



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:02 AM UTC

PDB ID : 5DJW / pdb_00005djw
Title : Crystal structure of Family 31 alpha-glucosidase (BT_3299) from Bacteroides thetaiotaomicron
Authors : Chaudet, M.M.; Rose, D.R.
Deposited on : 2015-09-02
Resolution : 2.70 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

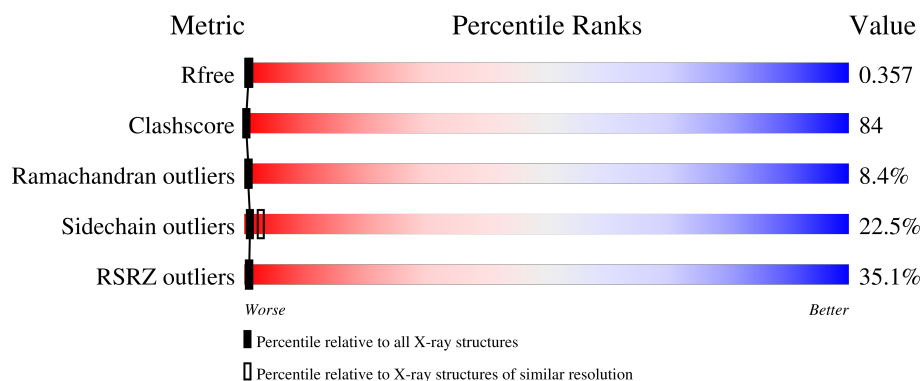
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	697	
1	B	697	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9139 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 Alpha-glucosidase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	588	Total	C	N	O	S	0	0	0
			4569	2924	782	843	20			
1	B	587	Total	C	N	O	S	0	0	0
			4547	2913	783	831	20			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8A2K6
A	685	HIS	-	expression tag	UNP Q8A2K6
A	686	HIS	-	expression tag	UNP Q8A2K6
A	687	HIS	-	expression tag	UNP Q8A2K6
A	688	HIS	-	expression tag	UNP Q8A2K6
A	689	HIS	-	expression tag	UNP Q8A2K6
A	690	HIS	-	expression tag	UNP Q8A2K6
A	691	LEU	-	expression tag	UNP Q8A2K6
A	692	ARG	-	expression tag	UNP Q8A2K6
A	693	VAL	-	expression tag	UNP Q8A2K6
A	694	PRO	-	expression tag	UNP Q8A2K6
A	695	ARG	-	expression tag	UNP Q8A2K6
A	696	GLY	-	expression tag	UNP Q8A2K6
A	697	SER	-	expression tag	UNP Q8A2K6
B	1	MET	-	initiating methionine	UNP Q8A2K6
B	685	HIS	-	expression tag	UNP Q8A2K6
B	686	HIS	-	expression tag	UNP Q8A2K6
B	687	HIS	-	expression tag	UNP Q8A2K6
B	688	HIS	-	expression tag	UNP Q8A2K6
B	689	HIS	-	expression tag	UNP Q8A2K6
B	690	HIS	-	expression tag	UNP Q8A2K6
B	691	LEU	-	expression tag	UNP Q8A2K6
B	692	ARG	-	expression tag	UNP Q8A2K6
B	693	VAL	-	expression tag	UNP Q8A2K6
B	694	PRO	-	expression tag	UNP Q8A2K6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	695	ARG	-	expression tag	UNP Q8A2K6
B	696	GLY	-	expression tag	UNP Q8A2K6
B	697	SER	-	expression tag	UNP Q8A2K6

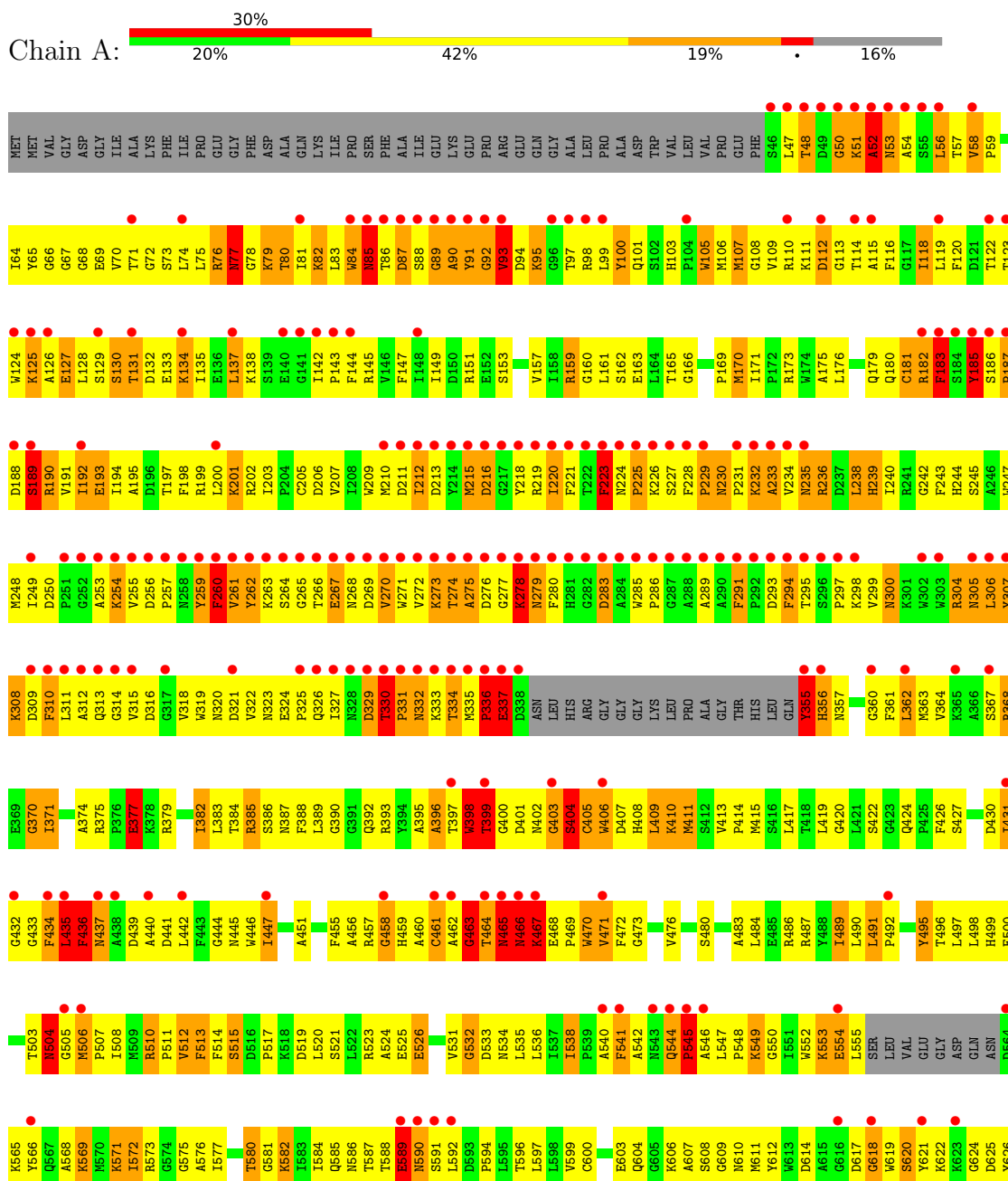
- Molecule 2 is water.

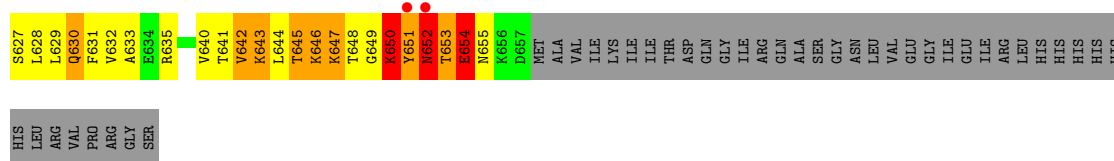
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	8	Total	O	0	0
			8	8		

3 Residue-property plots

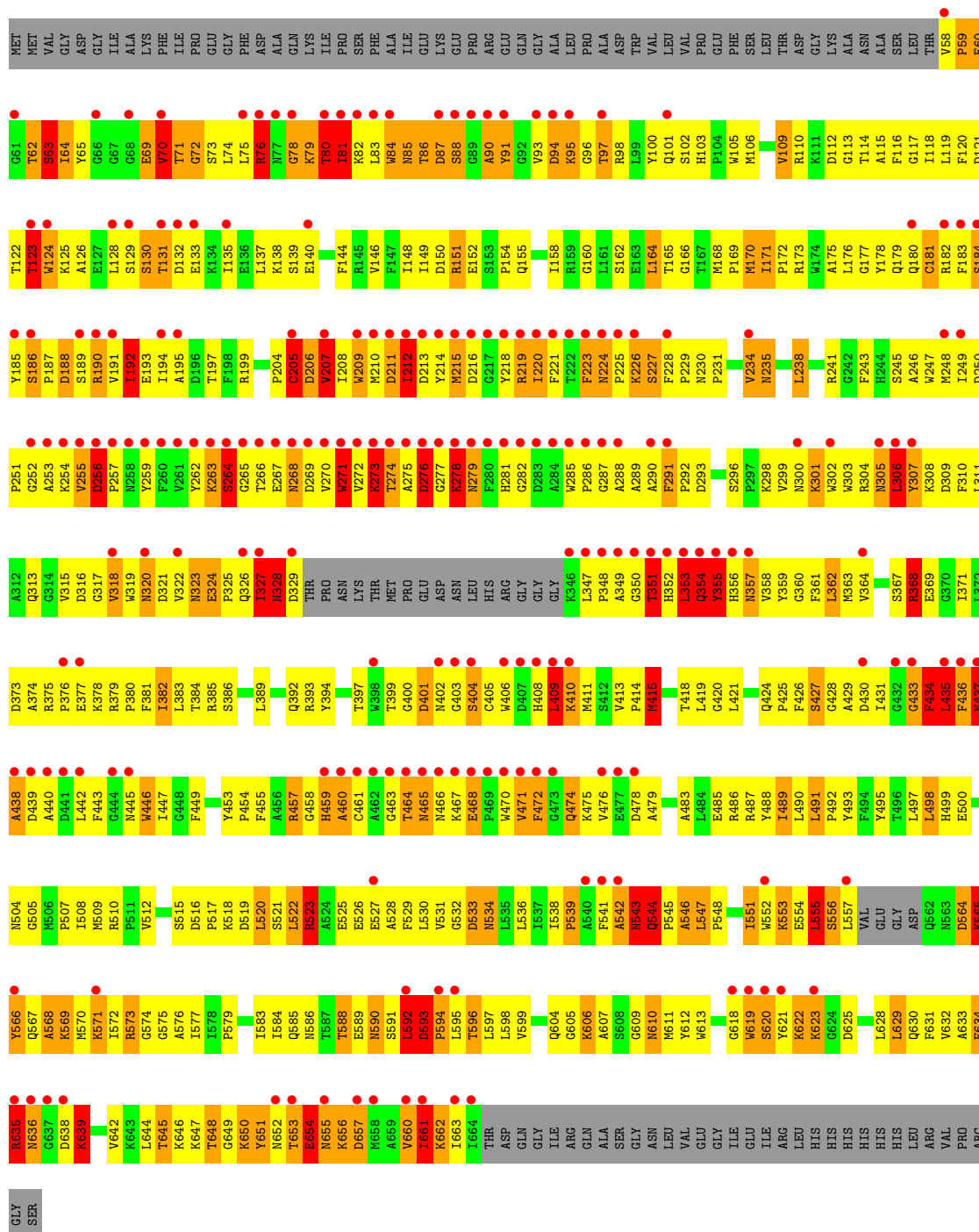
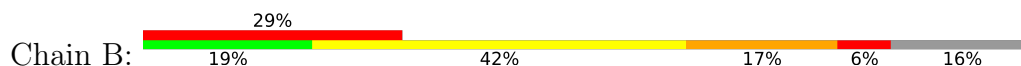
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Alpha-glucosidase II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.26Å 74.86Å 94.43Å 90.00° 95.70° 90.00°	Depositor
Resolution (Å)	47.55 – 2.70 47.55 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.55-2.70) 100.0 (47.55-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.330 , 0.390 0.314 , 0.357	Depositor DCC
R_{free} test set	1716 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 101.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	9139	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.64% 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	1.15	6/4694 (0.1%)	1.49	84/6370 (1.3%)
1	B	1.67	8/4672 (0.2%)	1.51	88/6342 (1.4%)
All	All	1.43	14/9366 (0.1%)	1.50	172/12712 (1.4%)

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	18
1	B	0	20
All	All	0	38

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	434	PHE	C-N	-81.29	0.19	1.33
1	B	594	PRO	C-N	22.21	1.64	1.33
1	A	50	GLY	C-N	16.85	1.55	1.33
1	B	91	TYR	CA-C	-7.58	1.42	1.52
1	B	597	LEU	C-O	-6.85	1.15	1.24
1	B	170	MET	C-O	-6.67	1.16	1.23
1	A	142	ILE	C-N	5.77	1.41	1.33
1	B	592	LEU	CA-C	-5.29	1.47	1.53
1	A	230	ASN	N-CA	-5.23	1.38	1.46
1	A	143	PRO	N-CD	5.20	1.55	1.47
1	A	545	PRO	N-CD	5.13	1.55	1.47
1	B	660	VAL	CA-C	5.09	1.59	1.52
1	B	206	ASP	N-CA	5.08	1.52	1.46
1	A	642	VAL	C-O	-5.01	1.19	1.24

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	GLY	N-CA-C	-22.86	87.19	112.33
1	A	50	GLY	O-C-N	-22.62	93.30	122.70
1	B	326	GLN	CA-C-N	19.44	156.97	121.97
1	B	326	GLN	C-N-CA	19.44	156.97	121.97
1	A	309	ASP	CB-CA-C	-18.14	82.94	111.06
1	B	62	THR	N-CA-C	15.57	127.96	111.14
1	A	50	GLY	CA-C-N	-15.48	98.92	121.05
1	A	50	GLY	C-N-CA	-15.48	98.92	121.05
1	A	225	PRO	CB-CA-C	-12.87	93.02	110.52
1	B	434	PHE	O-C-N	12.64	139.41	122.59
1	A	89	GLY	N-CA-C	-10.74	96.08	112.51
1	A	377	GLU	N-CA-C	10.74	126.06	111.24
1	B	434	PHE	CA-C-N	-10.47	101.54	121.54
1	B	434	PHE	C-N-CA	-10.47	101.54	121.54
1	B	109	VAL	N-CA-C	10.14	120.07	110.53
1	A	236	ARG	N-CA-C	-9.88	100.36	111.82
1	A	309	ASP	N-CA-C	9.83	123.67	112.57
1	B	206	ASP	N-CA-C	9.60	131.24	110.80
1	A	465	ASN	N-CA-C	9.34	122.85	110.53
1	B	326	GLN	O-C-N	-9.31	111.12	123.23
1	A	332	ASN	N-CA-C	9.13	124.06	111.74
1	A	620	SER	N-CA-C	-8.99	92.77	108.23
1	B	622	LYS	CA-C-N	8.78	132.05	120.28
1	B	622	LYS	C-N-CA	8.78	132.05	120.28
1	B	131	THR	N-CA-C	8.67	122.79	108.49
1	A	542	ALA	N-CA-C	8.49	122.70	109.96
1	A	356	HIS	N-CA-C	8.32	119.97	111.07
1	B	327	ILE	O-C-N	8.28	132.91	122.57
1	B	544	GLN	N-CA-C	-8.07	91.97	109.81
1	A	544	GLN	C-N-CD	8.00	138.19	120.60
1	B	327	ILE	CA-C-N	-7.99	110.92	122.67
1	B	327	ILE	C-N-CA	-7.99	110.92	122.67
1	B	401	ASP	N-CA-C	-7.97	96.25	109.24
1	B	80	THR	N-CA-C	7.94	123.01	112.13
1	B	306	LEU	CA-C-N	7.92	130.89	120.28
1	B	306	LEU	C-N-CA	7.92	130.89	120.28
1	A	544	GLN	N-CA-C	7.84	115.05	108.07
1	A	651	TYR	N-CA-C	7.79	118.53	108.24
1	A	307	TYR	N-CA-C	7.77	119.75	111.28
1	B	205	CYS	N-CA-C	7.75	120.17	107.23
1	B	209	TRP	N-CA-C	-7.75	100.28	110.43
1	B	227	SER	N-CA-C	-7.68	97.81	109.79
1	B	208	ILE	N-CA-C	-7.61	93.51	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	LEU	N-CA-C	7.58	119.32	111.14
1	A	336	PRO	CA-C-N	7.55	130.40	120.28
1	A	336	PRO	C-N-CA	7.55	130.40	120.28
1	A	260	PHE	N-CA-C	7.52	120.00	110.61
1	A	403	GLY	N-CA-C	-7.44	99.52	110.90
1	B	327	ILE	N-CA-C	7.37	124.67	109.34
1	A	399	THR	N-CA-C	7.33	120.18	111.02
1	A	405	CYS	N-CA-C	7.22	119.15	111.28
1	B	661	ILE	N-CA-C	7.18	124.28	109.34
1	B	255	VAL	N-CA-C	7.16	124.23	109.34
1	A	239	HIS	N-CA-C	7.04	120.35	111.69
1	B	415	MET	N-CA-C	7.00	118.70	111.14
1	B	278	LYS	N-CA-C	6.97	119.53	109.14
1	B	124	TRP	N-CA-C	6.93	119.98	109.23
1	A	52	ALA	CA-C-O	-6.92	110.61	120.51
1	A	642	VAL	N-CA-C	-6.92	98.15	108.46
1	B	76	ARG	N-CA-C	6.88	117.32	108.24
1	B	654	GLU	N-CA-C	6.83	120.50	111.28
1	A	51	LYS	O-C-N	-6.82	114.87	123.06
1	B	378	LYS	N-CA-C	-6.80	98.98	109.52
1	A	645	THR	N-CA-C	6.80	118.48	111.14
1	A	265	GLY	N-CA-C	-6.78	97.11	113.18
1	B	205	CYS	CA-C-N	6.78	134.49	121.54
1	B	205	CYS	C-N-CA	6.78	134.49	121.54
1	B	252	GLY	N-CA-C	6.77	120.87	112.14
1	B	326	GLN	N-CA-C	6.73	120.37	109.40
1	A	617	ASP	N-CA-C	6.71	118.99	110.61
1	B	91	TYR	N-CA-CB	6.66	121.74	110.49
1	A	142	ILE	CA-C-N	-6.62	112.95	119.76
1	A	142	ILE	C-N-CA	-6.62	112.95	119.76
1	B	410	LYS	N-CA-C	6.61	118.28	111.14
1	A	532	GLY	N-CA-C	6.60	124.06	114.10
1	B	192	ILE	N-CA-C	-6.58	100.16	109.63
1	B	85	ASN	N-CA-C	6.58	119.83	109.96
1	A	471	VAL	N-CA-C	6.55	116.69	110.53
1	B	81	ILE	N-CA-C	6.55	119.21	108.99
1	A	185	TYR	N-CA-C	6.52	121.60	112.93
1	A	305	ASN	N-CA-C	6.47	120.79	113.02
1	B	362	LEU	N-CA-C	6.45	118.10	111.14
1	A	329	ASP	N-CA-C	6.37	118.85	109.24
1	A	398	TRP	CB-CA-C	6.33	116.10	109.83
1	A	504	ASN	CA-C-N	6.31	127.67	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ASN	C-N-CA	6.31	127.67	120.53
1	B	238	LEU	N-CA-C	6.30	118.22	111.36
1	B	351	THR	N-CA-C	-6.30	100.94	110.70
1	A	565	LYS	N-CA-C	6.29	117.80	111.07
1	B	651	TYR	N-CA-C	6.24	118.09	109.29
1	B	368	ARG	N-CA-C	6.24	117.88	111.14
1	B	533	ASP	N-CA-C	6.23	117.87	111.14
1	A	310	PHE	CB-CA-C	-6.22	100.16	110.37
1	A	618	GLY	N-CA-C	-6.22	99.03	110.97
1	B	551	ILE	CA-C-N	6.21	132.43	121.80
1	B	551	ILE	C-N-CA	6.21	132.43	121.80
1	A	512	VAL	CA-C-N	6.19	129.19	120.28
1	A	512	VAL	C-N-CA	6.19	129.19	120.28
1	B	320	ASN	N-CA-C	6.14	118.42	108.41
1	A	534	ASN	N-CA-C	6.12	120.75	113.28
1	B	551	ILE	N-CA-C	6.12	117.65	108.96
1	B	207	VAL	N-CA-C	-6.09	101.73	109.58
1	B	599	VAL	N-CA-C	6.08	116.61	107.80
1	B	433	GLY	N-CA-C	6.07	127.56	113.18
1	A	310	PHE	CA-C-O	5.97	126.80	119.81
1	A	337	GLU	N-CA-C	5.94	117.76	111.28
1	B	289	ALA	N-CA-C	5.93	119.06	109.40
1	A	100	TYR	N-CA-C	5.90	117.71	111.28
1	B	534	ASN	N-CA-C	5.89	120.47	113.16
1	B	123	THR	N-CA-C	5.89	120.48	113.12
1	A	67	GLY	N-CA-C	5.87	123.42	115.32
1	A	404	SER	CA-C-N	5.85	128.12	120.28
1	A	404	SER	C-N-CA	5.85	128.12	120.28
1	A	589	GLU	CA-C-N	5.83	128.37	120.44
1	A	589	GLU	C-N-CA	5.83	128.37	120.44
1	B	273	LYS	N-CA-C	-5.83	101.67	110.70
1	A	470	TRP	N-CA-C	5.82	120.39	112.88
1	B	70	VAL	N-CA-C	5.82	121.45	109.34
1	A	483	ALA	N-CA-C	5.79	117.27	111.07
1	A	590	ASN	N-CA-C	5.79	117.39	111.14
1	B	553	LYS	N-CA-C	5.79	115.88	108.24
1	B	234	VAL	N-CA-C	5.75	117.17	110.62
1	A	130	SER	N-CA-C	5.74	119.66	107.67
1	A	91	TYR	N-CA-C	-5.70	98.66	110.80
1	B	305	ASN	N-CA-C	5.65	119.25	112.93
1	A	495	TYR	N-CA-C	5.64	117.51	111.36
1	A	153	SER	CA-C-N	5.63	125.16	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	SER	C-N-CA	5.63	125.16	119.19
1	B	199	ARG	N-CA-C	5.63	117.50	111.36
1	A	622	LYS	N-CA-C	-5.63	105.14	111.28
1	B	606	LYS	N-CA-C	5.61	117.80	108.99
1	A	545	PRO	CA-N-CD	-5.60	103.66	111.50
1	A	159	ARG	N-CA-C	-5.57	105.21	111.28
1	B	636	ASN	N-CA-C	5.57	122.66	110.80
1	A	85	ASN	N-CA-C	5.55	122.62	110.80
1	B	660	VAL	N-CA-C	5.53	120.83	109.34
1	B	328	ASN	N-CA-C	5.51	119.70	109.56
1	B	472	PHE	N-CA-C	-5.51	106.34	112.57
1	A	93	VAL	N-CA-C	5.50	120.77	109.34
1	B	594	PRO	N-CA-C	5.48	119.84	111.34
1	A	294	PHE	N-CA-C	-5.45	107.19	112.97
1	A	330	THR	C-N-CD	-5.45	102.67	125.00
1	B	78	GLY	N-CA-C	5.43	123.08	115.43
1	B	64	ILE	N-CA-C	5.42	116.39	108.53
1	B	596	THR	N-CA-C	5.42	117.35	109.71
1	A	508	ILE	N-CA-C	-5.41	105.10	110.62
1	B	324	GLU	N-CA-C	5.37	120.05	112.75
1	B	446	TRP	N-CA-C	5.37	116.94	111.14
1	A	355	TYR	CA-C-N	5.35	127.40	120.44
1	A	355	TYR	C-N-CA	5.35	127.40	120.44
1	B	296	SER	N-CA-C	5.35	116.62	109.83
1	B	269	ASP	N-CA-C	5.35	118.43	110.52
1	A	541	PHE	N-CA-C	5.27	122.02	110.80
1	B	291	PHE	N-CA-C	5.27	117.83	109.40
1	B	309	ASP	N-CA-C	5.25	116.81	111.14
1	B	590	ASN	N-CA-C	5.21	116.96	111.28
1	A	540	ALA	CA-C-N	5.20	131.47	121.54
1	A	540	ALA	C-N-CA	5.20	131.47	121.54
1	B	354	GLN	CA-C-N	5.16	131.40	121.54
1	B	354	GLN	C-N-CA	5.16	131.40	121.54
1	B	318	VAL	N-CA-C	5.14	115.52	108.12
1	B	409	LEU	N-CA-C	-5.11	105.71	111.28
1	B	91	TYR	N-CA-C	-5.11	99.92	110.80
1	A	370	GLY	N-CA-C	5.11	119.31	112.77
1	A	585	GLN	N-CA-C	5.08	116.90	111.36
1	B	518	LYS	N-CA-C	-5.08	107.58	112.97
1	A	331	PRO	CA-C-N	5.07	129.34	122.19
1	A	331	PRO	C-N-CA	5.07	129.34	122.19
1	A	291	PHE	N-CA-C	5.04	117.75	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	SER	N-CA-C	-5.04	105.91	111.71
1	A	216	ASP	N-CA-C	5.02	116.56	111.14
1	B	306	LEU	N-CA-C	-5.02	105.94	111.71

