6:SER:HB2	1:B:71:GLU:OE2	2.04	0.58
1:B:645:ARG:HH22	1:B:650:GLU:CD	2.11	0.58
1:C:80:GLU:H	1:C:80:GLU:CD	2.01	0.58
1:B:769:TRP:NE1	1:B:774:LYS:HG3	2.19	0.58
1:C:473:ARG:O	1:C:473:ARG:HD3	2.04	0.58
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.36	0.58
1:B:511:PRO:HA	1:B:516:PRO:HB3	1.84	0.58
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.39	0.58
1:A:645:ARG:HH22	1:A:650:GLU:CD	2.11	0.58
1:B:473:ARG:O	1:B:473:ARG:HD3	2.04	0.58
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.36	0.58
1:A:62:TRP:CD1	1:A:95:TYR:HB3	2.39	0.58
1:A:473:ARG:O	1:A:473:ARG:HD3	2.04	0.58
1:B:701:VAL:HG12	1:B:702:GLN:N	2.17	0.58
1:B:737:ILE:HG13	1:B:738:PRO:N	2.17	0.58
1:A:856:TYR:HD2	1:A:864:MET:HE1	1.68	0.58
1:D:336:ARG:NH2	1:D:338:GLU:OE1	2.36	0.58
1:D:473:ARG:HD3	1:D:473:ARG:O	2.04	0.58
1:D:737:ILE:HG13	1:D:738:PRO:N	2.17	0.58
1:A:769:TRP:NE1	1:A:774:LYS:HG3	2.19	0.58
1:C:427:THR:CA	1:C:436:MET:HE1	2.05	0.58
1:B:759:ASN:OD1	1:B:761:GLN:N	2.35	0.57
1:C:701:VAL:HG12	1:C:702:GLN:N	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:ARG:HH22	1:D:650:GLU:CD	2.11	0.57
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.19	0.57
1:A:429:ASP:OD1	1:A:430:PRO:HD2	2.04	0.57
1:B:316:HIS:HD2	1:B:317:THR:O	1.87	0.57
1:A:618:THR:HG22	1:A:912:ALA:HB1	1.86	0.57
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.57
1:B:856:TYR:HD2	1:B:864:MET:HE1	1.68	0.57
1:C:618:THR:HG22	1:C:912:ALA:HB1	1.86	0.57
1:D:6:SER:HB2	1:D:71:GLU:OE2	2.04	0.57
1:D:618:THR:HG22	1:D:912:ALA:HB1	1.86	0.57
1:A:6:SER:HB2	1:A:71:GLU:OE2	2.03	0.57
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.39	0.57
1:C:769:TRP:NE1	1:C:774:LYS:HG3	2.19	0.57
1:C:830:LEU:HD21	1:C:835:LEU:HB2	1.84	0.57
1:A:737:ILE:HG13	1:A:738:PRO:N	2.17	0.57
1:B:460:ASN:ND2	1:B:461:GLU:HG2	2.20	0.57
1:B:618:THR:HG22	1:B:912:ALA:HB1	1.86	0.57
1:C:62:TRP:CD1	1:C:95:TYR:HB3	2.39	0.57
1:C:134:LEU:HD12	1:C:134:LEU:H	1.69	0.57
1:C:26:ARG:HD2	1:C:169:SER:HA	1.87	0.57
1:C:429:ASP:OD1	1:C:430:PRO:HD2	2.04	0.57
1:D:140:ARG:NH1	1:D:170:GLU:OE1	2.31	0.57
1:D:316:HIS:HD2	1:D:317:THR:O	1.87	0.57
1:A:597:ASN:HD22	1:A:599:ARG:N	1.94	0.57
1:C:166:ARG:HD3	3:C:4137:HOH:O	2.05	0.57
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.40	0.57
1:A:316:HIS:HD2	1:A:317:THR:O	1.87	0.57
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.40	0.57
1:A:763:GLY:HA3	1:A:822:LEU:HD21	1.87	0.57
1:B:26:ARG:HD2	1:B:169:SER:HA	1.87	0.57
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.40	0.57
1:B:763:GLY:HA3	1:B:822:LEU:HD21	1.87	0.57
1:C:6:SER:HB2	1:C:71:GLU:OE2	2.03	0.57
1:C:460:ASN:ND2	1:C:461:GLU:HG2	2.20	0.57
1:A:460:ASN:ND2	1:A:461:GLU:HG2	2.20	0.57
1:B:360:HIS:CE1	1:B:361:PRO:HD2	2.40	0.56
1:A:166:ARG:HD3	3:A:4035:HOH:O	2.05	0.56
1:A:457:SER:HA	1:A:485:GLN:O	2.06	0.56
1:B:166:ARG:HD3	3:B:4097:HOH:O	2.05	0.56
1:B:834:VAL:HG12	1:B:835:LEU:N	2.19	0.56
1:D:460:ASN:ND2	1:D:461:GLU:HG2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:HIS:CE1	1:A:361:PRO:HD2	2.41	0.56
1:B:18:ASN:OD1	1:B:19:PRO:HD2	2.06	0.56
1:C:429:ASP:OD1	1:C:431[B]:ARG:HG3	2.05	0.56
1:C:763:GLY:HA3	1:C:822:LEU:HD21	1.87	0.56
1:D:763:GLY:HA3	1:D:822:LEU:HD21	1.87	0.56
1:D:18:ASN:OD1	1:D:19:PRO:HD2	2.06	0.56
1:A:26:ARG:HD2	1:A:169:SER:HA	1.87	0.56
1:C:834:VAL:HG12	1:C:835:LEU:N	2.19	0.56
1:D:38:ASN:HD21	1:D:41:GLU:H	1.53	0.56
1:D:166:ARG:HD3	3:D:4035:HOH:O	2.05	0.56
1:D:457:SER:HA	1:D:485:GLN:O	2.06	0.56
1:A:531:ARG:O	1:A:561:ARG:NH1	2.39	0.56
1:A:834:VAL:HG12	1:A:835:LEU:N	2.19	0.56
1:B:531:ARG:O	1:B:561:ARG:NH1	2.39	0.56
1:C:457:SER:HA	1:C:485:GLN:O	2.06	0.56
1:D:834:VAL:HG12	1:D:835:LEU:N	2.19	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:B:429:ASP:OD1	1:B:431[B]:ARG:HG3	2.05	0.56
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.36	0.56
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.40	0.56
1:D:134:LEU:HD12	1:D:134:LEU:H	1.69	0.56
1:D:429:ASP:OD1	1:D:431[B]:ARG:HG3	2.05	0.56
1:A:18:ASN:OD1	1:A:19:PRO:HD2	2.06	0.56
1:B:457:SER:HA	1:B:485:GLN:O	2.05	0.56
1:C:316:HIS:HD2	1:C:317:THR:O	1.88	0.56
1:C:833:ALA:HB1	1:C:858:ILE:O	2.06	0.56
1:A:429:ASP:OD1	1:A:431[B]:ARG:HG3	2.05	0.56
1:A:763:GLY:HA3	1:A:822:LEU:CD2	2.36	0.56
1:B:425:ARG:HH22	1:C:287:ASP:CG	2.14	0.56
1:D:429:ASP:OD1	1:D:430:PRO:HD2	2.04	0.55
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.74	0.55
1:B:425:ARG:NH2	1:C:287:ASP:OD2	2.39	0.55
1:C:360:HIS:CE1	1:C:361:PRO:HD2	2.41	0.55
1:D:395:HIS:ND1	1:D:396:PRO:HD2	2.22	0.55
1:A:100:TYR:HB2	1:A:203:TRP:CE3	2.42	0.55
1:A:833:ALA:HB1	1:A:858:ILE:O	2.06	0.55
1:C:100:TYR:HB2	1:C:203:TRP:CE3	2.42	0.55
1:D:763:GLY:HA3	1:D:822:LEU:CD2	2.36	0.55
1:B:38:ASN:HD21	1:B:41:GLU:H	1.53	0.55
1:B:134:LEU:HD12	1:B:134:LEU:H	1.69	0.55
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:833:ALA:HB1	1:B:858:ILE:O	2.06	0.55
1:C:395:HIS:ND1	1:C:396:PRO:HD2	2.22	0.55
1:C:531:ARG:O	1:C:561:ARG:NH1	2.39	0.55
1:A:140:ARG:NH1	1:A:170:GLU:OE1	2.31	0.55
1:B:100:TYR:HB2	1:B:203:TRP:CE3	2.42	0.55
1:C:18:ASN:OD1	1:C:19:PRO:HD2	2.06	0.55
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.55
1:D:360:HIS:CE1	1:D:361:PRO:HD2	2.41	0.55
1:A:662:PRO:C	1:A:663:LEU:HD23	2.32	0.55
1:A:942:ARG:HA	1:A:953:GLY:O	2.07	0.55
1:B:662:PRO:C	1:B:663:LEU:HD23	2.32	0.55
1:C:942:ARG:HA	1:C:953:GLY:O	2.07	0.55
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.36	0.55
1:C:786:ARG:HA	1:C:964:GLN:OE1	2.07	0.55
1:D:577:LYS:O	1:D:584:PRO:HA	2.06	0.55
1:D:668:VAL:HG13	1:D:669:PRO:HD2	1.89	0.55
1:D:833:ALA:HB1	1:D:858:ILE:O	2.06	0.55
1:B:90:TRP:HE1	1:B:96:ASP:CG	2.16	0.54
1:C:577:LYS:O	1:C:584:PRO:HA	2.06	0.54
1:D:531:ARG:O	1:D:561:ARG:NH1	2.39	0.54
1:A:786:ARG:HA	1:A:964:GLN:OE1	2.07	0.54
1:B:668:VAL:HG13	1:B:669:PRO:HD2	1.89	0.54
1:C:662:PRO:C	1:C:663:LEU:HD23	2.32	0.54
1:C:749:ILE:O	1:C:755:ARG:HG3	2.07	0.54
1:A:749:ILE:O	1:A:755:ARG:HG3	2.08	0.54
1:B:942:ARG:HA	1:B:953:GLY:O	2.07	0.54
1:D:100:TYR:HB2	1:D:203:TRP:CE3	2.42	0.54
1:B:786:ARG:HA	1:B:964:GLN:OE1	2.07	0.54
1:B:894:ARG:NH1	1:B:919:ASP:OD1	2.34	0.54
1:D:26:ARG:HD2	1:D:169:SER:HA	1.87	0.54
1:D:662:PRO:C	1:D:663:LEU:HD23	2.32	0.54
1:A:746:ASP:HA	1:A:760:ARG:CG	2.22	0.54
1:B:79:PRO:N	1:B:80:GLU:OE2	2.41	0.54
1:C:90:TRP:HE1	1:C:96:ASP:CG	2.16	0.54
1:D:79:PRO:N	1:D:80:GLU:OE2	2.41	0.54
1:D:942:ARG:HA	1:D:953:GLY:O	2.07	0.54
1:D:1020:TRP:CD1	1:D:1021:CYS:N	2.74	0.54
1:A:134:LEU:HD12	1:A:134:LEU:H	1.69	0.54
1:C:79:PRO:N	1:C:80:GLU:OE2	2.41	0.54
1:D:759:ASN:OD1	1:D:761:GLN:N	2.35	0.54
1:A:79:PRO:N	1:A:80:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TRP:HE1	1:A:96:ASP:CG	2.16	0.54
1:A:395:HIS:ND1	1:A:396:PRO:HD2	2.22	0.54
1:A:418:HIS:O	1:D:282:ARG:HD3	2.08	0.54
1:B:29:ALA:HA	3:B:4295:HOH:O	2.07	0.54
1:B:166:ARG:HG3	1:B:392:TYR:CB	2.38	0.54
1:C:668:VAL:HG13	1:C:669:PRO:HD2	1.89	0.54
1:D:38:ASN:ND2	1:D:41:GLU:N	2.48	0.54
1:D:749:ILE:O	1:D:755:ARG:HG3	2.08	0.54
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.38	0.54
1:C:38:ASN:HD21	1:C:41:GLU:H	1.53	0.54
1:D:29:ALA:HA	3:D:4347:HOH:O	2.07	0.54
1:C:30:HIS:HB2	1:C:31:PRO:CD	2.38	0.54
1:C:357:HIS:HD2	1:C:392:TYR:OH	1.91	0.54
1:C:903[A]:GLN:HB2	3:C:4239:HOH:O	2.08	0.54
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.74	0.54
1:D:786:ARG:HA	1:D:964:GLN:OE1	2.07	0.54
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.89	0.53
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.38	0.53
1:B:749:ILE:O	1:B:755:ARG:HG3	2.07	0.53
1:A:29:ALA:HA	3:A:4347:HOH:O	2.07	0.53
1:A:357:HIS:HD2	1:A:392:TYR:OH	1.91	0.53
1:A:903[A]:GLN:HB2	3:A:4157:HOH:O	2.09	0.53
1:D:90:TRP:HE1	1:D:96:ASP:CG	2.16	0.53
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.09	0.53
1:D:166:ARG:HG3	1:D:392:TYR:CB	2.38	0.53
1:B:1017:GLN:O	1:B:1018:LEU:HD23	2.09	0.53
1:B:742:THR:HG22	1:B:743:SER:H	1.74	0.53
1:C:6:SER:OG	1:C:9:VAL:HB	2.09	0.53
1:C:110:ASN:O	1:C:113:PHE:N	2.39	0.53
1:D:30:HIS:HB2	1:D:31:PRO:CD	2.38	0.53
1:C:894:ARG:NH1	1:C:919:ASP:OD1	2.34	0.53
1:D:357:HIS:HD2	1:D:392:TYR:OH	1.92	0.53
1:D:597:ASN:HD22	1:D:599:ARG:N	1.94	0.53
1:D:696:LEU:HD12	1:D:697:THR:H	1.74	0.53
1:B:597:ASN:HD22	1:B:599:ARG:N	1.94	0.53
1:D:654:TRP:CE2	1:D:666:GLY:HA3	2.44	0.53
1:B:356:ARG:HH22	1:B:367:MET:HE2	1.74	0.53
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.38	0.53
1:A:6:SER:OG	1:A:9:VAL:HB	2.09	0.52
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.09	0.52
1:A:356:ARG:HH22	1:A:367:MET:HE2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ALA:HA	3:C:4335:HOH:O	2.07	0.52
1:C:416:GLU:OE1	1:C:461:GLU:HG3	2.09	0.52
1:D:416:GLU:OE1	1:D:461:GLU:HG3	2.09	0.52
1:C:696:LEU:HD12	1:C:697:THR:H	1.74	0.52
1:C:959:ILE:HG23	1:C:959:ILE:O	2.09	0.52
1:C:1017:GLN:O	1:C:1018:LEU:HD23	2.09	0.52
1:D:742:THR:HG22	1:D:743:SER:H	1.74	0.52
1:A:416:GLU:OE1	1:A:461:GLU:HG3	2.09	0.52
1:A:920:LEU:HB3	1:A:921:PRO:CD	2.39	0.52
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.09	0.52
1:C:737:ILE:HG13	1:C:738:PRO:N	2.17	0.52
1:D:251:ARG:NH1	1:D:251:ARG:HG2	2.25	0.52
1:A:696:LEU:HD12	1:A:697:THR:H	1.74	0.52
1:B:959:ILE:HG23	1:B:959:ILE:O	2.09	0.52
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.09	0.52
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.09	0.52
1:D:356:ARG:HH22	1:D:367:MET:HE2	1.74	0.52
1:D:808:GLU:HA	1:D:808:GLU:OE1	2.10	0.52
1:B:696:LEU:HD12	1:B:697:THR:H	1.74	0.52
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.74	0.52
1:C:654:TRP:CE2	1:C:666:GLY:HA3	2.44	0.52
1:A:749:ILE:HD12	1:A:749:ILE:N	2.25	0.52
1:B:251:ARG:NH1	1:B:251:ARG:HG2	2.25	0.52
1:C:749:ILE:N	1:C:749:ILE:HD12	2.25	0.52
1:A:292:ARG:C	1:A:293:LEU:HD23	2.35	0.52
1:A:878:HIS:HB3	1:A:1009:LEU:O	2.10	0.52
1:A:959:ILE:HG23	1:A:959:ILE:O	2.09	0.52
1:B:357:HIS:HD2	1:B:392:TYR:OH	1.91	0.52
1:A:742:THR:HG22	1:A:743:SER:H	1.74	0.52
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.10	0.52
1:D:749:ILE:HD12	1:D:749:ILE:N	2.25	0.52
1:D:1017:GLN:O	1:D:1018:LEU:HD23	2.09	0.52
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.38	0.52
1:B:903[A]:GLN:HB2	3:B:4199:HOH:O	2.08	0.52
1:D:110:ASN:O	1:D:113:PHE:N	2.39	0.52
1:A:425:ARG:NH2	1:D:287:ASP:OD2	2.43	0.52
1:B:130:ASP:OD2	1:B:132:SER:OG	2.28	0.52
1:B:770:ILE:O	1:B:770:ILE:HG22	2.10	0.52
1:D:6:SER:OG	1:D:9:VAL:HB	2.09	0.52
1:D:130:ASP:OD2	1:D:132:SER:OG	2.28	0.52
1:D:148:SER:HB3	1:D:190:ARG:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:TRP:CE2	1:A:666:GLY:HA3	2.44	0.51
1:B:6:SER:OG	1:B:9:VAL:HB	2.09	0.51
1:C:742:THR:HG22	1:C:743:SER:H	1.74	0.51
1:D:542:MET:HA	1:D:604:ASN:HA	1.92	0.51
1:B:148:SER:HB3	1:B:190:ARG:O	2.10	0.51
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.92	0.51
1:B:749:ILE:N	1:B:749:ILE:HD12	2.25	0.51
1:C:292:ARG:C	1:C:293:LEU:HD23	2.35	0.51
1:C:878:HIS:HB3	1:C:1009:LEU:O	2.10	0.51
1:B:654:TRP:CE2	1:B:666:GLY:HA3	2.44	0.51
1:B:808:GLU:HA	1:B:808:GLU:OE1	2.10	0.51
1:C:542:MET:HA	1:C:604:ASN:HA	1.92	0.51
1:C:894:ARG:HD3	1:C:919:ASP:OD1	2.11	0.51
1:A:419:GLY:C	1:D:282:ARG:NH1	2.68	0.51
1:B:292:ARG:C	1:B:293:LEU:HD23	2.35	0.51
1:B:416:GLU:OE1	1:B:461:GLU:HG3	2.09	0.51
1:D:878:HIS:HB3	1:D:1009:LEU:O	2.10	0.51
1:D:959:ILE:HG23	1:D:959:ILE:O	2.09	0.51
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.25	0.51
1:A:282:ARG:NH1	1:D:419:GLY:C	2.68	0.51
1:B:878:HIS:HB3	1:B:1009:LEU:O	2.10	0.51
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.41	0.51
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.74	0.51
1:C:531:ARG:HB3	1:C:532:PRO:HD2	1.92	0.51
1:D:292:ARG:C	1:D:293:LEU:HD23	2.35	0.51
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.36	0.51
1:A:531:ARG:HB3	1:A:532:PRO:HD2	1.92	0.51
1:A:808:GLU:OE1	1:A:808:GLU:HA	2.10	0.51
1:C:38:ASN:ND2	1:C:41:GLU:N	2.48	0.51
1:D:230:ARG:HH11	1:D:230:ARG:CG	2.24	0.51
1:D:903[A]:GLN:HB2	3:D:4157:HOH:O	2.08	0.51
1:A:26:ARG:CD	1:A:169:SER:HB3	2.41	0.51
1:A:356:ARG:HD2	1:A:379:MET:HE1	1.92	0.51
1:B:822:LEU:HD12	1:B:824:GLN:H	1.76	0.51
1:C:148:SER:HB3	1:C:190:ARG:O	2.10	0.51
1:A:254:LEU:O	1:A:255:ARG:NH1	2.44	0.51
1:A:894:ARG:HD3	1:A:919:ASP:OD1	2.11	0.51
1:A:906:TYR:HB3	1:A:907:PRO:CD	2.41	0.51
1:C:597:ASN:HD22	1:C:599:ARG:N	1.94	0.51
1:B:26:ARG:CD	1:B:169:SER:HB3	2.41	0.51
1:B:254:LEU:C	1:B:255:ARG:HG2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:O	1:B:255:ARG:NH1	2.44	0.51
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.92	0.51
1:A:38:ASN:ND2	1:A:41:GLU:N	2.48	0.51
1:A:770:ILE:O	1:A:770:ILE:HG22	2.10	0.50
1:B:906:TYR:HB3	1:B:907:PRO:CD	2.41	0.50
1:C:26:ARG:CD	1:C:169:SER:HB3	2.41	0.50
1:C:95:TYR:CD1	1:C:95:TYR:N	2.79	0.50
1:D:254:LEU:O	1:D:255:ARG:NH1	2.44	0.50
1:D:894:ARG:NH1	1:D:919:ASP:OD1	2.34	0.50
1:A:134:LEU:N	1:A:134:LEU:CD1	2.73	0.50
1:A:282:ARG:CG	1:D:423:MET:HB2	2.42	0.50
1:A:881:ARG:HD3	1:A:987:ASP:CG	2.36	0.50
1:B:356:ARG:HD2	1:B:379:MET:HE1	1.92	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.92	0.50
1:D:65:ALA:HB1	1:D:66:PRO:CD	2.41	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.50
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.92	0.50
1:D:658:LEU:O	1:D:659:ASP:C	2.54	0.50
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.47	0.50
1:A:254:LEU:C	1:A:255:ARG:HG2	2.36	0.50
1:A:836:ILE:HG22	1:A:837:THR:N	2.26	0.50
1:B:881:ARG:HD3	1:B:987:ASP:CG	2.36	0.50
1:C:403:ASP:CG	1:C:451:PRO:HD2	2.36	0.50
1:D:356:ARG:HD2	1:D:379:MET:HE1	1.92	0.50
1:D:822:LEU:HD12	1:D:824:GLN:H	1.76	0.50
1:D:906:TYR:HB3	1:D:907:PRO:CD	2.41	0.50
1:A:38:ASN:HD21	1:A:41:GLU:H	1.53	0.50
1:A:767:GLN:CG	1:A:768:MET:N	2.75	0.50
1:B:134:LEU:N	1:B:134:LEU:CD1	2.73	0.50
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.24	0.50
1:D:770:ILE:O	1:D:770:ILE:HG22	2.10	0.50
1:D:881:ARG:HD3	1:D:987:ASP:CG	2.36	0.50
