



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:11 AM UTC

PDB ID : 5D06 / pdb_00005d06
Title : Crystal Structure of the Candida Glabrata Glycogen Debranching Enzyme
Authors : Zhai, L.; Xiang, S.
Deposited on : 2015-08-02
Resolution : 3.10 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

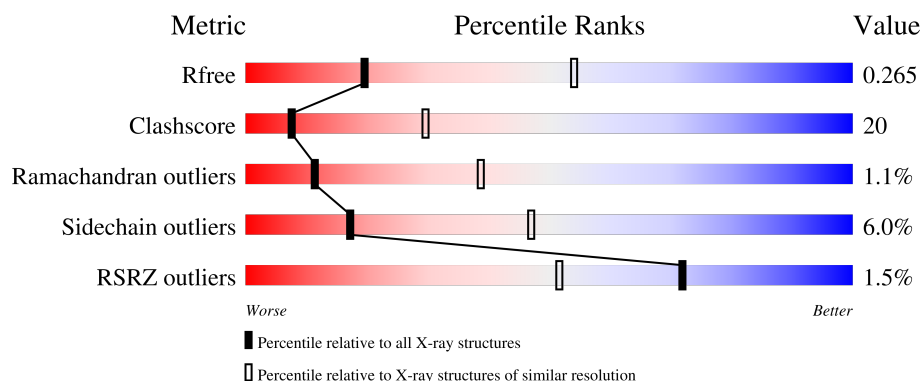
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	1528	% 66% 28% 5% .
1	B	1528	2% 62% 30% 5% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 24403 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.

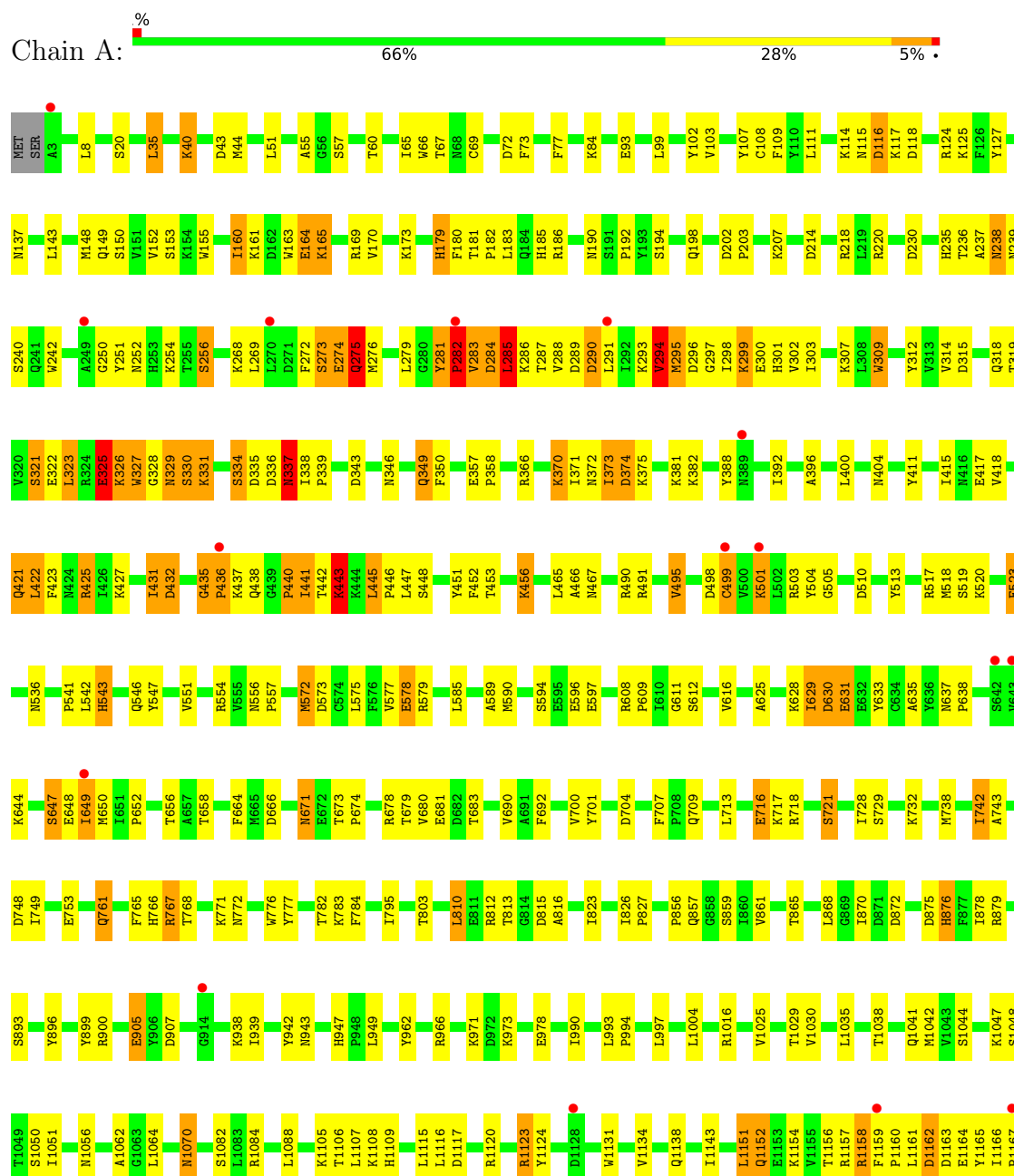
- Molecule 1 is a protein called Uncharacterized protein.

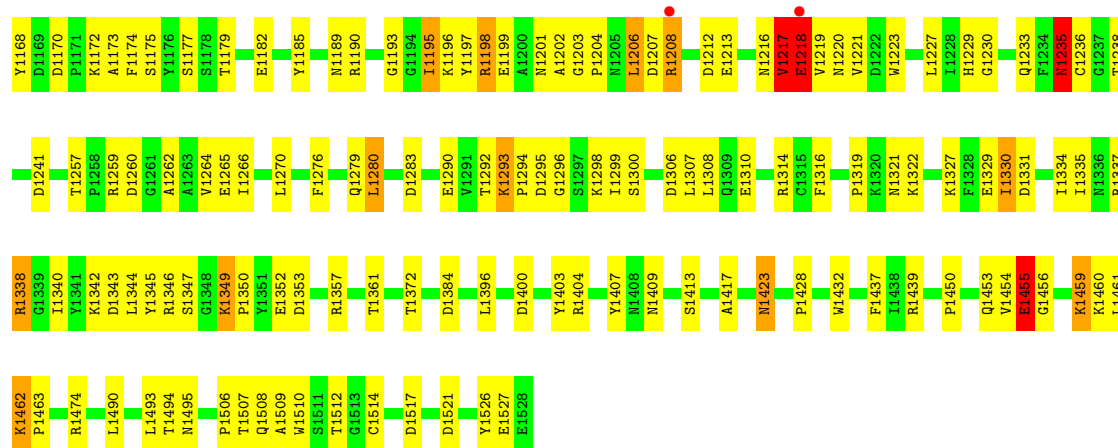
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1526	Total	C	N	O	S	0	0	0
			12278	7830	2065	2331	52			
1	B	1506	Total	C	N	O	S	0	0	0
			12125	7736	2038	2299	52			

3 Residue-property plots

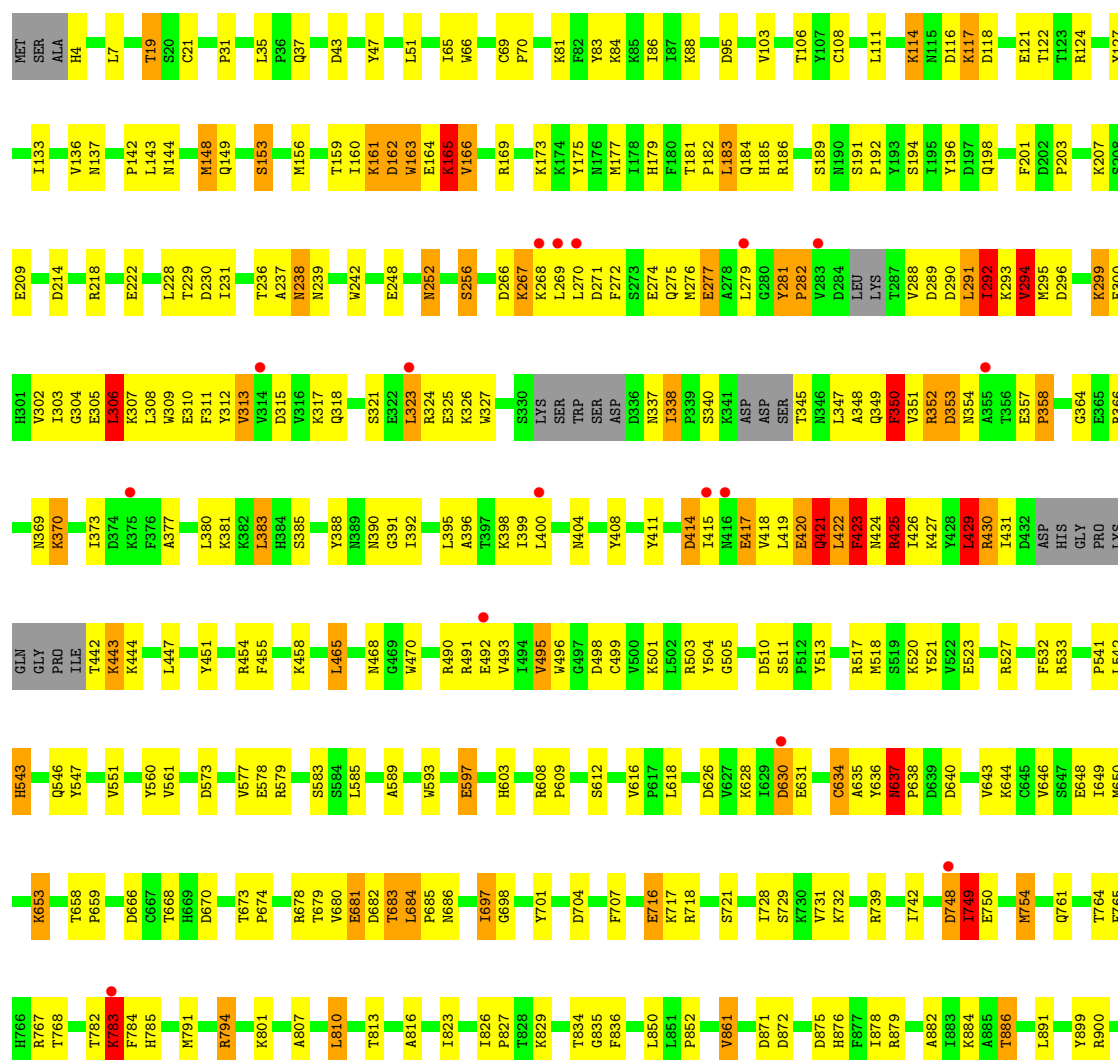
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

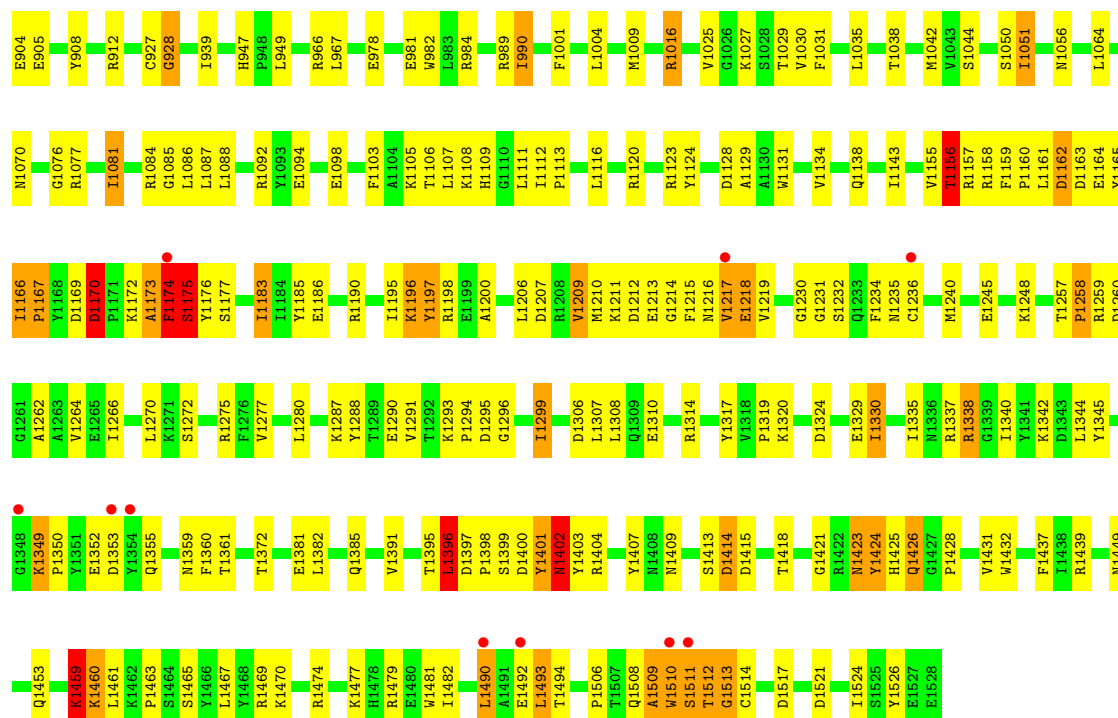
• Molecule 1: Uncharacterized protein





• Molecule 1: Uncharacterized protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.27Å 198.95Å 261.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.75 – 3.10 47.75 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.2 (47.75-3.10) 97.2 (47.75-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.234 , 0.268 0.234 , 0.265	Depositor DCC
R_{free} test set	2607 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24403	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	2/12589 (0.0%)	1.13	80/17071 (0.5%)
1	B	0.83	21/12427 (0.2%)	1.22	121/16845 (0.7%)
All	All	0.69	23/25016 (0.1%)	1.18	201/33916 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	8
All	All	0	15

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1174	PHE	CG-CD1	48.24	2.40	1.38
1	B	1174	PHE	CD2-CE2	18.56	1.94	1.38
1	B	1174	PHE	CG-CD2	16.00	1.72	1.38
1	B	1174	PHE	CB-CG	15.73	1.86	1.50
1	B	1174	PHE	CD1-CE1	13.82	1.80	1.38
1	B	1174	PHE	CE1-CZ	12.49	1.76	1.38
1	B	1174	PHE	CA-CB	10.33	1.71	1.53
1	B	1511	SER	N-CA	-9.06	1.35	1.46
1	B	1510	TRP	CA-C	-8.99	1.43	1.53
1	B	1512	THR	CA-C	-8.48	1.41	1.52
1	B	1174	PHE	CE2-CZ	8.02	1.62	1.38
1	B	1510	TRP	CB-CG	6.76	1.71	1.50
1	B	1156	THR	CA-CB	-5.93	1.44	1.53
1	B	423	PHE	CA-C	5.80	1.60	1.52
1	B	684	LEU	CA-C	5.67	1.58	1.52
1	B	1511	SER	CA-C	5.67	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1208	ARG	CG-CD	5.63	1.69	1.52
1	B	162	ASP	C-O	-5.63	1.16	1.24
1	B	1509	ALA	CA-C	-5.58	1.45	1.52
1	B	1174	PHE	CA-C	5.58	1.60	1.52
1	B	1510	TRP	CA-CB	5.57	1.66	1.51
1	B	1512	THR	CA-CB	5.48	1.62	1.53
1	A	1208	ARG	CA-CB	5.43	1.61	1.53