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	185	TYR	Peptide
1	A	235	ASN	Peptide
1	A	259	TYR	Peptide
1	A	330	THR	Peptide
1	A	336	PRO	Peptide
1	A	377	GLU	Peptide
1	A	396	ALA	Peptide
1	A	399	THR	Peptide
1	A	436	PHE	Peptide
1	A	458	GLY	Peptide
1	A	463	GLY	Peptide
1	A	464	THR	Peptide
1	A	50	GLY	Mainchain
1	A	504	ASN	Peptide
1	A	541	PHE	Peptide
1	A	620	SER	Peptide
1	A	652	ASN	Peptide
1	A	77	ASN	Peptide
1	B	188	ASP	Peptide
1	B	192	ILE	Peptide
1	B	205	CYS	Peptide
1	B	223	PHE	Peptide
1	B	256	ASP	Peptide
1	B	264	SER	Peptide
1	B	276	ASP	Peptide
1	B	306	LEU	Peptide
1	B	327	ILE	Mainchain
1	B	353	LEU	Mainchain
1	B	355	TYR	Peptide
1	B	434	PHE	Mainchain
1	B	544	GLN	Peptide
1	B	551	ILE	Peptide
1	B	593	ASP	Peptide
1	B	619	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	B	622	LYS	Peptide
1	B	635	ARG	Peptide
1	B	648	THR	Peptide
1	B	90	ALA	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4569	0	4348	758	5
1	B	4547	0	4344	734	1
2	A	15	0	0	8	1
2	B	8	0	0	3	0
All	All	9139	0	8692	1488	6

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 84.