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.50
1:D:26:ARG:CD	1:D:169:SER:HB3	2.41	0.50
1:A:230:ARG:HH11	1:A:230:ARG:CG	2.24	0.50
1:A:542:MET:HA	1:A:604:ASN:HA	1.92	0.50
1:B:403:ASP:CG	1:B:451:PRO:HD2	2.36	0.50
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.47	0.50
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.47	0.50
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.47	0.50
1:B:65:ALA:HB1	1:B:66:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:882:ILE:O	1:B:882:ILE:HG22	2.12	0.50
1:A:652:LEU:HD12	1:A:699:ARG:O	2.12	0.50
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.47	0.50
1:B:230:ARG:HH11	1:B:230:ARG:CG	2.24	0.50
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.47	0.50
1:B:433:LEU:O	1:B:437:SER:HB3	2.12	0.50
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.50
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.50
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.47	0.50
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.50
1:C:360:HIS:CG	1:C:361:PRO:HD2	2.47	0.50
1:C:767:GLN:CG	1:C:768:MET:N	2.75	0.50
1:B:894:ARG:HD3	1:B:919:ASP:OD1	2.11	0.50
1:D:95:TYR:CD1	1:D:95:TYR:N	2.79	0.50
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.47	0.50
1:D:403:ASP:CG	1:D:451:PRO:HD2	2.36	0.50
1:D:894:ARG:HD3	1:D:919:ASP:OD1	2.11	0.50
1:C:433:LEU:O	1:C:437:SER:HB3	2.12	0.49
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.49
1:A:148:SER:HB3	1:A:190:ARG:O	2.10	0.49
1:C:30:HIS:ND1	1:C:31:PRO:O	2.40	0.49
1:C:254:LEU:O	1:C:255:ARG:NH1	2.44	0.49
1:C:822:LEU:HD12	1:C:824:GLN:H	1.76	0.49
1:C:881:ARG:HD3	1:C:987:ASP:CG	2.36	0.49
1:A:12:GLN:HG3	1:A:13:ARG:N	2.27	0.49
1:A:77:ASP:C	1:A:78:LEU:HD23	2.37	0.49
1:A:638:VAL:O	1:A:677:LYS:HA	2.12	0.49
1:A:822:LEU:HD12	1:A:824:GLN:H	1.76	0.49
1:B:767:GLN:CG	1:B:768:MET:N	2.75	0.49
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.25	0.49
1:D:254:LEU:C	1:D:255:ARG:HG2	2.36	0.49
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.48	0.49
1:A:763:GLY:CA	1:A:822:LEU:HD21	2.42	0.49
1:C:77:ASP:C	1:C:78:LEU:HD23	2.37	0.49
1:D:638:VAL:O	1:D:677:LYS:HA	2.12	0.49
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.47	0.49
1:D:882:ILE:O	1:D:882:ILE:HG22	2.12	0.49
1:A:65:ALA:HB1	1:A:66:PRO:CD	2.41	0.49
1:A:272:ALA:HB1	1:A:273:PRO:CD	2.43	0.49
1:B:638:VAL:O	1:B:677:LYS:HA	2.12	0.49
1:B:763:GLY:CA	1:B:822:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TRP:HA	1:C:157:ARG:O	2.13	0.49
1:C:272:ALA:HB1	1:C:273:PRO:CD	2.43	0.49
1:C:595:THR:HG23	1:C:596:PRO:CA	2.43	0.49
1:C:638:VAL:O	1:C:677:LYS:HA	2.12	0.49
1:C:770:ILE:O	1:C:770:ILE:HG22	2.10	0.49
1:D:12:GLN:HG3	1:D:13:ARG:N	2.27	0.49
1:D:595:THR:HG23	1:D:596:PRO:CA	2.43	0.49
1:A:95:TYR:CD1	1:A:95:TYR:N	2.79	0.49
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.48	0.49
1:A:153:TRP:HA	1:A:157:ARG:O	2.13	0.49
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.48	0.49
1:B:153:TRP:HA	1:B:157:ARG:O	2.13	0.49
1:B:652:LEU:HD12	1:B:699:ARG:O	2.12	0.49
1:A:110:ASN:O	1:A:113:PHE:N	2.39	0.49
1:A:200:GLN:OE1	1:A:200:GLN:N	2.44	0.49
1:C:660:GLY:O	1:C:662:PRO:HD3	2.13	0.49
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.42	0.49
1:D:660:GLY:O	1:D:662:PRO:HD3	2.13	0.49
1:A:130:ASP:OD2	1:A:132:SER:OG	2.28	0.49
1:A:660:GLY:O	1:A:662:PRO:HD3	2.13	0.49
1:B:12:GLN:HG3	1:B:13:ARG:N	2.27	0.49
1:B:77:ASP:C	1:B:78:LEU:HD23	2.37	0.49
1:C:143:PHE:CD1	1:C:143:PHE:N	2.81	0.49
1:D:360:HIS:CG	1:D:361:PRO:HD2	2.47	0.49
1:D:767:GLN:CG	1:D:768:MET:N	2.75	0.49
1:C:130:ASP:OD2	1:C:132:SER:OG	2.28	0.49
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.48	0.49
1:C:830:LEU:HD22	1:C:835:LEU:HB2	1.95	0.49
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.41	0.49
1:C:938:ARG:NH2	3:C:4307:HOH:O	2.45	0.49
1:D:77:ASP:C	1:D:78:LEU:HD23	2.38	0.49
1:D:652:LEU:HD12	1:D:699:ARG:O	2.12	0.49
1:D:920:LEU:HB3	1:D:921:PRO:CD	2.39	0.49
1:B:595:THR:HG23	1:B:596:PRO:CA	2.43	0.49
1:B:938:ARG:NH2	3:B:4267:HOH:O	2.45	0.49
1:C:134:LEU:N	1:C:134:LEU:CD1	2.73	0.49
1:D:763:GLY:CA	1:D:822:LEU:HD21	2.42	0.49
1:D:836:ILE:HG22	1:D:837:THR:N	2.26	0.49
1:A:143:PHE:N	1:A:143:PHE:CD1	2.81	0.48
1:A:433:LEU:O	1:A:437:SER:HB3	2.12	0.48
1:A:651:LEU:HD12	1:A:651:LEU:HA	1.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:HIS:O	1:B:648:ASP:N	2.47	0.48
1:B:708:TRP:CE3	1:B:709:SER:HB3	2.48	0.48
1:C:835:LEU:CD1	1:C:857:ARG:HB2	2.43	0.48
1:C:836:ILE:HG22	1:C:837:THR:N	2.26	0.48
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.48	0.48
1:C:882:ILE:O	1:C:882:ILE:HG22	2.12	0.48
1:A:787:ALA:HA	1:A:788:PRO:HD3	1.66	0.48
1:C:12:GLN:HG3	1:C:13:ARG:N	2.27	0.48
1:C:652:LEU:HD12	1:C:699:ARG:O	2.12	0.48
1:D:143:PHE:N	1:D:143:PHE:CD1	2.81	0.48
1:D:153:TRP:HA	1:D:157:ARG:O	2.13	0.48
1:A:835:LEU:CD1	1:A:857:ARG:HB2	2.43	0.48
1:B:597:ASN:ND2	1:B:599:ARG:N	2.48	0.48
1:B:651:LEU:HD12	1:B:651:LEU:HA	1.46	0.48
1:B:660:GLY:O	1:B:662:PRO:HD3	2.13	0.48
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.44	0.48
1:B:835:LEU:CD1	1:B:857:ARG:HB2	2.43	0.48
1:D:433:LEU:O	1:D:437:SER:HB3	2.12	0.48
1:B:748:CYS:C	1:B:749:ILE:HD12	2.39	0.48
1:D:646:HIS:O	1:D:648:ASP:N	2.47	0.48
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.48
1:C:26:ARG:HD3	1:C:169:SER:HB3	1.96	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.65	0.48
1:C:257:THR:OG1	1:C:316:HIS:HE1	1.97	0.48
1:D:651:LEU:HD12	1:D:651:LEU:HA	1.46	0.48
1:A:595:THR:HG23	1:A:596:PRO:CA	2.43	0.48
1:A:651:LEU:HD23	1:A:653[A]:HIS:HE1	1.79	0.48
1:B:257:THR:OG1	1:B:316:HIS:HE1	1.97	0.48
1:C:646:HIS:O	1:C:648:ASP:N	2.46	0.48
1:C:651:LEU:HD23	1:C:653[A]:HIS:HE1	1.79	0.48
1:D:3:ILE:C	1:D:5:ASP:H	2.22	0.48
1:D:26:ARG:HD3	1:D:169:SER:HB3	1.96	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.40	0.48
1:D:251:ARG:HG2	1:D:251:ARG:HH11	1.79	0.48
1:A:3:ILE:C	1:A:5:ASP:H	2.22	0.48
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.49	0.48
1:A:513:PRO:O	1:A:514:ALA:HB3	2.14	0.48
1:A:597:ASN:ND2	1:A:599:ARG:N	2.48	0.48
1:A:599:ARG:HD2	1:A:600:GLN:OE1	2.14	0.48
1:A:646:HIS:O	1:A:648:ASP:N	2.46	0.48
1:A:894:ARG:NH1	1:A:919:ASP:OD1	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:TRP:HE1	1:C:604:ASN:HD22	1.62	0.48
1:C:599:ARG:HD2	1:C:600:GLN:OE1	2.14	0.48
1:C:856:TYR:HD2	1:C:864:MET:CE	2.27	0.48
1:D:748:CYS:C	1:D:749:ILE:HD12	2.39	0.48
1:A:257:THR:OG1	1:A:316:HIS:HE1	1.97	0.48
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.43	0.48
1:B:26:ARG:HD3	1:B:169:SER:HB3	1.96	0.48
1:B:143:PHE:CD1	1:B:143:PHE:N	2.81	0.48
1:B:147:ASN:HA	1:B:148:SER:HA	1.65	0.48
1:C:668:VAL:CG1	1:C:669:PRO:HD2	2.44	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:A:30:HIS:ND1	1:A:31:PRO:O	2.40	0.47
1:A:748:CYS:C	1:A:749:ILE:HD12	2.39	0.47
1:B:67:GLU:HG2	1:B:67:GLU:H	1.15	0.47
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.49	0.47
1:B:970:THR:CG2	1:B:975:LEU:HB2	2.44	0.47
1:C:573:GLN:HB2	1:C:602:CYS:O	2.14	0.47
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.49	0.47
1:D:910:LEU:HD12	1:D:910:LEU:C	2.39	0.47
1:A:210:ARG:NH1	1:A:358:GLU:OE1	2.47	0.47
1:A:668:VAL:HA	1:A:669:PRO:HD3	1.66	0.47
1:A:701:VAL:CG1	1:A:702:GLN:N	2.77	0.47
1:C:3:ILE:C	1:C:5:ASP:H	2.22	0.47
1:C:742:THR:CG2	1:C:743:SER:N	2.77	0.47
1:D:835:LEU:CD1	1:D:857:ARG:HB2	2.43	0.47
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:B:910:LEU:C	1:B:910:LEU:HD12	2.39	0.47
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.49	0.47
1:C:210:ARG:NH1	1:C:358:GLU:OE1	2.47	0.47
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.62	0.47
1:D:668:VAL:CG1	1:D:669:PRO:HD2	2.44	0.47
1:D:734:SER:HB2	1:D:860:GLY:HA3	1.95	0.47
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.62	0.47
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.15	0.47
1:A:830:LEU:HD22	1:A:835:LEU:HB2	1.95	0.47
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.48	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
1:C:910:LEU:C	1:C:910:LEU:HD12	2.39	0.47
1:D:210:ARG:NH1	1:D:358:GLU:OE1	2.47	0.47
1:D:599:ARG:HD2	1:D:600:GLN:OE1	2.14	0.47
1:D:856:TYR:HD2	1:D:864:MET:CE	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HA	1:A:19:PRO:HD3	1.56	0.47
1:A:423:MET:HB2	1:D:282:ARG:CG	2.43	0.47
1:A:856:TYR:HD2	1:A:864:MET:CE	2.27	0.47
1:A:970:THR:CG2	1:A:975:LEU:HB2	2.44	0.47
1:B:251:ARG:HG2	1:B:251:ARG:HH11	1.79	0.47
1:C:701:VAL:CG1	1:C:702:GLN:N	2.77	0.47
1:D:635:THR:OG1	1:D:681:GLU:HG3	2.15	0.47
1:D:651:LEU:HD23	1:D:653[A]:HIS:HE1	1.79	0.47
1:A:26:ARG:HD3	1:A:169:SER:HB3	1.96	0.47
1:A:658:LEU:O	1:A:659:ASP:C	2.54	0.47
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.97	0.47
1:A:882:ILE:HG22	1:A:882:ILE:O	2.12	0.47
1:B:110:ASN:O	1:B:113:PHE:N	2.39	0.47
1:B:651:LEU:HD23	1:B:653[A]:HIS:HE1	1.79	0.47
1:B:780:LEU:HA	1:B:886:CYS:HB3	1.97	0.47
1:B:856:TYR:HD2	1:B:864:MET:CE	2.27	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:D:780:LEU:HA	1:D:886:CYS:HB3	1.97	0.47
1:A:573:GLN:HB2	1:A:602:CYS:O	2.14	0.47
1:B:599:ARG:HD2	1:B:600:GLN:OE1	2.14	0.47
1:B:701:VAL:CG1	1:B:702:GLN:N	2.78	0.47
1:C:214:LEU:HD23	1:C:214:LEU:HA	1.61	0.47
1:C:513:PRO:O	1:C:514:ALA:HB3	2.14	0.47
1:C:661:LYS:HA	1:C:662:PRO:HD2	1.71	0.47
1:C:970:THR:CG2	1:C:975:LEU:HB2	2.44	0.47
1:D:257:THR:OG1	1:D:316:HIS:HE1	1.97	0.47
1:D:272:ALA:HB1	1:D:273:PRO:CD	2.43	0.47
1:D:830:LEU:HD22	1:D:835:LEU:HB2	1.95	0.47
1:D:938:ARG:NH2	3:D:4279:HOH:O	2.45	0.47
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.44	0.47
1:A:80:GLU:OE2	1:A:80:GLU:N	2.29	0.47
1:A:261:TRP:CD1	1:A:261:TRP:N	2.83	0.47
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.62	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.77	0.47
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.47
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.47	0.47
1:A:251:ARG:HG2	1:A:251:ARG:HH11	1.79	0.47
1:A:849:LEU:N	1:A:849:LEU:HD23	2.30	0.47
1:A:910:LEU:HD12	1:A:910:LEU:C	2.39	0.47
1:B:3:ILE:C	1:B:5:ASP:H	2.22	0.47
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:830:LEU:HD22	1:B:835:LEU:HB2	1.95	0.47
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.50	0.47
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.50	0.46
1:B:200:GLN:OE1	1:B:200:GLN:N	2.44	0.46
1:B:272:ALA:HB1	1:B:273:PRO:CD	2.43	0.46
1:D:441:THR:HG22	1:D:474:TRP:CH2	2.50	0.46
1:D:573:GLN:HB2	1:D:602:CYS:O	2.14	0.46
1:D:701:VAL:CG1	1:D:702:GLN:N	2.77	0.46
1:B:95:TYR:N	1:B:95:TYR:CD1	2.79	0.46
1:B:513:PRO:O	1:B:514:ALA:HB3	2.14	0.46
1:B:573:GLN:HB2	1:B:602:CYS:O	2.14	0.46
1:C:635:THR:OG1	1:C:681:GLU:HG3	2.15	0.46
1:D:230:ARG:HH11	1:D:230:ARG:HG2	1.81	0.46
1:D:234:ASP:O	1:D:235:PHE:HB2	2.15	0.46
1:A:230:ARG:HH11	1:A:230:ARG:HG2	1.81	0.46
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.97	0.46
1:A:429:ASP:OD1	1:A:431[A]:ARG:HG3	2.16	0.46
1:C:429:ASP:OD1	1:C:431[A]:ARG:HG3	2.16	0.46
1:D:834:VAL:CG1	1:D:835:LEU:N	2.79	0.46
1:A:11:LEU:HD11	1:A:187:MET:HE1	1.98	0.46
1:A:13:ARG:NH1	1:D:13:ARG:NH1	2.63	0.46
1:B:226:HIS:CD2	1:B:226:HIS:N	2.83	0.46
1:B:429:ASP:OD1	1:B:431[A]:ARG:HG3	2.16	0.46
1:B:429:ASP:HA	1:B:430:PRO:HD3	1.82	0.46
1:B:873:ALA:O	1:B:876:THR:HG22	2.16	0.46
1:C:226:HIS:N	1:C:226:HIS:CD2	2.83	0.46
1:C:227:VAL:HG12	1:C:228:ALA:N	2.31	0.46
1:C:1018:LEU:HD23	1:C:1018:LEU:HA	1.53	0.46
1:D:261:TRP:CD1	1:D:261:TRP:N	2.83	0.46
1:A:166:ARG:HG3	1:A:392:TYR:CG	2.51	0.46
1:B:234:ASP:O	1:B:235:PHE:HB2	2.15	0.46
1:B:441:THR:HG22	1:B:474:TRP:CH2	2.50	0.46
1:C:84:VAL:HG13	1:C:85:VAL:N	2.31	0.46
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.80	0.46
1:D:200:GLN:OE1	1:D:200:GLN:N	2.44	0.46
1:D:878:HIS:HA	1:D:879:PRO:HD3	1.69	0.46
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.97	0.46
1:A:742:THR:CG2	1:A:743:SER:N	2.77	0.46
1:B:166:ARG:HG3	1:B:392:TYR:CG	2.51	0.46
1:B:261:TRP:CD1	1:B:261:TRP:N	2.83	0.46
1:C:261:TRP:CD1	1:C:261:TRP:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.46
1:C:620:ALA:O	1:C:624:GLN:HG3	2.16	0.46
1:D:597:ASN:ND2	1:D:599:ARG:N	2.48	0.46
1:D:630:ARG:HE	1:D:630:ARG:HB3	1.31	0.46
1:A:436:MET:HE1	1:A:467:ASN:HD22	1.81	0.46
1:A:737:ILE:HA	1:A:738:PRO:HD3	1.78	0.46
1:B:620:ALA:O	1:B:624:GLN:HG3	2.16	0.46
1:B:635:THR:OG1	1:B:681:GLU:HG3	2.15	0.46
1:B:849:LEU:N	1:B:849:LEU:HD23	2.30	0.46
1:B:945:ASN:OD1	1:B:950:GLN:HB2	2.16	0.46
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.51	0.46
1:D:11:LEU:HD11	1:D:187:MET:HE1	1.98	0.46
1:D:227:VAL:HG12	1:D:228:ALA:N	2.31	0.46
1:D:873:ALA:O	1:D:876:THR:HG22	2.16	0.46
1:A:679:LEU:HA	1:A:679:LEU:HD23	1.13	0.46
1:B:111:PRO:HA	1:B:112:PRO:HA	1.57	0.46
1:B:369:GLU:O	1:B:373:VAL:HG23	2.16	0.46
1:B:742:THR:CG2	1:B:743:SER:N	2.77	0.46
1:B:834:VAL:CG1	1:B:835:LEU:N	2.79	0.46
1:C:141:ILE:CG1	1:C:142:ILE:N	2.79	0.46
1:D:127:PHE:HE2	1:D:184:LEU:HG	1.80	0.46
1:D:316:HIS:HB2	1:D:321:THR:O	2.16	0.46
1:D:701:VAL:O	1:D:703:PRO:HD3	2.16	0.46
1:D:894:ARG:NH2	1:D:921:PRO:HD3	2.31	0.46
1:B:701:VAL:O	1:B:703:PRO:HD3	2.16	0.46
1:C:441:THR:HG22	1:C:474:TRP:CH2	2.50	0.46
1:D:870:VAL:CG1	1:D:871:GLU:N	2.79	0.46
1:A:141:ILE:CG1	1:A:142:ILE:N	2.79	0.46
1:A:369:GLU:O	1:A:373:VAL:HG23	2.16	0.46
1:A:894:ARG:NH2	1:A:921:PRO:HD3	2.31	0.46
1:B:168:PRO:O	1:B:442:ARG:NH2	2.48	0.46
1:B:870:VAL:CG1	1:B:871:GLU:N	2.79	0.46
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.51	0.46
1:C:420:MET:HB3	1:C:420:MET:HE3	1.62	0.46
1:D:84:VAL:HG13	1:D:85:VAL:N	2.31	0.46
1:A:234:ASP:O	1:A:235:PHE:HB2	2.15	0.45
1:B:3:ILE:O	1:B:3:ILE:HD12	2.16	0.45
1:B:316:HIS:HB2	1:B:321:THR:O	2.16	0.45
1:C:230:ARG:HH11	1:C:230:ARG:HG2	1.81	0.45
1:C:234:ASP:O	1:C:235:PHE:HB2	2.15	0.45
1:C:834:VAL:CG1	1:C:835:LEU:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.52	0.45
1:A:3:ILE:HD12	1:A:3:ILE:O	2.16	0.45
1:A:38:ASN:ND2	1:A:41:GLU:HG3	2.32	0.45