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	TYR	CA-C-N	-16.43	99.30	119.84
1	A	281	TYR	C-N-CA	-16.43	99.30	119.84
1	B	353	ASP	N-CA-C	12.89	124.86	111.07
1	B	1174	PHE	CA-CB-CG	11.98	125.78	113.80
1	B	425	ARG	CB-CG-CD	11.79	138.41	111.30
1	B	281	TYR	CA-C-N	11.72	134.49	119.84
1	B	281	TYR	C-N-CA	11.72	134.49	119.84
1	B	1166	ILE	CA-C-N	-11.41	105.57	119.84
1	B	1166	ILE	C-N-CA	-11.41	105.57	119.84
1	B	1162	ASP	N-CA-C	11.33	118.07	108.78
1	B	1509	ALA	N-CA-C	-11.12	97.00	112.45
1	B	420	GLU	N-CA-C	10.94	123.29	111.36
1	A	1218	GLU	N-CA-C	10.87	122.30	107.73
1	B	1174	PHE	CB-CG-CD1	10.76	138.99	120.70
1	B	165	LYS	CA-C-N	10.35	133.60	120.56
1	B	165	LYS	C-N-CA	10.35	133.60	120.56
1	B	1513	GLY	N-CA-C	-10.19	100.50	112.73
1	B	1209	VAL	N-CA-C	9.82	123.04	113.71
1	A	443	LYS	N-CA-C	-9.78	100.69	111.36
1	B	1414	ASP	N-CA-C	9.71	124.74	113.19
1	A	1166	ILE	CA-C-N	-9.67	107.75	119.84
1	A	1166	ILE	C-N-CA	-9.67	107.75	119.84
1	A	290	ASP	N-CA-C	9.51	121.24	111.07
1	A	421	GLN	N-CA-C	-9.50	100.80	111.82
1	B	658	THR	CA-C-N	-9.38	112.91	119.66
1	B	658	THR	C-N-CA	-9.38	112.91	119.66
1	A	658	THR	CA-C-N	-9.08	113.12	119.66
1	A	658	THR	C-N-CA	-9.08	113.12	119.66
1	B	1512	THR	N-CA-CB	8.73	123.27	110.26
1	B	1512	THR	CB-CA-C	-8.46	94.12	110.11
1	B	165	LYS	CG-CD-CE	-8.24	92.35	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	THR	CA-C-N	-8.21	111.55	119.76
1	A	181	THR	C-N-CA	-8.21	111.55	119.76
1	B	414	ASP	N-CA-C	7.96	119.58	111.07
1	A	137	ASN	N-CA-C	-7.92	99.55	111.34
1	B	304	GLY	N-CA-C	7.91	122.22	112.73
1	A	422	LEU	N-CA-C	7.86	122.14	112.23
1	A	327	TRP	N-CA-C	-7.55	98.71	109.96
1	A	495	VAL	N-CA-C	7.46	119.82	109.45
1	A	431	ILE	CA-C-N	-7.37	111.58	122.41
1	A	431	ILE	C-N-CA	-7.37	111.58	122.41
1	B	1197	TYR	N-CA-C	7.34	119.31	108.60
1	A	1203	GLY	N-CA-C	-7.29	97.46	112.34
1	A	630	ASP	N-CA-C	-7.27	98.13	109.25
1	B	1174	PHE	N-CA-C	-7.27	95.32	110.80
1	B	1510	TRP	CA-CB-CG	7.26	127.40	113.60
1	A	274	GLU	N-CA-C	-7.24	105.07	114.04
1	A	1208	ARG	CB-CG-CD	7.22	127.91	111.30
1	A	504	TYR	N-CA-C	-7.21	100.14	110.59
1	B	927	CYS	N-CA-C	-7.19	104.13	113.12
1	B	338	ILE	N-CA-C	7.13	115.23	107.60
1	B	1175	SER	N-CA-C	7.12	125.97	110.80
1	A	1116	LEU	N-CA-C	-7.05	97.91	109.40
1	A	338	ILE	N-CA-C	7.05	114.53	107.55
1	B	1512	THR	CA-CB-CG2	7.01	122.41	110.50
1	A	284	ASP	N-CA-C	7.00	119.82	108.34
1	B	1163	ASP	N-CA-C	7.00	119.05	109.11
1	A	366	ARG	N-CA-C	6.98	118.89	111.28
1	B	1413	SER	N-CA-C	6.89	119.22	110.33
1	B	181	THR	CA-C-N	-6.85	112.91	119.76
1	B	181	THR	C-N-CA	-6.85	112.91	119.76
1	B	1173	ALA	N-CA-C	-6.85	102.18	112.04
1	A	1070	ASN	CB-CA-C	-6.83	108.69	116.54
1	B	352	ARG	CA-C-N	6.80	129.28	120.44
1	B	352	ARG	C-N-CA	6.80	129.28	120.44
1	B	1509	ALA	CA-C-O	6.80	128.29	120.00
1	A	435	GLY	CA-C-N	6.78	126.69	119.85
1	A	435	GLY	C-N-CA	6.78	126.69	119.85
1	B	1511	SER	N-CA-CB	-6.75	100.26	110.73
1	B	1051	ILE	N-CA-C	-6.73	106.44	112.90
1	A	294	VAL	CB-CA-C	-6.71	103.25	112.24
1	B	1177	SER	N-CA-C	6.70	120.19	110.28
1	A	876	HIS	CB-CA-C	-6.68	100.34	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	ASP	N-CA-C	6.64	120.32	109.76
1	A	630	ASP	CA-C-N	-6.60	110.50	121.92
1	A	630	ASP	C-N-CA	-6.60	110.50	121.92
1	B	1174	PHE	CB-CG-CD2	-6.58	109.50	120.70
1	B	783	LYS	N-CA-C	6.55	121.44	113.38
1	B	683	THR	N-CA-C	-6.52	103.44	111.33
1	B	504	TYR	N-CA-C	-6.52	101.14	110.59
1	A	153	SER	N-CA-C	6.51	118.93	111.11
1	B	748	ASP	N-CA-C	6.51	120.24	109.96
1	B	1209	VAL	CB-CA-C	-6.45	104.57	110.63
1	A	295	MET	N-CA-C	-6.45	105.05	113.17
1	A	1349	LYS	CA-C-N	6.43	127.88	119.84
1	A	1349	LYS	C-N-CA	6.43	127.88	119.84
1	B	1460	LYS	N-CA-C	-6.42	99.57	109.14
1	B	425	ARG	N-CA-C	6.41	124.45	110.80
1	B	421	GLN	CA-C-N	-6.40	109.32	121.54
1	B	421	GLN	C-N-CA	-6.40	109.32	121.54
1	B	1396	LEU	CD1-CG-CD2	-6.38	96.76	110.80
1	B	161	LYS	N-CA-C	-6.36	105.35	113.23
1	A	283	VAL	N-CA-C	-6.32	96.19	109.34
1	B	640	ASP	N-CA-C	6.30	120.19	111.55
1	B	289	ASP	CA-C-N	-6.26	112.84	122.60
1	B	289	ASP	C-N-CA	-6.26	112.84	122.60
1	B	352	ARG	N-CA-C	6.26	118.90	111.33
1	B	1510	TRP	CA-C-O	6.24	129.10	119.80
1	B	294	VAL	CB-CA-C	-6.18	101.16	111.29
1	B	1349	LYS	CA-C-N	6.18	127.56	119.84
1	B	1349	LYS	C-N-CA	6.18	127.56	119.84
1	B	277	GLU	CA-CB-CG	-6.18	101.75	114.10
1	B	1414	ASP	CA-C-N	-6.18	112.93	122.87
1	B	1414	ASP	C-N-CA	-6.18	112.93	122.87
1	A	1177	SER	N-CA-C	6.16	119.20	109.96
1	B	1402	ASN	N-CA-C	6.16	120.63	113.18
1	A	35	LEU	CA-C-N	-6.15	112.15	119.84
1	A	35	LEU	C-N-CA	-6.15	112.15	119.84
1	A	325	GLU	N-CA-C	6.15	119.89	112.38
1	B	1510	TRP	CB-CA-C	-6.14	107.74	116.34
1	B	681	GLU	N-CA-C	6.11	119.99	112.54
1	A	256	SER	CA-C-N	6.10	126.28	119.32
1	A	256	SER	C-N-CA	6.10	126.28	119.32
1	B	153	SER	N-CA-C	6.08	118.41	111.11
1	A	289	ASP	CA-C-N	6.07	128.34	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	289	ASP	C-N-CA	6.07	128.34	120.44
1	A	1170	ASP	N-CA-C	6.07	118.93	110.07
1	B	256	SER	CA-C-N	6.05	126.21	119.32
1	B	256	SER	C-N-CA	6.05	126.21	119.32
1	A	1152	GLN	CA-CB-CG	-6.02	102.07	114.10
1	A	644	LYS	N-CA-C	6.01	119.26	109.59
1	B	1401	TYR	N-CA-C	-6.01	105.95	113.28
1	B	1170	ASP	CA-C-N	-5.95	113.49	119.56
1	B	1170	ASP	C-N-CA	-5.95	113.49	119.56
1	A	1217	VAL	N-CA-C	-5.94	99.18	108.86
1	A	536	ASN	N-CA-CB	-5.93	103.14	111.62
1	B	928	GLY	N-CA-C	5.93	121.64	111.98
1	B	292	ILE	CA-CB-CG1	-5.91	100.35	110.40
1	A	1423	ASN	N-CA-C	5.88	119.99	112.34
1	B	313	VAL	N-CA-C	5.88	116.76	108.36
1	B	1359	ASN	N-CA-C	5.84	117.65	111.28
1	A	337	ASN	N-CA-C	-5.83	106.50	113.21
1	B	1070	ASN	CB-CA-C	-5.82	109.84	116.54
1	B	1116	LEU	N-CA-C	-5.79	99.97	109.40
1	A	160	ILE	N-CA-C	5.78	116.52	110.62
1	A	285	LEU	CB-CG-CD2	-5.78	93.38	110.70
1	B	1424	TYR	N-CA-C	5.73	118.27	111.33
1	B	495	VAL	N-CA-C	5.71	117.39	109.45
1	B	634	CYS	N-CA-C	5.70	118.17	108.02
1	B	421	GLN	N-CA-C	-5.68	106.02	113.17
1	B	370	LYS	N-CA-C	5.63	116.51	108.74
1	B	1426	GLN	CA-CB-CG	5.63	125.35	114.10
1	B	431	ILE	N-CA-C	-5.55	105.47	113.07
1	B	349	GLN	CA-CB-CG	5.54	125.19	114.10
1	B	659	PRO	O-C-N	5.54	123.75	121.15
1	B	1372	THR	CA-C-N	5.53	126.76	119.84
1	B	1372	THR	C-N-CA	5.53	126.76	119.84
1	A	323	LEU	N-CA-C	-5.52	106.48	113.43
1	A	495	VAL	CB-CA-C	-5.52	103.88	111.49
1	B	162	ASP	N-CA-C	-5.50	105.82	112.54
1	B	1217	VAL	CB-CA-C	-5.50	102.29	110.33
1	B	291	LEU	CA-CB-CG	5.50	135.56	116.30
1	A	373	ILE	N-CA-C	5.49	116.27	110.72
1	B	1183	ILE	N-CA-C	5.49	116.22	110.62
1	B	350	PHE	N-CA-C	-5.48	99.12	110.80
1	B	358	PRO	N-CA-C	5.48	119.82	111.11
1	A	445	LEU	CA-CB-CG	5.48	135.46	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	383	LEU	CA-CB-CG	-5.47	97.16	116.30
1	B	425	ARG	CA-C-N	5.46	129.64	121.77
1	B	425	ARG	C-N-CA	5.46	129.64	121.77
1	B	1143	ILE	N-CA-C	5.46	117.37	111.58
1	A	1372	THR	CA-C-N	5.42	126.62	119.84
1	A	1372	THR	C-N-CA	5.42	126.62	119.84
1	B	443	LYS	N-CA-C	5.42	119.00	112.93
1	B	1174	PHE	CE1-CZ-CE2	5.42	129.75	120.00
1	A	282	PRO	CA-C-N	-5.40	112.26	121.97
1	A	282	PRO	C-N-CA	-5.40	112.26	121.97
1	A	1217	VAL	CA-C-O	-5.36	115.06	121.28
1	A	432	ASP	N-CA-C	5.36	117.42	107.99
1	A	1151	LEU	CA-C-N	-5.35	114.11	122.73
1	A	1151	LEU	C-N-CA	-5.35	114.11	122.73
1	A	1293	LYS	CA-C-O	-5.35	115.35	120.97
1	B	684	LEU	CA-C-N	-5.35	113.15	119.84
1	B	684	LEU	C-N-CA	-5.35	113.15	119.84
1	B	1215	PHE	CA-C-N	-5.32	115.12	122.30
1	B	1215	PHE	C-N-CA	-5.32	115.12	122.30
1	A	1235	ASN	N-CA-C	5.29	116.85	108.96
1	A	370	LYS	N-CA-C	5.29	116.84	108.96
1	B	429	LEU	CA-CB-CG	5.28	134.77	116.30
1	B	1423	ASN	N-CA-C	5.28	119.20	112.34
1	B	1423	ASN	CA-C-N	5.26	127.58	120.38
1	B	1423	ASN	C-N-CA	5.26	127.58	120.38
1	B	1258	PRO	CA-C-N	-5.23	116.02	123.03
1	B	1258	PRO	C-N-CA	-5.23	116.02	123.03
1	A	1357	ARG	CA-C-N	-5.22	114.41	120.04
1	A	1357	ARG	C-N-CA	-5.22	114.41	120.04
1	B	347	LEU	N-CA-C	-5.21	105.52	111.14
1	A	1413	SER	N-CA-C	5.21	117.04	110.33
1	A	329	ASN	N-CA-C	5.18	120.61	110.56
1	A	1143	ILE	N-CA-C	5.17	117.06	111.58
1	B	912	ARG	N-CA-C	5.17	118.75	112.23
1	B	1512	THR	CA-CB-OG1	5.17	117.35	109.60
1	B	1162	ASP	CB-CA-C	-5.17	109.63	117.07
1	A	647	SER	N-CA-C	5.16	115.34	108.23
1	B	163	TRP	N-CA-C	5.08	117.94	111.69
1	B	1174	PHE	CD1-CG-CD2	-5.08	110.99	118.60
1	B	1169	ASP	N-CA-C	5.07	118.78	112.59
1	A	625	ALA	N-CA-C	-5.07	105.65	111.07
1	A	309	TRP	CA-CB-CG	-5.06	103.98	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	LYS	CD-CE-NZ	-5.06	95.72	111.90
1	A	275	GLN	N-CA-C	-5.04	105.97	111.82