All (1488) 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:A:84:TRP:CD1	1:A:85:ASN:H	1.12	1.64
1:A:272:VAL:CG1	1:A:336:PRO:HG2	1.40	1.51
1:B:553:LYS:CB	1:B:572:ILE:HG22	1.36	1.50
1:B:256:ASP:O	1:B:259:TYR:CD2	1.73	1.40
1:B:552:TRP:CB	1:B:571:LYS:HE2	1.49	1.39
1:A:256:ASP:O	1:A:259:TYR:CD2	1.73	1.39
1:B:181:CYS:SG	1:B:211:ASP:CB	2.12	1.37
1:A:324:GLU:OE2	1:A:385:ARG:NH1	1.57	1.37
1:A:84:TRP:CD1	1:A:85:ASN:N	1.89	1.36
1:A:101:GLN:NE2	1:A:387:ASN:HB3	1.41	1.35
1:A:280:PHE:CE1	1:A:336:PRO:HD2	1.67	1.30
1:B:379:ARG:NE	1:B:618:GLY:O	1.62	1.30
1:B:328:ASN:CB	1:B:348:PRO:HB3	1.59	1.29
1:B:406:TRP:CZ2	1:B:541:PHE:HD2	1.48	1.29
1:A:224:ASN:HB3	1:A:227:SER:CB	1.63	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG21	2:A:712:HOH:O	1.14	1.28
1:B:347:LEU:O	1:B:350:GLY:N	1.67	1.27
1:B:406:TRP:NE1	1:B:541:PHE:CE2	2.02	1.26
1:A:436:PHE:CZ	1:A:459:HIS:HE1	1.51	1.26
1:A:272:VAL:CG1	1:A:336:PRO:CG	2.14	1.25
1:A:379:ARG:NH2	1:A:618:GLY:O	1.69	1.25
1:B:188:ASP:OD1	1:B:191:VAL:HG22	1.33	1.24
1:A:436:PHE:HZ	1:A:459:HIS:CE1	1.56	1.24
1:B:219:ARG:NH1	1:B:254:LYS:HG2	1.50	1.23
1:A:436:PHE:CZ	1:A:459:HIS:CE1	2.25	1.22
1:B:214:TYR:OH	1:B:248:MET:O	1.52	1.22
1:A:193:GLU:O	1:A:197:THR:OG1	1.54	1.21
1:B:166:GLY:O	1:B:392:GLN:NE2	1.74	1.20
1:A:57:THR:HG23	1:A:134:LYS:CD	1.71	1.20
1:B:245:SER:OG	1:B:247:TRP:NE1	1.73	1.20
1:A:627:SER:HA	1:A:647:LYS:NZ	1.58	1.19
1:A:192:ILE:HG21	1:A:195:ALA:HB3	1.26	1.18
1:A:80:THR:HB	1:A:129:SER:CB	1.72	1.18
1:B:106:MET:HE2	1:B:128:LEU:HD22	1.22	1.17
1:A:86:THR:O	1:A:88:SER:N	1.77	1.17
1:A:272:VAL:CG2	1:A:280:PHE:HB2	1.74	1.17
1:A:233:ALA:CB	1:A:312:ALA:HA	1.72	1.17
1:A:272:VAL:HG13	1:A:336:PRO:CG	1.71	1.17
1:B:306:LEU:HD13	1:B:307:TYR:HA	1.17	1.17
1:A:225:PRO:O	1:A:229:PRO:HG3	1.43	1.16
1:B:406:TRP:CZ2	1:B:541:PHE:CD2	2.32	1.16
1:B:211:ASP:O	1:B:212:ILE:CG2	1.94	1.15
1:B:189:SER:O	1:B:191:VAL:N	1.76	1.15
1:B:178:TYR:HB3	1:B:205:CYS:HB3	1.15	1.15
1:B:406:TRP:NE1	1:B:541:PHE:CD2	2.16	1.14
1:A:224:ASN:HB3	1:A:227:SER:HB3	1.14	1.12
1:A:223:PHE:CZ	1:A:311:LEU:CB	2.32	1.12
1:A:57:THR:CG2	1:A:134:LYS:HD2	1.78	1.12
1:A:80:THR:HB	1:A:129:SER:CA	1.79	1.12
1:A:225:PRO:O	1:A:229:PRO:CG	1.96	1.12
1:B:263:LYS:HA	1:B:265:GLY:H	1.10	1.11
1:B:307:TYR:CD2	1:B:374:ALA:HB2	1.85	1.11
1:B:586:ASN:HB2	1:B:589:GLU:HG3	1.19	1.11
1:A:182:ARG:NH2	1:A:190:ARG:CB	2.13	1.10
1:A:256:ASP:O	1:A:259:TYR:HD2	1.15	1.10
1:B:553:LYS:CB	1:B:572:ILE:CG2	2.30	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ASP:O	1:B:259:TYR:CE2	2.05	1.09
1:A:101:GLN:NE2	1:A:387:ASN:CB	2.15	1.09
1:A:53:ASN:O	1:A:144:PHE:HZ	1.33	1.09
1:A:266:THR:O	1:A:267:GLU:HB2	1.46	1.09
1:A:627:SER:HA	1:A:647:LYS:HZ1	0.95	1.09
1:A:647:LYS:NZ	1:A:648:THR:O	1.85	1.09
1:B:186:SER:HB3	1:B:187:PRO:CD	1.82	1.08
1:A:87:ASP:HA	1:A:100:TYR:HE1	1.15	1.08
1:B:404:SER:O	1:B:442:LEU:CD2	2.02	1.08
1:B:552:TRP:CB	1:B:571:LYS:CE	2.32	1.08
1:A:272:VAL:HG22	1:A:280:PHE:HB2	1.09	1.07
1:B:219:ARG:NH1	1:B:254:LYS:CG	2.16	1.07
1:B:211:ASP:O	1:B:212:ILE:HG23	1.50	1.07
1:B:406:TRP:CE2	1:B:541:PHE:CD2	2.42	1.07
1:B:219:ARG:HH11	1:B:254:LYS:CG	1.67	1.07
1:A:84:TRP:HD1	1:A:85:ASN:N	1.38	1.07
1:A:84:TRP:CE2	1:A:356:HIS:CD2	2.43	1.07
1:A:294:PHE:HB3	1:A:362:LEU:HD22	1.36	1.07
1:A:80:THR:HB	1:A:129:SER:HA	1.34	1.07
1:B:186:SER:HB3	1:B:187:PRO:HD3	1.30	1.06
1:A:179:GLN:HB3	1:A:209:TRP:HE1	1.20	1.06
1:A:238:LEU:O	1:A:243:PHE:HB2	1.52	1.06
1:A:625:ASP:HA	1:A:651:TYR:CB	1.85	1.06
1:A:229:PRO:C	1:A:231:PRO:HD3	1.81	1.05
1:B:178:TYR:HB3	1:B:205:CYS:CB	1.85	1.05
1:B:328:ASN:HB2	1:B:348:PRO:HB3	1.11	1.05
1:A:625:ASP:CA	1:A:651:TYR:CB	2.34	1.05
1:A:460:ALA:HB3	1:A:467:LYS:HD3	1.39	1.05
1:A:229:PRO:C	1:A:231:PRO:CD	2.29	1.04
1:B:566:TYR:HA	1:B:567:GLN:HG2	1.36	1.04
1:A:86:THR:HG21	1:A:333:LYS:CB	1.88	1.04
1:A:192:ILE:O	1:A:194:ILE:N	1.90	1.04
1:B:194:ILE:CG2	1:B:470:TRP:HZ2	1.70	1.04
1:B:323:ASN:OD1	1:B:386:SER:HB3	1.58	1.04
1:A:280:PHE:CD1	1:A:336:PRO:HD2	1.91	1.04
1:B:194:ILE:HG22	1:B:470:TRP:CZ2	1.92	1.04
1:A:280:PHE:CE1	1:A:336:PRO:CD	2.42	1.03
1:A:506:MET:HB3	1:A:507:PRO:HD2	1.39	1.03
1:A:263:LYS:O	1:A:266:THR:CB	2.05	1.03
1:B:72:GLY:HA2	1:B:73:SER:HB2	1.39	1.03
1:B:210:MET:HB2	1:B:211:ASP:CB	1.88	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ASN:HB2	1:B:348:PRO:CB	1.90	1.02
1:B:328:ASN:CG	1:B:348:PRO:HB3	1.83	1.02
1:B:402:ASN:ND2	1:B:446:TRP:CH2	2.26	1.02
1:B:70:VAL:HG22	1:B:71:THR:H	1.25	1.02
1:B:139:SER:HB3	1:B:144:PHE:HE2	1.19	1.02
1:B:454:PRO:CD	1:B:509:MET:HE3	1.89	1.02
1:A:53:ASN:O	1:A:144:PHE:CZ	2.13	1.02
1:A:87:ASP:HA	1:A:100:TYR:CE1	1.95	1.02
1:A:233:ALA:HB2	1:A:312:ALA:HA	1.03	1.02
1:A:433:GLY:O	1:A:460:ALA:HA	1.55	1.02
1:A:119:LEU:HD13	1:A:389:LEU:HD21	1.41	1.01
1:B:270:VAL:CG2	1:B:292:PRO:HA	1.90	1.01
1:B:590:ASN:O	1:B:591:SER:OG	1.77	1.01
1:A:228:PHE:C	1:A:230:ASN:H	1.66	1.01
1:A:192:ILE:CG2	1:A:195:ALA:HB3	1.91	1.01
1:A:182:ARG:NH2	1:A:190:ARG:HB2	1.75	1.00
1:A:512:VAL:O	1:A:515:SER:OG	1.75	1.00
1:B:189:SER:O	1:B:191:VAL:HG13	1.60	1.00
1:A:506:MET:HB3	1:A:507:PRO:CD	1.90	1.00
1:B:221:PHE:CE1	1:B:306:LEU:HG	1.97	1.00
1:B:256:ASP:O	1:B:259:TYR:HD2	1.16	1.00
1:A:192:ILE:C	1:A:194:ILE:H	1.65	1.00
1:B:545:PRO:HG2	1:B:547:LEU:HD13	1.42	1.00
1:A:580:THR:OG1	1:A:596:THR:O	1.80	1.00
1:B:307:TYR:O	2:B:701:HOH:O	1.80	0.99
1:A:131:THR:HG22	1:A:132:ASP:H	1.24	0.99
1:A:512:VAL:HG13	1:A:548:PRO:HD3	1.42	0.99
1:A:101:GLN:HE21	1:A:387:ASN:HB3	0.83	0.99
1:A:248:MET:HB2	1:A:319:TRP:CZ2	1.98	0.99
1:B:522:LEU:O	1:B:523:ARG:HB2	1.61	0.99
1:A:78:GLY:HA2	1:A:131:THR:HA	1.42	0.98
1:A:219:ARG:HH22	1:A:256:ASP:CB	1.77	0.98
1:B:306:LEU:HD13	1:B:307:TYR:CA	1.93	0.98
1:B:188:ASP:OD1	1:B:191:VAL:CG2	2.12	0.98
1:A:182:ARG:HH22	1:A:190:ARG:CB	1.73	0.98
1:B:74:LEU:HD23	1:B:75:LEU:H	1.27	0.98
1:A:627:SER:CA	1:A:647:LYS:NZ	2.27	0.98
1:B:554:GLU:O	1:B:555:LEU:HB2	1.60	0.98
1:B:368:ARG:HG3	1:B:382:ILE:HG21	1.46	0.97
1:A:331:PRO:O	1:A:332:ASN:OD1	1.80	0.97
1:A:74:LEU:HD12	1:A:76:ARG:O	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:PRO:O	1:A:523:ARG:NH2	1.95	0.97
1:B:306:LEU:CD1	1:B:307:TYR:HA	1.94	0.97
1:A:225:PRO:C	1:A:229:PRO:HG3	1.88	0.96
1:B:248:MET:HB2	1:B:319:TRP:CZ2	2.00	0.96
1:A:101:GLN:HG2	1:A:387:ASN:N	1.79	0.96
1:B:194:ILE:CG2	1:B:470:TRP:CZ2	2.48	0.96
1:B:117:GLY:N	1:B:149:ILE:O	1.97	0.96
1:B:594:PRO:O	1:B:596:THR:N	1.97	0.95
1:B:406:TRP:HZ2	1:B:541:PHE:HD2	1.07	0.95
1:B:263:LYS:HA	1:B:265:GLY:N	1.79	0.95
1:B:573:ARG:HG2	1:B:573:ARG:HH11	1.30	0.95
1:A:525:GLU:OE1	1:A:545:PRO:HG2	1.65	0.95
1:A:119:LEU:CD1	1:A:389:LEU:HD21	1.97	0.95
1:A:86:THR:HG22	1:A:87:ASP:OD1	1.66	0.95
1:A:228:PHE:O	1:A:231:PRO:HD3	1.64	0.95
1:A:641:THR:HB	1:A:643:LYS:HE3	1.49	0.95
1:A:84:TRP:CG	1:A:85:ASN:H	1.83	0.94
1:A:224:ASN:HB3	1:A:227:SER:HB2	1.49	0.94
1:A:233:ALA:HB2	1:A:312:ALA:CA	1.96	0.94
1:B:118:ILE:HD11	1:B:120:PHE:CE1	2.01	0.94
1:B:328:ASN:CB	1:B:348:PRO:CB	2.42	0.94
1:A:272:VAL:HG11	1:A:336:PRO:CG	1.96	0.94
1:B:307:TYR:HD2	1:B:374:ALA:HB2	1.28	0.94
1:B:593:ASP:CB	1:B:594:PRO:HD3	1.97	0.94
1:B:512:VAL:HG23	1:B:528:ALA:O	1.68	0.94
1:A:101:GLN:HG2	1:A:387:ASN:H	1.33	0.94
1:B:555:LEU:HD23	1:B:570:MET:HE3	1.50	0.94
1:A:223:PHE:CE2	1:A:311:LEU:CB	2.51	0.93
1:B:219:ARG:HH12	1:B:254:LYS:HG2	1.33	0.93
1:B:402:ASN:HB2	1:B:430:ASP:HB2	1.47	0.93
1:A:272:VAL:HG11	1:A:336:PRO:HG2	1.49	0.93
1:A:179:GLN:OE1	1:A:455:PHE:HE1	1.52	0.93
1:A:256:ASP:O	1:A:259:TYR:CE2	2.21	0.93
1:A:275:ALA:O	1:A:277:GLY:N	2.00	0.93
1:B:211:ASP:C	1:B:212:ILE:HG22	1.92	0.93
1:B:245:SER:HG	1:B:247:TRP:NE1	1.65	0.93
1:A:277:GLY:O	1:A:278:LYS:HB2	1.66	0.93
1:A:179:GLN:HG2	1:A:207:VAL:HB	1.49	0.92
1:A:84:TRP:CZ3	1:A:356:HIS:HB2	2.04	0.92
1:B:434:PHE:HD2	1:B:435:LEU:HA	1.35	0.92
1:B:545:PRO:HG2	1:B:547:LEU:CD1	2.00	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:HE21	1:A:387:ASN:CB	1.77	0.91
1:B:593:ASP:HB2	1:B:594:PRO:HD3	1.51	0.91
1:A:182:ARG:HH21	1:A:190:ARG:HB2	1.34	0.91
1:B:170:MET:HE1	1:B:499:HIS:HA	1.53	0.91
1:B:415:MET:O	1:B:418:THR:HG22	1.70	0.91
1:B:454:PRO:HD3	1:B:509:MET:HE3	1.53	0.91
1:A:84:TRP:CE3	1:A:125:LYS:HG2	2.06	0.91
1:B:82:LYS:HG2	1:B:83:LEU:N	1.86	0.91
1:B:479:ALA:HB2	1:B:566:TYR:CD2	2.06	0.91
1:B:209:TRP:CB	1:B:246:ALA:HB3	2.00	0.91
1:B:306:LEU:HD21	1:B:310:PHE:HB3	1.51	0.90
1:A:224:ASN:CB	1:A:227:SER:HB3	2.00	0.90
1:A:269:ASP:HB2	1:A:279:ASN:HD22	1.34	0.90
1:A:329:ASP:OD1	1:A:330:THR:N	2.04	0.90
1:A:434:PHE:CD2	1:A:461:CYS:HB3	2.06	0.90
1:B:188:ASP:O	1:B:227:SER:OG	1.88	0.90
1:B:510:ARG:HB2	1:B:530:LEU:HB2	1.50	0.90
1:B:555:LEU:HD23	1:B:570:MET:CE	2.01	0.90
1:B:439:ASP:OD1	1:B:440:ALA:N	2.05	0.90
1:B:328:ASN:O	1:B:328:ASN:ND2	2.05	0.89
1:A:94:ASP:C	1:A:95:LYS:HG3	1.97	0.89
1:A:229:PRO:O	1:A:231:PRO:HD2	1.72	0.89
1:B:219:ARG:NH1	1:B:254:LYS:CD	2.34	0.89
1:A:101:GLN:CG	1:A:387:ASN:H	1.85	0.89
1:A:101:GLN:CG	1:A:387:ASN:N	2.35	0.89
1:A:610:ASN:O	2:A:701:HOH:O	1.91	0.89
1:B:353:LEU:C	1:B:354:GLN:HG2	1.98	0.89
1:B:194:ILE:O	1:B:197:THR:HB	1.72	0.89
1:A:230:ASN:N	1:A:231:PRO:HD3	1.87	0.89
1:A:625:ASP:C	1:A:651:TYR:CB	2.47	0.88
1:A:627:SER:CA	1:A:647:LYS:HZ1	1.82	0.88
1:A:549:LYS:HG3	1:A:550:GLY:N	1.88	0.88
1:A:119:LEU:HD11	1:A:389:LEU:CD2	2.04	0.88
1:B:454:PRO:HD2	1:B:509:MET:HE3	1.55	0.88
1:B:245:SER:O	1:B:316:ASP:O	1.91	0.88
1:A:653:THR:O	1:A:654:GLU:HB2	1.70	0.88
1:A:272:VAL:CG2	1:A:280:PHE:CB	2.51	0.88
1:B:347:LEU:O	1:B:350:GLY:CA	2.20	0.88
1:A:76:ARG:NH2	1:A:524:ALA:HB2	1.89	0.87
1:A:82:LYS:NZ	1:A:97:THR:HA	1.88	0.87
1:B:433:GLY:HA3	1:B:460:ALA:HB3	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:TRP:HZ2	1:B:541:PHE:CD2	1.81	0.87
1:B:525:GLU:OE1	1:B:545:PRO:O	1.93	0.87
1:B:86:THR:CG2	1:B:98:ARG:O	2.23	0.87
1:A:119:LEU:CD1	1:A:389:LEU:CD2	2.52	0.87
1:A:549:LYS:HG3	1:A:550:GLY:H	1.40	0.87
1:B:81:ILE:HG12	1:B:82:LYS:N	1.89	0.87
1:B:454:PRO:CD	1:B:509:MET:CE	2.52	0.86
1:B:546:ALA:O	1:B:547:LEU:HB2	1.74	0.86
1:A:86:THR:HG21	1:A:333:LYS:HB3	1.55	0.86
1:B:406:TRP:CE2	1:B:541:PHE:HD2	1.87	0.86
1:A:80:THR:CB	1:A:129:SER:HA	2.04	0.86
1:B:406:TRP:HE3	1:B:442:LEU:CD1	1.88	0.86
1:A:236:ARG:HG2	1:A:240:ILE:HG13	1.58	0.86
1:A:324:GLU:HG3	1:A:386:SER:OG	1.75	0.86
1:B:474:GLN:O	1:B:474:GLN:NE2	2.08	0.86
1:A:436:PHE:HE2	1:A:467:LYS:CB	1.88	0.86
1:A:500:GLU:O	1:A:505:GLY:N	2.08	0.86
1:A:286:PRO:HG2	1:A:289:ALA:HB2	1.57	0.86
1:A:413:VAL:HB	1:A:414:PRO:HD3	1.55	0.85
1:A:464:THR:HG22	1:A:465:ASN:H	1.41	0.85
1:B:194:ILE:HG21	1:B:470:TRP:HZ2	1.40	0.85
1:A:71:THR:CB	1:A:93:VAL:O	2.23	0.85
1:B:434:PHE:O	1:B:436:PHE:N	1.89	0.85
1:B:189:SER:C	1:B:191:VAL:H	1.85	0.85
1:A:229:PRO:C	1:A:231:PRO:HD2	2.00	0.85
1:B:436:PHE:O	1:B:438:ALA:N	2.09	0.85
1:A:186:SER:CB	1:A:187:PRO:HD3	2.07	0.84
1:B:64:ILE:H	1:B:76:ARG:HH21	1.25	0.84
1:B:454:PRO:HD3	1:B:509:MET:CE	2.06	0.84
1:A:462:ALA:C	1:A:463:GLY:O	2.01	0.84
1:A:228:PHE:O	1:A:230:ASN:N	2.10	0.84
1:A:577:ILE:O	2:A:702:HOH:O	1.95	0.84
1:A:330:THR:HB	1:A:331:PRO:HD2	1.58	0.84
1:B:211:ASP:O	1:B:212:ILE:HG22	1.72	0.84
1:A:182:ARG:NH2	1:A:190:ARG:CG	2.39	0.84
1:A:81:ILE:N	1:A:128:LEU:O	2.11	0.84
1:A:641:THR:HB	1:A:643:LYS:CE	2.08	0.84
1:B:210:MET:CB	1:B:211:ASP:CB	2.56	0.83
1:A:434:PHE:O	1:A:435:LEU:HB2	1.77	0.83
1:B:479:ALA:HB2	1:B:566:TYR:HD2	1.43	0.83
1:B:479:ALA:HA	1:B:566:TYR:CE2	2.14	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLN:O	2:B:702:HOH:O	1.94	0.83
1:A:182:ARG:HH22	1:A:190:ARG:HB3	1.40	0.83
1:A:273:LYS:O	1:A:275:ALA:N	2.11	0.83
1:A:406:TRP:CE3	1:A:442:LEU:HD13	2.13	0.83
1:B:139:SER:HB3	1:B:144:PHE:CE2	2.09	0.83
1:A:76:ARG:CZ	1:A:524:ALA:HB2	2.09	0.83
1:A:232:LYS:HA	1:A:311:LEU:HA	1.57	0.83
1:A:268:ASN:HB3	1:A:299:VAL:HG22	1.58	0.83
1:B:211:ASP:C	1:B:212:ILE:CG2	2.45	0.83
1:A:112:ASP:CG	1:A:113:GLY:H	1.86	0.82
1:B:165:THR:O	1:B:393:ARG:HD2	1.80	0.82
1:B:256:ASP:HB3	1:B:257:PRO:CD	2.09	0.82
1:A:466:ASN:HB3	1:A:471:VAL:HG11	1.62	0.82
1:B:277:GLY:C	1:B:278:LYS:HD3	2.04	0.82
1:A:192:ILE:CG2	1:A:195:ALA:CB	2.57	0.82
1:B:437:ASN:HA	1:B:465:ASN:OD1	1.78	0.82
1:A:272:VAL:HG13	1:A:336:PRO:HG2	0.83	0.82
1:B:270:VAL:HG22	1:B:292:PRO:HA	1.61	0.82
1:A:238:LEU:O	1:A:243:PHE:CB	2.28	0.82
1:A:269:ASP:HA	1:A:291:PHE:O	1.80	0.81
1:B:404:SER:O	1:B:442:LEU:HD22	1.80	0.81
1:B:62:THR:O	1:B:63:SER:HB2	1.79	0.81
1:B:209:TRP:HB2	1:B:246:ALA:HB3	1.61	0.81
1:A:272:VAL:HG13	1:A:336:PRO:O	1.81	0.81
1:B:270:VAL:HG22	1:B:271:TRP:N	1.93	0.81
1:B:479:ALA:CA	1:B:566:TYR:HE2	1.93	0.81
1:A:318:VAL:HG23	1:A:382:ILE:HD12	1.62	0.81
1:A:440:ALA:HB1	1:A:476:VAL:HG21	1.63	0.80
1:B:86:THR:HG21	1:B:98:ARG:O	1.81	0.80
1:B:406:TRP:HE3	1:B:442:LEU:HD13	1.44	0.80
1:A:259:TYR:O	1:A:260:PHE:HD1	1.64	0.80
1:B:132:ASP:O	1:B:133:GLU:HB2	1.80	0.80
1:B:414:PRO:HG3	1:B:526:GLU:HB3	1.64	0.80
1:B:404:SER:O	1:B:442:LEU:HD21	1.81	0.80
1:B:219:ARG:HH11	1:B:254:LYS:CD	1.93	0.79
1:B:74:LEU:CD2	1:B:75:LEU:H	1.94	0.79
1:B:322:VAL:O	1:B:324:GLU:N	2.15	0.79
1:A:280:PHE:CE2	1:A:335:MET:HB3	2.18	0.79
1:A:486:ARG:O	1:A:489:ILE:HG22	1.82	0.79
1:A:587:THR:O	1:A:590:ASN:HB2	1.82	0.79
1:B:132:ASP:O	1:B:133:GLU:CB	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ASN:N	1:A:231:PRO:CD	2.36	0.79
1:A:402:ASN:HB3	1:A:433:GLY:HA3	1.63	0.79
1:A:436:PHE:CE2	1:A:467:LYS:HB2	2.18	0.79
1:B:63:SER:HA	1:B:76:ARG:NH2	1.99	0.79
1:A:84:TRP:HD1	1:A:85:ASN:CA	1.96	0.78
1:A:268:ASN:CB	1:A:299:VAL:HG22	2.13	0.78
1:A:162:SER:O	1:A:166:GLY:N	2.16	0.78
1:B:256:ASP:CG	1:B:257:PRO:HD3	2.09	0.78
1:B:245:SER:HG	1:B:247:TRP:CD1	2.00	0.78
1:A:192:ILE:HG21	1:A:195:ALA:CB	2.10	0.78
1:A:219:ARG:NH2	1:A:256:ASP:CB	2.46	0.78
1:A:324:GLU:N	1:A:325:PRO:HA	1.97	0.78
1:B:256:ASP:CB	1:B:257:PRO:CD	2.61	0.78
1:A:283:ASP:H	1:A:327:ILE:HG23	1.48	0.78
1:B:507:PRO:O	1:B:510:ARG:NE	2.16	0.78
1:B:541:PHE:O	1:B:542:ALA:HB2	1.84	0.78
1:A:192:ILE:CG2	1:A:195:ALA:H	1.97	0.78
1:A:101:GLN:HG2	1:A:387:ASN:CA	2.14	0.78
1:A:436:PHE:HE2	1:A:467:LYS:HB2	1.48	0.78
1:A:308:LYS:HD2	1:A:371:ILE:HG12	1.66	0.77
1:B:212:ILE:HG13	1:B:213:ASP:N	1.98	0.77
1:B:479:ALA:CA	1:B:566:TYR:CE2	2.68	0.77
1:A:223:PHE:HZ	1:A:311:LEU:CB	1.97	0.77
1:B:454:PRO:HD2	1:B:509:MET:CE	2.14	0.77
1:A:436:PHE:CE2	1:A:460:ALA:HB2	2.20	0.77
1:B:256:ASP:HB3	1:B:257:PRO:HD2	1.66	0.77
1:A:274:THR:O	1:A:275:ALA:CB	2.33	0.77
1:A:285:TRP:HE1	1:A:322:VAL:HG21	1.49	0.77
1:A:305:ASN:OD1	1:A:307:TYR:HB3	1.84	0.77
1:B:402:ASN:ND2	1:B:446:TRP:CZ2	2.47	0.77
1:B:402:ASN:CB	1:B:430:ASP:HB2	2.14	0.77
1:A:225:PRO:CA	1:A:229:PRO:HG3	2.14	0.77
1:A:404:SER:HB2	1:A:436:PHE:HA	1.67	0.77
1:A:618:GLY:HA3	1:A:621:TYR:CE2	2.20	0.77
1:A:133:GLU:HA	1:A:134:LYS:HE3	1.66	0.76
1:A:207:VAL:HG13	1:A:244:HIS:O	1.84	0.76
1:A:262:TYR:CE1	1:A:264:SER:OG	2.38	0.76
1:A:430:ASP:HB3	1:A:459:HIS:HB3	1.68	0.76
1:B:525:GLU:OE2	1:B:527:GLU:CB	2.34	0.76
1:A:74:LEU:HD13	1:A:79:LYS:CE	2.16	0.76
1:A:272:VAL:HG22	1:A:280:PHE:CB	2.03	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:GLY:O	1:A:93:VAL:CB	2.33	0.76
1:A:436:PHE:CZ	1:A:460:ALA:HB2	2.19	0.76
1:A:431:ILE:CG2	1:A:446:TRP:HB3	2.16	0.76
1:A:618:GLY:HA3	1:A:621:TYR:CZ	2.21	0.75
1:B:406:TRP:CE3	1:B:442:LEU:CD1	2.69	0.75
1:B:126:ALA:HB1	1:B:137:LEU:HD21	1.67	0.75
1:A:324:GLU:CD	1:A:385:ARG:NH1	2.45	0.75
1:B:82:LYS:C	1:B:83:LEU:HD12	2.10	0.75
1:B:90:ALA:O	1:B:91:TYR:O	2.05	0.75
1:B:453:TYR:HA	1:B:509:MET:CE	2.15	0.75
1:B:210:MET:CA	1:B:211:ASP:CB	2.64	0.75
1:A:74:LEU:HD13	1:A:79:LYS:HE3	1.68	0.75
1:A:182:ARG:NH2	1:A:190:ARG:HG3	2.02	0.75
1:A:329:ASP:O	1:A:330:THR:OG1	2.05	0.75
1:B:464:THR:O	1:B:465:ASN:HB3	1.85	0.75
1:B:81:ILE:HG21	1:B:128:LEU:HB3	1.66	0.75
1:B:106:MET:HE3	1:B:135:ILE:HG13	1.68	0.75
1:B:586:ASN:HB2	1:B:589:GLU:CG	2.10	0.75
1:A:84:TRP:HA	1:A:357:ASN:OD1	1.87	0.75
1:B:91:TYR:CD2	1:B:415:MET:HE1	2.21	0.74
1:B:358:VAL:O	1:B:362:LEU:HG	1.87	0.74
1:A:274:THR:O	1:A:275:ALA:HB3	1.87	0.74
1:A:504:ASN:OD1	1:A:505:GLY:HA2	1.87	0.74
1:B:306:LEU:C	1:B:306:LEU:HD22	2.12	0.74
1:B:652:ASN:ND2	1:B:657:ASP:OD1	2.20	0.74
1:A:57:THR:HG23	1:A:134:LYS:HD2	0.85	0.74
1:A:84:TRP:CZ3	1:A:356:HIS:CB	2.71	0.74
1:B:78:GLY:O	1:B:79:LYS:HB2	1.86	0.74
1:B:245:SER:HG	1:B:247:TRP:HE1	1.24	0.74