1:A:226:HIS:CD2	1:A:226:HIS:N	2.83	0.45
1:A:441:THR:HG22	1:A:474:TRP:CH2	2.50	0.45
1:A:938:ARG:NH2	3:A:4279:HOH:O	2.45	0.45
1:B:38:ASN:ND2	1:B:41:GLU:HG3	2.31	0.45
1:B:80:GLU:OE2	1:B:80:GLU:N	2.29	0.45
1:B:436:MET:HE1	1:B:467:ASN:HD22	1.81	0.45
1:B:1018:LEU:HD23	1:B:1018:LEU:HA	1.53	0.45
1:C:242:ALA:O	1:C:290:THR:HA	2.16	0.45
1:C:701:VAL:O	1:C:703:PRO:HD3	2.16	0.45
1:D:226:HIS:N	1:D:226:HIS:CD2	2.83	0.45
1:D:369:GLU:O	1:D:373:VAL:HG23	2.16	0.45
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.52	0.45
1:D:945:ASN:OD1	1:D:950:GLN:HB2	2.16	0.45
1:A:227:VAL:HG12	1:A:228:ALA:N	2.31	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.16	0.45
1:A:834:VAL:CG1	1:A:835:LEU:N	2.79	0.45
1:A:1018:LEU:HD23	1:A:1018:LEU:HA	1.53	0.45
1:B:11:LEU:HD11	1:B:187:MET:HE1	1.98	0.45
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.45
1:B:287:ASP:CG	1:C:425:ARG:HH22	2.23	0.45
1:B:832:ASP:OD1	1:B:832:ASP:N	2.50	0.45
1:C:230:ARG:CG	1:C:230:ARG:NH1	2.79	0.45
1:C:369:GLU:O	1:C:373:VAL:HG23	2.16	0.45
1:D:531:ARG:CB	1:D:532:PRO:HD2	2.46	0.45
1:A:84:VAL:HG13	1:A:85:VAL:N	2.31	0.45
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.61	0.45
1:A:242:ALA:O	1:A:290:THR:HA	2.16	0.45
1:A:524:LEU:HB2	3:A:4198:HOH:O	2.16	0.45
1:A:620:ALA:O	1:A:624:GLN:HG3	2.16	0.45
1:B:141:ILE:CG1	1:B:142:ILE:N	2.79	0.45
1:B:242:ALA:O	1:B:290:THR:HA	2.16	0.45
1:B:352:ARG:O	1:B:385:ASN:HB2	2.17	0.45
1:B:531:ARG:CB	1:B:532:PRO:HD2	2.46	0.45
1:B:920:LEU:HB3	1:B:921:PRO:CD	2.39	0.45
1:B:925:MET:HE3	1:B:925:MET:HB3	1.82	0.45
1:C:67:GLU:HG2	1:C:67:GLU:H	1.15	0.45
1:C:80:GLU:OE2	1:C:80:GLU:N	2.29	0.45
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:873:ALA:O	1:C:876:THR:HG22	2.16	0.45
1:D:3:ILE:HD12	1:D:3:ILE:O	2.16	0.45
1:D:63:PHE:HB3	1:D:64:PRO:CD	2.45	0.45
1:D:620:ALA:O	1:D:624:GLN:HG3	2.16	0.45
1:A:352:ARG:O	1:A:385:ASN:HB2	2.17	0.45
1:A:559:TYR:HA	1:A:560:PRO:HD2	1.85	0.45
1:A:762:SER:C	1:A:822:LEU:HD23	2.42	0.45
1:A:915:PHE:O	1:A:916:ASP:HB2	2.17	0.45
1:B:579:ASP:CG	1:B:583:ASN:HB2	2.42	0.45
1:B:679:LEU:HA	1:B:679:LEU:HD23	1.13	0.45
1:C:38:ASN:ND2	1:C:41:GLU:HG3	2.32	0.45
1:C:63:PHE:HB3	1:C:64:PRO:CD	2.45	0.45
1:C:531:ARG:CB	1:C:532:PRO:HD2	2.46	0.45
1:C:762:SER:C	1:C:822:LEU:HD23	2.42	0.45
1:A:588:TYR:O	1:A:589:GLY:C	2.59	0.45
1:B:227:VAL:HG12	1:B:228:ALA:N	2.31	0.45
1:B:287:ASP:OD2	1:C:425:ARG:NH2	2.50	0.45
1:B:650:GLU:HA	1:B:701:VAL:O	2.17	0.45
1:B:762:SER:C	1:B:822:LEU:HD23	2.42	0.45
1:D:111:PRO:HA	1:D:112:PRO:HA	1.56	0.45
1:D:166:ARG:HG3	1:D:392:TYR:CG	2.51	0.45
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.45
1:A:945:ASN:OD1	1:A:950:GLN:HB2	2.16	0.45
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.95	0.45
1:B:878:HIS:HA	1:B:879:PRO:HD3	1.69	0.45
1:C:128:ASN:HD22	1:C:180:GLY:C	2.25	0.45
1:C:524:LEU:HB2	3:C:4262:HOH:O	2.16	0.45
1:C:579:ASP:CG	1:C:583:ASN:HB2	2.42	0.45
1:C:650:GLU:HA	1:C:701:VAL:O	2.17	0.45
1:D:38:ASN:ND2	1:D:41:GLU:HG3	2.32	0.45
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.80	0.45
1:D:757:GLN:HG2	1:D:758:PHE:N	2.31	0.45
1:A:128:ASN:HD22	1:A:180:GLY:C	2.25	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.16	0.45
1:B:84:VAL:HG13	1:B:85:VAL:N	2.31	0.45
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.99	0.45
1:B:90:TRP:C	1:B:90:TRP:CD1	2.95	0.45
1:B:894:ARG:NH2	1:B:921:PRO:HD3	2.31	0.45
1:C:3:ILE:HD12	1:C:3:ILE:O	2.16	0.45
1:C:11:LEU:HD11	1:C:187:MET:HE1	1.98	0.45
1:C:730:LEU:H	1:C:730:LEU:HG	1.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:ASP:OD1	1:C:832:ASP:N	2.49	0.45
1:D:143:PHE:O	1:D:168:PRO:HA	2.17	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.80	0.45
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.69	0.45
1:B:255:ARG:NH1	1:B:255:ARG:CG	2.79	0.45
1:B:420:MET:HB3	1:B:420:MET:HE3	1.62	0.45
1:B:915:PHE:O	1:B:916:ASP:HB2	2.17	0.45
1:C:849:LEU:N	1:C:849:LEU:HD23	2.30	0.45
1:D:429:ASP:OD1	1:D:431[A]:ARG:HG3	2.16	0.45
1:D:524:LEU:HB2	3:D:4198:HOH:O	2.16	0.45
1:A:90:TRP:CD1	1:A:90:TRP:C	2.95	0.45
1:A:399:TYR:CD1	1:A:399:TYR:N	2.85	0.45
1:B:128:ASN:HD22	1:B:180:GLY:C	2.25	0.45
1:B:230:ARG:HH11	1:B:230:ARG:HG2	1.81	0.45
1:B:599:ARG:HB2	1:B:600:GLN:H	1.54	0.45
1:C:945:ASN:OD1	1:C:950:GLN:HB2	2.16	0.45
1:D:441:THR:HG22	1:D:474:TRP:CZ3	2.52	0.45
1:D:832:ASP:OD1	1:D:832:ASP:N	2.50	0.45
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.99	0.44
1:B:38:ASN:ND2	1:B:41:GLU:N	2.48	0.44
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.99	0.44
1:C:118:ASN:HA	1:C:119:PRO:HD2	1.61	0.44
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.44
1:C:352:ARG:O	1:C:385:ASN:HB2	2.17	0.44
1:C:399:TYR:CD1	1:C:399:TYR:N	2.85	0.44
1:D:43:ARG:HD2	1:D:261:TRP:CD2	2.52	0.44
1:D:230:ARG:CG	1:D:230:ARG:NH1	2.79	0.44
1:D:352:ARG:O	1:D:385:ASN:HB2	2.17	0.44
1:D:1018:LEU:HD23	1:D:1018:LEU:HA	1.53	0.44
1:A:78:LEU:HB3	1:A:80:GLU:OE2	2.18	0.44
1:A:531:ARG:CB	1:A:532:PRO:HD2	2.46	0.44
1:A:645:ARG:NH2	1:A:650:GLU:CD	2.76	0.44
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.52	0.44
1:B:136:GLU:O	1:B:216:HIS:HE1	2.01	0.44
1:C:18:ASN:HA	1:C:19:PRO:HD3	1.56	0.44
1:C:166:ARG:HG3	1:C:392:TYR:CG	2.51	0.44
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.44
1:C:668:VAL:HA	1:C:669:PRO:HD3	1.66	0.44
1:C:894:ARG:NH2	1:C:921:PRO:HD3	2.31	0.44
1:D:141:ILE:CG1	1:D:142:ILE:N	2.79	0.44
1:D:650:GLU:HA	1:D:701:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:CG	1:A:230:ARG:NH1	2.79	0.44
1:A:708:TRP:CD1	1:A:708:TRP:N	2.85	0.44
1:A:870:VAL:CG1	1:A:871:GLU:N	2.79	0.44
1:A:989:PHE:CD1	1:A:989:PHE:N	2.86	0.44
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.52	0.44
1:B:786:ARG:HH11	1:B:990:HIS:CE1	2.36	0.44
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.52	0.44
1:C:316:HIS:HB2	1:C:321:THR:O	2.16	0.44
1:C:870:VAL:CG1	1:C:871:GLU:N	2.79	0.44
1:C:881:ARG:HD3	1:C:987:ASP:OD2	2.17	0.44
1:D:658:LEU:HD23	1:D:661:LYS:HZ3	1.83	0.44
1:D:849:LEU:N	1:D:849:LEU:HD23	2.30	0.44
1:A:136:GLU:O	1:A:216:HIS:HE1	2.01	0.44
1:A:579:ASP:CG	1:A:583:ASN:HB2	2.42	0.44
1:A:786:ARG:HH11	1:A:990:HIS:CE1	2.36	0.44
1:B:143:PHE:O	1:B:168:PRO:HA	2.17	0.44
1:C:395:HIS:CG	1:C:396:PRO:HD2	2.53	0.44
1:C:708:TRP:CD1	1:C:708:TRP:N	2.85	0.44
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.99	0.44
1:D:708:TRP:CD1	1:D:708:TRP:N	2.85	0.44
1:A:63:PHE:CD1	1:A:63:PHE:N	2.86	0.44
1:A:650:GLU:HA	1:A:701:VAL:O	2.17	0.44
1:B:441:THR:HG22	1:B:474:TRP:CZ3	2.52	0.44
1:B:947:GLY:HA3	1:B:948:PRO:HD2	1.89	0.44
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.51	0.44
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.78	0.44
1:C:989:PHE:CD1	1:C:989:PHE:N	2.86	0.44
1:D:78:LEU:HB3	1:D:80:GLU:OE2	2.18	0.44
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.00	0.44
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.61	0.44
1:A:168:PRO:O	1:A:442:ARG:NH2	2.48	0.44
1:A:395:HIS:HA	1:A:396:PRO:HD3	1.83	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.18	0.44
1:C:79:PRO:HB2	1:C:80:GLU:HG3	2.00	0.44
1:C:751:LEU:C	1:C:751:LEU:HD23	2.43	0.44
1:C:957:PHE:CD1	1:C:957:PHE:C	2.95	0.44
1:D:18:ASN:HA	1:D:19:PRO:HD3	1.56	0.44
1:D:242:ALA:O	1:D:290:THR:HA	2.16	0.44
1:D:588:TYR:O	1:D:589:GLY:C	2.59	0.44
1:A:645:ARG:NH2	1:A:650:GLU:OE1	2.51	0.44
1:A:751:LEU:C	1:A:751:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:TYR:CD1	1:B:399:TYR:N	2.85	0.44
1:B:524:LEU:HB2	3:B:4222:HOH:O	2.16	0.44
1:C:63:PHE:CD1	1:C:63:PHE:N	2.86	0.44
1:C:90:TRP:CD1	1:C:90:TRP:C	2.95	0.44
1:D:128:ASN:HD22	1:D:180:GLY:C	2.25	0.44
1:D:136:GLU:O	1:D:216:HIS:HE1	2.01	0.44
1:B:30:HIS:CE1	1:B:33:PHE:CD1	3.06	0.44
1:B:78:LEU:HB3	1:B:80:GLU:OE2	2.18	0.44
1:C:441:THR:HG22	1:C:474:TRP:CZ3	2.52	0.44
1:D:694:LEU:HD12	1:D:694:LEU:HA	1.82	0.44
1:D:762:SER:C	1:D:822:LEU:HD23	2.42	0.44
1:A:441:THR:HG22	1:A:474:TRP:CZ3	2.52	0.44
1:A:995:GLY:O	1:A:996:ASP:C	2.61	0.44
1:B:957:PHE:CD1	1:B:957:PHE:C	2.95	0.44
1:C:136:GLU:O	1:C:216:HIS:HE1	2.01	0.44
1:C:588:TYR:O	1:C:589:GLY:C	2.59	0.44
1:D:134:LEU:N	1:D:134:LEU:CD1	2.73	0.44
1:D:989:PHE:CD1	1:D:989:PHE:N	2.86	0.44
1:A:316:HIS:HB2	1:A:321:THR:O	2.16	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.43
1:A:832:ASP:OD1	1:A:832:ASP:N	2.50	0.43
1:B:881:ARG:HD3	1:B:987:ASP:OD2	2.18	0.43
1:C:145:GLY:HA3	1:C:210:ARG:HG3	2.00	0.43
1:C:786:ARG:HH11	1:C:990:HIS:CE1	2.36	0.43
1:C:915:PHE:O	1:C:916:ASP:HB2	2.17	0.43
1:D:90:TRP:CD1	1:D:90:TRP:C	2.95	0.43
1:D:751:LEU:HD23	1:D:751:LEU:C	2.43	0.43
1:A:30:HIS:CE1	1:A:33:PHE:CD1	3.06	0.43
1:A:227:VAL:CG1	1:A:240:LEU:HD11	2.48	0.43
1:B:630:ARG:HE	1:B:630:ARG:HB3	1.31	0.43
1:B:645:ARG:NH2	1:B:650:GLU:CD	2.76	0.43
1:B:645:ARG:NH2	1:B:650:GLU:OE1	2.51	0.43
1:B:647:SER:HG	1:B:672:VAL:H	1.65	0.43
1:B:989:PHE:CD1	1:B:989:PHE:N	2.86	0.43
1:C:255:ARG:NH1	1:C:255:ARG:CG	2.79	0.43
1:C:597:ASN:ND2	1:C:599:ARG:N	2.48	0.43
1:D:30:HIS:CE1	1:D:33:PHE:CD1	3.06	0.43
1:D:79:PRO:HB2	1:D:80:GLU:HG3	2.00	0.43
1:D:915:PHE:O	1:D:916:ASP:HB2	2.17	0.43
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.52	0.43
1:A:78:LEU:HA	1:A:79:PRO:HD2	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:THR:CG2	1:A:743:SER:H	2.31	0.43
1:B:395:HIS:CG	1:B:396:PRO:HD2	2.53	0.43
1:B:588:TYR:O	1:B:589:GLY:C	2.59	0.43
1:C:634:GLN:NE2	1:C:682:LEU:O	2.51	0.43
1:D:63:PHE:N	1:D:63:PHE:CD1	2.86	0.43
1:D:145:GLY:HA3	1:D:210:ARG:HG3	2.00	0.43
1:D:786:ARG:HH11	1:D:990:HIS:CE1	2.36	0.43
1:A:285:TYR:OH	1:D:424:ASN:HB3	2.19	0.43
1:A:881:ARG:HD3	1:A:987:ASP:OD2	2.17	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:B:433:LEU:HB3	1:B:434:PRO:HD3	2.00	0.43
1:B:682:LEU:HA	1:B:683:PRO:HD3	1.91	0.43
1:C:168:PRO:O	1:C:442:ARG:NH2	2.48	0.43
1:C:225:PHE:HA	1:C:243:GLU:O	2.19	0.43
1:C:657:ALA:O	1:C:694:LEU:HD12	2.18	0.43
1:D:399:TYR:CD1	1:D:399:TYR:N	2.85	0.43
1:D:881:ARG:HD3	1:D:987:ASP:OD2	2.18	0.43
1:A:67:GLU:HG2	1:A:67:GLU:H	1.15	0.43
1:A:79:PRO:HB2	1:A:80:GLU:HG3	2.00	0.43
1:A:143:PHE:O	1:A:168:PRO:HA	2.17	0.43
1:B:79:PRO:HB2	1:B:80:GLU:HG3	2.00	0.43
1:B:145:GLY:HA3	1:B:210:ARG:HG3	2.00	0.43
1:B:742:THR:CG2	1:B:743:SER:H	2.31	0.43
1:D:429:ASP:HA	1:D:430:PRO:HD3	1.82	0.43
1:D:507:ASP:C	1:D:519:SER:HB2	2.43	0.43
1:D:645:ARG:NH2	1:D:650:GLU:OE1	2.51	0.43
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.84	0.43
1:B:118:ASN:HA	1:B:119:PRO:HD2	1.61	0.43
1:B:657:ALA:O	1:B:694:LEU:HD12	2.18	0.43
1:B:751:LEU:C	1:B:751:LEU:HD23	2.43	0.43
1:C:176:PHE:CD1	1:C:176:PHE:N	2.87	0.43
1:C:217:LYS:HB3	1:C:218:PRO:HD2	2.00	0.43
1:C:482:ARG:HH11	1:C:482:ARG:HD2	1.57	0.43
1:C:878:HIS:HA	1:C:879:PRO:HD3	1.69	0.43
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.39	0.43
1:D:657:ALA:O	1:D:694:LEU:HD12	2.18	0.43
1:A:77:ASP:HA	3:A:4132:HOH:O	2.19	0.43
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.95	0.43
1:A:822:LEU:HD12	1:A:823:LEU:N	2.34	0.43
1:C:30:HIS:CE1	1:C:33:PHE:CD1	3.06	0.43
1:C:114:VAL:HA	1:C:115:PRO:HD3	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:GLN:OE1	1:C:200:GLN:N	2.44	0.43
1:C:429:ASP:HA	1:C:430:PRO:HD3	1.82	0.43
1:C:630:ARG:HE	1:C:630:ARG:HB3	1.31	0.43
1:C:645:ARG:NH2	1:C:650:GLU:OE2	2.45	0.43
1:C:679:LEU:HA	1:C:679:LEU:HD23	1.13	0.43
1:D:395:HIS:CG	1:D:396:PRO:HD2	2.53	0.43
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.66	0.43
1:A:217:LYS:HB3	1:A:218:PRO:HD2	2.00	0.43
1:A:420:MET:HE3	1:A:420:MET:HB3	1.62	0.43
1:A:630:ARG:HE	1:A:630:ARG:HB3	1.31	0.43
1:A:634:GLN:NE2	1:A:682:LEU:O	2.51	0.43
1:A:730:LEU:H	1:A:730:LEU:HG	1.41	0.43
1:B:708:TRP:CD1	1:B:708:TRP:N	2.85	0.43
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.80	0.43
1:D:354:VAL:HG22	1:D:355:ASN:N	2.34	0.43
1:A:105:TYR:HB3	1:A:106:PRO:HD2	2.01	0.43
1:A:251:ARG:HH11	1:A:251:ARG:CG	2.32	0.43
1:A:257:THR:HA	1:A:270:GLY:O	2.19	0.43
1:A:507:ASP:C	1:A:519:SER:HB2	2.44	0.43
1:A:687:GLN:HA	1:A:688:PRO:HD3	1.82	0.43
1:B:227:VAL:CG1	1:B:240:LEU:HD11	2.48	0.43
1:B:251:ARG:HH11	1:B:251:ARG:CG	2.32	0.43
1:B:634:GLN:NE2	1:B:682:LEU:O	2.51	0.43
1:C:734:SER:HB2	1:C:860:GLY:HA3	1.95	0.43
1:D:147:ASN:HA	1:D:148:SER:HA	1.65	0.43
1:D:685:LEU:CB	1:D:686:PRO:HD2	2.38	0.43
1:A:360:HIS:HA	1:A:361:PRO:HD3	1.89	0.43
1:A:570:TRP:CD1	1:A:571:VAL:HG22	2.54	0.43
1:B:30:HIS:ND1	1:B:31:PRO:O	2.40	0.43
1:B:63:PHE:CD1	1:B:63:PHE:N	2.86	0.43
1:B:187:MET:O	1:B:187:MET:HG3	2.19	0.43
1:B:622:HIS:HD2	1:B:625:GLN:OE1	2.02	0.43
1:C:840:HIS:ND1	1:C:840:HIS:N	2.67	0.43
1:D:105:TYR:HB3	1:D:106:PRO:HD2	2.01	0.43
1:D:257:THR:HA	1:D:270:GLY:O	2.19	0.43
1:D:622:HIS:HD2	1:D:625:GLN:OE1	2.02	0.43
1:D:988:GLY:C	1:D:989:PHE:CD1	2.97	0.43
1:A:145:GLY:HA3	1:A:210:ARG:HG3	2.01	0.42
1:A:395:HIS:CG	1:A:396:PRO:HD2	2.53	0.42
1:A:635:THR:HA	1:A:680:ILE:O	2.19	0.42
1:A:822:LEU:HD13	1:A:822:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:HA	3:B:4178:HOH:O	2.19	0.42
1:B:114:VAL:HA	1:B:115:PRO:HD3	1.77	0.42
1:B:257:THR:HA	1:B:270:GLY:O	2.19	0.42
1:C:187:MET:O	1:C:187:MET:HG3	2.19	0.42
1:D:579:ASP:CG	1:D:583:ASN:HB2	2.42	0.42
1:D:634:GLN:NE2	1:D:682:LEU:O	2.51	0.42
1:A:429:ASP:HA	1:A:430:PRO:HD3	1.82	0.42
1:B:507:ASP:C	1:B:519:SER:HB2	2.44	0.42
1:B:570:TRP:CD1	1:B:571:VAL:HG22	2.54	0.42
1:B:787:ALA:HA	1:B:788:PRO:HD3	1.66	0.42
1:C:507:ASP:C	1:C:519:SER:HB2	2.44	0.42
1:C:925:MET:HE3	1:C:925:MET:HB3	1.82	0.42
1:C:988:GLY:C	1:C:989:PHE:CD1	2.97	0.42
1:D:217:LYS:HB3	1:D:218:PRO:HD2	2.00	0.42
1:D:225:PHE:HA	1:D:243:GLU:O	2.19	0.42
1:A:225:PHE:HA	1:A:243:GLU:O	2.19	0.42
1:A:657:ALA:O	1:A:694:LEU:HD12	2.18	0.42
1:B:635:THR:HA	1:B:680:ILE:O	2.19	0.42
1:C:102:ASN:HD22	1:C:102:ASN:C	2.27	0.42
1:C:183:ARG:HH11	1:C:183:ARG:HD3	1.55	0.42
1:C:257:THR:HA	1:C:270:GLY:O	2.19	0.42
1:C:645:ARG:NH2	1:C:650:GLU:CD	2.76	0.42
1:D:187:MET:O	1:D:187:MET:HG3	2.19	0.42