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1158	ARG	Peptide
1	A	1217	VAL	Peptide
1	A	1218	GLU	Peptide
1	A	330	SER	Peptide
1	A	331	LYS	Peptide
1	A	436	PRO	Peptide
1	A	650	MET	Peptide
1	B	1174	PHE	Peptide
1	B	1218	GLU	Peptide
1	B	1509	ALA	Peptide
1	B	277	GLU	Peptide
1	B	306	LEU	Peptide
1	B	421	GLN	Peptide
1	B	442	THR	Peptide
1	B	783	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12278	0	11960	426	0
1	B	12125	0	11812	545	4
All	All	24403	0	23772	971	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (971) 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:1174:PHE:CZ	1:B:1174:PHE:CE1	1.76	1.68
1:B:1174:PHE:CE1	1:B:1174:PHE:CD1	1.80	1.64
1:B:1174:PHE:CG	1:B:1174:PHE:CB	1.86	1.56
1:B:1174:PHE:CE2	1:B:1174:PHE:CD2	1.94	1.55
1:B:1508:GLN:HB3	1:B:1510:TRP:HB3	1.21	1.16
1:B:1510:TRP:CE3	1:B:1511:SER:HB2	1.88	1.08
1:B:1174:PHE:CD1	1:B:1174:PHE:CG	2.40	1.08
1:B:425:ARG:HG2	1:B:426:ILE:N	1.69	1.07
1:B:678:ARG:HB2	1:B:783:LYS:HD3	1.30	1.07
1:B:1196:LYS:HG3	1:B:1218:GLU:HG3	1.33	1.02
1:A:282:PRO:HG2	1:A:294:VAL:HG22	1.40	1.02
1:B:165:LYS:HG3	1:B:166:VAL:H	0.89	1.02
1:A:1196:LYS:HA	1:A:1218:GLU:CG	1.90	1.01
1:B:1160:PRO:HG3	1:B:1164:GLU:H	1.28	0.99
1:B:165:LYS:HG3	1:B:166:VAL:N	1.72	0.98
1:B:682:ASP:HB2	1:B:783:LYS:HB3	1.43	0.98
1:A:1196:LYS:CA	1:A:1218:GLU:HG3	1.92	0.97
1:A:1361:THR:HG21	1:A:1437:PHE:HA	1.46	0.97
1:B:425:ARG:HG2	1:B:426:ILE:H	1.19	0.95
1:B:165:LYS:CG	1:B:166:VAL:H	1.80	0.95
1:B:1361:THR:HG21	1:B:1437:PHE:HA	1.46	0.95
1:B:1510:TRP:HE3	1:B:1511:SER:HB2	1.27	0.94
1:B:198:GLN:OE1	1:B:517:ARG:NH1	2.01	0.92
1:B:156:MET:O	1:B:165:LYS:NZ	2.03	0.92
1:B:422:LEU:HB3	1:B:425:ARG:HD3	1.53	0.90
1:B:468:ASN:HB3	1:B:501:LYS:HB2	1.54	0.90
1:B:679:THR:O	1:B:783:LYS:NZ	2.04	0.90
1:B:1035:LEU:HD22	1:B:1512:THR:HG22	1.55	0.89
1:A:1123:ARG:HH22	1:A:1207:ASP:HB2	1.38	0.89
1:B:1490:LEU:HB2	1:B:1510:TRP:CZ2	2.07	0.88
1:B:1320:LYS:O	1:B:1338:ARG:NH1	2.06	0.87
1:A:1196:LYS:HA	1:A:1218:GLU:HG3	0.96	0.87
1:A:400:LEU:O	1:A:404:ASN:ND2	2.08	0.86
1:B:425:ARG:HD2	1:B:426:ILE:HD12	1.57	0.86
1:A:349:GLN:O	1:A:349:GLN:HG2	1.76	0.85
1:A:432:ASP:OD1	1:A:435:GLY:N	2.07	0.85
1:B:1401:TYR:O	1:B:1404:ARG:NH2	2.09	0.85
1:A:283:VAL:HG11	1:A:441:ILE:HG12	1.57	0.84
1:B:742:ILE:HG21	1:B:767:ARG:HH21	1.41	0.84
1:B:1508:GLN:CB	1:B:1510:TRP:HB3	2.04	0.84
1:B:323:LEU:HD21	1:B:377:ALA:HB2	1.60	0.83
1:B:307:LYS:O	1:B:309:TRP:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1198:ARG:NH2	1:A:1212:ASP:O	2.11	0.83
1:A:1223:TRP:CD1	1:A:1293:LYS:HZ3	1.96	0.83
1:B:426:ILE:HA	1:B:429:LEU:HB2	1.60	0.83
1:B:608:ARG:HE	1:B:750:GLU:HB3	1.44	0.82
1:A:452:PHE:HA	1:A:466:ALA:HA	1.59	0.82
1:B:678:ARG:CB	1:B:783:LYS:HD3	2.10	0.82
1:B:1432:TRP:HB3	1:B:1511:SER:OG	1.80	0.82
1:B:313:VAL:HG13	1:B:404:ASN:HD22	1.44	0.82
1:A:721:SER:OG	1:A:823:ILE:O	1.97	0.82
1:A:328:GLY:H	1:A:331:LYS:HZ3	1.28	0.81
1:B:682:ASP:OD2	1:B:686:ASN:HB2	1.79	0.81
1:B:721:SER:OG	1:B:823:ILE:O	1.97	0.81
1:A:1204:PRO:HB2	1:A:1208:ARG:HH11	1.45	0.81
1:A:1204:PRO:HB2	1:A:1208:ARG:NH1	1.96	0.81
1:A:295:MET:SD	1:A:423:PHE:HB3	2.20	0.81
1:B:682:ASP:HB2	1:B:783:LYS:CB	2.10	0.80
1:B:1158:ARG:HA	1:B:1173:ALA:O	1.81	0.80
1:B:353:ASP:CG	1:B:354:ASN:HD22	1.89	0.80
1:B:353:ASP:OD1	1:B:354:ASN:N	2.15	0.80
1:A:1217:VAL:O	1:A:1218:GLU:HG2	1.81	0.79
1:B:1172:LYS:HA	1:B:1175:SER:HB3	1.64	0.79
1:A:186:ARG:NH2	1:A:202:ASP:OD2	2.16	0.78
1:B:1103:PHE:HB3	1:B:1112:ILE:HD11	1.66	0.78
1:A:251:TYR:HB2	1:A:501:LYS:HE2	1.66	0.78
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.65	0.78
1:A:1342:LYS:HE2	1:A:1353:ASP:HB3	1.65	0.77
1:A:325:GLU:N	1:A:325:GLU:OE1	2.17	0.77
1:A:72:ASP:OD1	1:A:73:PHE:N	2.15	0.77
1:A:1220:ASN:OD1	1:A:1221:VAL:N	2.13	0.77
1:B:520:LYS:HA	1:B:523:GLU:HB2	1.67	0.77
1:B:1217:VAL:HG13	1:B:1231:GLY:HA2	1.65	0.77
1:B:1508:GLN:HB3	1:B:1510:TRP:CB	2.10	0.77
1:A:326:LYS:CE	1:A:374:ASP:HB3	2.14	0.77
1:B:1197:TYR:H	1:B:1218:GLU:CD	1.92	0.77
1:A:1322:LYS:H	1:A:1322:LYS:HD2	1.49	0.77
1:A:1158:ARG:O	1:A:1159:PHE:HD2	1.68	0.76
1:A:442:THR:HG22	1:A:443:LYS:H	1.51	0.75
1:B:315:ASP:H	1:B:370:LYS:NZ	1.84	0.75
1:B:1510:TRP:CZ2	1:B:1512:THR:HG23	2.22	0.74
1:A:291:LEU:HA	1:A:294:VAL:HG23	1.69	0.74
1:A:748:ASP:OD1	1:A:749:ILE:N	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1396:LEU:HD23	1:B:1426:GLN:HB2	1.70	0.74
1:A:114:LYS:NZ	1:A:118:ASP:OD1	2.21	0.73
1:B:117:LYS:HD3	1:B:117:LYS:N	2.02	0.73
1:B:1196:LYS:CG	1:B:1218:GLU:HG3	2.14	0.73
1:B:1160:PRO:HG3	1:B:1164:GLU:N	2.03	0.73
1:A:1062:ALA:HB1	1:A:1510:TRP:HZ3	1.54	0.73
1:A:238:ASN:OD1	1:A:239:ASN:ND2	2.21	0.73
1:B:634:CYS:HB3	1:B:636:TYR:HE1	1.52	0.73
1:B:1400:ASP:OD2	1:B:1402:ASN:N	2.17	0.73
1:B:143:LEU:HD23	1:B:560:TYR:HE2	1.53	0.72
1:B:443:LYS:O	1:B:444:LYS:HG2	1.89	0.72
1:B:1108:LYS:HE2	1:B:1109:HIS:CE1	2.23	0.72
1:A:1108:LYS:HG2	1:A:1109:HIS:CD2	2.24	0.72
1:A:1259:ARG:NH2	1:A:1265:GLU:OE2	2.22	0.72
1:B:156:MET:HB3	1:B:165:LYS:HZ1	1.54	0.72
1:B:185:HIS:HB2	1:B:203:PRO:HD3	1.71	0.72
1:B:1165:TYR:O	1:B:1167:PRO:HD3	1.89	0.72
1:A:466:ALA:HB3	1:A:501:LYS:HE3	1.72	0.72
1:A:326:LYS:O	1:A:326:LYS:NZ	2.21	0.72
1:B:422:LEU:O	1:B:424:ASN:N	2.23	0.72
1:A:1316:PHE:O	1:A:1342:LYS:HB2	1.89	0.72
1:B:680:VAL:HG11	1:B:826:ILE:HD13	1.72	0.71
1:B:306:LEU:HD23	1:B:309:TRP:HE1	1.56	0.71
1:A:738:MET:HB3	1:A:776:TRP:CH2	2.26	0.71
1:A:1117:ASP:O	1:A:1120:ARG:HG2	1.91	0.71
1:A:1306:ASP:O	1:A:1310:GLU:HG3	1.91	0.70
1:B:1510:TRP:CG	1:B:1511:SER:H	1.88	0.70
1:B:1108:LYS:HD2	1:B:1159:PHE:CE2	2.27	0.70
1:B:636:TYR:CE1	1:B:643:VAL:HG13	2.27	0.70
1:A:335:ASP:OD1	1:A:336:ASP:N	2.24	0.70
1:A:680:VAL:HG11	1:A:826:ILE:HD13	1.74	0.70
1:A:962:TYR:CZ	1:A:966:ARG:HD3	2.27	0.70
1:B:1407:TYR:CE1	1:B:1424:TYR:HD1	2.10	0.69
1:B:169:ARG:NH1	1:B:701:TYR:OH	2.24	0.69
1:B:608:ARG:NE	1:B:750:GLU:HB3	2.07	0.69
1:B:143:LEU:HD23	1:B:560:TYR:CE2	2.28	0.69
1:A:251:TYR:HB2	1:A:501:LYS:CE	2.21	0.69
1:A:251:TYR:O	1:A:501:LYS:NZ	2.26	0.69
1:A:40:LYS:N	1:A:43:ASP:OD2	2.25	0.69
1:A:169:ARG:NH1	1:A:701:TYR:OH	2.25	0.69
1:A:328:GLY:N	1:A:331:LYS:HZ3	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ILE:HA	1:B:294:VAL:HG22	1.75	0.69
1:B:636:TYR:O	1:B:637:ASN:HB3	1.92	0.69
1:A:590:MET:HB2	1:A:671:ASN:HD22	1.57	0.69
1:B:306:LEU:HD23	1:B:309:TRP:NE1	2.08	0.69
1:B:716:GLU:OE2	1:B:718:ARG:NH1	2.25	0.69
1:A:629:ILE:HD13	1:A:631:GLU:HB2	1.73	0.68
1:B:420:GLU:HA	1:B:423:PHE:CB	2.23	0.68
1:B:513:TYR:CZ	1:B:517:ARG:HD3	2.29	0.68
1:B:1157:ARG:HH12	1:B:1186:GLU:CD	2.02	0.68
1:A:326:LYS:HE2	1:A:329:ASN:HB2	1.75	0.67
1:B:1432:TRP:N	1:B:1511:SER:HB3	2.10	0.67
1:A:1163:ASP:OD1	1:A:1190:ARG:NH2	2.28	0.67
1:B:238:ASN:OD1	1:B:239:ASN:ND2	2.25	0.67
1:B:1508:GLN:O	1:B:1510:TRP:HD1	1.76	0.67
1:A:1407:TYR:OH	1:A:1409:ASN:ND2	2.27	0.67
1:B:784:PHE:O	1:B:785:HIS:ND1	2.27	0.67
1:B:1213:GLU:HG3	1:B:1234:PHE:HB3	1.75	0.67
1:B:748:ASP:CG	1:B:749:ILE:H	2.00	0.67
1:A:572:MET:HE1	1:A:575:LEU:HD13	1.77	0.67
1:B:156:MET:C	1:B:165:LYS:HZ2	2.00	0.66
1:B:1156:THR:HG22	1:B:1156:THR:O	1.83	0.66
1:B:156:MET:HB3	1:B:165:LYS:NZ	2.09	0.66
1:B:290:ASP:OD1	1:B:293:LYS:HB2	1.96	0.66
1:B:520:LYS:HD2	1:B:520:LYS:O	1.96	0.66
1:B:1232:SER:N	1:B:1235:ASN:HD22	1.92	0.66
1:A:287:THR:HG22	1:A:288:VAL:H	1.60	0.65
1:B:292:ILE:HD13	1:B:427:LYS:HE2	1.76	0.65
1:A:1327:LYS:O	1:A:1327:LYS:HG2	1.97	0.65
1:B:299:LYS:HG2	1:B:300:GLU:N	2.10	0.65
1:A:179:HIS:NE2	1:A:230:ASP:OD1	2.26	0.65
1:B:162:ASP:O	1:B:165:LYS:NZ	2.21	0.65
1:B:1391:VAL:O	1:B:1431:VAL:HG13	1.97	0.65
1:A:240:SER:HB3	1:A:242:TRP:NE1	2.11	0.65
1:A:422:LEU:HA	1:A:425:ARG:HG3	1.79	0.65
1:A:150:SER:OG	1:A:700:VAL:HA	1.96	0.65
1:A:161:LYS:HD2	1:A:161:LYS:O	1.96	0.64
1:A:327:TRP:CE2	1:A:381:LYS:HE2	2.32	0.64
1:A:422:LEU:HG	1:A:425:ARG:HH21	1.62	0.64
1:B:268:LYS:O	1:B:268:LYS:HG3	1.95	0.64
1:B:1232:SER:OG	1:B:1235:ASN:ND2	2.31	0.64
1:A:520:LYS:HA	1:A:523:GLU:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:SER:OG	1:A:648:GLU:N	2.27	0.64
1:B:323:LEU:HD22	1:B:327:TRP:HE3	1.62	0.64
1:A:748:ASP:OD1	1:A:749:ILE:HG22	1.97	0.64
1:A:671:ASN:OD1	1:A:671:ASN:N	2.31	0.64
1:A:1108:LYS:HE3	1:A:1159:PHE:CD1	2.33	0.64
1:A:1219:VAL:HG22	1:A:1230:GLY:HA3	1.80	0.64
1:A:331:LYS:HB3	1:A:381:LYS:HZ2	1.63	0.63
1:A:452:PHE:CD1	1:A:466:ALA:HB2	2.33	0.63
1:B:1217:VAL:HG22	1:B:1235:ASN:CG	2.23	0.63
1:B:267:LYS:HE3	1:B:454:ARG:NH1	2.14	0.63
1:B:682:ASP:HB2	1:B:783:LYS:CD	2.28	0.63
1:B:1481:TRP:HB3	1:B:1490:LEU:HD21	1.80	0.63
1:A:284:ASP:OD1	1:A:440:PRO:HA	1.99	0.63
1:B:312:TYR:OH	1:B:414:ASP:OD2	2.15	0.63
1:B:451:TYR:CZ	1:B:491:ARG:HD2	2.34	0.63
1:B:267:LYS:HE3	1:B:454:ARG:HH11	1.64	0.62
1:B:1164:GLU:HG3	1:B:1165:TYR:O	1.99	0.62
1:B:628:LYS:HE2	1:B:630:ASP:O	2.00	0.62
1:B:682:ASP:HB2	1:B:783:LYS:HE3	1.81	0.62
1:A:1432:TRP:CG	1:A:1510:TRP:HD1	2.17	0.62
1:B:636:TYR:C	1:B:638:PRO:HD3	2.25	0.62
1:B:269:LEU:HA	1:B:272:PHE:HB3	1.82	0.62
1:B:317:LYS:O	1:B:321:SER:OG	2.15	0.62
1:A:273:SER:O	1:A:273:SER:OG	2.17	0.62
1:B:345:THR:O	1:B:348:ALA:HB3	2.00	0.62
1:B:116:ASP:HB2	1:B:117:LYS:NZ	2.15	0.62
1:B:318:GLN:HA	1:B:321:SER:HG	1.65	0.62
1:B:608:ARG:HE	1:B:750:GLU:CB	2.12	0.62
1:B:749:ILE:HG23	1:B:750:GLU:H	1.65	0.62
1:A:905:GLU:OE1	1:A:966:ARG:NH1	2.32	0.62
1:B:1159:PHE:HB3	1:B:1160:PRO:CD	2.30	0.62
1:B:1402:ASN:HB3	1:B:1426:GLN:HE21	1.63	0.62
1:B:1490:LEU:HB2	1:B:1510:TRP:CH2	2.34	0.62
1:B:1481:TRP:HB3	1:B:1490:LEU:CD2	2.30	0.62
1:A:327:TRP:CZ2	1:A:381:LYS:HE2	2.34	0.61
1:A:427:LYS:O	1:A:431:ILE:N	2.33	0.61
1:B:114:LYS:HE2	1:B:118:ASP:HA	1.82	0.61
1:B:148:MET:HE3	1:B:177:MET:HG2	1.82	0.61
1:B:423:PHE:HA	1:B:425:ARG:NH2	2.15	0.61
1:A:314:VAL:N	1:A:404:ASN:OD1	2.30	0.61
1:A:1160:PRO:HG2	1:A:1164:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ASP:CB	1:B:783:LYS:HB3	2.26	0.61
1:B:1293:LYS:HB3	1:B:1294:PRO:HD2	1.81	0.61
1:A:325:GLU:CD	1:A:326:LYS:HB3	2.25	0.61
1:A:513:TYR:CZ	1:A:517:ARG:HG3	2.35	0.61
1:B:417:GLU:OE1	1:B:417:GLU:N	2.33	0.61
1:B:1295:ASP:OD1	1:B:1296:GLY:N	2.32	0.61
1:B:323:LEU:HD22	1:B:327:TRP:CE3	2.34	0.61
1:B:369:ASN:C	1:B:370:LYS:HG2	2.25	0.61
1:B:505:GLY:HA3	1:B:510:ASP:HB3	1.83	0.61
1:A:1396:LEU:HD21	1:A:1400:ASP:HB3	1.81	0.61
1:B:1381:GLU:O	1:B:1385:GLN:HG3	2.00	0.61
1:A:326:LYS:HE3	1:A:374:ASP:HB3	1.82	0.61
1:B:185:HIS:CD2	1:B:196:TYR:CD1	2.89	0.61
1:B:875:ASP:OD2	1:B:879:ARG:NH1	2.34	0.61
1:A:1428:PRO:HB3	1:A:1493:LEU:HD21	1.82	0.61
1:B:182:PRO:HG2	1:B:192:PRO:O	2.01	0.60
1:B:1439:ARG:HD2	1:B:1521:ASP:OD2	2.02	0.60
1:A:422:LEU:HD23	1:A:425:ARG:HE	1.66	0.60
1:B:1510:TRP:CE2	1:B:1512:THR:HG23	2.36	0.60
1:A:1432:TRP:CB	1:A:1510:TRP:HD1	2.14	0.60
1:A:608:ARG:HD2	1:A:749:ILE:HG12	1.83	0.60
1:A:1490:LEU:HD12	1:A:1512:THR:HG22	1.83	0.60
1:B:1337:ARG:HD3	1:B:1382:LEU:HD22	1.83	0.60
1:B:1398:PRO:HA	1:B:1403:TYR:CD2	2.37	0.60
1:A:425:ARG:NH2	1:A:491:ARG:HB3	2.17	0.60
1:A:1195:ILE:HD12	1:A:1218:GLU:CD	2.27	0.60
1:B:422:LEU:CB	1:B:425:ARG:HD3	2.29	0.60
1:B:1105:LYS:HE2	1:B:1156:THR:O	2.01	0.60
