



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 5CSC / pdb_00005csc
Title : STRUCTURE OF AN OPEN FORM OF CHICKEN HEART CITRATE
SYNTHASE AT 2.8 ANGSTROMS RESOLUTION
Authors : Liao, D.-I.; Karpusas, M.; Remington, S.J.
Deposited on : 1990-05-07
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

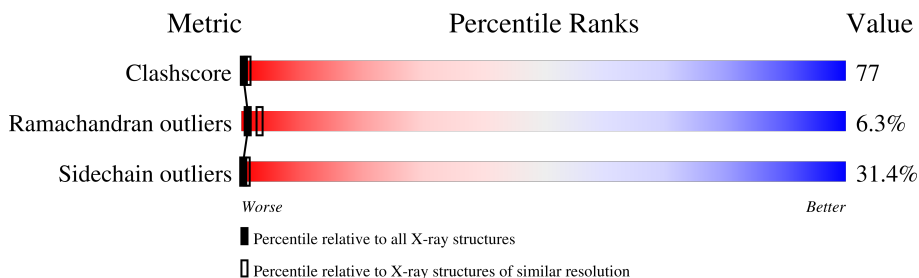
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	429	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6606 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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3303	2112	571	603	17			

- Molecule 2 is a protein called CITRATE SYNTHASE.

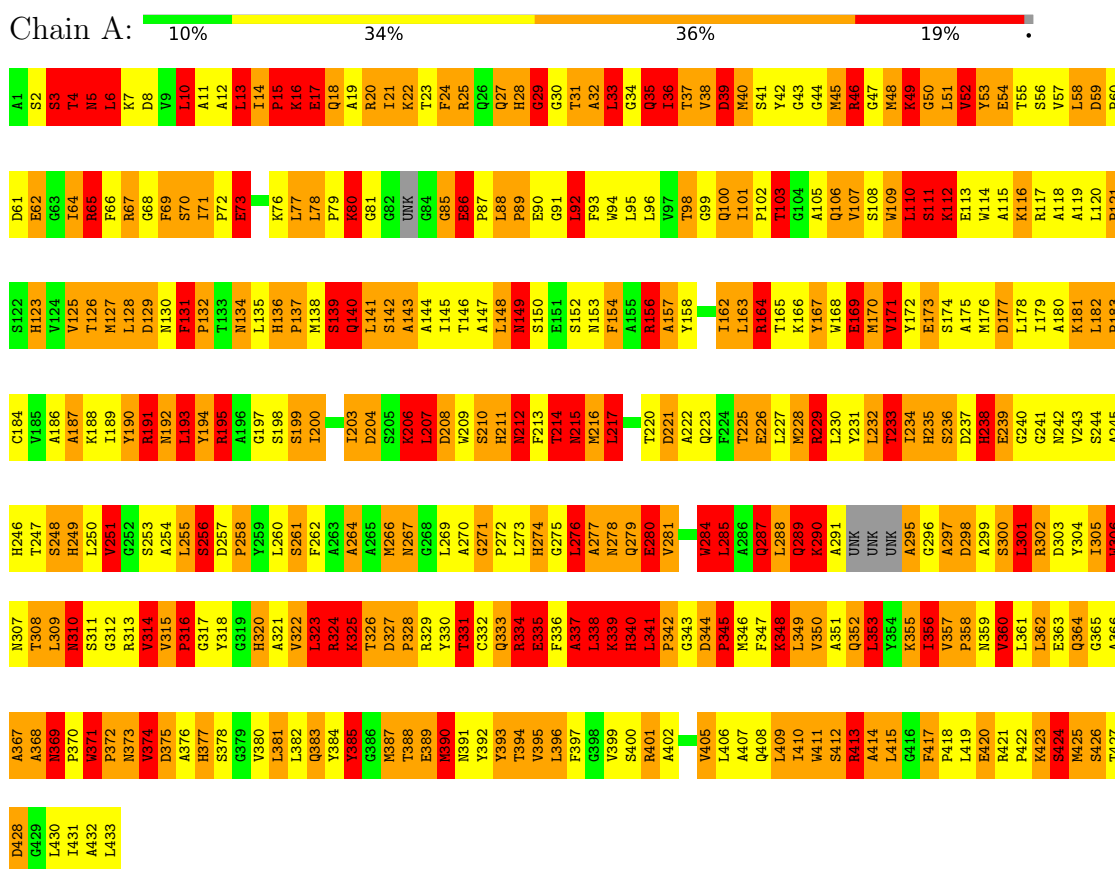
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	429	Total	C	N	O	S	0	0	0
			3303	2112	571	603	17			