1:B:470:TRP:C	1:B:472:PHE:H	1.94	0.74
1:B:428:GLY:HA3	1:B:455:PHE:O	1.87	0.74
1:B:575:GLY:HA2	1:B:606:LYS:O	1.87	0.74
1:B:379:ARG:CD	1:B:618:GLY:O	2.35	0.74
1:B:611:MET:HE3	1:B:631:PHE:HZ	1.51	0.74
1:A:179:GLN:OE1	1:A:455:PHE:CE1	2.40	0.73
1:A:581:GLY:O	1:A:582:LYS:HB3	1.86	0.73
1:B:459:HIS:CG	1:B:460:ALA:N	2.56	0.73
1:B:493:TYR:OH	1:B:531:VAL:O	2.04	0.73
1:B:379:ARG:CG	1:B:618:GLY:O	2.36	0.73
1:B:566:TYR:CA	1:B:567:GLN:HG2	2.15	0.73
1:A:171:ILE:HD12	1:A:175:ALA:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ASN:C	1:A:333:LYS:HG2	2.14	0.73
1:A:627:SER:CA	1:A:647:LYS:HZ3	1.98	0.73
1:B:307:TYR:HD2	1:B:374:ALA:CB	2.01	0.73
1:B:328:ASN:CG	1:B:348:PRO:CB	2.58	0.73
1:B:538:ILE:CD1	1:B:545:PRO:HG3	2.19	0.73
1:A:587:THR:HB	1:A:590:ASN:HD22	1.52	0.73
1:B:151:ARG:HH12	1:B:160:GLY:HA3	1.52	0.73
1:B:186:SER:CB	1:B:187:PRO:CD	2.60	0.73
1:B:87:ASP:HB3	1:B:324:GLU:OE1	1.88	0.73
1:B:224:ASN:H	1:B:225:PRO:HD2	1.52	0.73
1:A:538:ILE:HD12	1:A:569:LYS:HB3	1.69	0.73
1:B:83:LEU:N	1:B:83:LEU:HD12	2.02	0.73
1:B:256:ASP:C	1:B:259:TYR:CE2	2.66	0.73
1:B:402:ASN:HB2	1:B:430:ASP:CB	2.19	0.73
1:B:635:ARG:HE	1:B:636:ASN:HD22	1.35	0.73
1:A:436:PHE:CE1	1:A:459:HIS:CE1	2.77	0.73
1:B:93:VAL:O	1:B:97:THR:N	2.22	0.73
1:B:180:GLN:O	1:B:181:CYS:HB2	1.88	0.73
1:A:84:TRP:CZ3	1:A:125:LYS:HG2	2.23	0.72
1:B:204:PRO:CB	1:B:585:GLN:HA	2.18	0.72
1:B:166:GLY:HA3	1:B:393:ARG:HD2	1.71	0.72
1:A:84:TRP:O	1:A:85:ASN:HB2	1.89	0.72
1:A:179:GLN:HB3	1:A:209:TRP:NE1	2.02	0.72
1:A:436:PHE:CE2	1:A:460:ALA:CB	2.71	0.72
1:A:272:VAL:HG11	1:A:336:PRO:HG3	1.69	0.72
1:A:434:PHE:O	1:A:435:LEU:CB	2.36	0.72
1:A:236:ARG:NH1	1:B:661:ILE:HG23	2.04	0.72
1:A:266:THR:O	1:A:267:GLU:CB	2.32	0.72
1:A:506:MET:CB	1:A:507:PRO:CD	2.66	0.72
1:B:552:TRP:HA	1:B:571:LYS:HD3	1.72	0.72
1:B:590:ASN:C	1:B:591:SER:HG	1.92	0.72
1:A:80:THR:HA	1:A:129:SER:HA	1.70	0.72
1:B:545:PRO:O	1:B:546:ALA:CB	2.37	0.72
1:A:74:LEU:CD1	1:A:76:ARG:O	2.37	0.72
1:A:84:TRP:CH2	1:A:356:HIS:HB2	2.24	0.72
1:A:80:THR:CB	1:A:129:SER:CB	2.61	0.72
1:A:223:PHE:CD2	1:A:231:PRO:HB2	2.24	0.72
1:B:534:ASN:CG	1:B:576:ALA:HB1	2.14	0.72
1:B:62:THR:HB	1:B:64:ILE:HD11	1.72	0.71
1:B:527:GLU:CB	1:B:543:ASN:ND2	2.53	0.71
1:A:236:ARG:HG2	1:A:240:ILE:CG1	2.21	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ILE:HD11	1:B:120:PHE:HE1	1.54	0.71
1:B:431:ILE:HA	1:B:446:TRP:CE2	2.26	0.71
1:B:178:TYR:HB3	1:B:205:CYS:SG	2.30	0.71
1:A:84:TRP:HZ2	1:A:334:THR:CG2	2.03	0.71
1:A:397:THR:HG21	1:A:424:GLN:HG2	1.73	0.71
1:B:413:VAL:HB	1:B:414:PRO:HD3	1.73	0.71
1:B:100:TYR:HE2	1:B:400:GLY:HA2	1.55	0.71
1:B:270:VAL:CG2	1:B:292:PRO:CA	2.67	0.71
1:B:206:ASP:HB2	1:B:488:TYR:HH	1.55	0.70
1:A:84:TRP:HE3	1:A:125:LYS:HG2	1.52	0.70
1:A:225:PRO:O	1:A:229:PRO:HG2	1.91	0.70
1:B:209:TRP:HH2	1:B:459:HIS:CD2	2.10	0.70
1:A:73:SER:H	1:A:95:LYS:HE3	1.56	0.70
1:A:625:ASP:CB	1:A:651:TYR:CB	2.69	0.70
1:B:231:PRO:O	1:B:235:ASN:OD1	2.09	0.70
1:B:270:VAL:HG21	1:B:292:PRO:HB3	1.73	0.70
1:A:209:TRP:HE3	1:A:319:TRP:CE3	2.09	0.70
1:A:440:ALA:HB1	1:A:476:VAL:CG2	2.22	0.70
1:A:486:ARG:O	1:A:489:ILE:CG2	2.40	0.70
1:A:627:SER:CB	1:A:647:LYS:NZ	2.54	0.70
1:A:641:THR:HB	1:A:643:LYS:NZ	2.06	0.70
1:A:192:ILE:HG22	1:A:195:ALA:H	1.57	0.69
1:B:183:PHE:HA	1:B:212:ILE:H	1.54	0.69
1:B:459:HIS:CG	1:B:460:ALA:H	2.10	0.69
1:B:594:PRO:C	1:B:596:THR:H	1.98	0.69
1:A:224:ASN:CB	1:A:227:SER:CB	2.57	0.69
1:B:270:VAL:HG22	1:B:271:TRP:H	1.57	0.69
1:B:264:SER:OG	1:B:302:TRP:NE1	2.25	0.69
1:B:270:VAL:HG13	1:B:271:TRP:CE3	2.27	0.69
1:B:545:PRO:CG	1:B:547:LEU:CD1	2.70	0.69
1:B:81:ILE:HG12	1:B:82:LYS:H	1.55	0.69
1:B:184:SER:OG	1:B:185:TYR:N	2.24	0.69
1:A:84:TRP:CZ2	1:A:356:HIS:CD2	2.79	0.69
1:A:330:THR:CB	1:A:331:PRO:HD2	2.22	0.69
1:B:278:LYS:HD3	1:B:278:LYS:N	2.07	0.69
1:B:171:ILE:HD12	1:B:175:ALA:HB3	1.73	0.69
1:B:306:LEU:HD21	1:B:310:PHE:CB	2.23	0.69
1:B:436:PHE:C	1:B:438:ALA:H	2.00	0.69
1:A:409:LEU:HD23	1:A:410:LYS:N	2.08	0.69
1:A:434:PHE:CD2	1:A:461:CYS:CB	2.75	0.69
1:B:485:GLU:O	1:B:489:ILE:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:TRP:CB	1:B:571:LYS:CD	2.71	0.69
1:A:191:VAL:O	1:A:192:ILE:HB	1.92	0.69
1:B:298:LYS:O	1:B:301:LYS:HE3	1.94	0.69
1:A:232:LYS:HA	1:A:311:LEU:CA	2.18	0.68
1:A:232:LYS:O	1:A:233:ALA:HB3	1.92	0.68
1:A:266:THR:CB	1:A:268:ASN:OD1	2.41	0.68
1:B:64:ILE:O	1:B:74:LEU:CD2	2.41	0.68
1:A:466:ASN:O	1:A:467:LYS:HB3	1.92	0.68
1:B:520:LEU:HD12	1:B:520:LEU:N	2.09	0.68
1:B:552:TRP:CB	1:B:571:LYS:HD3	2.23	0.68
1:A:90:ALA:C	1:A:92:GLY:H	2.01	0.68
1:A:228:PHE:C	1:A:230:ASN:N	2.34	0.68
1:A:538:ILE:CG2	1:A:544:GLN:O	2.41	0.68
1:B:406:TRP:CE3	1:B:442:LEU:HD12	2.28	0.68
1:A:84:TRP:HZ2	1:A:334:THR:HG21	1.59	0.68
1:A:131:THR:HG22	1:A:132:ASP:N	2.04	0.68
1:A:307:TYR:O	1:A:310:PHE:HD2	1.76	0.68
1:B:64:ILE:N	1:B:76:ARG:HH21	1.91	0.68
1:B:189:SER:C	1:B:191:VAL:N	2.48	0.68
1:B:215:MET:HB2	1:B:218:TYR:HA	1.76	0.68
1:B:248:MET:HB2	1:B:319:TRP:CE2	2.29	0.68
1:B:300:ASN:O	1:B:304:ARG:N	2.25	0.68
1:B:277:GLY:C	1:B:278:LYS:CD	2.66	0.68
1:A:538:ILE:HG21	1:A:544:GLN:O	1.94	0.68
1:A:577:ILE:HB	1:A:609:GLY:HA3	1.75	0.68
1:B:210:MET:HA	1:B:211:ASP:CB	2.24	0.68
1:B:453:TYR:HA	1:B:509:MET:HE2	1.75	0.68
1:A:86:THR:HG21	1:A:333:LYS:HB2	1.74	0.67
1:A:202:ARG:HD3	1:B:583:ILE:HD12	1.75	0.67
1:A:628:LEU:HB3	1:A:648:THR:HB	1.75	0.67
1:B:474:GLN:O	1:B:478:ASP:OD2	2.12	0.67
1:A:84:TRP:CD2	1:A:356:HIS:CD2	2.81	0.67
1:A:68:GLY:HA2	1:A:422:SER:CB	2.25	0.67
1:B:70:VAL:HG22	1:B:71:THR:N	2.03	0.67
1:B:245:SER:O	1:B:316:ASP:C	2.36	0.67
1:A:649:GLY:O	1:A:650:LYS:HB2	1.93	0.67
1:B:63:SER:HA	1:B:76:ARG:HH21	1.58	0.67
1:A:426:PHE:CE2	1:A:455:PHE:HB2	2.30	0.67
1:A:586:ASN:OD1	1:A:588:THR:HB	1.93	0.67
1:B:63:SER:H	1:B:76:ARG:HH22	1.43	0.67
1:B:81:ILE:CG2	1:B:128:LEU:CB	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASP:HB3	1:B:519:ASP:HB2	1.77	0.67
1:A:307:TYR:HA	1:A:310:PHE:CE2	2.29	0.67
1:A:462:ALA:O	1:A:463:GLY:C	2.36	0.67
1:B:178:TYR:CB	1:B:205:CYS:HB3	2.08	0.67
1:B:347:LEU:O	1:B:350:GLY:HA2	1.95	0.67
1:A:171:ILE:HD12	1:A:175:ALA:CB	2.24	0.67
1:A:379:ARG:CZ	1:A:618:GLY:O	2.42	0.67
1:B:256:ASP:CB	1:B:257:PRO:HD3	2.24	0.67
1:A:106:MET:O	1:A:107:MET:HB3	1.92	0.66
1:A:308:LYS:HD2	1:A:371:ILE:CG1	2.25	0.66
1:A:128:LEU:HD23	1:A:137:LEU:HB2	1.77	0.66
1:A:239:HIS:HE1	1:A:316:ASP:OD2	1.76	0.66
1:A:460:ALA:CB	1:A:467:LYS:HD3	2.22	0.66
1:B:193:GLU:HB3	1:B:195:ALA:HB3	1.78	0.66
1:B:204:PRO:HB2	1:B:584:ILE:O	1.95	0.66
1:B:209:TRP:HB3	1:B:246:ALA:HB3	1.73	0.66
1:B:434:PHE:CD2	1:B:435:LEU:HA	2.25	0.66
1:A:491:LEU:HD21	1:A:590:ASN:OD1	1.95	0.66
1:A:126:ALA:O	1:A:127:GLU:HB2	1.95	0.66
1:B:256:ASP:C	1:B:259:TYR:HE2	2.01	0.66
1:B:307:TYR:HD1	1:B:307:TYR:H	1.44	0.66
1:B:605:GLY:O	1:B:606:LYS:HG3	1.96	0.66
1:A:165:THR:CG2	1:A:390:GLY:HA2	2.26	0.66
1:A:128:LEU:CD2	1:A:137:LEU:HB2	2.26	0.66
1:A:575:GLY:HA2	1:A:606:LYS:O	1.95	0.66
1:B:81:ILE:CG2	1:B:128:LEU:HB3	2.25	0.66
1:A:589:GLU:OE1	2:A:703:HOH:O	2.12	0.66
1:B:78:GLY:O	1:B:79:LYS:CB	2.44	0.66
1:B:367:SER:O	1:B:371:ILE:HD12	1.96	0.66
1:B:479:ALA:HB2	1:B:566:TYR:CE2	2.31	0.66
1:B:573:ARG:NH1	1:B:574:GLY:O	2.29	0.66
1:A:552:TRP:O	1:A:572:ILE:O	2.14	0.66
1:B:459:HIS:ND1	1:B:460:ALA:N	2.43	0.66
1:B:545:PRO:O	1:B:546:ALA:HB2	1.95	0.66
1:A:272:VAL:CG2	1:A:280:PHE:CA	2.74	0.66
1:A:500:GLU:O	1:A:505:GLY:CA	2.44	0.66
1:A:512:VAL:CG1	1:A:548:PRO:HD3	2.22	0.66
1:B:612:TYR:OH	1:B:621:TYR:HB3	1.96	0.66
1:A:500:GLU:O	1:A:505:GLY:HA3	1.96	0.65
1:B:538:ILE:HD12	1:B:545:PRO:HG3	1.77	0.65
1:B:606:LYS:NZ	1:B:634:GLU:HG3	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:CYS:O	1:A:406:TRP:HB2	1.94	0.65
1:A:464:THR:CG2	1:A:465:ASN:H	2.10	0.65
1:B:81:ILE:HG21	1:B:128:LEU:CB	2.26	0.65
1:B:483:ALA:O	1:B:486:ARG:HB2	1.97	0.65
1:B:228:PHE:N	1:B:229:PRO:HD3	2.12	0.65
1:B:557:LEU:H	1:B:557:LEU:HD12	1.61	0.65
1:B:124:TRP:O	1:B:140:GLU:CB	2.44	0.65
1:B:270:VAL:CG2	1:B:271:TRP:N	2.59	0.65
1:B:512:VAL:CG2	1:B:528:ALA:O	2.43	0.65
1:B:100:TYR:CE2	1:B:400:GLY:HA2	2.31	0.65
1:A:248:MET:HB2	1:A:319:TRP:CH2	2.32	0.65
1:A:654:GLU:C	1:A:655:ASN:HD22	2.03	0.65
1:B:479:ALA:CB	1:B:566:TYR:CD2	2.79	0.65
1:B:64:ILE:H	1:B:76:ARG:NH2	1.94	0.65
1:B:522:LEU:N	1:B:522:LEU:HD23	2.12	0.65
1:A:84:TRP:CE2	1:A:356:HIS:HD2	2.14	0.65
1:B:82:LYS:HE2	1:B:84:TRP:HB3	1.78	0.65
1:A:538:ILE:CD1	1:A:569:LYS:HB3	2.27	0.65
1:B:554:GLU:O	1:B:555:LEU:CB	2.41	0.65
1:B:63:SER:CA	1:B:76:ARG:NH2	2.60	0.64
1:A:74:LEU:HD22	1:A:79:LYS:HD2	1.79	0.64
1:A:84:TRP:CD1	1:A:85:ASN:CA	2.75	0.64
1:A:84:TRP:HD1	1:A:85:ASN:HA	1.62	0.64
1:B:91:TYR:CD2	1:B:415:MET:CE	2.81	0.64
1:B:118:ILE:CD1	1:B:120:PHE:CE1	2.79	0.64
1:B:593:ASP:CB	1:B:594:PRO:CD	2.70	0.64
1:A:84:TRP:O	1:A:85:ASN:CB	2.45	0.64
1:B:520:LEU:HD12	1:B:520:LEU:H	1.61	0.64
1:A:306:LEU:HA	1:A:374:ALA:HB2	1.77	0.64
1:A:626:TYR:O	1:A:650:LYS:N	2.31	0.64
1:B:609:GLY:O	1:B:631:PHE:N	2.16	0.64
1:B:115:ALA:HB3	1:B:154:PRO:HA	1.79	0.64
1:B:638:ASP:CG	1:B:639:LYS:HG2	2.22	0.64
1:A:80:THR:CA	1:A:129:SER:HA	2.27	0.64
1:B:165:THR:O	1:B:393:ARG:CD	2.46	0.64
1:A:261:VAL:CG1	1:A:262:TYR:N	2.59	0.64
1:A:618:GLY:CA	1:A:621:TYR:CZ	2.79	0.64
1:B:90:ALA:O	1:B:91:TYR:C	2.41	0.64
1:B:406:TRP:HZ2	1:B:541:PHE:HB2	1.63	0.64
1:B:517:PRO:O	1:B:523:ARG:NH2	2.31	0.64
1:A:84:TRP:CD2	1:A:356:HIS:HD2	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:LYS:O	1:A:112:ASP:O	2.16	0.63
1:A:165:THR:O	1:A:393:ARG:NH1	2.29	0.63
1:A:105:TRP:CE2	1:A:161:LEU:HD22	2.34	0.63
1:A:465:ASN:C	1:A:466:ASN:OD1	2.42	0.63
1:B:81:ILE:HG22	1:B:128:LEU:O	1.98	0.63
1:A:52:ALA:O	1:A:53:ASN:ND2	2.32	0.63
1:A:420:GLY:HA3	1:A:507:PRO:HG3	1.80	0.63
1:B:181:CYS:O	1:B:459:HIS:CD2	2.51	0.63
1:A:211:ASP:O	1:A:212:ILE:HG22	1.98	0.63
1:A:461:CYS:SG	1:A:462:ALA:N	2.72	0.63
1:B:566:TYR:N	1:B:567:GLN:HA	2.12	0.63
1:B:106:MET:HE1	1:B:129:SER:O	1.99	0.63
1:A:101:GLN:HG3	1:A:387:ASN:N	2.14	0.63
1:A:552:TRP:CH2	1:A:573:ARG:HG3	2.34	0.63
1:B:117:GLY:O	1:B:148:ILE:HA	1.98	0.63
1:B:188:ASP:OD2	1:B:192:ILE:CD1	2.46	0.63
1:B:255:VAL:O	1:B:255:VAL:HG23	1.99	0.62
1:A:215:MET:HE3	1:A:218:TYR:HA	1.80	0.62
1:B:206:ASP:HB2	1:B:488:TYR:OH	1.98	0.62
1:B:434:PHE:HD2	1:B:435:LEU:CA	2.08	0.62
1:B:435:LEU:O	1:B:436:PHE:CB	2.48	0.62
1:A:133:GLU:CA	1:A:134:LYS:HE3	2.29	0.62
1:B:305:ASN:ND2	1:B:307:TYR:CE1	2.67	0.62
1:B:579:PRO:HB2	1:B:611:MET:HE2	1.81	0.62
1:B:590:ASN:O	1:B:590:ASN:ND2	2.29	0.62
1:A:99:LEU:N	1:A:99:LEU:HD12	2.13	0.62
1:B:557:LEU:HD12	1:B:557:LEU:N	2.15	0.62
1:A:462:ALA:O	1:A:463:GLY:O	2.17	0.62
1:B:132:ASP:O	1:B:133:GLU:HG2	1.99	0.62
1:B:279:ASN:OD1	1:B:279:ASN:N	2.33	0.62
1:B:82:LYS:HG2	1:B:83:LEU:H	1.64	0.62
1:B:509:MET:HG3	1:B:529:PHE:CD2	2.35	0.62
1:A:182:ARG:O	1:A:183:PHE:HB2	2.00	0.62
1:A:272:VAL:HG21	1:A:280:PHE:HA	1.81	0.62
1:A:307:TYR:O	1:A:310:PHE:CD2	2.53	0.62
1:A:322:VAL:HG13	1:A:326:GLN:OE1	2.00	0.62
1:B:194:ILE:HG22	1:B:470:TRP:CH2	2.33	0.62
1:B:263:LYS:CA	1:B:265:GLY:H	2.00	0.62
1:B:264:SER:HG	1:B:302:TRP:NE1	1.97	0.62
1:B:431:ILE:HA	1:B:446:TRP:NE1	2.15	0.62
1:A:151:ARG:HH12	1:A:160:GLY:HA3	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ALA:C	1:A:235:ASN:H	2.08	0.62
1:B:86:THR:HG22	1:B:98:ARG:O	1.99	0.62
1:B:512:VAL:HG13	1:B:548:PRO:HG3	1.82	0.61
1:A:65:TYR:O	1:A:106:MET:HG2	2.00	0.61
1:A:74:LEU:HD13	1:A:79:LYS:CD	2.30	0.61
1:A:397:THR:HG23	1:A:424:GLN:NE2	2.15	0.61
1:B:223:PHE:CB	1:B:224:ASN:HA	2.29	0.61
1:B:369:GLU:O	1:B:373:ASP:HB2	2.00	0.61
1:B:109:VAL:O	1:B:110:ARG:HB3	1.99	0.61
1:B:185:TYR:O	1:B:212:ILE:HD13	2.00	0.61
1:B:188:ASP:HB3	1:B:189:SER:HA	1.81	0.61
1:B:270:VAL:CG2	1:B:271:TRP:H	2.13	0.61
1:B:305:ASN:ND2	1:B:307:TYR:HE1	1.97	0.61
1:A:431:ILE:HG22	1:A:446:TRP:HB3	1.80	0.61
1:A:286:PRO:CG	1:A:289:ALA:HB2	2.31	0.61
1:B:171:ILE:HB	1:B:172:PRO:HD2	1.82	0.61
1:B:151:ARG:HH12	1:B:160:GLY:CA	2.12	0.61
1:B:247:TRP:CD1	1:B:315:VAL:HG13	2.36	0.61
1:A:101:GLN:NE2	1:A:387:ASN:HB2	2.14	0.61
1:B:479:ALA:N	1:B:566:TYR:HE2	1.98	0.61
1:B:519:ASP:OD1	1:B:521:SER:N	2.32	0.61
1:B:590:ASN:C	1:B:591:SER:OG	2.37	0.61
1:B:651:TYR:CG	1:B:652:ASN:N	2.68	0.61
1:A:230:ASN:HD21	1:A:234:VAL:CB	2.14	0.60
1:A:430:ASP:HB3	1:A:459:HIS:CB	2.30	0.60
1:A:431:ILE:HG22	1:A:431:ILE:O	2.01	0.60
1:A:625:ASP:HB3	1:A:651:TYR:CB	2.31	0.60
1:B:162:SER:HB2	1:B:504:ASN:O	2.00	0.60
1:B:173:ARG:NH1	1:B:495:TYR:CE2	2.68	0.60
1:B:285:TRP:HB2	1:B:286:PRO:HD3	1.83	0.60
1:B:611:MET:HE3	1:B:631:PHE:CZ	2.35	0.60
1:A:86:THR:O	1:A:87:ASP:C	2.45	0.60
1:B:64:ILE:HG12	1:B:76:ARG:NH2	2.16	0.60
1:B:101:GLN:HB3	1:B:103:HIS:CE1	2.37	0.60
1:A:627:SER:CB	1:A:647:LYS:HE2	2.30	0.60
1:A:269:ASP:HB2	1:A:279:ASN:ND2	2.14	0.60
1:B:267:GLU:O	1:B:268:ASN:CB	2.49	0.60
1:B:593:ASP:HB3	1:B:594:PRO:HD3	1.83	0.60
1:A:231:PRO:C	1:A:233:ALA:H	2.09	0.60
1:A:330:THR:HB	1:A:331:PRO:CD	2.31	0.60
1:A:192:ILE:C	1:A:194:ILE:N	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:PHE:O	1:A:231:PRO:CD	2.46	0.60
1:A:257:PRO:HA	1:A:259:TYR:CE2	2.37	0.60
1:A:231:PRO:O	1:A:311:LEU:CB	2.50	0.60
1:A:233:ALA:C	1:A:235:ASN:N	2.56	0.60
1:A:94:ASP:O	1:A:95:LYS:CB	2.49	0.60
1:B:106:MET:HE3	1:B:135:ILE:CG1	2.32	0.60
1:A:89:GLY:O	1:A:90:ALA:HB2	2.01	0.60
1:A:185:TYR:O	1:A:187:PRO:O	2.19	0.60
1:A:582:LYS:HE2	1:A:594:PRO:HD2	1.82	0.60
1:B:552:TRP:CA	1:B:571:LYS:HD3	2.32	0.60
1:A:90:ALA:C	1:A:92:GLY:N	2.55	0.60
1:A:410:LYS:HZ3	1:A:413:VAL:HG21	1.67	0.60
1:B:573:ARG:HG2	1:B:573:ARG:NH1	2.05	0.60
1:A:629:LEU:HD22	1:A:644:LEU:HD11	1.83	0.59
1:B:545:PRO:CG	1:B:547:LEU:HD11	2.31	0.59
1:A:264:SER:C	1:A:266:THR:N	2.60	0.59
1:B:257:PRO:HA	1:B:259:TYR:CE2	2.38	0.59
1:A:280:PHE:CZ	1:A:335:MET:HA	2.38	0.59
1:B:264:SER:HG	1:B:302:TRP:CD1	2.21	0.59
1:B:74:LEU:HD23	1:B:75:LEU:N	2.08	0.59
1:B:579:PRO:CB	1:B:611:MET:HE2	2.32	0.59
1:B:352:HIS:O	1:B:353:LEU:CB	2.50	0.59
1:A:431:ILE:HG23	1:A:446:TRP:HB3	1.83	0.59
1:A:431:ILE:C	1:A:459:HIS:CD2	2.80	0.59
1:A:432:GLY:HA3	1:A:459:HIS:NE2	2.18	0.59
1:B:402:ASN:HB2	1:B:430:ASP:OD2	2.02	0.59
1:A:64:ILE:O	1:A:77:ASN:ND2	2.28	0.58
1:A:209:TRP:HH2	1:A:383:LEU:CD1	2.15	0.58
1:B:177:GLY:H	1:B:487:ARG:HH21	1.50	0.58
1:A:410:LYS:NZ	1:A:413:VAL:HG21	2.18	0.58
1:B:285:TRP:N	1:B:286:PRO:HD2	2.17	0.58
1:B:590:ASN:C	1:B:590:ASN:HD22	2.08	0.58
1:A:51:LYS:O	1:A:52:ALA:O	2.21	0.58
1:A:126:ALA:HB3	1:A:137:LEU:HD11	1.85	0.58
1:A:280:PHE:CD1	1:A:336:PRO:CD	2.77	0.58
1:A:362:LEU:HD23	1:A:362:LEU:O	2.02	0.58
1:A:652:ASN:O	1:A:653:THR:OG1	2.20	0.58
1:B:64:ILE:O	1:B:74:LEU:HD21	2.03	0.58
1:B:128:LEU:HG	1:B:137:LEU:HD12	1.84	0.58
1:B:266:THR:O	1:B:267:GLU:HB3	2.02	0.58
1:B:180:GLN:OE1	1:B:181:CYS:HA	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:C	1:A:134:LYS:HE3	2.28	0.58
1:A:464:THR:HG22	1:A:465:ASN:N	2.14	0.58
1:B:126:ALA:CB	1:B:137:LEU:HD21	2.34	0.58
1:B:219:ARG:NH1	1:B:254:LYS:HD2	2.19	0.58
1:B:364:VAL:HG21	1:B:384:THR:HB	1.84	0.58
1:B:381:PHE:CE1	1:B:383:LEU:HD21	2.38	0.58
1:A:262:TYR:O	1:A:262:TYR:HD1	1.85	0.58
1:B:270:VAL:O	1:B:271:TRP:CB	2.51	0.58
1:A:88:SER:CB	1:A:98:ARG:O	2.52	0.58
1:B:204:PRO:HB2	1:B:585:GLN:HA	1.86	0.58
1:B:307:TYR:CD2	1:B:374:ALA:CB	2.73	0.58
1:B:479:ALA:CB	1:B:566:TYR:CE2	2.86	0.58
1:B:507:PRO:O	1:B:510:ARG:CD	2.52	0.58
1:B:638:ASP:C	1:B:639:LYS:HG2	2.28	0.58
1:A:624:GLY:O	1:A:650:LYS:O	2.21	0.58
1:B:220:ILE:HG21	1:B:250:ASP:O	2.04	0.58
1:A:635:ARG:HB2	1:A:640:VAL:HG22	1.86	0.58
1:B:223:PHE:HB2	1:B:224:ASN:HA	1.84	0.58
1:A:74:LEU:O	1:A:75:LEU:C	2.46	0.57
1:A:84:TRP:CG	1:A:85:ASN:N	2.48	0.57
1:A:165:THR:O	1:A:165:THR:HG22	2.03	0.57
1:A:399:THR:O	1:A:399:THR:HG22	2.03	0.57
1:A:451:ALA:O	1:A:487:ARG:HD2	2.04	0.57
1:B:178:TYR:CB	1:B:205:CYS:SG	2.92	0.57
1:B:270:VAL:HG21	1:B:292:PRO:CB	2.34	0.57
1:B:59:PRO:HB2	1:B:62:THR:OG1	2.03	0.57
1:B:257:PRO:CA	1:B:259:TYR:CE2	2.87	0.57
1:B:566:TYR:N	1:B:566:TYR:CD1	2.72	0.57
1:B:594:PRO:C	1:B:596:THR:N	2.59	0.57
1:A:210:MET:HG3	1:A:247:TRP:CH2	2.39	0.57
1:A:112:ASP:CG	1:A:113:GLY:N	2.57	0.57
1:A:259:TYR:O	1:A:260:PHE:CD1	2.53	0.57
1:A:398:TRP:HH2	1:A:401:ASP:OD1	1.86	0.57
1:B:577:ILE:HG13	1:B:607:ALA:HB1	1.85	0.57
1:A:538:ILE:HD12	1:A:569:LYS:CB	2.33	0.57
1:B:328:ASN:HB2	1:B:348:PRO:CA	2.35	0.57
1:B:453:TYR:HA	1:B:509:MET:HE1	1.85	0.57