1:A:236:THR:HG21	1:A:242:TRP:CZ2	2.37	0.59
1:A:321:SER:OG	1:A:322:GLU:N	2.33	0.59
1:A:520:LYS:HA	1:A:523:GLU:CG	2.32	0.59
1:B:900:ARG:NH1	1:B:904:GLU:O	2.34	0.59
1:A:421:GLN:O	1:A:425:ARG:HG2	2.02	0.59
1:B:1138:GLN:HE22	1:B:1275:ARG:HH21	1.49	0.59
1:A:198:GLN:NE2	1:A:236:THR:OG1	2.35	0.59
1:B:1035:LEU:CD2	1:B:1512:THR:HG22	2.31	0.59
1:B:1508:GLN:O	1:B:1510:TRP:CD1	2.55	0.59
1:A:441:ILE:O	1:A:442:THR:OG1	2.18	0.59
1:B:1211:LYS:HB2	1:B:1213:GLU:CD	2.28	0.59
1:A:328:GLY:H	1:A:331:LYS:NZ	1.99	0.59
1:A:1108:LYS:HE3	1:A:1159:PHE:HD1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1295:ASP:OD1	1:A:1296:GLY:N	2.34	0.59
1:A:1350:PRO:O	1:A:1353:ASP:HB2	2.02	0.59
1:A:281:TYR:CE2	1:A:293:LYS:HD3	2.37	0.58
1:A:1204:PRO:CB	1:A:1208:ARG:HG2	2.33	0.58
1:A:1229:HIS:HE1	1:A:1346:ARG:HG2	1.68	0.58
1:B:420:GLU:HA	1:B:423:PHE:HB2	1.84	0.58
1:B:1166:ILE:HD12	1:B:1166:ILE:N	2.18	0.58
1:A:330:SER:C	1:A:331:LYS:HD3	2.28	0.58
1:A:185:HIS:HB2	1:A:203:PRO:HD3	1.85	0.58
1:B:1213:GLU:HG3	1:B:1234:PHE:CB	2.33	0.58
1:B:1314:ARG:NH1	1:B:1329:GLU:OE2	2.35	0.58
1:B:1402:ASN:HB3	1:B:1426:GLN:NE2	2.18	0.58
1:A:766:HIS:CE1	1:A:865:THR:HG21	2.38	0.58
1:B:420:GLU:HA	1:B:423:PHE:HB3	1.85	0.58
1:B:682:ASP:HB2	1:B:783:LYS:CE	2.33	0.58
1:B:421:GLN:HE22	1:B:492:GLU:CG	2.16	0.58
1:B:673:THR:HG21	1:B:707:PHE:O	2.02	0.58
1:B:425:ARG:CG	1:B:426:ILE:N	2.57	0.58
1:A:765:PHE:HE2	1:A:767:ARG:HB2	1.68	0.58
1:B:1407:TYR:OH	1:B:1409:ASN:OD1	2.21	0.58
1:A:326:LYS:NZ	1:A:374:ASP:HB3	2.18	0.58
1:A:1217:VAL:HG12	1:A:1235:ASN:OD1	2.04	0.58
1:B:398:LYS:HG3	1:B:399:ILE:N	2.18	0.58
1:A:1439:ARG:HD2	1:A:1521:ASP:OD2	2.04	0.57
1:B:315:ASP:HB2	1:B:370:LYS:HZ1	1.68	0.57
1:A:1292:THR:HG22	1:A:1298:LYS:NZ	2.18	0.57
1:A:283:VAL:CG1	1:A:441:ILE:HG12	2.32	0.57
1:A:309:TRP:CD1	1:A:411:TYR:HH	2.22	0.57
1:A:1299:ILE:HG22	1:A:1300:SER:O	2.04	0.57
1:B:1403:TYR:O	1:B:1404:ARG:HD3	2.03	0.57
1:A:1041:GLN:OE1	1:A:1507:THR:HG21	2.05	0.57
1:A:1220:ASN:CG	1:A:1221:VAL:H	2.07	0.57
1:B:682:ASP:CB	1:B:783:LYS:HD2	2.35	0.57
1:B:1272:SER:HB2	1:B:1275:ARG:NH2	2.20	0.57
1:A:1204:PRO:HB3	1:A:1208:ARG:HG2	1.85	0.57
1:B:309:TRP:CD1	1:B:411:TYR:CE1	2.93	0.57
1:B:312:TYR:HE2	1:B:411:TYR:HD1	1.52	0.57
1:A:312:TYR:HE2	1:A:411:TYR:HD1	1.52	0.57
1:B:315:ASP:H	1:B:370:LYS:HZ3	1.53	0.57
1:A:1417:ALA:O	1:A:1423:ASN:ND2	2.37	0.57
1:B:1510:TRP:CG	1:B:1511:SER:N	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1105:LYS:NZ	1:A:1158:ARG:HE	2.03	0.56
1:A:1106:THR:O	1:A:1124:TYR:OH	2.05	0.56
1:A:1190:ARG:HG3	1:A:1195:ILE:HG22	1.87	0.56
1:A:276:MET:HA	1:A:279:LEU:HG	1.88	0.56
1:A:423:PHE:O	1:A:427:LYS:HG3	2.06	0.56
1:A:630:ASP:OD1	1:A:635:ALA:HB3	2.06	0.56
1:A:1038:THR:HG21	1:A:1512:THR:OG1	2.06	0.56
1:B:682:ASP:OD1	1:B:685:PRO:HG2	2.05	0.56
1:A:1195:ILE:HD11	1:A:1219:VAL:HB	1.87	0.56
1:B:313:VAL:HG21	1:B:408:TYR:CE1	2.40	0.56
1:A:290:ASP:N	1:A:290:ASP:OD1	2.37	0.56
1:B:292:ILE:HD13	1:B:427:LYS:CE	2.35	0.56
1:B:1160:PRO:HG2	1:B:1162:ASP:C	2.29	0.56
1:B:1195:ILE:O	1:B:1218:GLU:HB3	2.05	0.56
1:A:466:ALA:H	1:A:501:LYS:NZ	2.03	0.56
1:A:1117:ASP:HB3	1:A:1120:ARG:O	2.06	0.56
1:B:1361:THR:HG21	1:B:1437:PHE:CA	2.29	0.56
1:B:505:GLY:HA3	1:B:510:ASP:CB	2.36	0.56
1:A:893:SER:HA	1:A:896:TYR:CD2	2.40	0.56
1:B:121:GLU:HG2	1:B:122:THR:H	1.71	0.55
1:B:315:ASP:CB	1:B:370:LYS:NZ	2.68	0.55
1:A:1197:TYR:CD2	1:A:1218:GLU:OE2	2.59	0.55
1:B:1510:TRP:CE3	1:B:1511:SER:CB	2.77	0.55
1:A:312:TYR:CE2	1:A:411:TYR:HD1	2.25	0.55
1:B:704:ASP:OD2	1:B:732:LYS:HG3	2.07	0.55
1:B:1396:LEU:HD11	1:B:1400:ASP:HB3	1.88	0.55
1:B:1482:ILE:HB	1:B:1490:LEU:CD1	2.36	0.55
1:A:1342:LYS:HZ2	1:A:1345:TYR:HA	1.72	0.55
1:B:1217:VAL:HG22	1:B:1235:ASN:ND2	2.22	0.55
1:B:1330:ILE:HD11	1:B:1335:ILE:HD12	1.89	0.55
1:B:65:ILE:HG12	1:B:111:LEU:HD22	1.88	0.55
1:B:1245:GLU:HG2	1:B:1245:GLU:O	2.07	0.55
1:B:1050:SER:HB2	1:B:1056:ASN:HA	1.87	0.55
1:B:1350:PRO:O	1:B:1353:ASP:HB2	2.07	0.55
1:A:326:LYS:NZ	1:A:331:LYS:NZ	2.55	0.55
1:B:1428:PRO:HB3	1:B:1493:LEU:HD21	1.88	0.55
1:A:505:GLY:HA3	1:A:510:ASP:HB3	1.87	0.55
1:A:519:SER:O	1:A:523:GLU:HG2	2.06	0.55
1:B:307:LYS:C	1:B:309:TRP:H	2.15	0.55
1:B:717:LYS:HD2	1:B:717:LYS:O	2.06	0.55
1:B:679:THR:C	1:B:783:LYS:HZ3	2.04	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1158:ARG:HA	1:A:1173:ALA:O	2.07	0.54
1:A:1361:THR:HG21	1:A:1437:PHE:CA	2.28	0.54
1:A:1450:PRO:HA	1:A:1453:GLN:OE1	2.07	0.54
1:B:1418:THR:HA	1:B:1423:ASN:HB2	1.87	0.54
1:B:1465:SER:O	1:B:1469:ARG:HG2	2.07	0.54
1:A:242:TRP:NE1	1:A:517:ARG:HH22	2.05	0.54
1:A:273:SER:HA	1:A:276:MET:HB3	1.90	0.54
1:A:1493:LEU:HD23	1:A:1494:THR:N	2.22	0.54
1:B:1403:TYR:C	1:B:1404:ARG:HD3	2.33	0.54
1:A:251:TYR:HD1	1:A:501:LYS:HD3	1.73	0.54
1:A:692:PHE:C	1:A:767:ARG:HH21	2.15	0.54
1:B:1396:LEU:HD12	1:B:1396:LEU:C	2.32	0.54
1:A:65:ILE:HG12	1:A:111:LEU:HD22	1.90	0.54
1:A:114:LYS:HZ1	1:A:118:ASP:CG	2.14	0.54
1:A:1342:LYS:HD3	1:A:1344:LEU:O	2.07	0.54
1:B:184:GLN:HA	1:B:201:PHE:HA	1.90	0.54
1:B:291:LEU:O	1:B:294:VAL:HG13	2.08	0.54
1:B:353:ASP:CG	1:B:354:ASN:N	2.65	0.54
1:B:1157:ARG:NH1	1:B:1186:GLU:OE2	2.37	0.54
1:B:218:ARG:O	1:B:222:GLU:HG2	2.08	0.54
1:B:327:TRP:HZ3	1:B:392:ILE:HG21	1.72	0.54
1:B:391:GLY:O	1:B:395:LEU:HB2	2.08	0.54
1:B:116:ASP:HB2	1:B:117:LYS:HZ2	1.73	0.53
1:B:718:ARG:HH21	1:B:823:ILE:HG13	1.73	0.53
1:B:1510:TRP:CD2	1:B:1512:THR:N	2.76	0.53
1:B:276:MET:O	1:B:279:LEU:HB3	2.08	0.53
1:B:1210:MET:HE1	1:B:1234:PHE:O	2.09	0.53
1:B:256:SER:O	1:B:256:SER:OG	2.23	0.53
1:B:276:MET:O	1:B:279:LEU:N	2.37	0.53
1:B:1031:PHE:CG	1:B:1479:ARG:HG3	2.43	0.53
1:B:1398:PRO:HA	1:B:1403:TYR:CG	2.43	0.53
1:B:1404:ARG:HB2	1:B:1423:ASN:OD1	2.08	0.53
1:A:1432:TRP:HB3	1:A:1510:TRP:HD1	1.73	0.53
1:B:19:THR:HG22	1:B:21:CYS:O	2.07	0.53
1:B:1170:ASP:HB2	1:B:1172:LYS:H	1.74	0.53
1:A:466:ALA:H	1:A:501:LYS:HZ2	1.56	0.53
1:A:1050:SER:OG	1:A:1051:ILE:N	2.39	0.53
1:B:248:GLU:HA	1:B:252:ASN:HD21	1.74	0.53
1:B:761:GLN:O	1:B:782:THR:HG22	2.09	0.53
1:A:315:ASP:O	1:A:319:THR:OG1	2.24	0.53
1:A:1292:THR:HG22	1:A:1298:LYS:HZ2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD22	1:B:653:LYS:HB2	1.91	0.53
1:B:470:TRP:HZ3	1:B:496:TRP:HE1	1.56	0.53
1:B:1160:PRO:O	1:B:1176:TYR:OH	2.05	0.53
1:B:1166:ILE:HD11	1:B:1200:ALA:HB1	1.90	0.53
1:B:1186:GLU:O	1:B:1190:ARG:HB2	2.09	0.53
1:B:1213:GLU:HG2	1:B:1214:GLY:N	2.23	0.53
1:A:1279:GLN:NE2	1:A:1283:ASP:OD2	2.42	0.53
1:B:1474:ARG:HG2	1:B:1474:ARG:HH11	1.73	0.53
1:B:185:HIS:HD2	1:B:196:TYR:CD1	2.26	0.53
1:B:395:LEU:O	1:B:398:LYS:HG2	2.09	0.53
1:B:748:ASP:CG	1:B:749:ILE:HG22	2.33	0.53
1:B:1077:ARG:O	1:B:1081:ILE:HD12	2.09	0.53
1:B:1209:VAL:HG11	1:B:1245:GLU:HG3	1.91	0.53
1:B:1337:ARG:HD2	1:B:1340:ILE:HD11	1.90	0.53
1:A:630:ASP:HB3	1:A:633:TYR:HA	1.90	0.53
1:B:313:VAL:HG13	1:B:404:ASN:ND2	2.18	0.53
1:B:589:ALA:HB3	1:B:666:ASP:HA	1.91	0.53
1:A:1107:LEU:C	1:A:1157:ARG:HH22	2.17	0.52
1:B:420:GLU:O	1:B:423:PHE:HB3	2.10	0.52
1:B:593:TRP:CD1	1:B:597:GLU:HG3	2.44	0.52
1:A:589:ALA:HB3	1:A:666:ASP:HA	1.91	0.52
1:A:1432:TRP:HB3	1:A:1510:TRP:CD1	2.45	0.52
1:B:1160:PRO:HG3	1:B:1164:GLU:HB3	1.89	0.52
1:A:1172:LYS:HA	1:A:1175:SER:HB2	1.92	0.52
1:B:422:LEU:O	1:B:425:ARG:HB3	2.09	0.52
1:B:939:ILE:HD11	1:B:947:HIS:CD2	2.44	0.52
1:B:981:GLU:OE1	1:B:984:ARG:NH2	2.39	0.52
1:B:1453:GLN:HB3	1:B:1461:LEU:HD23	1.91	0.52
1:A:678:ARG:HB3	1:A:784:PHE:HA	1.91	0.52
1:A:1204:PRO:O	1:A:1208:ARG:HG3	2.10	0.52
1:A:1217:VAL:O	1:A:1218:GLU:CG	2.55	0.52
1:B:323:LEU:O	1:B:327:TRP:N	2.42	0.52
1:B:603:HIS:O	1:B:754:MET:HE1	2.09	0.52
1:A:182:PRO:HG2	1:A:192:PRO:O	2.09	0.52
1:A:281:TYR:HE2	1:A:293:LYS:HD3	1.74	0.52
1:B:1352:GLU:HA	1:B:1355:GLN:HG3	1.90	0.52
1:B:1431:VAL:C	1:B:1511:SER:HB3	2.35	0.52
1:A:673:THR:HG21	1:A:707:PHE:O	2.10	0.52
1:B:1106:THR:O	1:B:1124:TYR:OH	2.16	0.52
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.90	0.52
1:A:337:ASN:HB3	1:A:350:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ILE:HG12	1:A:993:LEU:HD22	1.91	0.52
1:A:1494:THR:HG22	1:A:1495:ASN:O	2.10	0.52
1:B:816:ALA:HB2	1:B:826:ILE:HG13	1.91	0.52
1:B:1160:PRO:CG	1:B:1164:GLU:HB3	2.39	0.52
1:B:1262:ALA:HB3	1:B:1345:TYR:HB3	1.91	0.52
1:A:1156:THR:HG21	1:A:1174:PHE:CD1	2.45	0.52
1:A:505:GLY:HA3	1:A:510:ASP:CB	2.40	0.52
1:A:1259:ARG:HH21	1:A:1265:GLU:CD	2.18	0.52
1:A:1260:ASP:OD1	1:A:1347:SER:HB2	2.09	0.52
1:A:1270:LEU:HD23	1:A:1308:LEU:HD11	1.92	0.52
1:A:296:ASP:HB3	1:A:299:LYS:HE3	1.92	0.51
1:A:716:GLU:CD	1:A:718:ARG:HH21	2.18	0.51
1:A:870:ILE:HD11	1:A:997:LEU:CD1	2.40	0.51
1:A:1107:LEU:O	1:A:1157:ARG:NH2	2.43	0.51
1:B:1432:TRP:N	1:B:1511:SER:CB	2.73	0.51
1:A:288:VAL:N	1:A:290:ASP:OD1	2.43	0.51
1:A:1109:HIS:CG	1:A:1197:TYR:CE2	2.98	0.51
1:A:323:LEU:C	1:A:325:GLU:OE1	2.53	0.51
1:A:452:PHE:CE1	1:A:466:ALA:HB2	2.45	0.51
1:A:466:ALA:HB3	1:A:501:LYS:CE	2.39	0.51
1:A:629:ILE:HG22	1:A:649:ILE:HA	1.91	0.51
1:B:813:THR:O	1:B:827:PRO:HG2	2.10	0.51
1:A:1259:ARG:HH12	1:A:1343:ASP:CG	2.18	0.51
1:A:1346:ARG:HG3	1:A:1346:ARG:O	2.09	0.51
1:B:1329:GLU:OE1	1:B:1329:GLU:N	2.43	0.51
1:A:813:THR:O	1:A:827:PRO:HG2	2.11	0.51
1:B:160:ILE:C	1:B:163:TRP:H	2.19	0.51
1:A:287:THR:HB	1:A:290:ASP:CG	2.36	0.51
1:A:1474:ARG:HG2	1:A:1474:ARG:HH11	1.76	0.51
1:B:323:LEU:HG	1:B:373:ILE:HG23	1.92	0.51
1:B:419:LEU:O	1:B:423:PHE:N	2.38	0.51
1:B:682:ASP:HA	1:B:685:PRO:HD2	1.93	0.51
1:B:1196:LYS:HA	1:B:1218:GLU:CD	2.36	0.51
1:B:1198:ARG:HG2	1:B:1216:ASN:HB3	1.93	0.51
1:B:236:THR:HG21	1:B:242:TRP:CZ2	2.46	0.51
1:A:72:ASP:HA	1:A:102:TYR:CE2	2.46	0.51
1:A:240:SER:HB3	1:A:242:TRP:CD1	2.46	0.51
1:A:337:ASN:O	1:A:339:PRO:HD3	2.11	0.51
1:A:1160:PRO:CG	1:A:1164:GLU:HB3	2.41	0.51
1:A:1474:ARG:HG2	1:A:1474:ARG:NH1	2.26	0.51
1:B:252:ASN:OD1	1:B:465:LEU:HD22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:LEU:HG	1:B:398:LYS:HZ2	1.76	0.51
1:B:765:PHE:HE2	1:B:767:ARG:HB2	1.76	0.51
1:A:322:GLU:O	1:A:373:ILE:HG21	2.11	0.50
1:B:1463:PRO:HD3	1:B:1526:TYR:CE1	2.46	0.50
1:A:1432:TRP:CG	1:A:1510:TRP:CD1	2.98	0.50
1:A:312:TYR:HE2	1:A:411:TYR:CD1	2.30	0.50
1:B:165:LYS:HD2	1:B:166:VAL:HG23	1.93	0.50
1:B:268:LYS:O	1:B:269:LEU:HD23	2.10	0.50
1:B:513:TYR:OH	1:B:517:ARG:HD3	2.10	0.50
1:B:836:PHE:CD1	1:B:852:PRO:HD3	2.46	0.50
1:A:242:TRP:CG	1:A:517:ARG:HH12	2.29	0.50
1:B:1185:TYR:CG	1:B:1288:TYR:HD2	2.30	0.50
1:A:114:LYS:NZ	1:A:118:ASP:HA	2.27	0.50
1:A:160:ILE:O	1:A:163:TRP:HB2	2.11	0.50
1:A:1029:THR:HG22	1:A:1030:VAL:H	1.77	0.50
1:A:1403:TYR:O	1:A:1404:ARG:HD3	2.11	0.50
1:B:191:SER:HB3	1:B:498:ASP:OD2	2.12	0.50
1:B:315:ASP:H	1:B:370:LYS:HZ1	1.59	0.50
1:B:1404:ARG:O	1:B:1423:ASN:ND2	2.42	0.50
1:B:1432:TRP:CA	1:B:1511:SER:HB3	2.42	0.50
1:A:296:ASP:CB	1:A:299:LYS:HE3	2.42	0.50
1:A:629:ILE:CD1	1:A:631:GLU:HB2	2.39	0.50
1:A:704:ASP:OD2	1:A:732:LYS:HG3	2.11	0.50
1:B:513:TYR:CE2	1:B:517:ARG:HD3	2.47	0.50
1:B:541:PRO:HB2	1:B:543:HIS:CE1	2.46	0.50
1:B:681:GLU:HA	1:B:810:LEU:HD23	1.93	0.50
1:A:198:GLN:HG3	1:A:518:MET:HE1	1.94	0.50
1:A:411:TYR:CZ	1:A:415:ILE:HG13	2.47	0.50