1:D:864:MET:HE3	1:D:864:MET:HB2	1.67	0.42
1:A:622:HIS:HD2	1:A:625:GLN:OE1	2.02	0.42
1:A:988:GLY:C	1:A:989:PHE:CD1	2.97	0.42
1:B:278:ILE:HD12	1:B:278:ILE:HA	1.88	0.42
1:C:124:SER:HA	1:C:184:LEU:O	2.20	0.42
1:C:227:VAL:CG1	1:C:240:LEU:HD11	2.48	0.42
1:C:576:ILE:HD13	1:C:584:PRO:HB2	2.02	0.42
1:C:822:LEU:HD12	1:C:823:LEU:N	2.34	0.42
1:D:479:ASP:HA	1:D:480:PRO:HD2	1.73	0.42
1:A:38:ASN:ND2	1:A:38:ASN:C	2.77	0.42
1:A:102:ASN:C	1:A:102:ASN:HD22	2.27	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:A:282:ARG:NH1	1:D:418:HIS:O	2.52	0.42
1:A:354:VAL:HG22	1:A:355:ASN:N	2.34	0.42
1:A:925:MET:HE3	1:A:925:MET:HB3	1.82	0.42
1:B:38:ASN:ND2	1:B:38:ASN:C	2.77	0.42
1:B:52[A]:ARG:HH11	1:B:52[A]:ARG:HD3	1.65	0.42
1:B:737:ILE:HA	1:B:738:PRO:HD3	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:635:THR:HA	1:C:680:ILE:O	2.19	0.42
1:D:102:ASN:C	1:D:102:ASN:HD22	2.27	0.42
1:D:576:ILE:HD13	1:D:584:PRO:HB2	2.02	0.42
1:A:187:MET:O	1:A:187:MET:HG3	2.19	0.42
1:A:255:ARG:NH1	1:A:255:ARG:CG	2.79	0.42
1:A:858:ILE:HG12	1:A:864:MET:HB3	2.02	0.42
1:B:472:TYR:O	1:B:476:LYS:HG2	2.20	0.42
1:B:988:GLY:C	1:B:989:PHE:CD1	2.97	0.42
1:C:274:PHE:HB3	1:C:286:ALA:O	2.20	0.42
1:C:570:TRP:CD1	1:C:571:VAL:HG22	2.54	0.42
1:C:742:THR:CG2	1:C:743:SER:H	2.31	0.42
1:D:420:MET:HB3	1:D:420:MET:HE3	1.62	0.42
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.42
1:A:105:TYR:HA	1:A:106:PRO:HD3	1.91	0.42
1:A:274:PHE:HB3	1:A:286:ALA:O	2.20	0.42
1:A:568:TRP:CD1	1:A:568:TRP:C	2.98	0.42
1:B:105:TYR:HB3	1:B:106:PRO:HD2	2.01	0.42
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.84	0.42
1:C:77:ASP:HA	3:C:4218:HOH:O	2.19	0.42
1:C:479:ASP:HA	1:C:480:PRO:HD2	1.73	0.42
1:C:995:GLY:O	1:C:996:ASP:C	2.61	0.42
1:D:38:ASN:ND2	1:D:38:ASN:C	2.77	0.42
1:D:214:LEU:HD23	1:D:214:LEU:HA	1.61	0.42
1:D:570:TRP:CD1	1:D:571:VAL:HG22	2.54	0.42
1:D:708:TRP:CD1	1:D:708:TRP:H	2.38	0.42
1:B:685:LEU:CB	1:B:686:PRO:HD2	2.38	0.42
1:B:822:LEU:HD12	1:B:823:LEU:N	2.34	0.42
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.78	0.42
1:C:354:VAL:HG22	1:C:355:ASN:N	2.34	0.42
1:C:622:HIS:HD2	1:C:625:GLN:OE1	2.02	0.42
1:C:757:GLN:HG2	1:C:758:PHE:N	2.31	0.42
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.66	0.42
1:D:251:ARG:HH11	1:D:251:ARG:CG	2.32	0.42
1:D:274:PHE:HB3	1:D:286:ALA:O	2.20	0.42
1:D:645:ARG:NH2	1:D:650:GLU:CD	2.76	0.42
1:D:822:LEU:HD12	1:D:823:LEU:N	2.34	0.42
1:D:835:LEU:HA	1:D:835:LEU:HD12	1.90	0.42
1:A:424:ASN:HD22	1:A:424:ASN:HA	1.40	0.42
1:B:11:LEU:N	1:B:11:LEU:HD23	2.35	0.42
1:B:217:LYS:HB3	1:B:218:PRO:HD2	2.01	0.42
1:B:274:PHE:HB3	1:B:286:ALA:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:HD23	1:B:308:LEU:HA	1.80	0.42
1:C:63:PHE:CB	1:C:64:PRO:CD	2.98	0.42
1:C:251:ARG:HH11	1:C:251:ARG:CG	2.32	0.42
1:D:635:THR:HA	1:D:680:ILE:O	2.19	0.42
1:D:840:HIS:ND1	1:D:840:HIS:N	2.67	0.42
1:D:858:ILE:HG12	1:D:864:MET:HB3	2.02	0.42
1:A:11:LEU:N	1:A:11:LEU:HD23	2.35	0.42
1:A:441:THR:O	1:A:445:GLN:HG3	2.20	0.42
1:A:474:TRP:CZ2	1:A:478:VAL:HG21	2.55	0.42
1:B:102:ASN:HD22	1:B:102:ASN:C	2.27	0.42
1:B:124:SER:HA	1:B:184:LEU:O	2.20	0.42
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.42
1:C:472:TYR:O	1:C:476:LYS:HG2	2.20	0.42
1:C:474:TRP:CZ2	1:C:478:VAL:HG21	2.55	0.42
1:C:651:LEU:HD12	1:C:651:LEU:HA	1.46	0.42
1:C:856:TYR:CD1	1:C:856:TYR:N	2.88	0.42
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.84	0.42
1:D:378:LEU:HA	1:D:378:LEU:HD23	1.75	0.42
1:D:856:TYR:N	1:D:856:TYR:CD1	2.88	0.42
1:A:111:PRO:HA	1:A:112:PRO:HA	1.56	0.41
1:A:645:ARG:NH2	1:A:650:GLU:OE2	2.46	0.41
1:A:856:TYR:CD1	1:A:856:TYR:N	2.88	0.41
1:B:262:GLN:O	1:B:262:GLN:HG2	2.19	0.41
1:B:576:ILE:HD13	1:B:584:PRO:HB2	2.02	0.41
1:C:38:ASN:ND2	1:C:38:ASN:C	2.77	0.41
1:D:128:ASN:ND2	1:D:180:GLY:C	2.78	0.41
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.41
1:A:7:LEU:HD23	1:A:7:LEU:HA	1.85	0.41
1:A:176:PHE:CD1	1:A:176:PHE:N	2.87	0.41
1:A:647:SER:HG	1:A:672:VAL:H	1.65	0.41
1:A:658:LEU:HD23	1:A:661:LYS:HZ2	1.85	0.41
1:A:721:ARG:HE	1:B:874:SER:CB	2.32	0.41
1:A:757:GLN:HG2	1:A:758:PHE:N	2.31	0.41
1:A:965:GLN:O	1:A:966:GLN:C	2.62	0.41
1:B:176:PHE:CD1	1:B:176:PHE:N	2.87	0.41
1:B:288:ARG:HH11	1:B:288:ARG:HD3	1.48	0.41
1:C:105:TYR:HB3	1:C:106:PRO:HD2	2.01	0.41
1:C:128:ASN:ND2	1:C:180:GLY:C	2.78	0.41
1:C:227:VAL:CG1	1:C:228:ALA:N	2.83	0.41
1:C:395:HIS:HA	1:C:396:PRO:HD3	1.83	0.41
1:C:473:ARG:HD3	1:C:473:ARG:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:ARG:HB2	1:C:600:GLN:H	1.54	0.41
1:D:141:ILE:HG12	1:D:142:ILE:N	2.35	0.41
1:D:262:GLN:O	1:D:262:GLN:HG2	2.19	0.41
1:D:473:ARG:HD3	1:D:473:ARG:C	2.45	0.41
1:D:474:TRP:CZ2	1:D:478:VAL:HG21	2.55	0.41
1:D:559:TYR:HB2	1:D:562:LEU:CD1	2.47	0.41
1:D:995:GLY:O	1:D:996:ASP:C	2.61	0.41
1:A:141:ILE:HG12	1:A:142:ILE:N	2.35	0.41
1:A:524:LEU:O	1:A:561:ARG:NH2	2.50	0.41
1:B:23:GLN:HG2	3:B:4413:HOH:O	2.20	0.41
1:B:128:ASN:ND2	1:B:180:GLY:C	2.78	0.41
1:C:141:ILE:HG12	1:C:142:ILE:N	2.35	0.41
1:C:262:GLN:O	1:C:262:GLN:HG2	2.19	0.41
1:C:568:TRP:CD1	1:C:568:TRP:C	2.98	0.41
1:C:578:TYR:HA	1:C:583:ASN:O	2.20	0.41
1:C:858:ILE:HG12	1:C:864:MET:HB3	2.02	0.41
1:D:407:LEU:HD23	1:D:407:LEU:HA	1.86	0.41
1:D:835:LEU:HD12	1:D:857:ARG:HB2	2.03	0.41
1:A:23:GLN:HG2	3:A:7533:HOH:O	2.20	0.41
1:A:63:PHE:CB	1:A:64:PRO:CD	2.98	0.41
1:A:682:LEU:HA	1:A:683:PRO:HD3	1.91	0.41
1:A:835:LEU:HD12	1:A:857:ARG:HB2	2.03	0.41
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.56	0.41
1:B:41:GLU:HG2	1:B:46:ARG:NH1	2.35	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD2	1.58	0.41
1:B:250:LEU:HD23	1:B:250:LEU:HA	1.90	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.86	0.41
1:B:559:TYR:HA	1:B:560:PRO:HD2	1.85	0.41
1:D:41:GLU:HG2	1:D:46:ARG:NH1	2.35	0.41
1:D:524:LEU:O	1:D:561:ARG:NH2	2.50	0.41
1:D:568:TRP:CD1	1:D:568:TRP:C	2.98	0.41
1:D:742:THR:CG2	1:D:743:SER:H	2.32	0.41
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.55	0.41
1:A:599:ARG:HB2	1:A:600:GLN:H	1.54	0.41
1:B:63:PHE:CB	1:B:64:PRO:CD	2.98	0.41
1:B:822:LEU:HD13	1:B:822:LEU:HA	1.79	0.41
1:D:77:ASP:HA	3:D:4132:HOH:O	2.19	0.41
1:D:124:SER:HA	1:D:184:LEU:O	2.20	0.41
1:D:352:ARG:NH2	1:D:641:GLU:OE1	2.54	0.41
1:D:559:TYR:HA	1:D:560:PRO:HD2	1.86	0.41
1:D:965:GLN:O	1:D:966:GLN:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.41
1:A:957:PHE:CD1	1:A:957:PHE:C	2.95	0.41
1:B:272:ALA:HA	1:B:273:PRO:HD3	1.88	0.41
1:B:354:VAL:HG22	1:B:355:ASN:N	2.34	0.41
1:B:649:ASN:O	1:B:702:GLN:HG3	2.21	0.41
1:B:856:TYR:CD1	1:B:856:TYR:N	2.88	0.41
1:C:11:LEU:N	1:C:11:LEU:HD23	2.35	0.41
1:C:736:ALA:C	1:C:737:ILE:HG22	2.46	0.41
1:C:892:ALA:HB3	1:C:946:TYR:CE1	2.56	0.41
1:A:278:ILE:HD12	1:A:278:ILE:HA	1.88	0.41
1:A:380:LYS:HE3	1:A:406:GLY:O	2.21	0.41
1:A:578:TYR:HA	1:A:583:ASN:O	2.20	0.41
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.45	0.41
1:B:69:VAL:HG13	1:B:70:PRO:HD2	2.03	0.41
1:B:352:ARG:NH2	1:B:641:GLU:OE1	2.54	0.41
1:B:473:ARG:HD3	1:B:473:ARG:C	2.45	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.03	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:B:655:MET:O	1:B:696:LEU:HD12	2.21	0.41
1:B:708:TRP:CD1	1:B:708:TRP:H	2.38	0.41
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.56	0.41
1:C:26:ARG:HD2	1:C:169:SER:HB3	2.02	0.41
1:C:41:GLU:HG2	1:C:46:ARG:NH1	2.35	0.41
1:C:559:TYR:HB2	1:C:562:LEU:CD1	2.47	0.41
1:C:649:ASN:O	1:C:702:GLN:HG3	2.21	0.41
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.91	0.41
1:C:970:THR:HG22	1:C:972:HIS:O	2.21	0.41
1:D:63:PHE:CB	1:D:64:PRO:CD	2.98	0.41
1:A:62:TRP:C	1:A:63:PHE:CD1	2.99	0.41
1:A:227:VAL:CG1	1:A:228:ALA:N	2.83	0.41
1:A:282:ARG:HG3	1:D:423:MET:HB2	2.03	0.41
1:A:454:ILE:C	1:A:455:ILE:HG13	2.46	0.41
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.38	0.41
1:A:840:HIS:N	1:A:840:HIS:ND1	2.67	0.41
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.36	0.41
1:A:949:HIS:CD2	1:A:1020:TRP:NE1	2.79	0.41
1:C:441:THR:O	1:C:445:GLN:HG3	2.20	0.41
1:C:511:PRO:HA	1:C:516:PRO:CB	2.51	0.41
1:C:708:TRP:CD1	1:C:708:TRP:H	2.38	0.41
1:D:26:ARG:HD2	1:D:169:SER:HB3	2.02	0.41
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:454:ILE:C	1:D:455:ILE:HG13	2.46	0.41
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.36	0.41
1:A:41:GLU:HG2	1:A:46:ARG:NH1	2.35	0.41
1:A:63:PHE:HB3	1:A:64:PRO:CD	2.45	0.41
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.56	0.41
1:A:262:GLN:O	1:A:262:GLN:HG2	2.19	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.41
1:A:649:ASN:O	1:A:702:GLN:HG3	2.21	0.41
1:A:655:MET:O	1:A:696:LEU:HD12	2.21	0.41
1:A:708:TRP:CD1	1:A:708:TRP:H	2.38	0.41
1:A:778:THR:HG22	1:A:779:PRO:N	2.35	0.41
1:A:970:THR:HG22	1:A:972:HIS:O	2.21	0.41
1:B:105:TYR:HA	1:B:106:PRO:HD3	1.91	0.41
1:B:225:PHE:C	1:B:226:HIS:CD2	2.99	0.41
1:B:474:TRP:CZ2	1:B:478:VAL:HG21	2.55	0.41
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.81	0.41
1:B:778:THR:HG22	1:B:779:PRO:N	2.35	0.41
1:B:858:ILE:HG12	1:B:864:MET:HB3	2.02	0.41
1:B:965:GLN:O	1:B:966:GLN:C	2.62	0.41
1:C:62:TRP:C	1:C:63:PHE:CD1	2.99	0.41
1:C:305:ILE:HA	1:C:306:PRO:HD2	1.88	0.41
1:C:380:LYS:HE3	1:C:406:GLY:O	2.21	0.41
1:C:524:LEU:O	1:C:561:ARG:NH2	2.50	0.41
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.03	0.41
1:C:652:LEU:O	1:C:667:GLU:HA	2.20	0.41
1:C:835:LEU:HD12	1:C:857:ARG:HB2	2.03	0.41
1:D:11:LEU:N	1:D:11:LEU:HD23	2.35	0.41
1:D:114:VAL:HA	1:D:115:PRO:HD3	1.77	0.41
1:D:168:PRO:O	1:D:442:ARG:NH2	2.48	0.41
1:D:336:ARG:NH2	1:D:338:GLU:CD	2.79	0.41
1:D:649:ASN:O	1:D:702:GLN:HG3	2.21	0.41
1:D:655:MET:O	1:D:696:LEU:HD12	2.21	0.41
1:D:778:THR:CG2	1:D:779:PRO:CD	2.99	0.41
1:D:778:THR:HG22	1:D:779:PRO:N	2.35	0.41
1:D:917:ARG:NH2	1:D:943:GLU:OE1	2.54	0.41
1:A:26:ARG:HD2	1:A:169:SER:HB3	2.02	0.41
1:A:161:TYR:OH	1:A:163:GLN:NE2	2.50	0.41
1:A:378:LEU:HA	1:A:378:LEU:HD23	1.75	0.41
1:A:868:VAL:HG12	1:A:869:ASP:N	2.36	0.41
1:B:581:ASN:HD22	1:B:583:ASN:ND2	2.19	0.41
1:B:868:VAL:HG12	1:B:869:ASP:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.84	0.41
1:D:176:PHE:CD1	1:D:176:PHE:N	2.87	0.41
1:D:578:TYR:HA	1:D:583:ASN:O	2.21	0.41
1:D:736:ALA:C	1:D:737:ILE:HG22	2.46	0.41
1:D:970:THR:HG22	1:D:972:HIS:O	2.21	0.41
1:A:128:ASN:ND2	1:A:180:GLY:C	2.78	0.40
1:A:149:ALA:O	1:A:150:PHE:HB3	2.21	0.40
1:A:576:ILE:HD13	1:A:584:PRO:HB2	2.02	0.40
1:B:18:ASN:HA	1:B:19:PRO:HD3	1.56	0.40
1:B:26:ARG:HD2	1:B:169:SER:HB3	2.02	0.40
1:B:141:ILE:HG12	1:B:142:ILE:N	2.35	0.40
1:B:840:HIS:ND1	1:B:840:HIS:N	2.67	0.40
1:B:995:GLY:O	1:B:996:ASP:C	2.61	0.40
1:C:352:ARG:NH2	1:C:641:GLU:OE1	2.54	0.40
1:D:69:VAL:HG13	1:D:70:PRO:HD2	2.03	0.40
1:A:272:ALA:CB	1:A:273:PRO:CD	2.99	0.40
1:A:278:ILE:N	1:A:278:ILE:HD13	2.37	0.40
1:A:436:MET:HE3	1:A:467:ASN:ND2	2.29	0.40
1:A:473:ARG:HD3	1:A:473:ARG:C	2.45	0.40
1:A:917:ARG:NH2	1:A:943:GLU:OE1	2.54	0.40
1:A:956:GLN:CD	1:A:956:GLN:N	2.79	0.40
1:B:214:LEU:HA	1:B:214:LEU:HD23	1.61	0.40
1:B:380:LYS:HE3	1:B:406:GLY:O	2.21	0.40
1:B:568:TRP:CD1	1:B:568:TRP:C	2.98	0.40
1:C:23:GLN:HG2	3:C:4454:HOH:O	2.20	0.40
1:C:149:ALA:O	1:C:150:PHE:HB3	2.21	0.40
1:C:956:GLN:CD	1:C:956:GLN:N	2.79	0.40
1:D:23:GLN:HG2	3:D:7533:HOH:O	2.20	0.40
1:D:647:SER:HG	1:D:672:VAL:H	1.65	0.40
1:D:956:GLN:CD	1:D:956:GLN:N	2.79	0.40
1:A:502:MET:HA	1:A:537:GLU:O	2.22	0.40
1:B:272:ALA:CB	1:B:273:PRO:CD	2.99	0.40
1:B:780:LEU:HA	1:B:780:LEU:HD12	1.89	0.40
1:C:89:ASN:O	1:C:92:MET:HB2	2.21	0.40
1:C:407:LEU:HD23	1:C:407:LEU:HA	1.86	0.40
1:C:502:MET:HA	1:C:537:GLU:O	2.22	0.40
1:D:62:TRP:C	1:D:63:PHE:CD1	2.99	0.40
1:A:90:TRP:NE1	1:A:96:ASP:OD1	2.55	0.40
1:A:147:ASN:HA	1:A:148:SER:HA	1.65	0.40
1:A:244:VAL:O	1:A:288:ARG:HA	2.22	0.40
1:A:736:ALA:C	1:A:737:ILE:HG22	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:TRP:C	1:B:63:PHE:CD1	2.99	0.40
1:B:336:ARG:NH2	1:B:338:GLU:CD	2.79	0.40
1:B:578:TYR:HA	1:B:583:ASN:O	2.21	0.40
1:B:970:THR:HG22	1:B:972:HIS:O	2.21	0.40
1:C:38:ASN:HD21	1:C:41:GLU:N	2.17	0.40
1:C:65:ALA:CB	1:C:66:PRO:CD	3.00	0.40
1:D:89:ASN:O	1:D:92:MET:HB2	2.22	0.40
1:D:227:VAL:CG1	1:D:240:LEU:HD11	2.48	0.40
1:D:702:GLN:O	1:D:712:GLY:N	2.50	0.40
1:D:868:VAL:HG12	1:D:869:ASP:N	2.36	0.40
1:A:100:TYR:O	1:A:597:ASN:HB2	2.22	0.40
1:A:225:PHE:C	1:A:226:HIS:CD2	2.99	0.40
1:B:436:MET:HE3	1:B:467:ASN:ND2	2.29	0.40
1:B:844:HIS:ND1	1:B:845:GLN:HG2	2.36	0.40
1:B:956:GLN:CD	1:B:956:GLN:N	2.79	0.40
1:C:244:VAL:O	1:C:288:ARG:HA	2.22	0.40
1:C:336:ARG:NH2	1:C:338:GLU:CD	2.79	0.40
1:C:486:TYR:CE2	1:C:488:GLY:HA3	2.56	0.40
1:C:559:TYR:HA	1:C:560:PRO:HD2	1.86	0.40
1:C:702:GLN:O	1:C:712:GLY:N	2.50	0.40
1:C:778:THR:HG22	1:C:779:PRO:N	2.35	0.40
1:C:868:VAL:HG12	1:C:869:ASP:N	2.36	0.40
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.54	0.40
1:D:237:ARG:CB	1:D:237:ARG:NH1	2.79	0.40
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.03	0.40
1:D:679:LEU:C	1:D:680:ILE:HG13	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	21	51
1	B	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	21	51
1	C	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	21	51
1	D	1026/1021 (100%)	953 (93%)	67 (6%)	6 (1%)	21	51
All	All	4104/4084 (100%)	3812 (93%)	268 (6%)	24 (1%)	21	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	SER
1	B	647	SER
1	C	647	SER
1	D	647	SER
1	A	77	ASP
1	A	601	PHE
1	B	77	ASP
1	B	601	PHE
1	C	77	ASP
1	C	601	PHE
1	D	77	ASP
1	D	601	PHE
1	A	164	ASP
1	B	164	ASP
1	C	164	ASP
1	D	164	ASP
1	A	690	SER
1	B	690	SER
1	C	690	SER
1	D	690	SER
1	A	10	VAL
1	B	10	VAL
1	C	10	VAL
1	D	10	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	880/873 (101%)	746 (85%)	134 (15%)	3	10
1	B	880/873 (101%)	746 (85%)	134 (15%)	3	10
1	C	880/873 (101%)	746 (85%)	134 (15%)	3	10
1	D	880/873 (101%)	746 (85%)	134 (15%)	3	10
All	All	3520/3492 (101%)	2984 (85%)	536 (15%)	3	10