1:B:507:PRO:O	1:B:510:ARG:HD3	2.05	0.57
1:B:81:ILE:CG2	1:B:128:LEU:O	2.52	0.57
1:B:379:ARG:HG3	1:B:618:GLY:O	2.04	0.57
1:A:406:TRP:CD1	1:A:409:LEU:HD22	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:THR:HA	1:B:352:HIS:NE2	2.16	0.57
1:A:209:TRP:HH2	1:A:383:LEU:HD12	1.69	0.57
1:A:440:ALA:CB	1:A:476:VAL:HG21	2.34	0.57
1:A:573:ARG:O	1:A:576:ALA:HB3	2.04	0.57
1:B:183:PHE:HA	1:B:212:ILE:N	2.18	0.57
1:B:629:LEU:CD2	1:B:647:LYS:HD2	2.35	0.57
1:B:629:LEU:HD22	1:B:647:LYS:HD2	1.86	0.57
1:A:66:GLY:HA3	1:A:106:MET:HA	1.87	0.57
1:A:120:PHE:HB3	1:A:144:PHE:CE1	2.40	0.57
1:B:94:ASP:O	1:B:96:GLY:N	2.32	0.57
1:B:298:LYS:HA	1:B:301:LYS:CE	2.34	0.57
1:B:298:LYS:HA	1:B:301:LYS:HE3	1.85	0.57
1:B:474:GLN:HE21	1:B:474:GLN:HA	1.70	0.57
1:A:78:GLY:CA	1:A:131:THR:HA	2.28	0.56
1:A:118:ILE:CG1	1:A:120:PHE:CE1	2.87	0.56
1:A:226:LYS:C	1:A:228:PHE:H	2.11	0.56
1:B:488:TYR:HD2	1:B:584:ILE:CG2	2.17	0.56
1:B:542:ALA:O	1:B:543:ASN:O	2.23	0.56
1:A:330:THR:CB	1:A:331:PRO:CD	2.77	0.56
1:A:597:LEU:HD21	1:A:631:PHE:CD1	2.40	0.56
1:B:72:GLY:HA2	1:B:73:SER:CB	2.16	0.56
1:A:53:ASN:O	1:A:54:ALA:HB2	2.05	0.56
1:A:82:LYS:NZ	1:A:97:THR:CA	2.66	0.56
1:A:85:ASN:HB3	1:A:99:LEU:O	2.05	0.56
1:A:94:ASP:O	1:A:95:LYS:HB2	2.05	0.56
1:A:170:MET:HE2	1:A:498:LEU:HG	1.87	0.56
1:A:259:TYR:CE2	1:A:262:TYR:CD1	2.92	0.56
1:A:432:GLY:HA3	1:A:436:PHE:HE1	1.69	0.56
1:A:456:ALA:HA	2:A:704:HOH:O	2.05	0.56
1:B:213:ASP:HB3	1:B:218:TYR:CE1	2.41	0.56
1:B:434:PHE:CD2	1:B:434:PHE:C	2.83	0.56
1:B:467:LYS:O	1:B:468:GLU:CB	2.53	0.56
1:B:470:TRP:C	1:B:472:PHE:N	2.58	0.56
1:B:472:PHE:O	1:B:476:VAL:HG21	2.05	0.56
1:A:72:GLY:C	1:A:74:LEU:H	2.14	0.56
1:A:236:ARG:NE	1:A:240:ILE:HD11	2.20	0.56
1:A:360:GLY:O	1:A:364:VAL:HG12	2.06	0.56
1:A:525:GLU:OE1	1:A:545:PRO:CG	2.47	0.56
1:B:541:PHE:O	1:B:542:ALA:CB	2.50	0.56
1:A:388:PHE:CD1	1:A:389:LEU:N	2.73	0.56
1:A:633:ALA:HB2	1:A:642:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:ND2	1:B:446:TRP:HH2	1.99	0.56
1:A:444:GLY:O	1:A:566:TYR:HB3	2.05	0.56
1:B:132:ASP:O	1:B:133:GLU:CG	2.54	0.56
1:B:536:LEU:HD21	1:B:548:PRO:HD2	1.87	0.56
1:B:555:LEU:O	1:B:557:LEU:N	2.36	0.56
1:B:606:LYS:HZ3	1:B:634:GLU:HG3	1.70	0.56
1:A:552:TRP:CZ2	1:A:573:ARG:HG3	2.41	0.56
1:A:304:ARG:HB2	1:A:370:GLY:HA2	1.88	0.56
1:B:375:ARG:HG2	1:B:376:PRO:HD2	1.87	0.56
1:B:553:LYS:CB	1:B:572:ILE:H	2.19	0.56
1:A:125:LYS:CE	1:A:355:TYR:HA	2.36	0.56
1:A:618:GLY:N	1:A:621:TYR:OH	2.39	0.56
1:B:190:ARG:HG2	1:B:194:ILE:HG12	1.88	0.56
1:B:212:ILE:HG13	1:B:213:ASP:H	1.71	0.56
1:B:306:LEU:HD13	1:B:307:TYR:N	2.21	0.56
1:B:430:ASP:O	1:B:431:ILE:HB	2.06	0.56
1:B:638:ASP:C	1:B:639:LYS:CG	2.79	0.56
1:B:117:GLY:O	1:B:149:ILE:N	2.38	0.55
1:B:135:ILE:HG23	1:B:135:ILE:O	2.06	0.55
1:A:86:THR:HG21	1:A:333:LYS:CG	2.36	0.55
1:A:403:GLY:HA2	1:A:435:LEU:HB3	1.89	0.55
1:B:70:VAL:O	1:B:415:MET:HG3	2.06	0.55
1:A:123:THR:HG23	1:A:355:TYR:HD2	1.72	0.55
1:A:532:GLY:O	1:A:533:ASP:HB2	2.05	0.55
1:A:627:SER:CB	1:A:647:LYS:CE	2.84	0.55
1:B:403:GLY:HA3	1:B:408:HIS:ND1	2.21	0.55
1:B:101:GLN:HB3	1:B:103:HIS:HE1	1.70	0.55
1:B:262:TYR:O	1:B:263:LYS:CB	2.53	0.55
1:B:270:VAL:HG23	1:B:292:PRO:HA	1.85	0.55
1:B:635:ARG:O	1:B:635:ARG:HG3	2.07	0.55
1:A:224:ASN:CB	1:A:227:SER:HB2	2.29	0.55
1:A:436:PHE:CE2	1:A:467:LYS:CB	2.76	0.55
1:A:94:ASP:C	1:A:95:LYS:CG	2.67	0.55
1:B:654:GLU:N	1:B:655:ASN:HA	2.21	0.55
1:A:149:ILE:CG2	1:A:151:ARG:HG3	2.37	0.55
1:A:355:TYR:CD1	1:A:355:TYR:N	2.72	0.55
1:A:496:THR:HA	1:A:612:TYR:HB3	1.88	0.55
1:A:572:ILE:HD13	1:A:600:CYS:HB2	1.89	0.55
1:A:611:MET:HE2	1:A:629:LEU:HD12	1.88	0.55
1:B:500:GLU:O	1:B:504:ASN:HB2	2.06	0.55
1:A:432:GLY:HA3	1:A:459:HIS:CE1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:HB2	1:B:461:CYS:HB2	1.87	0.55
1:B:248:MET:HG3	1:B:319:TRP:NE1	2.22	0.55
1:A:70:VAL:O	1:A:415:MET:HE2	2.06	0.55
1:A:262:TYR:CD1	1:A:262:TYR:C	2.85	0.55
1:A:272:VAL:HG21	1:A:280:PHE:CA	2.35	0.55
1:B:181:CYS:O	1:B:459:HIS:HD2	1.90	0.55
1:A:125:LYS:HE3	1:A:355:TYR:HA	1.89	0.55
1:A:433:GLY:O	1:A:460:ALA:CA	2.43	0.55
1:A:233:ALA:HB3	1:A:312:ALA:HA	1.82	0.54
1:A:308:LYS:HB3	1:A:315:VAL:CG1	2.37	0.54
1:A:531:VAL:HB	1:A:535:LEU:HD23	1.89	0.54
1:B:188:ASP:OD2	1:B:192:ILE:HD12	2.07	0.54
1:B:285:TRP:HB2	1:B:286:PRO:CD	2.36	0.54
1:B:584:ILE:HG13	1:B:589:GLU:HB2	1.89	0.54
1:A:507:PRO:O	1:A:510:ARG:NE	2.26	0.54
1:B:403:GLY:C	1:B:405:CYS:H	2.15	0.54
1:B:406:TRP:CZ2	1:B:541:PHE:HB2	2.42	0.54
1:A:84:TRP:CD1	1:A:85:ASN:HA	2.40	0.54
1:A:151:ARG:HH12	1:A:160:GLY:CA	2.21	0.54
1:B:69:GLU:HB3	1:B:101:GLN:HB2	1.88	0.54
1:B:118:ILE:HD11	1:B:146:VAL:HG13	1.90	0.54
1:B:534:ASN:ND2	1:B:576:ALA:HB1	2.21	0.54
1:A:441:ASP:O	1:A:445:ASN:ND2	2.35	0.54
1:A:212:ILE:CG2	1:A:213:ASP:N	2.70	0.54
1:A:245:SER:O	1:A:316:ASP:HB2	2.08	0.54
1:A:264:SER:C	1:A:266:THR:H	2.15	0.54
1:B:158:ILE:HG21	1:B:507:PRO:CD	2.37	0.54
1:B:255:VAL:HG21	1:B:281:HIS:CD2	2.43	0.54
1:B:459:HIS:O	1:B:460:ALA:CB	2.56	0.54
1:A:330:THR:CG2	2:A:712:HOH:O	1.97	0.54
1:A:457:ARG:HG2	1:A:458:GLY:O	2.07	0.54
1:B:458:GLY:O	1:B:459:HIS:HB2	2.07	0.54
1:B:633:ALA:HB2	1:B:642:VAL:HG22	1.90	0.54
1:A:100:TYR:CG	1:A:385:ARG:HD3	2.43	0.54
1:A:406:TRP:CD2	1:A:442:LEU:HD13	2.42	0.54
1:A:618:GLY:N	1:A:621:TYR:CZ	2.76	0.54
1:A:85:ASN:OD1	1:A:88:SER:CB	2.56	0.54
1:A:383:LEU:CD2	1:A:396:ALA:HB3	2.37	0.54
1:A:440:ALA:HB2	1:A:472:PHE:HB3	1.91	0.54
1:B:118:ILE:CG1	1:B:120:PHE:CE1	2.91	0.54
1:B:612:TYR:HB2	1:B:628:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:TRP:HD1	1:B:446:TRP:O	1.91	0.53
1:A:504:ASN:OD1	1:A:505:GLY:CA	2.56	0.53
1:B:555:LEU:HD23	1:B:570:MET:HE2	1.87	0.53
1:A:192:ILE:HG23	1:A:195:ALA:H	1.71	0.53
1:A:210:MET:HG3	1:A:247:TRP:CZ3	2.43	0.53
1:B:187:PRO:HA	1:B:188:ASP:C	2.33	0.53
1:A:69:GLU:C	1:A:70:VAL:CG1	2.82	0.53
1:A:236:ARG:HD3	1:B:661:ILE:HG12	1.91	0.53
1:B:219:ARG:HH11	1:B:254:LYS:HD2	1.69	0.53
1:B:291:PHE:CD1	1:B:291:PHE:N	2.76	0.53
1:A:72:GLY:HA3	1:A:95:LYS:HG2	1.89	0.53
1:A:84:TRP:CZ2	1:A:356:HIS:CG	2.97	0.53
1:A:402:ASN:OD1	1:A:408:HIS:HB3	2.08	0.53
1:B:299:VAL:O	1:B:303:TRP:N	2.29	0.53
1:A:119:LEU:HD11	1:A:389:LEU:HD23	1.88	0.53
1:A:379:ARG:HE	1:A:618:GLY:C	2.16	0.53
1:A:436:PHE:HE2	1:A:467:LYS:HB3	1.72	0.53
1:B:74:LEU:CD2	1:B:75:LEU:N	2.68	0.53
1:B:434:PHE:HD2	1:B:434:PHE:C	2.17	0.53
1:B:651:TYR:CD2	1:B:652:ASN:N	2.68	0.53
1:A:101:GLN:CD	1:A:387:ASN:CB	2.80	0.53
1:A:272:VAL:HG21	1:A:280:PHE:CB	2.39	0.53
1:B:254:LYS:HE2	1:B:286:PRO:O	2.09	0.53
1:B:270:VAL:O	1:B:271:TRP:HB2	2.07	0.53
1:B:273:LYS:O	1:B:352:HIS:HE1	1.92	0.53
1:A:186:SER:CB	1:A:187:PRO:CD	2.85	0.53
1:A:229:PRO:CA	1:A:231:PRO:HD3	2.38	0.53
1:B:257:PRO:C	1:B:259:TYR:CE2	2.87	0.53
1:B:512:VAL:HG12	1:B:522:LEU:HD13	1.90	0.53
1:A:262:TYR:HD1	1:A:262:TYR:C	2.17	0.52
1:B:555:LEU:HB3	1:B:570:MET:HE2	1.90	0.52
1:B:633:ALA:CB	1:B:642:VAL:HG22	2.40	0.52
1:A:464:THR:CG2	1:A:465:ASN:N	2.72	0.52
1:A:630:GLN:HB3	1:A:645:THR:OG1	2.09	0.52
1:B:59:PRO:O	1:B:60:GLU:HB2	2.09	0.52
1:A:79:LYS:HZ2	1:A:95:LYS:HD3	1.74	0.52
1:A:236:ARG:O	1:A:240:ILE:HG13	2.09	0.52
1:A:306:LEU:CD1	1:A:374:ALA:HA	2.39	0.52
1:A:468:GLU:HB2	1:A:471:VAL:HG23	1.91	0.52
1:A:627:SER:HB3	1:A:647:LYS:HE2	1.91	0.52
1:A:101:GLN:HG3	1:A:387:ASN:H	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:O	1:A:243:PHE:CA	2.57	0.52
1:A:519:ASP:OD1	1:A:521:SER:N	2.42	0.52
1:A:587:THR:HB	1:A:590:ASN:ND2	2.21	0.52
1:B:189:SER:O	1:B:191:VAL:CG1	2.44	0.52
1:A:91:TYR:O	1:A:92:GLY:C	2.53	0.52
1:A:111:LYS:HG2	1:A:520:LEU:HD11	1.92	0.52
1:A:361:PHE:CD1	1:A:361:PHE:C	2.87	0.52
1:B:181:CYS:O	1:B:459:HIS:HB2	2.10	0.52
1:B:459:HIS:CE1	1:B:460:ALA:HA	2.44	0.52
1:A:379:ARG:NH2	1:A:614:ASP:OD2	2.41	0.52
1:A:72:GLY:HA2	1:A:411:MET:HE2	1.91	0.52
1:A:268:ASN:O	1:A:293:ASP:CB	2.58	0.52
1:A:466:ASN:OD1	1:A:466:ASN:N	2.43	0.52
1:B:65:TYR:OH	1:B:523:ARG:HG2	2.09	0.52
1:B:225:PRO:O	1:B:226:LYS:O	2.28	0.52
1:A:587:THR:CB	1:A:590:ASN:HD22	2.22	0.52
1:B:90:ALA:C	1:B:91:TYR:O	2.51	0.52
1:B:216:ASP:C	1:B:218:TYR:H	2.17	0.52
1:B:285:TRP:CB	1:B:286:PRO:CD	2.88	0.52
1:A:407:ASP:O	1:A:411:MET:HB2	2.10	0.51
1:A:627:SER:HB2	1:A:647:LYS:CE	2.40	0.51
1:B:91:TYR:CE2	1:B:415:MET:CE	2.93	0.51
1:B:182:ARG:HE	1:B:466:ASN:HA	1.73	0.51
1:A:160:GLY:HA2	1:A:163:GLU:CD	2.35	0.51
1:A:232:LYS:O	1:A:233:ALA:CB	2.57	0.51
1:B:534:ASN:CG	1:B:576:ALA:CB	2.83	0.51
1:B:619:TRP:CD1	1:B:623:LYS:HZ1	2.28	0.51
1:A:108:GLY:O	1:A:115:ALA:HA	2.11	0.51
1:B:323:ASN:OD1	1:B:360:GLY:HA3	2.10	0.51
1:A:209:TRP:CH2	1:A:383:LEU:HD12	2.44	0.51
1:A:293:ASP:O	1:A:299:VAL:HB	2.11	0.51
1:B:123:THR:CG2	1:B:124:TRP:HE3	2.23	0.51
1:B:158:ILE:HG21	1:B:507:PRO:HD2	1.91	0.51
1:B:307:TYR:N	1:B:307:TYR:CD1	2.78	0.51
1:A:210:MET:HE2	1:A:247:TRP:CH2	2.45	0.51
1:B:510:ARG:NH1	1:B:533:ASP:OD1	2.43	0.51
1:B:632:VAL:O	1:B:642:VAL:HG13	2.11	0.51
1:A:145:ARG:HE	1:A:147:PHE:HE2	1.58	0.51
1:A:165:THR:HG21	1:A:390:GLY:HA2	1.91	0.51
1:A:497:LEU:HD11	1:A:532:GLY:HA3	1.92	0.51
1:A:621:TYR:HB2	1:A:625:ASP:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:SER:O	1:B:228:PHE:HB2	2.09	0.51
1:B:270:VAL:O	1:B:271:TRP:CG	2.64	0.51
1:B:411:MET:C	1:B:414:PRO:HD2	2.34	0.51
1:A:230:ASN:ND2	1:A:234:VAL:CB	2.74	0.51
1:A:245:SER:CB	1:A:314:GLY:O	2.58	0.51
1:A:511:PRO:HG2	1:A:514:PHE:CG	2.46	0.51
1:A:627:SER:HB2	1:A:647:LYS:HE2	1.92	0.51
1:B:251:PRO:HG3	1:B:363:MET:SD	2.51	0.51
1:B:350:GLY:O	1:B:352:HIS:N	2.39	0.51
1:B:584:ILE:CG1	1:B:589:GLU:HB2	2.41	0.51
1:A:69:GLU:C	1:A:70:VAL:HG13	2.35	0.51
1:A:105:TRP:HH2	1:A:157:VAL:CG1	2.24	0.51
1:A:225:PRO:HA	1:A:229:PRO:HG3	1.88	0.51
1:B:543:ASN:O	1:B:545:PRO:HD3	2.11	0.51
1:A:101:GLN:HG3	1:A:386:SER:HA	1.93	0.51
1:A:209:TRP:CE3	1:A:319:TRP:CE3	2.96	0.51
1:A:304:ARG:HB3	1:A:370:GLY:CA	2.41	0.51
1:A:405:CYS:SG	1:A:408:HIS:ND1	2.84	0.51
1:B:204:PRO:HB3	1:B:585:GLN:CD	2.36	0.51
1:B:353:LEU:O	1:B:354:GLN:HG2	2.11	0.51
1:B:487:ARG:O	1:B:490:LEU:HB2	2.11	0.51
1:B:542:ALA:C	1:B:543:ASN:OD1	2.54	0.51
1:A:101:GLN:HG2	1:A:387:ASN:C	2.35	0.51
1:A:126:ALA:CB	1:A:137:LEU:HD11	2.41	0.51
1:B:509:MET:HG3	1:B:529:PHE:HD2	1.73	0.51
1:A:48:THR:CB	1:A:53:ASN:HB2	2.41	0.50
1:A:607:ALA:HB3	1:A:633:ALA:HB3	1.92	0.50
1:B:86:THR:O	1:B:100:TYR:CD1	2.63	0.50
1:B:534:ASN:OD1	1:B:573:ARG:NE	2.44	0.50
1:A:472:PHE:HB2	1:A:476:VAL:HG21	1.92	0.50
1:B:321:ASP:O	1:B:322:VAL:HB	2.11	0.50
1:B:557:LEU:N	1:B:557:LEU:CD1	2.73	0.50
1:A:457:ARG:N	2:A:704:HOH:O	2.36	0.50
1:A:641:THR:CB	1:A:643:LYS:NZ	2.67	0.50
1:B:406:TRP:CZ3	1:B:442:LEU:HD12	2.46	0.50
1:B:516:ASP:HB3	1:B:519:ASP:CB	2.39	0.50
1:A:179:GLN:CB	1:A:209:TRP:HE1	2.08	0.50
1:A:324:GLU:N	1:A:325:PRO:CA	2.72	0.50
1:A:384:THR:HG22	1:A:395:ALA:HB1	1.93	0.50
1:A:552:TRP:HB3	1:A:571:LYS:HB3	1.92	0.50
1:B:348:PRO:O	1:B:348:PRO:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LYS:C	1:B:566:TYR:CD1	2.90	0.50
1:B:567:GLN:O	1:B:568:ALA:HB3	2.12	0.50
1:A:120:PHE:HB2	1:A:137:LEU:HD22	1.92	0.50
1:B:63:SER:CA	1:B:76:ARG:HH21	2.22	0.50
1:B:248:MET:HG2	1:B:249:ILE:N	2.26	0.50
1:B:485:GLU:HG2	1:B:583:ILE:CG2	2.41	0.50
1:B:649:GLY:O	1:B:650:LYS:CB	2.59	0.50
1:A:545:PRO:O	1:A:546:ALA:C	2.51	0.50
1:B:72:GLY:CA	1:B:73:SER:HB2	2.24	0.50
1:B:350:GLY:C	1:B:352:HIS:N	2.69	0.50
1:B:62:THR:O	1:B:63:SER:CB	2.54	0.49
1:A:180:GLN:HG3	1:A:181:CYS:N	2.27	0.49
1:A:236:ARG:HG2	1:A:240:ILE:CD1	2.42	0.49
1:B:361:PHE:CZ	1:B:394:TYR:HE2	2.30	0.49
1:B:364:VAL:CG2	1:B:384:THR:HB	2.42	0.49
1:A:181:CYS:HB3	1:A:209:TRP:HB2	1.95	0.49
1:A:414:PRO:HG3	1:A:526:GLU:HB2	1.94	0.49
1:B:83:LEU:N	1:B:83:LEU:CD1	2.73	0.49
1:B:182:ARG:NE	1:B:466:ASN:HA	2.27	0.49
1:A:77:ASN:ND2	1:A:77:ASN:N	2.60	0.49
1:A:182:ARG:HD3	1:A:194:ILE:HG13	1.95	0.49
1:B:270:VAL:HG13	1:B:271:TRP:CD2	2.48	0.49
1:B:402:ASN:HB2	1:B:430:ASP:CG	2.38	0.49
1:A:84:TRP:NE1	1:A:356:HIS:CD2	2.80	0.49
1:B:64:ILE:N	1:B:76:ARG:NH2	2.56	0.49
1:B:94:ASP:C	1:B:96:GLY:H	2.20	0.49
1:B:228:PHE:N	1:B:229:PRO:CD	2.75	0.49
1:B:257:PRO:HA	1:B:259:TYR:HE2	1.76	0.49
1:A:280:PHE:CE1	1:A:336:PRO:HD3	2.41	0.49
1:A:420:GLY:CA	1:A:507:PRO:HG3	2.43	0.49
1:B:179:GLN:OE1	1:B:455:PHE:HE1	1.95	0.49
1:B:311:LEU:HD23	1:B:315:VAL:HB	1.93	0.49
1:A:192:ILE:CG2	1:A:195:ALA:N	2.73	0.49
1:B:212:ILE:CG1	1:B:213:ASP:N	2.73	0.49
1:B:379:ARG:CG	1:B:619:TRP:HA	2.43	0.49
1:B:436:PHE:C	1:B:438:ALA:N	2.59	0.49
1:B:437:ASN:O	1:B:438:ALA:HB3	2.11	0.49
1:B:592:LEU:O	1:B:592:LEU:HG	2.13	0.49
1:B:593:ASP:HB3	1:B:594:PRO:CD	2.41	0.49
1:B:604:GLN:HA	1:B:604:GLN:NE2	2.28	0.49
1:A:125:LYS:HE2	1:A:356:HIS:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:VAL:HG13	1:B:71:THR:N	2.28	0.49
1:B:109:VAL:HB	1:B:523:ARG:NH1	2.28	0.49
1:B:379:ARG:HG3	1:B:619:TRP:HA	1.95	0.49
1:A:84:TRP:CH2	1:A:356:HIS:CB	2.96	0.49
1:A:105:TRP:CZ2	1:A:161:LEU:HD22	2.47	0.49
1:A:170:MET:CE	1:A:498:LEU:HG	2.42	0.49
1:A:619:TRP:O	1:A:621:TYR:CD1	2.66	0.49
1:B:204:PRO:HB3	1:B:585:GLN:HA	1.92	0.49
1:B:219:ARG:HH11	1:B:254:LYS:CB	2.23	0.49
1:B:565:LYS:C	1:B:566:TYR:HD1	2.20	0.49
1:A:100:TYR:CD1	1:A:385:ARG:HD3	2.47	0.49
1:A:410:LYS:HZ3	1:A:413:VAL:CG2	2.26	0.49
1:A:459:HIS:ND1	1:A:460:ALA:HB2	2.28	0.49
1:A:503:THR:HG23	1:A:504:ASN:N	2.27	0.49
1:B:653:THR:C	1:B:654:GLU:HG2	2.36	0.48
1:A:173:ARG:HH21	1:A:590:ASN:HB3	1.78	0.48
1:A:261:VAL:HG13	1:A:262:TYR:N	2.28	0.48
1:A:466:ASN:O	1:A:467:LYS:NZ	2.34	0.48
1:B:443:PHE:CD2	1:B:472:PHE:CE2	3.01	0.48
1:A:72:GLY:C	1:A:74:LEU:N	2.70	0.48
1:A:111:LYS:C	1:A:112:ASP:O	2.55	0.48
1:A:336:PRO:HG2	1:A:336:PRO:O	2.12	0.48
1:B:356:HIS:O	1:B:357:ASN:HB2	2.12	0.48
1:B:459:HIS:ND1	1:B:460:ALA:HA	2.28	0.48
1:A:383:LEU:HD23	1:A:396:ALA:HB3	1.95	0.48
1:B:181:CYS:O	1:B:459:HIS:CB	2.62	0.48
1:B:471:VAL:HG12	1:B:471:VAL:O	2.13	0.48
1:A:304:ARG:CB	1:A:370:GLY:CA	2.91	0.48
1:A:434:PHE:N	1:A:434:PHE:CD1	2.82	0.48
1:A:572:ILE:O	1:A:572:ILE:HG23	2.14	0.48
1:B:115:ALA:CB	1:B:154:PRO:HA	2.41	0.48
1:B:118:ILE:CG1	1:B:120:PHE:CZ	2.97	0.48
1:B:171:ILE:HD12	1:B:175:ALA:CB	2.42	0.48
1:B:634:GLU:O	1:B:635:ARG:CG	2.62	0.48
1:A:82:LYS:HD2	1:A:98:ARG:H	1.78	0.48
1:A:84:TRP:HA	1:A:357:ASN:CG	2.38	0.48
1:A:332:ASN:C	1:A:333:LYS:CG	2.81	0.48
1:B:536:LEU:CD2	1:B:548:PRO:HD2	2.44	0.48
1:A:86:THR:CG2	1:A:333:LYS:HB3	2.37	0.48
1:A:173:ARG:HD3	1:A:495:TYR:CE2	2.49	0.48
1:A:307:TYR:HA	1:A:310:PHE:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LYS:H	1:A:308:LYS:HG3	1.52	0.48
1:A:456:ALA:CA	2:A:704:HOH:O	2.60	0.48
1:B:446:TRP:CD1	1:B:446:TRP:C	2.92	0.48
1:B:472:PHE:O	1:B:476:VAL:CG2	2.61	0.48
1:A:192:ILE:HG22	1:A:195:ALA:N	2.26	0.48
1:B:63:SER:N	1:B:76:ARG:HH22	2.10	0.48
1:B:188:ASP:HB3	1:B:189:SER:CA	2.43	0.48
1:B:351:THR:O	1:B:351:THR:OG1	2.32	0.48
1:B:610:ASN:HA	1:B:629:LEU:O	2.13	0.48
1:A:170:MET:HE3	1:A:499:HIS:HA	1.96	0.48
1:B:118:ILE:HD13	1:B:148:ILE:CG1	2.43	0.48
1:B:454:PRO:HD3	1:B:509:MET:HE2	1.91	0.48
1:A:72:GLY:HA3	1:A:95:LYS:CG	2.43	0.47
1:A:382:ILE:HG13	1:A:383:LEU:N	2.29	0.47
1:A:413:VAL:HB	1:A:414:PRO:CD	2.36	0.47
1:B:118:ILE:CD1	1:B:146:VAL:HG13	2.44	0.47
1:B:173:ARG:O	1:B:176:LEU:HB2	2.14	0.47
1:B:285:TRP:CB	1:B:286:PRO:HD3	2.44	0.47
1:B:449:PHE:CB	1:B:539:PRO:HG3	2.43	0.47
1:A:68:GLY:N	1:A:422:SER:OG	2.44	0.47
1:A:259:TYR:CE1	1:A:262:TYR:O	2.67	0.47
1:A:312:ALA:HB2	1:A:315:VAL:H	1.79	0.47
1:A:587:THR:CB	1:A:590:ASN:ND2	2.77	0.47
1:B:171:ILE:O	1:B:379:ARG:NH1	2.43	0.47
1:B:224:ASN:H	1:B:225:PRO:CD	2.26	0.47
1:B:247:TRP:HD1	1:B:315:VAL:HG13	1.79	0.47
1:B:158:ILE:HD11	1:B:421:LEU:CD2	2.43	0.47
1:B:248:MET:HB2	1:B:319:TRP:CH2	2.45	0.47
1:A:278:LYS:HD3	1:A:279:ASN:OD1	2.15	0.47
1:A:285:TRP:N	1:A:286:PRO:CD	2.77	0.47
1:A:367:SER:CB	1:A:382:ILE:HD13	2.45	0.47
1:A:436:PHE:CE2	1:A:460:ALA:HB1	2.49	0.47
1:A:459:HIS:ND1	1:A:459:HIS:C	2.73	0.47
1:A:329:ASP:C	1:A:330:THR:HG1	2.15	0.47
1:A:379:ARG:NE	1:A:618:GLY:O	2.47	0.47
1:A:489:ILE:HG13	1:A:489:ILE:O	2.13	0.47
1:B:75:LEU:N	1:B:75:LEU:HD22	2.30	0.47
1:B:443:PHE:CD2	1:B:472:PHE:HE2	2.32	0.47
1:B:474:GLN:NE2	1:B:474:GLN:C	2.73	0.47
1:A:431:ILE:C	1:A:459:HIS:NE2	2.73	0.47
1:A:465:ASN:O	1:A:466:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:324:GLU:N	1:B:325:PRO:HA	2.30	0.47
1:B:420:GLY:HA3	1:B:507:PRO:HB3	1.96	0.47
1:B:527:GLU:CB	1:B:543:ASN:HD22	2.28	0.47