1:B:423:PHE:HA	1:B:425:ARG:CZ	2.42	0.50
1:B:1131:TRP:CD1	1:B:1266:ILE:HG23	2.47	0.50
1:A:325:GLU:HG2	1:A:326:LYS:HB3	1.94	0.50
1:A:812:ARG:NH2	1:A:815:ASP:OD1	2.45	0.50
1:B:1042:MET:HE3	1:B:1508:GLN:C	2.35	0.50
1:B:274:GLU:H	1:B:274:GLU:CD	2.19	0.50
1:B:1219:VAL:HG22	1:B:1230:GLY:HA3	1.94	0.50
1:B:1431:VAL:CG1	1:B:1510:TRP:HZ3	2.25	0.50
1:A:939:ILE:HD11	1:A:947:HIS:CD2	2.46	0.49
1:A:1262:ALA:HB3	1:A:1345:TYR:HB3	1.93	0.49
1:A:453:THR:N	1:A:465:LEU:O	2.30	0.49
1:A:1198:ARG:HA	1:A:1216:ASN:HA	1.93	0.49
1:A:1259:ARG:NH1	1:A:1343:ASP:OD2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1402:ASN:N	1:B:1402:ASN:HD22	2.11	0.49
1:B:1431:VAL:HG11	1:B:1510:TRP:HZ3	1.78	0.49
1:A:273:SER:HA	1:A:276:MET:CB	2.42	0.49
1:A:447:LEU:HD12	1:A:448:SER:HB3	1.95	0.49
1:B:303:ILE:O	1:B:306:LEU:HD22	2.12	0.49
1:A:283:VAL:HG11	1:A:441:ILE:CG1	2.35	0.49
1:A:418:VAL:HG22	1:A:490:ARG:HA	1.94	0.49
1:A:1105:LYS:NZ	1:A:1158:ARG:HH21	2.11	0.49
1:A:1330:ILE:HD12	1:A:1331:ASP:N	2.28	0.49
1:B:742:ILE:HG21	1:B:767:ARG:NH2	2.20	0.49
1:B:882:ALA:HB2	1:B:982:TRP:CZ2	2.47	0.49
1:A:285:LEU:HD21	1:A:290:ASP:OD2	2.13	0.49
1:A:1462:LYS:HG3	1:A:1463:PRO:N	2.28	0.49
1:B:679:THR:OG1	1:B:783:LYS:HE2	2.12	0.49
1:B:1213:GLU:CG	1:B:1214:GLY:N	2.76	0.49
1:A:8:LEU:HB2	1:A:652:PRO:HG2	1.94	0.49
1:B:148:MET:HE2	1:B:179:HIS:HB2	1.95	0.49
1:B:162:ASP:O	1:B:165:LYS:HG2	2.12	0.49
1:B:886:THR:OG1	1:B:1009:MET:HE1	2.13	0.49
1:B:1185:TYR:HE1	1:B:1290:GLU:O	1.95	0.49
1:A:816:ALA:HB2	1:A:826:ILE:HG13	1.95	0.49
1:A:1105:LYS:HE2	1:A:1156:THR:O	2.12	0.49
1:B:274:GLU:CD	1:B:275:GLN:H	2.20	0.49
1:A:1229:HIS:CE1	1:A:1346:ARG:HG2	2.48	0.49
1:B:274:GLU:HG2	1:B:275:GLN:HG3	1.95	0.49
1:B:318:GLN:HA	1:B:321:SER:OG	2.12	0.48
1:B:1432:TRP:CA	1:B:1511:SER:CB	2.91	0.48
1:A:1161:LEU:HD23	1:A:1161:LEU:O	2.13	0.48
1:A:1223:TRP:HD1	1:A:1293:LYS:HZ3	1.51	0.48
1:A:1330:ILE:HD11	1:A:1335:ILE:HD12	1.94	0.48
1:B:1396:LEU:CD2	1:B:1426:GLN:HB2	2.40	0.48
1:B:1407:TYR:CZ	1:B:1424:TYR:HD1	2.30	0.48
1:B:1459:LYS:HD2	1:B:1459:LYS:HA	1.36	0.48
1:A:326:LYS:HZ3	1:A:331:LYS:NZ	2.11	0.48
1:A:1223:TRP:CD1	1:A:1293:LYS:NZ	2.76	0.48
1:B:127:TYR:HB2	1:B:578:GLU:HG2	1.94	0.48
1:B:315:ASP:CB	1:B:370:LYS:HZ1	2.27	0.48
1:B:357:GLU:HB3	1:B:358:PRO:HD2	1.95	0.48
1:A:738:MET:HE2	1:A:776:TRP:CE2	2.48	0.48
1:B:309:TRP:HE3	1:B:311:PHE:HB2	1.77	0.48
1:B:312:TYR:CE2	1:B:411:TYR:HD1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLN:HE22	1:B:492:GLU:HG2	1.78	0.48
1:A:1115:LEU:HB3	1:A:1123:ARG:HB3	1.95	0.48
1:B:231:ILE:HD12	1:B:532:PHE:CG	2.48	0.48
1:B:338:ILE:HG23	1:B:383:LEU:HD22	1.96	0.48
1:B:682:ASP:H	1:B:783:LYS:HE3	1.77	0.48
1:B:1287:LYS:HE3	1:B:1288:TYR:CE1	2.49	0.48
1:B:1291:VAL:HB	1:B:1299:ILE:HG13	1.96	0.48
1:A:357:GLU:HB3	1:A:358:PRO:HD2	1.95	0.48
1:A:1238:THR:HG21	1:A:1259:ARG:HE	1.78	0.48
1:B:422:LEU:HA	1:B:425:ARG:HB3	1.96	0.48
1:B:717:LYS:HD2	1:B:717:LYS:C	2.37	0.48
1:B:1259:ARG:HB3	1:B:1344:LEU:HD21	1.96	0.48
1:B:728:ILE:HD11	1:B:810:LEU:HD22	1.95	0.48
1:A:299:LYS:HD2	1:A:300:GLU:HB3	1.95	0.48
1:A:252:ASN:OD1	1:A:254:LYS:HB2	2.14	0.48
1:A:683:THR:HG22	1:A:728:ILE:HG13	1.96	0.48
1:B:159:THR:O	1:B:163:TRP:CD1	2.67	0.48
1:B:1400:ASP:OD2	1:B:1401:TYR:N	2.47	0.48
1:A:761:GLN:O	1:A:782:THR:OG1	2.30	0.48
1:B:274:GLU:OE1	1:B:274:GLU:N	2.47	0.48
1:B:396:ALA:O	1:B:400:LEU:HG	2.13	0.48
1:B:871:ASP:OD1	1:B:872:ASP:N	2.47	0.48
1:B:1230:GLY:O	1:B:1260:ASP:HA	2.13	0.48
1:A:907:ASP:OD1	1:A:1047:LYS:HB2	2.14	0.47
1:A:1082:SER:OG	1:A:1510:TRP:HB3	2.13	0.47
1:A:251:TYR:CD1	1:A:503:ARG:HB2	2.49	0.47
1:A:326:LYS:CE	1:A:329:ASN:HB2	2.42	0.47
1:A:326:LYS:O	1:A:331:LYS:NZ	2.44	0.47
1:B:1272:SER:HB2	1:B:1275:ARG:HH22	1.79	0.47
1:B:1449:ASN:O	1:B:1453:GLN:NE2	2.46	0.47
1:A:326:LYS:NZ	1:A:331:LYS:HZ2	2.13	0.47
1:A:1154:LYS:HB2	1:A:1154:LYS:HE2	1.65	0.47
1:B:161:LYS:N	1:B:161:LYS:HD3	2.28	0.47
1:B:749:ILE:HG23	1:B:750:GLU:HG2	1.96	0.47
1:B:900:ARG:HH22	1:B:908:TYR:HE1	1.63	0.47
1:B:1342:LYS:HB2	1:B:1353:ASP:O	2.14	0.47
1:A:256:SER:O	1:A:256:SER:OG	2.24	0.47
1:A:1293:LYS:HG3	1:A:1294:PRO:N	2.29	0.47
1:B:35:LEU:CD1	1:B:133:ILE:HD13	2.45	0.47
1:B:315:ASP:OD2	1:B:318:GLN:HB3	2.15	0.47
1:B:470:TRP:HZ3	1:B:496:TRP:NE1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1064:LEU:O	1:A:1506:PRO:HD2	2.14	0.47
1:B:1197:TYR:O	1:B:1218:GLU:OE2	2.33	0.47
1:A:269:LEU:HA	1:A:272:PHE:HB3	1.97	0.47
1:A:440:PRO:HB2	1:A:441:ILE:H	1.44	0.47
1:A:947:HIS:CD2	1:A:949:LEU:H	2.33	0.47
1:A:1138:GLN:HG3	1:A:1276:PHE:CD1	2.50	0.47
1:A:1349:LYS:HG3	1:A:1352:GLU:HG3	1.97	0.47
1:B:236:THR:HG21	1:B:242:TRP:CH2	2.50	0.47
1:A:165:LYS:HD2	1:A:165:LYS:HA	1.57	0.47
1:A:235:HIS:CG	1:A:499:CYS:HB3	2.50	0.47
1:A:284:ASP:HB3	1:A:438:GLN:HE21	1.78	0.47
1:A:334:SER:HA	1:A:382:LYS:NZ	2.29	0.47
1:A:1048:SER:HB2	1:A:1070:ASN:ND2	2.29	0.47
1:A:1084:ARG:HG3	1:A:1088:LEU:HD12	1.97	0.47
1:A:1342:LYS:NZ	1:A:1345:TYR:HA	2.29	0.47
1:B:350:PHE:O	1:B:353:ASP:CG	2.58	0.47
1:B:381:LYS:HA	1:B:385:SER:O	2.15	0.47
1:B:679:THR:N	1:B:783:LYS:HE2	2.29	0.47
1:B:682:ASP:HB2	1:B:783:LYS:HD2	1.95	0.47
1:B:1107:LEU:HD22	1:B:1183:ILE:HG23	1.97	0.47
1:B:1159:PHE:HB3	1:B:1160:PRO:HD2	1.94	0.47
1:B:1397:ASP:OD2	1:B:1399:SER:OG	2.28	0.47
1:A:66:TRP:CH2	1:A:84:LYS:HG3	2.50	0.47
1:A:728:ILE:HD11	1:A:810:LEU:HD22	1.96	0.47
1:A:966:ARG:NH1	1:A:966:ARG:HB3	2.30	0.47
1:B:377:ALA:O	1:B:381:LYS:HG2	2.15	0.47
1:A:312:TYR:CD2	1:A:411:TYR:HB2	2.50	0.47
1:A:1109:HIS:CE1	1:A:1163:ASP:HB3	2.50	0.47
1:B:31:PRO:O	1:B:47:TYR:OH	2.23	0.47
1:B:148:MET:HA	1:B:177:MET:O	2.15	0.47
1:B:311:PHE:HE2	1:B:364:GLY:O	1.98	0.47
1:B:315:ASP:HB2	1:B:370:LYS:NZ	2.30	0.47
1:B:324:ARG:HB2	1:B:388:TYR:CZ	2.50	0.47
1:B:518:MET:HA	1:B:521:TYR:HB3	1.97	0.47
1:B:648:GLU:OE2	1:B:876:HIS:HD2	1.97	0.47
1:A:251:TYR:CD1	1:A:501:LYS:HD3	2.50	0.47
1:A:1062:ALA:HB1	1:A:1510:TRP:CZ3	2.42	0.47
1:B:163:TRP:HA	1:B:165:LYS:NZ	2.30	0.47
1:B:443:LYS:HA	1:B:443:LYS:HD2	1.74	0.47
1:B:634:CYS:HB3	1:B:636:TYR:CE1	2.40	0.47
1:B:1108:LYS:HD2	1:B:1159:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLY:HA3	1:A:465:LEU:HD13	1.98	0.46
1:B:194:SER:OG	1:B:498:ASP:OD2	2.31	0.46
1:B:682:ASP:O	1:B:683:THR:C	2.56	0.46
1:B:1112:ILE:HG13	1:B:1113:PRO:HD2	1.97	0.46
1:B:307:LYS:C	1:B:309:TRP:N	2.72	0.46
1:B:395:LEU:HG	1:B:398:LYS:NZ	2.31	0.46
1:B:451:TYR:CD1	1:B:495:VAL:HG21	2.50	0.46
1:B:1198:ARG:NH1	1:B:1212:ASP:O	2.49	0.46
1:A:268:LYS:O	1:A:269:LEU:HD23	2.15	0.46
1:A:1157:ARG:HH11	1:A:1157:ARG:HG3	1.80	0.46
1:A:1204:PRO:O	1:A:1208:ARG:CG	2.63	0.46
1:A:170:VAL:HA	1:A:173:LYS:HE2	1.98	0.46
1:A:329:ASN:H	1:A:331:LYS:NZ	2.13	0.46
1:A:1342:LYS:CE	1:A:1353:ASP:HB3	2.40	0.46
1:B:66:TRP:CZ3	1:B:84:LYS:HB2	2.51	0.46
1:B:353:ASP:OD2	1:B:354:ASN:ND2	2.46	0.46
1:B:707:PHE:CD1	1:B:823:ILE:HD11	2.51	0.46
1:A:251:TYR:H	1:A:501:LYS:HD3	1.81	0.46
1:A:1179:THR:OG1	1:A:1182:GLU:HG2	2.16	0.46
1:B:310:GLU:H	1:B:310:GLU:CD	2.23	0.46
1:B:1109:HIS:O	1:B:1111:LEU:HD13	2.15	0.46
1:A:541:PRO:HB2	1:A:543:HIS:CE1	2.50	0.46
1:A:893:SER:HA	1:A:896:TYR:HD2	1.81	0.46
1:A:1035:LEU:O	1:A:1038:THR:HB	2.16	0.46
1:B:173:LYS:HE2	1:B:175:TYR:HE2	1.81	0.46
1:B:267:LYS:HE2	1:B:267:LYS:HB3	1.66	0.46
1:B:491:ARG:HA	1:B:491:ARG:HD3	1.79	0.46
1:B:573:ASP:O	1:B:577:VAL:HG23	2.16	0.46
1:A:161:LYS:HA	1:A:164:GLU:HB2	1.98	0.46
1:A:287:THR:HG22	1:A:288:VAL:N	2.27	0.46
1:A:331:LYS:HD2	1:A:331:LYS:HA	1.60	0.46
1:A:466:ALA:C	1:A:501:LYS:HG3	2.40	0.46
1:A:542:LEU:O	1:A:546:GLN:HG3	2.16	0.46
1:A:594:SER:OG	1:A:596:GLU:HG2	2.16	0.46
1:B:136:VAL:HG13	1:B:137:ASN:H	1.81	0.46
1:B:296:ASP:HB3	1:B:299:LYS:HD3	1.96	0.46
1:B:327:TRP:CZ3	1:B:392:ILE:HG21	2.51	0.46
1:A:279:LEU:HD12	1:A:279:LEU:O	2.16	0.46
1:B:1064:LEU:O	1:B:1506:PRO:HD2	2.15	0.46
1:A:275:GLN:N	1:A:275:GLN:OE1	2.49	0.46
1:A:417:GLU:O	1:A:421:GLN:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:MET:HB3	1:A:776:TRP:CZ2	2.50	0.46
1:B:309:TRP:CD1	1:B:411:TYR:HE1	2.34	0.46
1:B:312:TYR:CD2	1:B:411:TYR:HB2	2.51	0.46
1:B:503:ARG:NH2	1:B:511:SER:OG	2.49	0.46
1:B:635:ALA:C	1:B:636:TYR:HD1	2.24	0.46
1:B:748:ASP:OD1	1:B:749:ILE:N	2.40	0.46
1:B:1174:PHE:CZ	1:B:1174:PHE:CD1	2.97	0.46
1:B:1349:LYS:HG3	1:B:1352:GLU:HG3	1.98	0.46
1:A:1123:ARG:NH2	1:A:1207:ASP:HB2	2.19	0.46
1:B:891:LEU:HD23	1:B:891:LEU:HA	1.81	0.46
1:A:127:TYR:HB2	1:A:578:GLU:HG2	1.98	0.45
1:A:1158:ARG:O	1:A:1159:PHE:CD2	2.59	0.45
1:B:149:GLN:HG2	1:B:175:TYR:CE1	2.51	0.45
1:B:1185:TYR:CE1	1:B:1290:GLU:O	2.69	0.45
1:B:1206:LEU:HD12	1:B:1207:ASP:N	2.31	0.45
1:A:329:ASN:H	1:A:331:LYS:HZ3	1.63	0.45
1:A:742:ILE:HG22	1:A:743:ALA:N	2.30	0.45
1:A:1508:GLN:NE2	1:A:1510:TRP:CH2	2.85	0.45
1:B:429:LEU:O	1:B:430:ARG:HB2	2.15	0.45
1:B:1270:LEU:HD23	1:B:1308:LEU:HD11	1.98	0.45
1:A:325:GLU:OE2	1:A:326:LYS:HB3	2.16	0.45
1:B:307:LYS:O	1:B:310:GLU:OE1	2.35	0.45
1:B:682:ASP:C	1:B:684:LEU:N	2.72	0.45
1:B:1432:TRP:HA	1:B:1511:SER:HB3	1.98	0.45
1:A:435:GLY:HA2	1:A:436:PRO:HD2	1.77	0.45
1:B:350:PHE:O	1:B:351:VAL:C	2.59	0.45
1:B:424:ASN:OD1	1:B:424:ASN:O	2.34	0.45
1:B:1196:LYS:HE2	1:B:1218:GLU:HB2	1.98	0.45
1:A:679:THR:HG21	1:A:783:LYS:HE3	1.98	0.45
1:A:896:TYR:HD1	1:A:900:ARG:HD3	1.80	0.45
1:B:1407:TYR:CZ	1:B:1424:TYR:CD1	3.04	0.45
1:B:1510:TRP:NE1	1:B:1512:THR:HG23	2.31	0.45
1:A:713:LEU:H	1:A:713:LEU:HD12	1.81	0.45
1:A:1131:TRP:CD1	1:A:1266:ILE:HG23	2.52	0.45
1:B:266:ASP:HB3	1:B:454:ARG:HH22	1.82	0.45
1:B:312:TYR:HE2	1:B:411:TYR:CD1	2.34	0.45
1:B:928:GLY:CA	1:B:966:ARG:HH12	2.30	0.45
1:B:947:HIS:CD2	1:B:949:LEU:H	2.34	0.45
1:B:1108:LYS:HD2	1:B:1159:PHE:CD2	2.51	0.45
1:B:1128:ASP:OD1	1:B:1129:ALA:N	2.49	0.45
1:B:1211:LYS:HB2	1:B:1213:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1235:ASN:O	1:B:1258:PRO:HB3	2.16	0.45
1:A:681:GLU:HA	1:A:810:LEU:HD23	1.97	0.45
1:B:1421:GLY:O	1:B:1424:TYR:HB2	2.17	0.45
1:B:1467:LEU:O	1:B:1470:LYS:HB2	2.17	0.45
1:A:761:GLN:HE21	1:A:761:GLN:HB3	1.44	0.45
1:B:183:LEU:N	1:B:184:GLN:OE1	2.50	0.45
1:B:267:LYS:O	1:B:271:ASP:HB2	2.17	0.45
1:B:1161:LEU:O	1:B:1161:LEU:HD23	2.17	0.45
1:A:325:GLU:CG	1:A:326:LYS:HB3	2.47	0.45
1:A:649:ILE:H	1:A:649:ILE:HG13	1.56	0.45
1:B:179:HIS:NE2	1:B:533:ARG:HD2	2.32	0.45
1:A:302:VAL:HG23	1:A:303:ILE:H	1.82	0.44
1:A:664:PHE:CE2	1:A:690:VAL:HG22	2.52	0.44
1:A:1042:MET:HE3	1:A:1509:ALA:N	2.32	0.44
1:A:1193:GLY:O	1:A:1294:PRO:HD3	2.17	0.44
1:B:1397:ASP:OD2	1:B:1399:SER:N	2.48	0.44
1:A:938:LYS:HE2	1:A:942:TYR:HE2	1.83	0.44
1:A:1454:VAL:HG12	1:A:1455:GLU:N	2.32	0.44
1:B:1087:LEU:HA	1:B:1092:ARG:HB2	1.99	0.44
1:A:575:LEU:HD11	1:A:579:ARG:NH2	2.33	0.44
1:A:649:ILE:HD12	1:A:649:ILE:O	2.16	0.44
1:A:1050:SER:HB2	1:A:1056:ASN:HA	1.98	0.44
1:B:186:ARG:HD2	1:B:192:PRO:HA	1.99	0.44
1:B:350:PHE:CD1	1:B:353:ASP:OD2	2.70	0.44
1:B:421:GLN:HE22	1:B:492:GLU:CA	2.30	0.44
1:B:451:TYR:CE1	1:B:491:ARG:HD2	2.53	0.44
1:B:1029:THR:HG22	1:B:1030:VAL:N	2.33	0.44
1:A:69:CYS:SG	1:A:107:TYR:HB3	2.58	0.44
1:A:1107:LEU:O	1:A:1157:ARG:NH1	2.48	0.44