All (536) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	12	GLN
1	A	24	LEU
1	A	37	ARG
1	A	38	ASN
1	A	39	SER
1	A	49	GLN
1	A	67	GLU
1	A	71	GLU
1	A	72	SER
1	A	80	GLU
1	A	84	VAL
1	A	85	VAL
1	A	90	TRP
1	A	114	VAL
1	A	116	THR
1	A	134	LEU
1	A	135	GLN
1	A	136	GLU
1	A	138	GLN
1	A	148	SER
1	A	169	SER
1	A	187	MET
1	A	190	ARG
1	A	202	MET
1	A	210	ARG
1	A	211	ASP
1	A	214	LEU
1	A	219	THR
1	A	223	SER
1	A	230	ARG
1	A	237	ARG
1	A	245	GLN

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Mol	Chain	Res	Type
1	A	246	MET
1	A	249	GLU
1	A	251	ARG
1	A	255	ARG
1	A	259	SER
1	A	269	SER
1	A	277	GLU
1	A	278	ILE
1	A	279	ILE
1	A	282	ARG
1	A	288	ARG
1	A	291	LEU
1	A	310	ARG
1	A	322	LEU
1	A	324	GLU
1	A	333	ARG
1	A	347	LYS
1	A	357	HIS
1	A	385	ASN
1	A	424	ASN
1	A	437	SER
1	A	448	ARG
1	A	473	ARG
1	A	481	SER
1	A	519	SER
1	A	521	LYS
1	A	525	SER
1	A	526	LEU
1	A	529	GLU
1	A	533	LEU
1	A	545	SER
1	A	546	LEU
1	A	554	GLN
1	A	571	VAL
1	A	576	ILE
1	A	580	GLU
1	A	581	ASN
1	A	599	ARG
1	A	600	GLN
1	A	630	ARG
1	A	645	ARG
1	A	647	SER