1:B:538:ILE:HG23	1:B:538:ILE:O	2.15	0.47
1:B:259:TYR:HE1	1:B:263:LYS:CB	2.28	0.47
1:B:259:TYR:CE1	1:B:262:TYR:O	2.68	0.47
1:B:270:VAL:CG2	1:B:292:PRO:HB3	2.44	0.47
1:B:415:MET:O	1:B:418:THR:CG2	2.53	0.47
1:B:449:PHE:HB3	1:B:539:PRO:HG3	1.97	0.47
1:A:171:ILE:HG13	1:A:498:LEU:HD21	1.96	0.47
1:A:398:TRP:HE3	1:A:398:TRP:O	1.98	0.47
1:B:246:ALA:HA	1:B:317:GLY:O	2.15	0.47
1:A:120:PHE:CB	1:A:137:LEU:HD22	2.45	0.47
1:A:402:ASN:HB3	1:A:433:GLY:CA	2.38	0.47
1:A:457:ARG:HG2	1:A:458:GLY:N	2.30	0.47
1:A:519:ASP:OD1	1:A:521:SER:HB2	2.15	0.47
1:B:272:VAL:O	1:B:274:THR:N	2.47	0.47
1:B:430:ASP:O	1:B:457:ARG:O	2.32	0.47
1:B:488:TYR:HB3	1:B:584:ILE:HG22	1.97	0.47
1:B:498:LEU:HA	1:B:508:ILE:HD11	1.97	0.47
1:A:76:ARG:HH11	1:A:523:ARG:HB3	1.80	0.46
1:A:86:THR:CG2	1:A:87:ASP:N	2.77	0.46
1:A:124:TRP:CZ2	1:A:355:TYR:CE1	3.03	0.46
1:A:209:TRP:N	1:A:209:TRP:CD1	2.83	0.46
1:B:304:ARG:O	1:B:307:TYR:HB3	2.15	0.46
1:A:93:VAL:O	1:A:411:MET:HE1	2.15	0.46
1:A:131:THR:CG2	1:A:132:ASP:H	2.05	0.46
1:A:262:TYR:HE1	1:A:264:SER:HG	1.59	0.46
1:A:272:VAL:CG1	1:A:336:PRO:CB	2.87	0.46
1:A:405:CYS:O	1:A:406:TRP:CB	2.63	0.46
1:A:293:ASP:C	1:A:295:THR:H	2.23	0.46
1:A:432:GLY:CA	1:A:436:PHE:HE1	2.28	0.46
1:A:627:SER:HB2	1:A:647:LYS:NZ	2.29	0.46
1:A:312:ALA:HB2	1:A:315:VAL:N	2.30	0.46
1:A:460:ALA:HB3	1:A:467:LYS:CD	2.28	0.46
1:B:94:ASP:C	1:B:96:GLY:N	2.74	0.46
1:B:257:PRO:CA	1:B:259:TYR:HE2	2.26	0.46
1:B:404:SER:C	1:B:442:LEU:HD21	2.41	0.46
1:B:566:TYR:C	1:B:567:GLN:HG2	2.41	0.46
1:A:76:ARG:NH1	1:A:523:ARG:HB3	2.30	0.46
1:A:86:THR:HG22	1:A:87:ASP:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:GLN:HA	1:A:395:ALA:O	2.16	0.46
1:A:471:VAL:C	1:A:473:GLY:H	2.24	0.46
1:A:506:MET:CB	1:A:507:PRO:HD2	2.26	0.46
1:B:409:LEU:HB2	1:B:446:TRP:CE3	2.50	0.46
1:A:447:ILE:HD12	1:A:447:ILE:HA	1.71	0.46
1:A:544:GLN:CB	1:A:545:PRO:HA	2.45	0.46
1:B:630:GLN:HG2	1:B:645:THR:OG1	2.16	0.46
1:A:81:ILE:O	1:A:128:LEU:N	2.48	0.46
1:A:431:ILE:HG13	1:A:447:ILE:HD13	1.97	0.46
1:A:118:ILE:HG12	1:A:120:PHE:CE1	2.50	0.46
1:A:253:ALA:O	1:A:289:ALA:HA	2.15	0.46
1:A:436:PHE:CD2	1:A:460:ALA:HB1	2.51	0.46
1:B:86:THR:HG23	1:B:88:SER:OG	2.15	0.46
1:B:87:ASP:OD1	1:B:87:ASP:N	2.38	0.46
1:B:162:SER:OG	1:B:505:GLY:HA3	2.14	0.46
1:B:285:TRP:N	1:B:286:PRO:CD	2.78	0.46
1:B:612:TYR:OH	1:B:621:TYR:CB	2.64	0.46
1:A:89:GLY:HA3	1:A:100:TYR:CE2	2.51	0.46
1:A:245:SER:CB	1:A:247:TRP:HE1	2.29	0.46
1:A:486:ARG:C	1:A:489:ILE:HG22	2.39	0.46
1:A:627:SER:CB	1:A:647:LYS:HZ3	2.23	0.46
1:A:176:LEU:HD11	1:A:495:TYR:HD1	1.81	0.46
1:A:190:ARG:HD2	1:A:193:GLU:OE1	2.15	0.46
1:A:233:ALA:O	1:A:235:ASN:N	2.49	0.46
1:B:612:TYR:CD1	1:B:612:TYR:C	2.93	0.46
1:A:431:ILE:O	1:A:459:HIS:NE2	2.49	0.45
1:A:465:ASN:HB3	1:A:466:ASN:OD1	2.16	0.45
1:A:491:LEU:CB	1:A:492:PRO:HD3	2.46	0.45
1:A:536:LEU:HD23	1:A:571:LYS:HD3	1.98	0.45
1:A:581:GLY:O	1:A:582:LYS:CB	2.58	0.45
1:A:628:LEU:N	1:A:647:LYS:HZ3	2.13	0.45
1:B:112:ASP:HB2	1:B:114:THR:H	1.80	0.45
1:B:356:HIS:O	1:B:357:ASN:CB	2.65	0.45
1:B:634:GLU:O	1:B:635:ARG:HG3	2.15	0.45
1:A:306:LEU:HD12	1:A:374:ALA:HA	1.99	0.45
1:A:375:ARG:HD2	1:A:375:ARG:C	2.41	0.45
1:B:486:ARG:O	1:B:489:ILE:HG13	2.16	0.45
1:A:194:ILE:HD12	1:A:470:TRP:HZ2	1.81	0.45
1:A:278:LYS:CD	1:A:279:ASN:H	2.30	0.45
1:B:126:ALA:HB1	1:B:137:LEU:CD2	2.41	0.45
1:B:162:SER:CB	1:B:504:ASN:O	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:HD2	1:B:613:TRP:CH2	2.50	0.45
1:B:304:ARG:HG2	1:B:369:GLU:HB2	1.97	0.45
1:B:424:GLN:O	1:B:424:GLN:HG3	2.14	0.45
1:B:530:LEU:HB3	1:B:532:GLY:O	2.15	0.45
1:B:635:ARG:HE	1:B:636:ASN:ND2	2.09	0.45
1:A:77:ASN:N	1:A:77:ASN:HD22	2.14	0.45
1:A:179:GLN:CG	1:A:207:VAL:HB	2.33	0.45
1:B:328:ASN:ND2	1:B:328:ASN:C	2.73	0.45
1:B:620:SER:HB3	1:B:621:TYR:H	1.59	0.45
1:A:203:ILE:CG2	1:A:484:LEU:HD12	2.47	0.45
1:A:236:ARG:HE	1:A:240:ILE:HD11	1.82	0.45
1:A:272:VAL:CG1	1:A:336:PRO:HG3	2.24	0.45
1:B:91:TYR:CE2	1:B:415:MET:HE1	2.51	0.45
1:A:431:ILE:HG23	1:A:446:TRP:CB	2.46	0.45
1:A:467:LYS:HB3	1:A:467:LYS:NZ	2.32	0.45
1:B:168:MET:HA	1:B:392:GLN:O	2.17	0.45
1:B:605:GLY:C	1:B:606:LYS:HG3	2.41	0.45
1:A:72:GLY:CA	1:A:411:MET:HE2	2.47	0.45
1:A:73:SER:N	1:A:95:LYS:HE3	2.29	0.45
1:A:130:SER:HB3	1:A:135:ILE:HA	1.99	0.45
1:A:270:VAL:HG12	1:A:293:ASP:HA	1.98	0.45
1:B:116:PHE:HA	1:B:150:ASP:HA	1.98	0.45
1:B:183:PHE:HA	1:B:212:ILE:CA	2.46	0.45
1:B:262:TYR:O	1:B:262:TYR:CD2	2.70	0.45
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.78	0.45
1:A:84:TRP:CH2	1:A:356:HIS:CG	3.05	0.45
1:A:293:ASP:O	1:A:299:VAL:CB	2.64	0.45
1:B:91:TYR:CE2	1:B:415:MET:HE3	2.51	0.45
1:B:223:PHE:HB2	1:B:224:ASN:CA	2.47	0.45
1:A:271:TRP:O	1:A:337:GLU:OE2	2.34	0.45
1:A:361:PHE:CD2	1:A:388:PHE:HB3	2.52	0.45
1:A:434:PHE:CE2	1:A:461:CYS:CB	3.00	0.45
1:B:273:LYS:O	1:B:352:HIS:CE1	2.70	0.45
1:B:382:ILE:O	1:B:383:LEU:HD23	2.17	0.45
1:B:437:ASN:CA	1:B:465:ASN:OD1	2.57	0.45
1:A:231:PRO:C	1:A:233:ALA:N	2.74	0.44
1:A:324:GLU:OE2	1:A:385:ARG:HD2	2.17	0.44
1:A:409:LEU:HA	1:A:446:TRP:CZ2	2.52	0.44
1:A:410:LYS:O	1:A:414:PRO:HD2	2.18	0.44
1:A:426:PHE:CD2	1:A:455:PHE:HB2	2.50	0.44
1:B:245:SER:OG	1:B:247:TRP:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASN:OD1	1:B:360:GLY:CA	2.65	0.44
1:A:248:MET:HB2	1:A:319:TRP:CE2	2.47	0.44
1:A:402:ASN:O	1:A:434:PHE:O	2.34	0.44
1:A:627:SER:HB2	1:A:647:LYS:HZ3	1.83	0.44
1:B:458:GLY:O	1:B:459:HIS:CB	2.66	0.44
1:B:499:HIS:CE1	1:B:612:TYR:CE2	3.05	0.44
1:B:474:GLN:NE2	1:B:474:GLN:CA	2.80	0.44
1:A:86:THR:CG2	1:A:87:ASP:OD1	2.53	0.44
1:A:89:GLY:O	1:A:90:ALA:CB	2.65	0.44
1:A:236:ARG:HH11	1:B:661:ILE:HG23	1.78	0.44
1:B:270:VAL:CG2	1:B:292:PRO:CB	2.96	0.44
1:B:270:VAL:HG23	1:B:293:ASP:H	1.83	0.44
1:B:652:ASN:ND2	1:B:656:LYS:O	2.51	0.44
1:A:320:ASN:CG	1:A:363:MET:HE2	2.43	0.44
1:A:398:TRP:O	1:A:398:TRP:CE3	2.70	0.44
1:A:513:PHE:CD1	1:A:513:PHE:C	2.96	0.44
1:A:520:LEU:HD23	1:A:520:LEU:HA	1.80	0.44
1:B:102:SER:C	1:B:103:HIS:ND1	2.75	0.44
1:B:257:PRO:O	1:B:259:TYR:CE2	2.70	0.44
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.83	0.44
1:A:74:LEU:HD11	1:A:77:ASN:CG	2.42	0.44
1:A:297:PRO:HA	1:A:300:ASN:ND2	2.33	0.44
1:B:424:GLN:HA	1:B:425:PRO:HD3	1.88	0.44
1:A:256:ASP:HA	1:A:257:PRO:HD3	1.86	0.44
1:B:62:THR:HB	1:B:64:ILE:CD1	2.46	0.44
1:B:93:VAL:O	1:B:97:THR:CA	2.65	0.44
1:B:180:GLN:O	1:B:181:CYS:CB	2.60	0.44
1:B:419:LEU:HD13	1:B:427:SER:HB3	2.00	0.44
1:B:520:LEU:N	1:B:520:LEU:CD1	2.79	0.44
1:B:577:ILE:HA	1:B:598:LEU:O	2.18	0.44
1:A:538:ILE:O	1:A:568:ALA:HB1	2.17	0.44
1:A:577:ILE:HB	1:A:609:GLY:CA	2.47	0.44
1:B:229:PRO:HD2	1:B:230:ASN:H	1.83	0.44
1:A:182:ARG:O	1:A:183:PHE:CB	2.66	0.44
1:A:211:ASP:OD1	1:A:212:ILE:HB	2.18	0.44
1:B:224:ASN:O	1:B:228:PHE:O	2.36	0.44
1:B:433:GLY:HA3	1:B:460:ALA:CB	2.40	0.44
1:B:446:TRP:O	1:B:446:TRP:CD1	2.70	0.44
1:B:541:PHE:O	1:B:541:PHE:CD1	2.70	0.44
1:A:173:ARG:HG2	1:A:491:LEU:HD11	1.99	0.43
1:A:275:ALA:C	1:A:277:GLY:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLU:HB2	1:A:546:ALA:HB3	1.99	0.43
1:B:193:GLU:C	1:B:195:ALA:N	2.74	0.43
1:B:493:TYR:O	1:B:497:LEU:HG	2.18	0.43
1:A:83:LEU:O	1:A:84:TRP:HB2	2.17	0.43
1:A:466:ASN:CB	1:A:471:VAL:HG11	2.39	0.43
1:B:224:ASN:HB3	1:B:225:PRO:HD3	2.00	0.43
1:B:459:HIS:O	1:B:460:ALA:HB3	2.19	0.43
1:B:661:ILE:H	1:B:661:ILE:HG13	1.56	0.43
1:A:107:MET:HA	1:A:116:PHE:O	2.18	0.43
1:A:525:GLU:CD	1:A:545:PRO:HD2	2.43	0.43
1:B:274:THR:CG2	1:B:275:ALA:N	2.80	0.43
1:B:306:LEU:HD22	1:B:306:LEU:O	2.17	0.43
1:B:320:ASN:O	1:B:385:ARG:N	2.38	0.43
1:A:413:VAL:O	1:A:417:LEU:HG	2.19	0.43
1:A:525:GLU:OE2	1:A:545:PRO:CD	2.66	0.43
1:A:629:LEU:HD22	1:A:644:LEU:HD21	1.99	0.43
1:B:227:SER:O	1:B:228:PHE:CB	2.63	0.43
1:A:126:ALA:O	1:A:127:GLU:CB	2.66	0.43
1:A:305:ASN:O	1:A:306:LEU:CB	2.66	0.43
1:B:59:PRO:O	1:B:60:GLU:CB	2.65	0.43
1:B:491:LEU:N	1:B:492:PRO:CD	2.81	0.43
1:B:538:ILE:CG2	1:B:569:LYS:HB2	2.49	0.43
1:A:84:TRP:HA	1:A:357:ASN:ND2	2.33	0.43
1:A:84:TRP:HA	1:A:357:ASN:HD21	1.83	0.43
1:A:197:THR:O	1:A:201:LYS:HG3	2.18	0.43
1:A:577:ILE:HG12	1:A:599:VAL:HG22	2.00	0.43
1:B:179:GLN:HA	1:B:207:VAL:O	2.17	0.43
1:B:282:GLY:O	1:B:288:ALA:HA	2.18	0.43
1:B:305:ASN:HD21	1:B:307:TYR:HE1	1.67	0.43
1:B:436:PHE:O	1:B:437:ASN:C	2.61	0.43
1:B:606:LYS:HZ1	1:B:634:GLU:HG3	1.81	0.43
1:B:635:ARG:HE	1:B:636:ASN:HB2	1.83	0.43
1:A:466:ASN:O	1:A:467:LYS:CB	2.64	0.43
1:B:121:ASP:O	1:B:144:PHE:HB2	2.18	0.43
1:B:118:ILE:HG13	1:B:120:PHE:CZ	2.54	0.43
1:B:169:PRO:HD2	2:B:704:HOH:O	2.19	0.43
1:B:623:LYS:HB2	1:B:625:ASP:H	1.84	0.43
1:A:397:THR:O	1:A:398:TRP:CD1	2.71	0.43
1:B:180:GLN:O	1:B:209:TRP:O	2.36	0.43
1:B:180:GLN:OE1	1:B:181:CYS:N	2.51	0.43
1:B:210:MET:HB3	1:B:210:MET:HE3	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:CYS:HB3	1:B:463:GLY:H	1.83	0.43
1:A:304:ARG:HB3	1:A:370:GLY:HA3	2.01	0.43
1:A:313:GLN:HG3	1:A:313:GLN:O	2.19	0.43
1:B:132:ASP:C	1:B:133:GLU:HG2	2.44	0.43
1:B:426:PHE:CE2	1:B:455:PHE:HB2	2.54	0.43
1:B:443:PHE:CG	1:B:472:PHE:CE2	3.07	0.43
1:B:479:ALA:CB	1:B:566:TYR:HD2	2.19	0.43
1:A:238:LEU:O	1:A:243:PHE:N	2.52	0.42
1:A:434:PHE:CE2	1:A:461:CYS:HB2	2.54	0.42
1:B:85:ASN:HB2	1:B:356:HIS:HD2	1.84	0.42
1:B:91:TYR:CG	1:B:415:MET:HE1	2.53	0.42
1:B:275:ALA:O	1:B:276:ASP:C	2.62	0.42
1:B:415:MET:C	1:B:418:THR:HG22	2.40	0.42
1:B:586:ASN:HB3	1:B:588:THR:H	1.84	0.42
1:A:105:TRP:CH2	1:A:157:VAL:CG1	3.01	0.42
1:A:420:GLY:C	1:A:507:PRO:HG3	2.43	0.42
1:A:587:THR:HG22	1:A:590:ASN:HD21	1.84	0.42
1:A:649:GLY:O	1:A:650:LYS:CB	2.65	0.42
1:B:248:MET:HB3	1:B:248:MET:HE2	1.77	0.42
1:B:307:TYR:HD2	1:B:374:ALA:CA	2.31	0.42
1:A:271:TRP:CD1	1:A:271:TRP:N	2.84	0.42
1:A:319:TRP:CD1	1:A:321:ASP:HB2	2.54	0.42
1:A:367:SER:HB3	1:A:382:ILE:HD13	2.01	0.42
1:A:503:THR:CG2	1:A:504:ASN:N	2.82	0.42
1:B:204:PRO:C	1:B:205:CYS:SG	3.02	0.42
1:B:253:ALA:HB3	1:B:290:ALA:HB3	2.00	0.42
1:B:255:VAL:HG12	1:B:262:TYR:CE1	2.54	0.42
1:B:277:GLY:CA	1:B:278:LYS:HD3	2.49	0.42
1:A:58:VAL:CG2	1:A:116:PHE:HZ	2.32	0.42
1:A:84:TRP:CZ2	1:A:334:THR:HG21	2.46	0.42
1:A:159:ARG:HG2	1:A:504:ASN:HB2	2.01	0.42
1:A:199:ARG:NH2	1:A:242:GLY:O	2.51	0.42
1:A:300:ASN:O	1:A:304:ARG:HG2	2.20	0.42
1:A:331:PRO:C	1:A:332:ASN:OD1	2.58	0.42
1:A:402:ASN:CB	1:A:433:GLY:HA3	2.42	0.42
1:B:59:PRO:HD3	1:B:133:GLU:O	2.19	0.42
1:B:81:ILE:CG2	1:B:128:LEU:HB2	2.49	0.42
1:B:85:ASN:OD1	1:B:100:TYR:O	2.37	0.42
1:B:209:TRP:HE1	1:B:457:ARG:HD2	1.85	0.42
1:B:223:PHE:CB	1:B:224:ASN:CA	2.96	0.42
1:B:635:ARG:CD	1:B:639:LYS:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:H	1:A:134:LYS:HD3	1.85	0.42
1:A:254:LYS:HA	1:A:289:ALA:HA	2.01	0.42
1:A:645:THR:O	1:A:646:LYS:HD2	2.19	0.42
1:B:158:ILE:HD11	1:B:421:LEU:HD22	2.01	0.42
1:B:183:PHE:HA	1:B:212:ILE:HA	2.01	0.42
1:B:193:GLU:OE1	1:B:241:ARG:NH1	2.53	0.42
1:B:493:TYR:HE2	1:B:531:VAL:HG12	1.85	0.42
1:A:133:GLU:C	1:A:134:LYS:HG2	2.44	0.42
1:A:439:ASP:OD1	1:A:439:ASP:N	2.47	0.42
1:A:506:MET:HE2	1:A:506:MET:HB2	1.62	0.42
1:A:525:GLU:CD	1:A:545:PRO:HG2	2.41	0.42
1:B:575:GLY:C	1:B:607:ALA:HA	2.45	0.42
1:A:82:LYS:HB2	1:A:98:ARG:CB	2.50	0.42
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.84	0.42
1:B:122:THR:HB	1:B:144:PHE:CD2	2.54	0.42
1:B:224:ASN:HB3	1:B:225:PRO:CD	2.49	0.42
1:B:431:ILE:HD13	1:B:447:ILE:HD12	2.01	0.42
1:B:527:GLU:CB	1:B:543:ASN:CG	2.93	0.42
1:A:226:LYS:C	1:A:228:PHE:N	2.77	0.42
1:B:112:ASP:CB	1:B:114:THR:H	2.32	0.42
1:B:231:PRO:HB2	1:B:313:GLN:HB3	2.02	0.42
1:B:371:ILE:HG21	1:B:380:PRO:HB3	2.01	0.42
1:A:249:ILE:HG22	1:A:250:ASP:N	2.34	0.42
1:A:272:VAL:HG13	1:A:336:PRO:CB	2.39	0.42
1:A:323:ASN:C	1:A:325:PRO:HA	2.42	0.42
1:A:536:LEU:HB3	1:A:571:LYS:HB2	2.02	0.42
1:B:368:ARG:HD2	1:B:394:TYR:O	2.19	0.42
1:A:58:VAL:HG13	1:A:59:PRO:O	2.19	0.42
1:A:103:HIS:HB3	1:A:389:LEU:HD13	2.01	0.42
1:A:162:SER:O	1:A:166:GLY:CA	2.68	0.42
1:A:198:PHE:CD1	1:A:205:CYS:HB2	2.55	0.42
1:A:254:LYS:HB2	1:A:286:PRO:HB2	2.02	0.42
1:A:307:TYR:HA	1:A:310:PHE:HE2	1.81	0.42
1:A:308:LYS:HE2	1:A:308:LYS:HB2	1.77	0.42
1:A:397:THR:CG2	1:A:424:GLN:HG2	2.45	0.42
1:A:490:LEU:HD23	1:A:490:LEU:HA	1.80	0.42
1:A:525:GLU:OE2	1:A:545:PRO:HD2	2.20	0.42
1:A:627:SER:C	1:A:647:LYS:HZ3	2.27	0.42
1:B:80:THR:OG1	1:B:130:SER:OG	2.07	0.42
1:B:81:ILE:HG23	1:B:128:LEU:CB	2.48	0.42
1:A:94:ASP:O	1:A:95:LYS:CG	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:HA	1:A:134:LYS:CE	2.44	0.41
1:A:220:ILE:O	1:A:221:PHE:HB2	2.19	0.41
1:A:465:ASN:C	1:A:466:ASN:CG	2.86	0.41
1:A:500:GLU:C	1:A:505:GLY:HA3	2.45	0.41
1:A:587:THR:HG22	1:A:590:ASN:ND2	2.34	0.41
1:B:131:THR:O	1:B:132:ASP:C	2.63	0.41
1:B:406:TRP:HZ2	1:B:541:PHE:CB	2.30	0.41
1:A:68:GLY:HA2	1:A:422:SER:OG	2.20	0.41
1:A:242:GLY:HA3	1:A:586:ASN:ND2	2.35	0.41
1:A:324:GLU:CD	1:A:324:GLU:H	2.28	0.41
1:B:238:LEU:O	1:B:243:PHE:HB2	2.19	0.41
1:B:485:GLU:HG2	1:B:583:ILE:HG23	2.02	0.41
1:B:538:ILE:HD11	1:B:545:PRO:HG3	2.00	0.41
1:B:621:TYR:CD1	1:B:621:TYR:N	2.88	0.41
1:B:158:ILE:HG21	1:B:507:PRO:HD3	2.02	0.41
1:B:189:SER:OG	1:B:190:ARG:N	2.53	0.41
1:B:348:PRO:HA	1:B:349:ALA:HA	1.57	0.41
1:B:249:ILE:HG22	1:B:250:ASP:N	2.35	0.41
1:B:406:TRP:NE1	1:B:541:PHE:HE2	1.95	0.41
1:B:649:GLY:O	1:B:650:LYS:HB2	2.20	0.41
1:A:225:PRO:C	1:A:229:PRO:CG	2.68	0.41
1:B:109:VAL:HB	1:B:523:ARG:HH11	1.85	0.41
1:B:323:ASN:O	1:B:359:TYR:HD2	2.04	0.41
1:A:278:LYS:HD3	1:A:279:ASN:H	1.85	0.41
1:B:109:VAL:HG12	1:B:113:GLY:HA2	2.03	0.41
1:B:187:PRO:HA	1:B:188:ASP:O	2.21	0.41
1:A:182:ARG:HH21	1:A:190:ARG:CB	2.00	0.41
1:A:361:PHE:HD2	1:A:388:PHE:HB3	1.85	0.41
1:A:468:GLU:OE1	1:A:470:TRP:NE1	2.54	0.41
1:A:586:ASN:OD1	1:A:588:THR:CB	2.65	0.41
1:B:285:TRP:C	1:B:287:GLY:H	2.29	0.41
1:B:298:LYS:CA	1:B:301:LYS:HE3	2.50	0.41
1:B:464:THR:O	1:B:465:ASN:CB	2.60	0.41
1:B:653:THR:HB	1:B:654:GLU:HG2	2.02	0.41
1:A:465:ASN:O	1:A:466:ASN:CG	2.64	0.41
1:A:469:PRO:HD2	1:A:470:TRP:CZ3	2.56	0.41
1:B:474:GLN:HE21	1:B:474:GLN:CA	2.33	0.41
1:A:134:LYS:CE	1:A:134:LYS:N	2.83	0.41
1:A:181:CYS:O	1:A:182:ARG:HB2	2.19	0.41
1:A:189:SER:HB2	1:A:190:ARG:H	1.69	0.41
1:A:191:VAL:O	1:A:192:ILE:CB	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:LEU:HB3	1:A:492:PRO:HD3	2.02	0.41
1:A:552:TRP:O	1:A:553:LYS:C	2.63	0.41
1:B:227:SER:C	1:B:228:PHE:CD2	2.99	0.41
1:B:270:VAL:HB	1:B:299:VAL:HG22	2.02	0.41
1:B:375:ARG:HA	1:B:376:PRO:HD2	1.77	0.41
1:A:268:ASN:O	1:A:293:ASP:HB2	2.21	0.41
1:A:304:ARG:HG2	1:A:304:ARG:H	1.58	0.41
1:A:368:ARG:HB2	1:A:382:ILE:HG21	2.03	0.41
1:B:253:ALA:H	1:B:290:ALA:H	1.68	0.41
1:B:257:PRO:C	1:B:259:TYR:CD2	2.99	0.41
1:B:272:VAL:C	1:B:274:THR:N	2.78	0.41
1:B:318:VAL:O	1:B:382:ILE:HA	2.21	0.41
1:B:328:ASN:O	1:B:329:ASP:CB	2.69	0.41
1:B:429:ALA:HB3	1:B:453:TYR:CZ	2.56	0.41
1:B:547:LEU:HA	1:B:548:PRO:HD3	1.96	0.41
1:A:53:ASN:OD1	1:A:138:LYS:HG2	2.21	0.40
1:A:434:PHE:N	1:A:434:PHE:HD1	2.19	0.40
1:B:94:ASP:O	1:B:95:LYS:HB3	2.21	0.40
1:B:421:LEU:HD23	1:B:421:LEU:HA	1.82	0.40
1:A:98:ARG:C	1:A:99:LEU:HD12	2.46	0.40
1:A:249:ILE:CG2	1:A:250:ASP:N	2.83	0.40
1:B:179:GLN:HA	1:B:207:VAL:HG23	1.44	0.40
1:A:123:THR:CG2	1:A:355:TYR:HD2	2.33	0.40
1:A:133:GLU:C	1:A:134:LYS:CG	2.94	0.40
1:A:180:GLN:O	1:A:209:TRP:HD1	2.04	0.40
1:A:652:ASN:C	1:A:653:THR:HG1	2.28	0.40
1:B:70:VAL:CG2	1:B:71:THR:H	2.02	0.40
1:B:176:LEU:HD11	1:B:498:LEU:HD22	2.03	0.40
1:A:308:LYS:HB3	1:A:315:VAL:HG11	2.02	0.40
1:A:312:ALA:HB3	1:A:313:GLN:HA	1.32	0.40
1:A:411:MET:C	1:A:414:PRO:HD2	2.47	0.40
1:A:169:PRO:HG2	1:A:393:ARG:O	2.22	0.40
1:A:254:LYS:HG2	1:A:255:VAL:H	1.86	0.40
1:A:262:TYR:HE1	1:A:264:SER:OG	1.98	0.40
1:B:75:LEU:N	1:B:75:LEU:CD2	2.84	0.40
1:B:418:THR:HG23	1:B:419:LEU:N	2.36	0.40
1:B:470:TRP:O	1:B:472:PHE:N	2.55	0.40
1:B:543:ASN:C	1:B:545:PRO:N	2.80	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:OE1	1:A:653:THR:OG1[2_557]	0.80	1.40
1:A:521:SER:OG	1:B:377:GLU:CB[2_557]	1.36	0.84
1:A:554:GLU:CD	1:A:653:THR:OG1[2_557]	1.72	0.48
1:A:554:GLU:OE2	1:A:652:ASN:O[2_557]	1.90	0.30
1:A:554:GLU:OE1	1:A:653:THR:CB[2_557]	1.98	0.22
2:A:714:HOH:O	2:A:715:HOH:O[2_547]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	582/697 (84%)	471 (81%)	66 (11%)	45 (8%)	1	1
1	B	581/697 (83%)	464 (80%)	64 (11%)	53 (9%)	0	0
All	All	1163/1394 (83%)	935 (80%)	130 (11%)	98 (8%)	0	1