1:A:1223:TRP:HD1	1:A:1293:LYS:NZ	2.15	0.44
1:B:81:LYS:HG2	1:B:83:TYR:CZ	2.53	0.44
1:B:184:GLN:O	1:B:186:ARG:HG2	2.17	0.44
1:B:1324:ASP:OD2	1:B:1324:ASP:N	2.50	0.44
1:A:388:TYR:HA	1:A:392:ILE:HG13	1.99	0.44
1:A:1029:THR:HG22	1:A:1030:VAL:N	2.33	0.44
1:B:117:LYS:N	1:B:117:LYS:CD	2.76	0.44
1:B:189:SER:OG	1:B:498:ASP:CG	2.61	0.44
1:B:1094:GLU:O	1:B:1098:GLU:HG2	2.16	0.44
1:B:1185:TYR:CG	1:B:1288:TYR:CD2	3.05	0.44
1:A:57:SER:O	1:A:60:THR:OG1	2.33	0.44
1:B:761:GLN:HE21	1:B:761:GLN:HB3	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ALA:O	1:A:400:LEU:HG	2.17	0.44
1:A:1108:LYS:NZ	1:A:1164:GLU:O	2.47	0.44
1:B:148:MET:HE1	1:B:228:LEU:HD11	1.99	0.44
1:A:182:PRO:HD3	1:A:230:ASP:HB2	1.99	0.44
1:A:186:ARG:HD2	1:A:190:ASN:OD1	2.18	0.44
1:B:108:CYS:HB3	1:B:127:TYR:CD2	2.52	0.44
1:B:1085:GLY:HA3	1:B:1513:GLY:CA	2.48	0.44
1:A:35:LEU:HD12	1:A:35:LEU:H	1.83	0.44
1:A:108:CYS:HB3	1:A:127:TYR:CD2	2.52	0.44
1:A:609:PRO:O	1:A:612:SER:HB2	2.18	0.44
1:A:875:ASP:OD2	1:A:879:ARG:NH1	2.51	0.44
1:A:1105:LYS:HZ3	1:A:1158:ARG:HE	1.66	0.44
1:A:1514:CYS:O	1:A:1517:ASP:HB2	2.18	0.44
1:B:520:LYS:NZ	1:B:527:ARG:NH2	2.66	0.44
1:B:782:THR:OG1	1:B:783:LYS:N	2.49	0.44
1:B:834:THR:HG22	1:B:835:GLY:H	1.83	0.44
1:B:1320:LYS:HB3	1:B:1320:LYS:HE3	1.84	0.44
1:A:291:LEU:HA	1:A:294:VAL:CG2	2.45	0.43
1:B:43:ASP:OD1	1:B:43:ASP:N	2.49	0.43
1:B:307:LYS:HG2	1:B:310:GLU:OE2	2.18	0.43
1:B:351:VAL:HG21	1:B:399:ILE:HD13	1.99	0.43
1:B:415:ILE:HG22	1:B:418:VAL:HG21	2.01	0.43
1:B:631:GLU:HB2	1:B:650:MET:SD	2.58	0.43
1:B:637:ASN:OD1	1:B:637:ASN:C	2.61	0.43
1:A:326:LYS:HZ1	1:A:331:LYS:HZ2	1.64	0.43
1:B:674:PRO:HB3	1:B:783:LYS:NZ	2.33	0.43
1:B:899:TYR:O	1:B:900:ARG:HB2	2.19	0.43
1:A:637:ASN:HA	1:A:638:PRO:HD3	1.85	0.43
1:A:1455:GLU:CD	1:A:1455:GLU:H	2.25	0.43
1:B:163:TRP:C	1:B:165:LYS:H	2.25	0.43
1:B:404:ASN:OD1	1:B:404:ASN:N	2.52	0.43
1:B:542:LEU:O	1:B:546:GLN:HG3	2.18	0.43
1:B:928:GLY:HA2	1:B:966:ARG:NH1	2.33	0.43
1:B:1042:MET:HE3	1:B:1508:GLN:O	2.19	0.43
1:A:66:TRP:O	1:A:109:PHE:HA	2.18	0.43
1:A:143:LEU:HD23	1:A:143:LEU:O	2.18	0.43
1:A:899:TYR:O	1:A:900:ARG:HB2	2.19	0.43
1:A:962:TYR:O	1:A:966:ARG:HG3	2.19	0.43
1:B:114:LYS:HE2	1:B:118:ASP:CA	2.45	0.43
1:B:270:LEU:C	1:B:443:LYS:HZ1	2.25	0.43
1:B:425:ARG:CD	1:B:426:ILE:HD12	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:900:ARG:HD3	1:B:900:ARG:HA	1.74	0.43
1:B:1084:ARG:HG3	1:B:1088:LEU:HD12	2.00	0.43
1:A:312:TYR:CE2	1:A:411:TYR:CD1	3.05	0.43
1:A:1185:TYR:CE1	1:A:1189:ASN:HB2	2.53	0.43
1:A:1456:GLY:HA3	1:A:1460:LYS:O	2.18	0.43
1:B:637:ASN:N	1:B:638:PRO:HD3	2.34	0.43
1:B:1050:SER:OG	1:B:1051:ILE:N	2.52	0.43
1:A:947:HIS:HD2	1:A:949:LEU:H	1.67	0.43
1:B:794:ARG:HH21	1:B:850:LEU:HD21	1.84	0.43
1:A:67:THR:HG21	1:A:99:LEU:HD22	2.00	0.43
1:A:856:PRO:O	1:A:859:SER:OG	2.24	0.43
1:A:1201:ASN:HB2	1:A:1206:LEU:HD11	2.00	0.43
1:B:414:ASP:O	1:B:417:GLU:HG2	2.19	0.43
1:B:835:GLY:HA3	1:B:852:PRO:HB3	2.00	0.43
1:A:326:LYS:HZ3	1:A:331:LYS:HZ1	1.67	0.43
1:A:1293:LYS:HD2	1:A:1294:PRO:HD2	1.99	0.43
1:A:1463:PRO:HD3	1:A:1526:TYR:CE1	2.54	0.43
1:B:327:TRP:CE3	1:B:388:TYR:CD1	3.07	0.43
1:B:422:LEU:CA	1:B:425:ARG:HD3	2.48	0.43
1:B:426:ILE:HD13	1:B:447:LEU:HD11	1.99	0.43
1:B:455:PHE:HE2	1:B:465:LEU:HG	1.82	0.43
1:B:1031:PHE:CD1	1:B:1479:ARG:HG3	2.54	0.43
1:A:302:VAL:HG23	1:A:303:ILE:N	2.34	0.43
1:A:594:SER:OG	1:A:597:GLU:HG3	2.19	0.43
1:B:106:THR:HG21	1:B:579:ARG:O	2.18	0.43
1:B:214:ASP:O	1:B:218:ARG:HB2	2.19	0.43
1:B:1108:LYS:HD3	1:B:1124:TYR:CE1	2.54	0.43
1:B:1160:PRO:HG2	1:B:1162:ASP:O	2.19	0.43
1:A:1337:ARG:HB2	1:A:1340:ILE:HD12	2.01	0.43
1:B:318:GLN:O	1:B:318:GLN:HG2	2.18	0.43
1:B:728:ILE:O	1:B:731:VAL:N	2.49	0.43
1:A:285:LEU:HD21	1:A:290:ASP:CB	2.48	0.42
1:A:290:ASP:CG	1:A:291:LEU:N	2.78	0.42
1:A:868:LEU:O	1:A:994:PRO:HD3	2.18	0.42
1:A:1223:TRP:NE1	1:A:1293:LYS:HZ3	2.15	0.42
1:B:697:ILE:HD11	1:B:739:ARG:NE	2.35	0.42
1:B:1131:TRP:HA	1:B:1134:VAL:HG12	2.00	0.42
1:B:1493:LEU:HD23	1:B:1494:THR:N	2.34	0.42
1:A:446:PRO:HG2	1:A:448:SER:O	2.19	0.42
1:A:1322:LYS:H	1:A:1322:LYS:CD	2.27	0.42
1:B:493:VAL:HG12	1:B:495:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:O	1:A:554:ARG:NH1	2.52	0.42
1:A:451:TYR:CD1	1:A:495:VAL:HG11	2.55	0.42
1:B:237:ALA:C	1:B:239:ASN:H	2.27	0.42
1:B:395:LEU:HA	1:B:398:LYS:HG2	2.00	0.42
1:B:1248:LYS:NZ	1:B:1414:ASP:HB3	2.34	0.42
1:B:1514:CYS:O	1:B:1517:ASP:HB2	2.19	0.42
1:A:307:LYS:C	1:A:309:TRP:H	2.26	0.42
1:A:611:GLY:N	1:A:753:GLU:OE1	2.52	0.42
1:B:682:ASP:CG	1:B:686:ASN:HB2	2.40	0.42
1:A:295:MET:HA	1:A:298:ILE:HB	2.02	0.42
1:A:447:LEU:HD12	1:A:448:SER:N	2.34	0.42
1:B:69:CYS:HA	1:B:70:PRO:HD2	1.92	0.42
1:B:281:TYR:HA	1:B:282:PRO:HD3	1.60	0.42
1:B:142:PRO:C	1:B:144:ASN:H	2.28	0.42
1:B:966:ARG:CG	1:B:967:LEU:N	2.83	0.42
1:B:1174:PHE:CB	1:B:1174:PHE:CD2	2.93	0.42
1:A:115:ASN:OD1	1:A:116:ASP:N	2.51	0.42
1:A:214:ASP:O	1:A:218:ARG:HB2	2.19	0.42
1:B:51:LEU:HD13	1:B:65:ILE:HD13	2.02	0.42
1:B:136:VAL:HG13	1:B:137:ASN:N	2.34	0.42
1:B:1240:MET:HA	1:B:1425:HIS:CE1	2.54	0.42
1:B:1306:ASP:O	1:B:1310:GLU:HG3	2.20	0.42
1:A:237:ALA:C	1:A:239:ASN:H	2.27	0.42
1:A:417:GLU:HG3	1:A:490:ARG:CZ	2.49	0.42
1:B:325:GLU:OE2	1:B:326:LYS:HG2	2.18	0.42
1:A:547:TYR:O	1:A:551:VAL:HG23	2.19	0.42
1:A:1120:ARG:O	1:A:1120:ARG:CG	2.66	0.42
1:A:1190:ARG:HG3	1:A:1195:ILE:CG2	2.49	0.42
1:B:149:GLN:HG2	1:B:175:TYR:CD1	2.55	0.42
1:B:153:SER:HA	1:B:156:MET:SD	2.60	0.42
1:B:541:PRO:HB2	1:B:543:HIS:HE1	1.85	0.42
1:B:682:ASP:CB	1:B:783:LYS:CD	2.95	0.42
1:A:1195:ILE:O	1:A:1218:GLU:HB3	2.20	0.42
1:B:834:THR:HG22	1:B:835:GLY:N	2.35	0.42
1:A:51:LEU:HD13	1:A:65:ILE:HD13	2.01	0.41
1:A:1151:LEU:HD11	1:A:1280:LEU:HD21	2.01	0.41
1:A:1319:PRO:O	1:A:1338:ARG:HB2	2.20	0.41
1:B:229:THR:OG1	1:B:230:ASP:O	2.34	0.41
1:B:426:ILE:HA	1:B:429:LEU:CB	2.43	0.41
1:B:490:ARG:NH2	1:B:492:GLU:OE2	2.53	0.41
1:B:674:PRO:C	1:B:679:THR:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:ILE:HD13	1:B:767:ARG:HE	1.84	0.41
1:B:891:LEU:HD13	1:B:1092:ARG:HD3	2.01	0.41
1:B:947:HIS:HD2	1:B:949:LEU:H	1.68	0.41
1:B:1196:LYS:HA	1:B:1218:GLU:CG	2.49	0.41
1:B:1510:TRP:CG	1:B:1512:THR:H	2.37	0.41
1:A:194:SER:HB3	1:A:498:ASP:HB3	2.01	0.41
1:A:573:ASP:O	1:A:577:VAL:HG23	2.20	0.41
1:B:315:ASP:HB3	1:B:370:LYS:NZ	2.35	0.41
1:B:966:ARG:HG3	1:B:967:LEU:N	2.31	0.41
1:B:1105:LYS:HG2	1:B:1155:VAL:HB	2.02	0.41
1:A:203:PRO:O	1:A:207:LYS:NZ	2.53	0.41
1:B:182:PRO:HD3	1:B:230:ASP:HB2	2.02	0.41
1:B:313:VAL:HG21	1:B:408:TYR:CD1	2.55	0.41
1:B:989:ARG:HE	1:B:989:ARG:HB2	1.62	0.41
1:B:1077:ARG:NE	1:B:1128:ASP:OD2	2.53	0.41
1:B:1395:THR:HB	1:B:1425:HIS:O	2.20	0.41
1:A:286:LYS:HG2	1:A:438:GLN:OE1	2.21	0.41
1:A:287:THR:C	1:A:290:ASP:OD1	2.63	0.41
1:A:681:GLU:HB2	1:A:783:LYS:HG2	2.02	0.41
1:A:905:GLU:OE2	1:A:966:ARG:HD2	2.19	0.41
1:A:1107:LEU:HB3	1:A:1157:ARG:NH1	2.36	0.41
1:A:1218:GLU:HB3	1:A:1219:VAL:H	1.44	0.41
1:A:1264:VAL:HG23	1:A:1343:ASP:O	2.20	0.41
1:B:267:LYS:HD2	1:B:454:ARG:HD2	2.02	0.41
1:B:1198:ARG:HD3	1:B:1216:ASN:ND2	2.35	0.41
1:B:1248:LYS:HZ2	1:B:1414:ASP:N	2.18	0.41
1:A:456:LYS:CD	1:A:456:LYS:N	2.83	0.41
1:B:520:LYS:NZ	1:B:527:ARG:HH22	2.17	0.41
1:B:1035:LEU:O	1:B:1038:THR:HB	2.20	0.41
1:B:1086:LEU:HD21	1:B:1512:THR:OG1	2.20	0.41
1:A:149:GLN:HG2	1:A:170:VAL:HG11	2.01	0.41
1:A:284:ASP:CG	1:A:440:PRO:HA	2.46	0.41
1:A:1107:LEU:HB3	1:A:1157:ARG:CZ	2.51	0.41
1:B:307:LYS:HB3	1:B:366:ARG:HH21	1.85	0.41
1:B:875:ASP:O	1:B:879:ARG:HG3	2.21	0.41
1:B:1396:LEU:HD12	1:B:1397:ASP:O	2.20	0.41
1:A:20:SER:HB2	1:A:656:THR:OG1	2.20	0.41
1:A:297:GLY:O	1:A:301:HIS:HB2	2.20	0.41
1:A:343:ASP:CG	1:A:346:ASN:HB2	2.46	0.41
1:A:1198:ARG:HB2	1:A:1216:ASN:HB3	2.02	0.41
1:A:1199:GLU:O	1:A:1202:ALA:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:O	1:B:303:ILE:C	2.64	0.41
1:B:547:TYR:O	1:B:551:VAL:HG23	2.20	0.41
1:B:1317:TYR:CE2	1:B:1319:PRO:HA	2.56	0.41
1:A:152:VAL:HB	1:A:155:TRP:CE3	2.55	0.41
1:A:349:GLN:O	1:A:350:PHE:C	2.63	0.41
1:B:88:LYS:HE2	1:B:95:ASP:OD1	2.21	0.41
1:B:636:TYR:N	1:B:636:TYR:CD1	2.87	0.41
1:B:680:VAL:CG1	1:B:826:ILE:HD13	2.47	0.41
1:B:794:ARG:HE	1:B:850:LEU:HD21	1.86	0.41
1:A:55:ALA:HB2	1:A:93:GLU:C	2.46	0.41
1:A:180:PHE:HB3	1:A:183:LEU:HD13	2.02	0.41
1:A:285:LEU:CD2	1:A:290:ASP:OD2	2.69	0.41
1:A:772:ASN:HB3	1:A:872:ASP:OD1	2.21	0.41
1:A:1196:LYS:HD2	1:A:1218:GLU:HB2	2.03	0.41
1:B:323:LEU:HD21	1:B:377:ALA:CB	2.40	0.41
1:B:340:SER:OG	1:B:383:LEU:HD21	2.21	0.41
1:B:626:ASP:CG	1:B:1027:LYS:HE2	2.45	0.41
1:B:697:ILE:HG22	1:B:698:GLY:N	2.35	0.41
1:B:784:PHE:C	1:B:785:HIS:ND1	2.78	0.41
1:B:990:ILE:HG12	1:B:1001:PHE:HB3	2.03	0.41
1:B:1009:MET:HE3	1:B:1009:MET:O	2.21	0.41
1:B:1076:GLY:HA2	1:B:1103:PHE:CE2	2.55	0.41
1:B:1158:ARG:O	1:B:1159:PHE:HD1	2.04	0.41
1:B:1432:TRP:CB	1:B:1511:SER:OG	2.61	0.41
1:A:319:THR:OG1	1:A:370:LYS:HE3	2.21	0.41
1:A:1131:TRP:HA	1:A:1134:VAL:HG12	2.01	0.41
1:B:380:LEU:HD22	1:B:395:LEU:HD23	2.03	0.41
1:B:718:ARG:HH21	1:B:823:ILE:CG1	2.34	0.41
1:B:1460:LYS:HE2	1:B:1460:LYS:HB3	1.94	0.41
1:A:44:MET:HE3	1:A:44:MET:HB2	1.85	0.40
1:A:185:HIS:CD2	1:A:186:ARG:N	2.89	0.40
1:A:307:LYS:C	1:A:309:TRP:N	2.78	0.40
1:A:318:GLN:C	1:A:321:SER:OG	2.64	0.40
1:A:674:PRO:O	1:A:679:THR:N	2.54	0.40
1:B:160:ILE:O	1:B:163:TRP:HB2	2.21	0.40
1:B:303:ILE:HA	1:B:306:LEU:HD21	2.02	0.40
1:A:556:ASN:HA	1:A:557:PRO:HD2	1.89	0.40
1:A:1236:CYS:HB3	1:A:1241:ASP:HB2	2.02	0.40
1:A:1384:ASP:OD1	1:A:1474:ARG:CZ	2.68	0.40
1:B:293:LYS:HD2	1:B:293:LYS:HA	1.88	0.40
1:B:323:LEU:O	1:B:323:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:PRO:O	1:B:612:SER:HB2	2.19	0.40
1:A:878:ILE:HG21	1:A:1004:LEU:HD23	2.03	0.40
1:A:1185:TYR:HE1	1:A:1290:GLU:O	2.05	0.40
1:A:1193:GLY:C	1:A:1294:PRO:HD3	2.46	0.40
1:B:350:PHE:O	1:B:352:ARG:N	2.54	0.40
1:B:561:VAL:H	1:B:583:SER:HG	1.70	0.40
1:B:1277:VAL:HA	1:B:1280:LEU:HB2	2.04	0.40
1:B:1432:TRP:HA	1:B:1511:SER:CB	2.51	0.40
1:A:370:LYS:CD	1:A:371:ILE:H	2.35	0.40
1:A:425:ARG:NH2	1:A:491:ARG:CB	2.84	0.40
1:A:612:SER:OG	1:A:943:ASN:ND2	2.55	0.40
1:A:761:GLN:CD	1:A:857:GLN:HE21	2.30	0.40
1:A:777:TYR:CE1	1:A:795:ILE:HD13	2.57	0.40
1:A:876:HIS:CD2	1:A:876:HIS:C	2.98	0.40
1:A:1108:LYS:CE	1:A:1159:PHE:HD1	2.33	0.40
1:B:668:THR:C	1:B:670:ASP:H	2.29	0.40
1:B:749:ILE:HG13	1:B:750:GLU:N	2.37	0.40
1:B:878:ILE:HG21	1:B:1004:LEU:HD23	2.04	0.40
1:B:1264:VAL:HG11	1:B:1360:PHE:HA	2.04	0.40
1:B:1407:TYR:CE1	1:B:1424:TYR:CD1	3.00	0.40
1:A:284:ASP:OD2	1:A:438:GLN:HG3	2.22	0.40
1:A:372:ASN:ND2	1:A:375:LYS:HD2	2.37	0.40
1:A:1314:ARG:NH1	1:A:1329:GLU:HG3	2.36	0.40
1:B:182:PRO:HB2	1:B:184:GLN:OE1	2.22	0.40
1:B:807:ALA:HB2	1:B:861:VAL:HG13	2.04	0.40
1:B:1016:ARG:HH11	1:B:1016:ARG:HD3	1.76	0.40
1:B:1209:VAL:HG11	1:B:1245:GLU:CG	2.51	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1174:PHE:CG	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CD1	1:B:1174:PHE:CD1[3_656]	1.88	0.32
1:B:1174:PHE:CG	1:B:1174:PHE:CG[3_656]	1.91	0.29
1:B:116:ASP:O	1:B:390:ASN:ND2[4_567]	2.13	0.07