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Mol	Chain	Res	Type
1	A	655	MET
1	A	661	LYS
1	A	665	SER
1	A	672	VAL
1	A	675	GLN
1	A	687	GLN
1	A	690	SER
1	A	698	VAL
1	A	719	GLN
1	A	721	ARG
1	A	728	VAL
1	A	730	LEU
1	A	734	SER
1	A	737	ILE
1	A	741	THR
1	A	743	SER
1	A	746	ASP
1	A	750	GLU
1	A	755	ARG
1	A	761	GLN
1	A	765	LEU
1	A	766	SER
1	A	768	MET
1	A	770	ILE
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	797	GLU
1	A	800	ARG
1	A	801	ILE
1	A	811	LYS
1	A	817	GLN
1	A	822	LEU
1	A	824	GLN
1	A	830	LEU
1	A	836	ILE
1	A	843	GLN
1	A	845	GLN
1	A	856	TYR
1	A	857	ARG
1	A	858	ILE
1	A	866	ILE

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Mol	Chain	Res	Type
1	A	867	THR
1	A	874	SER
1	A	881	ARG
1	A	894	ARG
1	A	917	ARG
1	A	934	GLU
1	A	937	LEU
1	A	938	ARG
1	A	950	GLN
1	A	969	GLU
1	A	986	ILE
1	A	991	MET
1	A	1004	SER
1	A	1006	GLU
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	3	ILE
1	B	12	GLN
1	B	24	LEU
1	B	37	ARG
1	B	38	ASN
1	B	39	SER
1	B	49	GLN
1	B	67	GLU
1	B	71	GLU
1	B	72	SER
1	B	80	GLU
1	B	84	VAL
1	B	85	VAL
1	B	90	TRP
1	B	114	VAL
1	B	116	THR
1	B	134	LEU
1	B	135	GLN
1	B	136	GLU
1	B	138	GLN
1	B	148	SER
1	B	169	SER
1	B	187	MET
1	B	190	ARG
1	B	202	MET