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	TRP
1	A	87	ASP
1	A	90	ALA
1	A	93	VAL
1	A	112	ASP
1	A	127	GLU
1	A	193	GLU
1	A	229	PRO
1	A	274	THR
1	A	275	ALA
1	A	276	ASP
1	A	278	LYS
1	A	437	ASN
1	A	467	LYS
1	A	506	MET

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Mol	Chain	Res	Type
1	A	545	PRO
1	A	650	LYS
1	A	654	GLU
1	B	59	PRO
1	B	72	GLY
1	B	181	CYS
1	B	190	ARG
1	B	211	ASP
1	B	212	ILE
1	B	215	MET
1	B	226	LYS
1	B	263	LYS
1	B	268	ASN
1	B	271	TRP
1	B	323	ASN
1	B	327	ILE
1	B	353	LEU
1	B	355	TYR
1	B	434	PHE
1	B	435	LEU
1	B	437	ASN
1	B	542	ALA
1	B	546	ALA
1	B	564	ASP
1	B	565	LYS
1	B	593	ASP
1	B	595	LEU
1	B	663	ILE
1	A	52	ALA
1	A	53	ASN
1	A	56	LEU
1	A	85	ASN
1	A	92	GLY
1	A	182	ARG
1	A	400	GLY
1	A	406	TRP
1	A	435	LEU
1	B	60	GLU
1	B	63	SER
1	B	79	LYS
1	B	460	ALA
1	B	468	GLU