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	1524/1528 (100%)	1376 (90%)	133 (9%)	15 (1%)	12	41
1	B	1496/1528 (98%)	1337 (89%)	140 (9%)	19 (1%)	9	35
All	All	3020/3056 (99%)	2713 (90%)	273 (9%)	34 (1%)	11	39

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	PRO
1	A	437	LYS
1	A	440	PRO
1	A	1165	TYR
1	A	1167	PRO
1	A	1455	GLU
1	A	1459	LYS
1	B	238	ASN
1	B	282	PRO
1	B	308	LEU
1	B	423	PHE
1	B	430	ARG
1	B	637	ASN
1	B	1167	PRO
1	B	1175	SER
1	A	124	ARG
1	A	238	ASN
1	A	501	LYS
1	B	1459	LYS
1	A	326	LYS
1	A	1162	ASP
1	B	37	GLN
1	B	422	LEU
1	B	729	SER
1	A	729	SER

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Mol	Chain	Res	Type
1	B	124	ARG
1	B	165	LYS
1	A	321	SER
1	B	299	LYS
1	B	425	ARG
1	A	1168	TYR
1	B	294	VAL
1	B	350	PHE
1	B	749	ILE

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	1344/1346 (100%)	1263 (94%)	81 (6%)	17	47
1	B	1327/1346 (99%)	1249 (94%)	78 (6%)	18	48
All	All	2671/2692 (99%)	2512 (94%)	159 (6%)	17	47