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Mol	Chain	Res	Type
1	B	210	ARG
1	B	211	ASP
1	B	214	LEU
1	B	219	THR
1	B	223	SER
1	B	230	ARG
1	B	237	ARG
1	B	245	GLN
1	B	246	MET
1	B	249	GLU
1	B	251	ARG
1	B	255	ARG
1	B	259	SER
1	B	269	SER
1	B	277	GLU
1	B	278	ILE
1	B	279	ILE
1	B	282	ARG
1	B	288	ARG
1	B	291	LEU
1	B	310	ARG
1	B	322	LEU
1	B	324	GLU
1	B	333	ARG
1	B	347	LYS
1	B	357	HIS
1	B	385	ASN
1	B	424	ASN
1	B	437	SER
1	B	448	ARG
1	B	473	ARG
1	B	481	SER
1	B	519	SER
1	B	521	LYS
1	B	525	SER
1	B	526	LEU
1	B	529	GLU
1	B	533	LEU
1	B	545	SER
1	B	546	LEU
1	B	554	GLN
1	B	571	VAL

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Mol	Chain	Res	Type
1	B	576	ILE
1	B	580	GLU
1	B	581	ASN
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	645	ARG
1	B	647	SER
1	B	655	MET
1	B	661	LYS
1	B	665	SER
1	B	672	VAL
1	B	675	GLN
1	B	687	GLN
1	B	690	SER
1	B	698	VAL
1	B	719	GLN
1	B	721	ARG
1	B	728	VAL
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	741	THR
1	B	743	SER
1	B	746	ASP
1	B	750	GLU
1	B	755	ARG
1	B	761	GLN
1	B	765	LEU
1	B	766	SER
1	B	768	MET
1	B	770	ILE
1	B	772	ASP
1	B	773	LYS
1	B	774	LYS
1	B	797	GLU
1	B	800	ARG
1	B	801	ILE
1	B	811	LYS
1	B	817	GLN
1	B	822	LEU
1	B	824	GLN