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Mol	Chain	Res	Type
1	B	523	ARG
1	B	555	LEU
1	B	568	ALA
1	B	639	LYS
1	B	657	ASP
1	A	48	THR
1	A	95	LYS
1	A	131	THR
1	A	187	PRO
1	A	189	SER
1	A	233	ALA
1	A	466	ASN
1	A	554	GLU
1	A	582	LYS
1	B	84	TRP
1	B	97	THR
1	B	184	SER
1	B	224	ASN
1	B	438	ALA
1	B	459	HIS
1	B	543	ASN
1	B	635	ARG
1	B	650	LYS
1	B	662	LYS
1	A	183	PHE
1	A	223	PHE
1	A	232	LYS
1	A	273	LYS
1	B	125	LYS
1	A	107	MET
1	A	192	ILE
1	A	336	PRO
1	B	186	SER
1	B	471	VAL
1	B	544	GLN
1	B	547	LEU
1	B	556	SER
1	A	330	THR
1	B	436	PHE
1	A	431	ILE
1	B	539	PRO

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	464/579 (80%)	360 (78%)	104 (22%)	1	3
1	B	462/579 (80%)	358 (78%)	104 (22%)	1	3
All	All	926/1158 (80%)	718 (78%)	208 (22%)	1	3

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	56	LEU
1	A	58	VAL
1	A	76	ARG
1	A	77	ASN
1	A	79	LYS
1	A	80	THR
1	A	82	LYS
1	A	85	ASN
1	A	105	TRP
1	A	109	VAL
1	A	110	ARG
1	A	114	THR
1	A	118	ILE
1	A	122	THR
1	A	125	LYS
1	A	134	LYS
1	A	137	LEU
1	A	170	MET
1	A	181	CYS
1	A	183	PHE
1	A	185	TYR
1	A	188	ASP
1	A	189	SER
1	A	190	ARG
1	A	200	LEU
1	A	201	LYS

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Mol	Chain	Res	Type
1	A	206	ASP
1	A	212	ILE
1	A	215	MET
1	A	216	ASP
1	A	220	ILE
1	A	223	PHE
1	A	238	LEU
1	A	254	LYS
1	A	260	PHE
1	A	261	VAL
1	A	262	TYR
1	A	267	GLU
1	A	270	VAL
1	A	278	LYS
1	A	279	ASN
1	A	283	ASP
1	A	298	LYS
1	A	300	ASN
1	A	304	ARG
1	A	306	LEU
1	A	308	LYS
1	A	334	THR
1	A	337	GLU
1	A	355	TYR
1	A	362	LEU
1	A	368	ARG
1	A	371	ILE
1	A	377	GLU
1	A	382	ILE
1	A	385	ARG
1	A	398	TRP
1	A	404	SER
1	A	409	LEU
1	A	410	LYS
1	A	411	MET
1	A	419	LEU
1	A	427	SER
1	A	434	PHE
1	A	435	LEU
1	A	436	PHE
1	A	437	ASN
1	A	447	ILE

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Mol	Chain	Res	Type
1	A	461	CYS
1	A	465	ASN
1	A	466	ASN
1	A	467	LYS
1	A	480	SER
1	A	489	ILE
1	A	491	LEU
1	A	510	ARG
1	A	513	PHE
1	A	515	SER
1	A	526	GLU
1	A	538	ILE
1	A	547	LEU
1	A	549	LYS
1	A	553	LYS
1	A	555	LEU
1	A	569	LYS
1	A	571	LYS
1	A	572	ILE
1	A	580	THR
1	A	584	ILE
1	A	589	GLU
1	A	592	LEU
1	A	603	GLU
1	A	604	GLN
1	A	608	SER
1	A	630	GLN
1	A	632	VAL
1	A	643	LYS
1	A	646	LYS
1	A	647	LYS
1	A	650	LYS
1	A	652	ASN
1	A	653	THR
1	A	654	GLU
1	B	58	VAL
1	B	63	SER
1	B	69	GLU
1	B	70	VAL
1	B	71	THR
1	B	76	ARG
1	B	80	THR

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Mol	Chain	Res	Type
1	B	81	ILE
1	B	86	THR
1	B	87	ASP
1	B	88	SER
1	B	94	ASP
1	B	95	LYS
1	B	105	TRP
1	B	119	LEU
1	B	123	THR
1	B	130	SER
1	B	138	LYS
1	B	151	ARG
1	B	152	GLU
1	B	155	GLN
1	B	164	LEU
1	B	171	ILE
1	B	192	ILE
1	B	207	VAL
1	B	212	ILE
1	B	219	ARG
1	B	220	ILE
1	B	234	VAL
1	B	235	ASN
1	B	256	ASP
1	B	264	SER
1	B	271	TRP
1	B	273	LYS
1	B	274	THR
1	B	276	ASP
1	B	278	LYS
1	B	279	ASN
1	B	301	LYS
1	B	306	LEU
1	B	307	TYR
1	B	308	LYS
1	B	328	ASN
1	B	351	THR
1	B	354	GLN
1	B	355	TYR
1	B	357	ASN
1	B	368	ARG
1	B	382	ILE

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Mol	Chain	Res	Type
1	B	389	LEU
1	B	397	THR
1	B	399	THR
1	B	401	ASP
1	B	404	SER
1	B	409	LEU
1	B	410	LYS
1	B	415	MET
1	B	427	SER
1	B	434	PHE
1	B	435	LEU
1	B	437	ASN
1	B	445	ASN
1	B	457	ARG
1	B	464	THR
1	B	465	ASN
1	B	474	GLN
1	B	475	LYS
1	B	489	ILE
1	B	491	LEU
1	B	498	LEU
1	B	515	SER
1	B	520	LEU
1	B	522	LEU
1	B	523	ARG
1	B	543	ASN
1	B	544	GLN
1	B	555	LEU
1	B	556	SER
1	B	564	ASP
1	B	565	LYS
1	B	566	TYR
1	B	569	LYS
1	B	571	LYS
1	B	573	ARG
1	B	588	THR
1	B	592	LEU
1	B	610	ASN
1	B	620	SER
1	B	623	LYS
1	B	629	LEU
1	B	634	GLU

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Mol	Chain	Res	Type
1	B	635	ARG
1	B	639	LYS
1	B	644	LEU
1	B	645	THR
1	B	646	LYS
1	B	648	THR
1	B	653	THR
1	B	654	GLU
1	B	655	ASN
1	B	656	LYS
1	B	660	VAL
1	B	661	ILE
1	B	662	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	230	ASN
1	A	235	ASN
1	A	239	HIS
1	A	244	HIS
1	A	258	ASN
1	A	328	ASN
1	A	356	HIS
1	A	424	GLN
1	A	655	ASN
1	B	244	HIS
1	B	281	HIS
1	B	300	ASN
1	B	305	ASN
1	B	352	HIS
1	B	354	GLN
1	B	466	ASN
1	B	474	GLN
1	B	543	ASN
1	B	604	GLN
1	B	636	ASN
1	B	655	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	594:PRO	C	595:LEU	N	1.64
1	B	434:PHE	C	435:LEU	N	0.19

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	588/697 (84%)	1.66	211 (35%)	1 0	10, 42, 120, 162	0
1	B	587/697 (84%)	1.59	202 (34%)	1 1	11, 43, 110, 166	0
All	All	1175/1394 (84%)	1.62	413 (35%)	1 1	10, 42, 117, 166	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLY	8.4
1	A	264	SER	7.5
1	A	261	VAL	7.5
1	B	265	GLY	7.0
1	A	544	GLN	6.5
1	B	215	MET	6.3
1	A	280	PHE	6.2
1	B	432	GLY	6.2
1	B	355	TYR	6.1
1	B	637	GLY	6.0
1	A	48	THR	6.0
1	A	54	ALA	6.0
1	A	291	PHE	5.9
1	A	265	GLY	5.8
1	A	91	TYR	5.7
1	A	55	SER	5.7
1	B	621	TYR	5.6
1	A	266	THR	5.5
1	A	312	ALA	5.5
1	A	292	PRO	5.5
1	A	290	ALA	5.4
1	A	335	MET	5.4
1	A	277	GLY	5.4
1	A	288	ALA	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	259	TYR	5.3
1	A	274	THR	5.2
1	A	275	ALA	5.2
1	A	336	PRO	5.2
1	A	260	PHE	5.2
1	A	281	HIS	5.2
1	B	346	LYS	5.1
1	B	222	THR	5.1
1	B	277	GLY	5.1
1	A	337	GLU	5.1
1	B	437	ASN	5.1
1	A	219	ARG	5.1
1	A	93	VAL	5.1
1	A	218	TYR	5.1
1	A	271	TRP	5.0
1	A	272	VAL	5.0
1	A	50	GLY	5.0
1	A	233	ALA	5.0
1	A	223	PHE	4.9
1	B	376	PRO	4.9
1	B	566	TYR	4.9
1	A	338	ASP	4.8
1	B	218	TYR	4.8
1	B	274	THR	4.8
1	A	262	TYR	4.7
1	B	268	ASN	4.6
1	A	258	ASN	4.6
1	A	216	ASP	4.6
1	B	212	ILE	4.6
1	B	619	TRP	4.6
1	B	351	THR	4.6
1	A	435	LEU	4.5
1	B	260	PHE	4.5
1	A	263	LYS	4.5
1	A	222	THR	4.5
1	A	53	ASN	4.4
1	A	289	ALA	4.4
1	B	349	ALA	4.4
1	A	231	PRO	4.4
1	B	184	SER	4.4
1	B	463	GLY	4.4
1	A	253	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	348	PRO	4.3
1	B	211	ASP	4.3
1	A	270	VAL	4.3
1	A	267	GLU	4.2
1	B	76	ARG	4.2
1	B	462	ALA	4.2
1	B	284	ALA	4.2
1	B	464	THR	4.2
1	B	210	MET	4.2
1	A	259	TYR	4.1
1	B	350	GLY	4.1
1	B	442	LEU	4.1
1	B	261	VAL	4.1
1	B	285	TRP	4.0
1	A	276	ASP	4.0
1	A	310	PHE	4.0
1	A	254	LYS	4.0
1	B	186	SER	4.0
1	B	327	ILE	4.0
1	B	258	ASN	4.0
1	B	620	SER	4.0
1	B	228	PHE	4.0
1	A	217	GLY	3.9
1	A	228	PHE	3.9
1	A	355	TYR	3.9
1	B	275	ALA	3.9
1	A	187	PRO	3.9
1	B	404	SER	3.9
1	B	262	TYR	3.8
1	B	270	VAL	3.8
1	B	461	CYS	3.8
1	A	273	LYS	3.8
1	A	279	ASN	3.8
1	B	267	GLU	3.8
1	B	435	LEU	3.8
1	A	221	PHE	3.8
1	A	302	TRP	3.8
1	A	306	LEU	3.8
1	A	437	ASN	3.7
1	B	356	HIS	3.7
1	A	220	ILE	3.7
1	A	189	SER	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	252	GLY	3.7
1	B	255	VAL	3.7
1	B	286	PRO	3.7
1	B	84	TRP	3.7
1	B	288	ALA	3.7
1	A	257	PRO	3.7
1	B	272	VAL	3.7
1	A	326	GLN	3.7
1	A	112	ASP	3.7
1	B	305	ASN	3.7
1	A	307	TYR	3.7
1	A	252	GLY	3.7
1	A	296	SER	3.6
1	A	183	PHE	3.6
1	A	327	ILE	3.5
1	A	131	THR	3.5
1	B	209	TRP	3.5
1	B	271	TRP	3.5
1	B	264	SER	3.5
1	A	334	THR	3.5
1	A	618	GLY	3.5
1	B	257	PRO	3.5
1	B	280	PHE	3.5
1	B	81	ILE	3.5
1	B	266	THR	3.5
1	B	658	MET	3.5
1	B	77	ASN	3.5
1	B	58	VAL	3.5
1	B	281	HIS	3.5
1	A	461	CYS	3.5
1	B	213	ASP	3.5
1	B	253	ALA	3.5
1	A	185	TYR	3.4
1	A	232	LYS	3.4
1	A	214	TYR	3.4
1	B	80	THR	3.4
1	B	287	GLY	3.4
1	B	91	TYR	3.4
1	A	330	THR	3.4
1	A	52	ALA	3.4
1	B	403	GLY	3.4
1	B	660	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	227	SER	3.4
1	B	472	PHE	3.4
1	B	326	GLN	3.3
1	A	255	VAL	3.3
1	A	251	PRO	3.3
1	B	291	PHE	3.3
1	A	46	SER	3.3
1	B	595	LEU	3.3
1	A	56	LEU	3.3
1	A	284	ALA	3.3
1	A	440	ALA	3.3
1	B	216	ASP	3.3
1	B	276	ASP	3.3
1	B	460	ALA	3.2
1	B	664	ILE	3.2
1	A	465	ASN	3.2
1	B	279	ASN	3.2
1	B	542	ALA	3.2
1	A	506	MET	3.2
1	B	278	LYS	3.2
1	A	438	ALA	3.2
1	A	328	ASN	3.2
1	B	132	ASP	3.2
1	A	313	GLN	3.2
1	B	124	TRP	3.2
1	A	268	ASN	3.1
1	A	125	LYS	3.1
1	A	97	THR	3.1
1	A	184	SER	3.1
1	B	194	ILE	3.1
1	B	269	ASP	3.1
1	A	47	LEU	3.1
1	A	92	GLY	3.1
1	A	90	ALA	3.1
1	B	540	ALA	3.1
1	B	541	PHE	3.1
1	B	407	ASP	3.1
1	B	527	GLU	3.1
1	A	325	PRO	3.1
1	A	331	PRO	3.1
1	B	653	THR	3.1
1	A	540	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	623	LYS	3.1
1	A	229	PRO	3.1
1	B	180	GLN	3.1
1	B	354	GLN	3.1
1	B	467	LYS	3.1
1	A	51	LYS	3.0
1	B	440	ALA	3.0
1	B	93	VAL	3.0
1	B	283	ASP	3.0
1	A	294	PHE	3.0
1	A	406	TRP	3.0
1	B	406	TRP	3.0
1	A	88	SER	3.0
1	B	129	SER	3.0
1	A	58	VAL	3.0
1	A	119	LEU	2.9
1	B	661	ILE	2.9
1	B	352	HIS	2.9
1	B	552	TRP	2.9
1	B	224	ASN	2.9
1	B	445	ASN	2.9
1	A	432	GLY	2.9
1	B	290	ALA	2.9
1	A	234	VAL	2.9
1	B	183	PHE	2.9
1	B	471	VAL	2.9
1	B	476	VAL	2.9
1	B	353	LEU	2.9
1	B	140	GLU	2.9
1	A	295	THR	2.9
1	A	126	ALA	2.9
1	B	234	VAL	2.9
1	A	225	PRO	2.9
1	A	309	ASP	2.9
1	B	214	TYR	2.9
1	B	273	LYS	2.9
1	A	315	VAL	2.9
1	A	434	PHE	2.9
1	A	545	PRO	2.8
1	A	142	ILE	2.8
1	A	141	GLY	2.8
1	A	188	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	87	ASP	2.8
1	A	466	ASN	2.8
1	A	360	GLY	2.8
1	A	285	TRP	2.8
1	A	367	SER	2.8
1	B	254	LYS	2.8
1	B	75	LEU	2.8
1	A	123	THR	2.8
1	A	464	THR	2.8
1	B	97	THR	2.8
1	B	205	CYS	2.8
1	B	182	ARG	2.8
1	A	278	LYS	2.8
1	B	663	ILE	2.8
1	A	89	GLY	2.8
1	B	78	GLY	2.8
1	B	433	GLY	2.8
1	B	473	GLY	2.8
1	B	329	ASP	2.8
1	B	263	LYS	2.7
1	B	128	LEU	2.7
1	B	347	LEU	2.7
1	B	256	ASP	2.7
1	A	144	PHE	2.7
1	A	505	GLY	2.7
1	A	87	ASP	2.7
1	A	399	THR	2.7
1	A	462	ALA	2.7
1	B	219	ARG	2.7
1	B	436	PHE	2.7
1	A	74	LEU	2.7
1	A	311	LEU	2.7
1	A	235	ASN	2.7
1	A	554	GLU	2.7
1	A	71	THR	2.7
1	A	333	LYS	2.7
1	B	225	PRO	2.7
1	A	458	GLY	2.7
1	A	283	ASP	2.7
1	B	478	ASP	2.7
1	B	307	TYR	2.6
1	A	99	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	306	LEU	2.6
1	B	459	HIS	2.6
1	B	357	ASN	2.6
1	B	402	ASN	2.6
1	B	409	LEU	2.6
1	A	110	ARG	2.6
1	A	96	GLY	2.6
1	A	403	GLY	2.6
1	B	226	LYS	2.6
1	B	468	GLU	2.6
1	A	115	ALA	2.6
1	A	256	ASP	2.6
1	A	148	ILE	2.6
1	A	137	LEU	2.6
1	A	49	ASP	2.6
1	A	621	TYR	2.6
1	B	217	GLY	2.6
1	A	590	ASN	2.6
1	A	104	PRO	2.5
1	B	90	ALA	2.5
1	A	365	LYS	2.5
1	B	408	HIS	2.5
1	B	195	ALA	2.5
1	A	114	THR	2.5
1	B	83	LEU	2.5
1	A	215	MET	2.5
1	B	318	VAL	2.5
1	B	465	ASN	2.5
1	A	442	LEU	2.5
1	A	591	SER	2.5
1	A	213	ASP	2.5
1	A	329	ASP	2.5
1	B	470	TRP	2.5
1	A	616	GLY	2.5
1	B	131	THR	2.4
1	A	592	LEU	2.4
1	B	249	ILE	2.4
1	A	211	ASP	2.4
1	A	356	HIS	2.4
1	A	546	ALA	2.4
1	A	86	THR	2.4
1	B	88	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	638	ASP	2.4
1	A	143	PRO	2.4
1	A	200	LEU	2.4
1	B	466	ASN	2.4
1	B	636	ASN	2.4
1	A	589	GLU	2.4
1	A	210	MET	2.4
1	B	248	MET	2.4
1	B	135	ILE	2.4
1	B	557	LEU	2.4
1	A	332	ASN	2.4
1	A	321	ASP	2.4
1	B	94	ASP	2.4
1	B	657	ASP	2.4
1	B	398	TRP	2.4
1	B	618	GLY	2.4
1	B	190	ARG	2.4
1	B	364	VAL	2.4
1	A	566	TYR	2.3
1	A	305	ASN	2.3
1	B	469	PRO	2.3
1	A	317	GLY	2.3
1	B	68	GLY	2.3
1	A	362	LEU	2.3
1	B	320	ASN	2.3
1	A	226	LYS	2.3
1	A	286	PRO	2.3
1	B	635	ARG	2.3
1	A	212	ILE	2.3
1	A	651	TYR	2.3
1	A	224	ASN	2.3
1	B	594	PRO	2.3
1	A	84	TRP	2.3
1	B	82	LYS	2.3
1	B	123	THR	2.3
1	A	85	ASN	2.3
1	B	441	ASP	2.3
1	B	592	LEU	2.3
1	A	249	ILE	2.2
1	B	438	ALA	2.2
1	A	134	LYS	2.2
1	A	122	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	543	ASN	2.2
1	A	269	ASP	2.2
1	B	101	GLN	2.2
1	B	95	LYS	2.2
1	A	140	GLU	2.2
1	B	185	TYR	2.2
1	A	293	ASP	2.2
1	A	564	ASP	2.2
1	B	282	GLY	2.2
1	B	571	LYS	2.2
1	A	81	ILE	2.2
1	A	182	ARG	2.2
1	A	186	SER	2.2
1	B	322	VAL	2.2
1	B	302	TRP	2.2
1	B	652	ASN	2.2
1	A	287	GLY	2.2
1	A	314	GLY	2.2
1	A	471	VAL	2.2
1	A	303	TRP	2.1
1	A	492	PRO	2.1
1	A	467	LYS	2.1
1	B	89	GLY	2.1
1	A	129	SER	2.1
1	A	431	ILE	2.1
1	B	189	SER	2.1
1	B	133	GLU	2.1
1	A	98	ARG	2.1
1	B	410	LYS	2.1
1	A	652	ASN	2.1
1	B	66	GLY	2.1
1	B	444	GLY	2.1
1	B	191	VAL	2.1
1	B	623	LYS	2.1
1	B	430	ASP	2.1
1	B	477	GLU	2.1
1	A	124	TRP	2.1
1	A	298	LYS	2.1
1	B	61	GLY	2.1
1	A	192	ILE	2.1
1	B	70	VAL	2.1
1	B	223	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	THR	2.0
1	B	655	ASN	2.0
1	B	220	ILE	2.0
1	B	207	VAL	2.0
1	A	541	PHE	2.0
1	B	221	PHE	2.0
1	B	377	GLU	2.0
1	B	439	ASP	2.0
1	A	297	PRO	2.0
1	A	447	ILE	2.0
1	B	300	ASN	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.