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LYS
1	A	103	VAL
1	A	116	ASP
1	A	117	LYS
1	A	125	LYS
1	A	148	MET
1	A	164	GLU
1	A	165	LYS
1	A	179	HIS
1	A	220	ARG
1	A	273	SER
1	A	274	GLU
1	A	275	GLN
1	A	285	LEU

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Mol	Chain	Res	Type
1	A	294	VAL
1	A	299	LYS
1	A	325	GLU
1	A	334	SER
1	A	337	ASN
1	A	349	GLN
1	A	374	ASP
1	A	425	ARG
1	A	441	ILE
1	A	443	LYS
1	A	445	LEU
1	A	456	LYS
1	A	467	ASN
1	A	499	CYS
1	A	523	GLU
1	A	543	HIS
1	A	572	MET
1	A	578	GLU
1	A	585	LEU
1	A	616	VAL
1	A	628	LYS
1	A	629	ILE
1	A	631	GLU
1	A	649	ILE
1	A	671	ASN
1	A	709	GLN
1	A	716	GLU
1	A	717	LYS
1	A	721	SER
1	A	742	ILE
1	A	761	GLN
1	A	767	ARG
1	A	768	THR
1	A	771	LYS
1	A	803	THR
1	A	810	LEU
1	A	861	VAL
1	A	905	GLU
1	A	971	LYS
1	A	973	LYS
1	A	978	GLU
1	A	990	ILE

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Mol	Chain	Res	Type
1	A	1016	ARG
1	A	1025	VAL
1	A	1044	SER
1	A	1123	ARG
1	A	1152	GLN
1	A	1162	ASP
1	A	1195	ILE
1	A	1198	ARG
1	A	1206	LEU
1	A	1213	GLU
1	A	1227	LEU
1	A	1233	GLN
1	A	1235	ASN
1	A	1257	THR
1	A	1280	LEU
1	A	1307	LEU
1	A	1321	ASN
1	A	1330	ILE
1	A	1334	ILE
1	A	1338	ARG
1	A	1455	GLU
1	A	1459	LYS
1	A	1461	LEU
1	A	1462	LYS
1	A	1527	GLU
1	B	4	HIS
1	B	19	THR
1	B	86	ILE
1	B	103	VAL
1	B	114	LYS
1	B	117	LYS
1	B	148	MET
1	B	164	GLU
1	B	166	VAL
1	B	183	LEU
1	B	207	LYS
1	B	209	GLU
1	B	252	ASN
1	B	267	LYS
1	B	288	VAL
1	B	292	ILE
1	B	295	MET

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Mol	Chain	Res	Type
1	B	305	GLU
1	B	306	LEU
1	B	323	LEU
1	B	337	ASN
1	B	417	GLU
1	B	425	ARG
1	B	429	LEU
1	B	458	LYS
1	B	465	LEU
1	B	499	CYS
1	B	543	HIS
1	B	585	LEU
1	B	597	GLU
1	B	616	VAL
1	B	618	LEU
1	B	637	ASN
1	B	644	LYS
1	B	646	VAL
1	B	649	ILE
1	B	653	LYS
1	B	697	ILE
1	B	716	GLU
1	B	749	ILE
1	B	754	MET
1	B	764	THR
1	B	768	THR
1	B	791	MET
1	B	794	ARG
1	B	801	LYS
1	B	810	LEU
1	B	829	LYS
1	B	861	VAL
1	B	884	LYS
1	B	886	THR
1	B	905	GLU
1	B	978	GLU
1	B	990	ILE
1	B	1016	ARG
1	B	1025	VAL
1	B	1044	SER
1	B	1081	ILE
1	B	1120	ARG

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Mol	Chain	Res	Type
1	B	1123	ARG
1	B	1156	THR
1	B	1170	ASP
1	B	1196	LYS
1	B	1236	CYS
1	B	1257	THR
1	B	1299	ILE
1	B	1307	LEU
1	B	1330	ILE
1	B	1338	ARG
1	B	1396	LEU
1	B	1402	ASN
1	B	1415	ASP
1	B	1459	LYS
1	B	1477	LYS
1	B	1490	LEU
1	B	1492	GLU
1	B	1493	LEU
1	B	1524	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	198	GLN
1	A	224	ASN
1	A	234	ASN
1	A	235	HIS
1	A	337	ASN
1	A	390	ASN
1	A	536	ASN
1	A	669	HIS
1	A	675	ASN
1	A	857	GLN
1	A	947	HIS
1	A	1056	ASN
1	A	1070	ASN
1	A	1309	GLN
1	A	1385	GLN
1	A	1409	ASN
1	A	1442	HIS
1	A	1445	ASN

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Mol	Chain	Res	Type
1	B	144	ASN
1	B	185	HIS
1	B	224	ASN
1	B	235	HIS
1	B	241	GLN
1	B	252	ASN
1	B	354	ASN
1	B	421	GLN
1	B	424	ASN
1	B	661	HIS
1	B	669	HIS
1	B	675	ASN
1	B	876	HIS
1	B	895	ASN
1	B	947	HIS
1	B	1056	ASN
1	B	1070	ASN
1	B	1235	ASN
1	B	1385	GLN
1	B	1402	ASN
1	B	1445	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1526/1528 (99%)	0.09	18 (1%) 76 58	52, 93, 140, 187	0
1	B	1506/1528 (98%)	0.17	26 (1%) 69 48	47, 87, 148, 190	0
All	All	3032/3056 (99%)	0.13	44 (1%) 72 52	47, 90, 146, 190	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1510	TRP	5.6
1	B	1490	LEU	5.1
1	B	323	LEU	3.3
1	B	415	ILE	3.2
1	A	270	LEU	3.2
1	B	630	ASP	3.1
1	B	1217	VAL	3.0
1	A	1128	ASP	2.9
1	B	1348	GLY	2.9
1	B	270	LEU	2.8
1	B	748	ASP	2.7
1	A	436	PRO	2.7
1	A	499	CYS	2.7
1	B	783	LYS	2.6
1	B	1353	ASP	2.6
1	A	501	LYS	2.5
1	B	375	LYS	2.4
1	A	1208	ARG	2.4
1	B	400	LEU	2.4
1	B	355	ALA	2.4
1	B	314	VAL	2.3
1	B	268	LYS	2.3
1	B	1354	TYR	2.3
1	B	416	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	643	VAL	2.3
1	B	1174	PHE	2.3
1	B	283	VAL	2.2
1	A	282	PRO	2.2
1	A	914	GLY	2.2
1	A	1167	PRO	2.2
1	A	642	SER	2.2
1	B	1492	GLU	2.1
1	A	291	LEU	2.1
1	B	279	LEU	2.1
1	A	3	ALA	2.1
1	A	1218	GLU	2.1
1	A	1159	PHE	2.1
1	B	492	GLU	2.1
1	B	1511	SER	2.0
1	A	389	ASN	2.0
1	B	1236	CYS	2.0
1	B	269	LEU	2.0
1	A	649	ILE	2.0
1	A	249	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.