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Mol	Chain	Res	Type
1	B	830	LEU
1	B	836	ILE
1	B	843	GLN
1	B	845	GLN
1	B	856	TYR
1	B	857	ARG
1	B	858	ILE
1	B	866	ILE
1	B	867	THR
1	B	874	SER
1	B	881	ARG
1	B	894	ARG
1	B	917	ARG
1	B	934	GLU
1	B	937	LEU
1	B	938	ARG
1	B	950	GLN
1	B	969	GLU
1	B	986	ILE
1	B	991	MET
1	B	1004	SER
1	B	1006	GLU
1	B	1017	GLN
1	B	1018	LEU
1	B	1023	LYS
1	C	3	ILE
1	C	12	GLN
1	C	24	LEU
1	C	37	ARG
1	C	38	ASN
1	C	39	SER
1	C	49	GLN
1	C	67	GLU
1	C	71	GLU
1	C	72	SER
1	C	80	GLU
1	C	84	VAL
1	C	85	VAL
1	C	90	TRP
1	C	114	VAL
1	C	116	THR
1	C	134	LEU

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Mol	Chain	Res	Type
1	C	135	GLN
1	C	136	GLU
1	C	138	GLN
1	C	148	SER
1	C	169	SER
1	C	187	MET
1	C	190	ARG
1	C	202	MET
1	C	210	ARG
1	C	211	ASP
1	C	214	LEU
1	C	219	THR
1	C	223	SER
1	C	230	ARG
1	C	237	ARG
1	C	245	GLN
1	C	246	MET
1	C	249	GLU
1	C	251	ARG
1	C	255	ARG
1	C	259	SER
1	C	269	SER
1	C	277	GLU
1	C	278	ILE
1	C	279	ILE
1	C	282	ARG
1	C	288	ARG
1	C	291	LEU
1	C	310	ARG
1	C	322	LEU
1	C	324	GLU
1	C	333	ARG
1	C	347	LYS
1	C	357	HIS
1	C	385	ASN
1	C	424	ASN
1	C	437	SER
1	C	448	ARG
1	C	473	ARG
1	C	481	SER
1	C	519	SER
1	C	521	LYS

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Mol	Chain	Res	Type
1	C	525	SER
1	C	526	LEU
1	C	529	GLU
1	C	533	LEU
1	C	545	SER
1	C	546	LEU
1	C	554	GLN
1	C	571	VAL
1	C	576	ILE
1	C	580	GLU
1	C	581	ASN
1	C	599	ARG
1	C	600	GLN
1	C	630	ARG
1	C	645	ARG
1	C	647	SER
1	C	655	MET
1	C	661	LYS
1	C	665	SER
1	C	672	VAL
1	C	675	GLN
1	C	687	GLN
1	C	690	SER
1	C	698	VAL
1	C	719	GLN
1	C	721	ARG
1	C	728	VAL
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	741	THR
1	C	743	SER
1	C	746	ASP
1	C	750	GLU
1	C	755	ARG
1	C	761	GLN
1	C	765	LEU
1	C	766	SER
1	C	768	MET
1	C	770	ILE
1	C	772	ASP
1	C	773	LYS

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Mol	Chain	Res	Type
1	C	774	LYS
1	C	797	GLU
1	C	800	ARG
1	C	801	ILE
1	C	811	LYS
1	C	817	GLN
1	C	822	LEU
1	C	824	GLN
1	C	830	LEU
1	C	836	ILE
1	C	843	GLN
1	C	845	GLN
1	C	856	TYR
1	C	857	ARG
1	C	858	ILE
1	C	866	ILE
1	C	867	THR
1	C	874	SER
1	C	881	ARG
1	C	894	ARG
1	C	917	ARG
1	C	934	GLU
1	C	937	LEU
1	C	938	ARG
1	C	950	GLN
1	C	969	GLU
1	C	986	ILE
1	C	991	MET
1	C	1004	SER
1	C	1006	GLU
1	C	1017	GLN
1	C	1018	LEU
1	C	1023	LYS
1	D	3	ILE
1	D	12	GLN
1	D	24	LEU
1	D	37	ARG
1	D	38	ASN
1	D	39	SER
1	D	49	GLN
1	D	67	GLU
1	D	71	GLU

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Mol	Chain	Res	Type
1	D	72	SER
1	D	80	GLU
1	D	84	VAL
1	D	85	VAL
1	D	90	TRP
1	D	114	VAL
1	D	116	THR
1	D	134	LEU
1	D	135	GLN
1	D	136	GLU
1	D	138	GLN
1	D	148	SER
1	D	169	SER
1	D	187	MET
1	D	190	ARG
1	D	202	MET
1	D	210	ARG
1	D	211	ASP
1	D	214	LEU
1	D	219	THR
1	D	223	SER
1	D	230	ARG
1	D	237	ARG
1	D	245	GLN
1	D	246	MET
1	D	249	GLU
1	D	251	ARG
1	D	255	ARG
1	D	259	SER
1	D	269	SER
1	D	277	GLU
1	D	278	ILE
1	D	279	ILE
1	D	282	ARG
1	D	288	ARG
1	D	291	LEU
1	D	310	ARG
1	D	322	LEU
1	D	324	GLU
1	D	333	ARG
1	D	347	LYS
1	D	357	HIS

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Mol	Chain	Res	Type
1	D	385	ASN
1	D	424	ASN
1	D	437	SER
1	D	448	ARG
1	D	473	ARG
1	D	481	SER
1	D	519	SER
1	D	521	LYS
1	D	525	SER
1	D	526	LEU
1	D	529	GLU
1	D	533	LEU
1	D	545	SER
1	D	546	LEU
1	D	554	GLN
1	D	571	VAL
1	D	576	ILE
1	D	580	GLU
1	D	581	ASN
1	D	599	ARG
1	D	600	GLN
1	D	630	ARG
1	D	645	ARG
1	D	647	SER
1	D	655	MET
1	D	661	LYS
1	D	665	SER
1	D	672	VAL
1	D	675	GLN
1	D	687	GLN
1	D	690	SER
1	D	698	VAL
1	D	719	GLN
1	D	721	ARG
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	741	THR
1	D	743	SER
1	D	746	ASP
1	D	750	GLU

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Mol	Chain	Res	Type
1	D	755	ARG
1	D	761	GLN
1	D	765	LEU
1	D	766	SER
1	D	768	MET
1	D	770	ILE
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	797	GLU
1	D	800	ARG
1	D	801	ILE
1	D	811	LYS
1	D	817	GLN
1	D	822	LEU
1	D	824	GLN
1	D	830	LEU
1	D	836	ILE
1	D	843	GLN
1	D	845	GLN
1	D	856	TYR
1	D	857	ARG
1	D	858	ILE
1	D	866	ILE
1	D	867	THR
1	D	874	SER
1	D	881	ARG
1	D	894	ARG
1	D	917	ARG
1	D	934	GLU
1	D	937	LEU
1	D	938	ARG
1	D	950	GLN
1	D	969	GLU
1	D	986	ILE
1	D	991	MET
1	D	1004	SER
1	D	1006	GLU
1	D	1017	GLN
1	D	1018	LEU
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	50	GLN
1	A	102	ASN
1	A	128	ASN
1	A	216	HIS
1	A	226	HIS
1	A	266	GLN
1	A	316	HIS
1	A	357	HIS
1	A	363	HIS
1	A	385	ASN
1	A	424	ASN
1	A	445	GLN
1	A	467	ASN
1	A	554	GLN
1	A	581	ASN
1	A	597	ASN
1	A	604	ASN
1	A	622	HIS
1	A	623	GLN
1	A	624	GLN
1	A	634	GLN
1	A	824	GLN
1	A	890	GLN
1	A	949	HIS
1	A	990	HIS
1	A	1017	GLN
1	B	38	ASN
1	B	102	ASN
1	B	128	ASN
1	B	216	HIS
1	B	226	HIS
1	B	266	GLN
1	B	316	HIS
1	B	357	HIS
1	B	363	HIS
1	B	424	ASN
1	B	467	ASN
1	B	554	GLN
1	B	581	ASN
1	B	597	ASN
1	B	604	ASN

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Mol	Chain	Res	Type
1	B	622	HIS
1	B	624	GLN
1	B	634	GLN
1	B	824	GLN
1	B	890	GLN
1	B	949	HIS
1	B	990	HIS
1	B	1017	GLN
1	C	38	ASN
1	C	50	GLN
1	C	102	ASN
1	C	128	ASN
1	C	216	HIS
1	C	226	HIS
1	C	266	GLN
1	C	316	HIS
1	C	357	HIS
1	C	363	HIS
1	C	385	ASN
1	C	424	ASN
1	C	445	GLN
1	C	467	ASN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	604	ASN
1	C	622	HIS
1	C	624	GLN
1	C	634	GLN
1	C	718	GLN
1	C	824	GLN
1	C	890	GLN
1	C	949	HIS
1	C	990	HIS
1	C	1017	GLN
1	D	38	ASN
1	D	50	GLN
1	D	102	ASN
1	D	128	ASN
1	D	216	HIS
1	D	226	HIS
1	D	266	GLN

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Mol	Chain	Res	Type
1	D	316	HIS
1	D	357	HIS
1	D	363	HIS
1	D	385	ASN
1	D	424	ASN
1	D	445	GLN
1	D	467	ASN
1	D	554	GLN
1	D	581	ASN
1	D	597	ASN
1	D	604	ASN
1	D	622	HIS
1	D	624	GLN
1	D	634	GLN
1	D	817	GLN
1	D	824	GLN
1	D	890	GLN
1	D	949	HIS
1	D	990	HIS
1	D	1017	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1021/1021 (100%)	-0.64	1 (0%) 92 90	8, 29, 69, 100	26 (2%)
1	B	1021/1021 (100%)	-0.61	0 100 100	8, 29, 69, 100	26 (2%)
1	C	1021/1021 (100%)	-0.70	1 (0%) 92 90	8, 29, 69, 100	26 (2%)
1	D	1021/1021 (100%)	-0.70	2 (0%) 91 88	8, 29, 69, 100	26 (2%)
All	All	4084/4084 (100%)	-0.66	4 (0%) 92 90	8, 29, 69, 100	104 (2%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	3.9
1	D	319	ASP	2.7
1	C	581	ASN	2.1
1	D	744	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	3001	1/1	0.97	0.05	28,28,28,28	0
2	MG	C	3002	1/1	0.97	0.07	31,31,31,31	0
2	MG	D	3002	1/1	0.97	0.05	31,31,31,31	0
2	MG	B	3002	1/1	0.98	0.04	31,31,31,31	0
2	MG	C	3001	1/1	0.99	0.03	28,28,28,28	0
2	MG	B	3001	1/1	0.99	0.04	28,28,28,28	0
2	MG	D	3001	1/1	0.99	0.02	28,28,28,28	0
2	MG	A	3002	1/1	0.99	0.07	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.