3 Residue-property plots

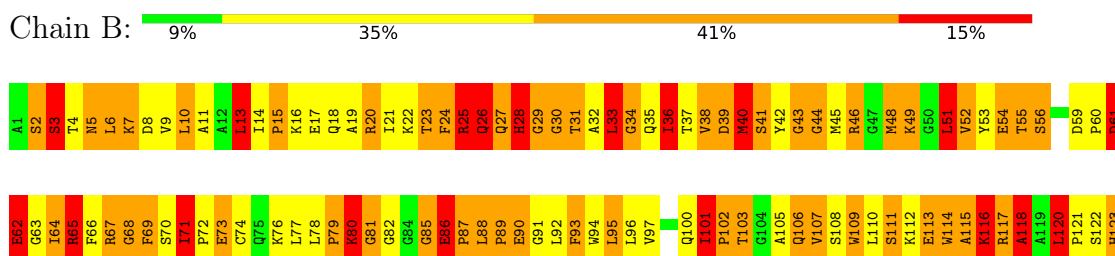
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

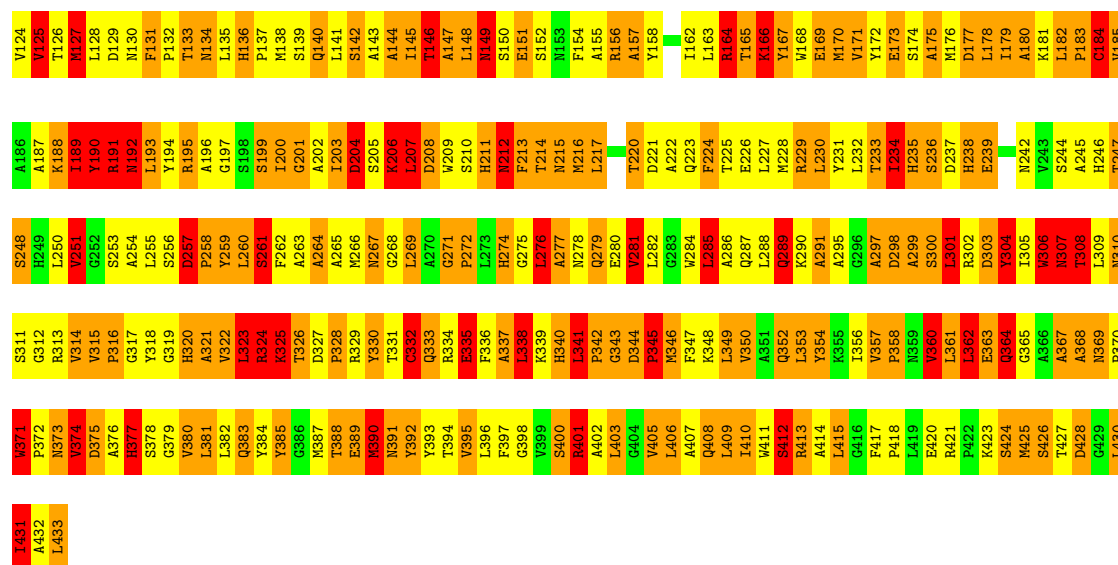
Note EDS was not executed.

• Molecule 1: CITRATE SYNTHASE



• Molecule 2: CITRATE SYNTHASE





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	58.85Å 58.85Å 259.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6606	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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	2.47	173/3383 (5.1%)	2.55	273/4594 (5.9%)
2	B	2.59	207/3383 (6.1%)	2.58	295/4594 (6.4%)
All	All	2.53	380/6766 (5.6%)	2.57	568/9188 (6.2%)

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	7	5
2	B	5	3
All	All	12	8

All (380) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	ALA	CA-C	-14.71	1.38	1.53
1	A	366	ALA	C-N	12.16	1.43	1.33
2	B	177	ASP	C-O	-11.02	1.10	1.24
1	A	78	LEU	C-N	10.80	1.46	1.33
2	B	368	ALA	CA-C	10.64	1.67	1.52
2	B	320	HIS	CE1-NE2	10.37	1.43	1.32
2	B	304	TYR	C-N	10.25	1.46	1.34
2	B	369	ASN	N-CA	-10.18	1.35	1.46
2	B	24	PHE	C-N	10.16	1.47	1.33
2	B	211	HIS	N-CA	-10.03	1.34	1.46
2	B	278	ASN	C-N	9.83	1.46	1.33
2	B	178	LEU	C-O	-9.77	1.12	1.24
1	A	350	VAL	CA-C	9.44	1.64	1.52
2	B	95	LEU	C-N	9.42	1.46	1.34
2	B	44	GLY	C-N	9.37	1.46	1.33
1	A	156	ARG	N-CA	-9.23	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	235	HIS	CA-C	-9.14	1.40	1.52
2	B	20	ARG	NE-CZ	9.07	1.43	1.33
1	A	225	THR	CA-C	-9.03	1.40	1.52
2	B	173	GLU	CA-C	-8.97	1.41	1.52
1	A	277	ALA	N-CA	8.93	1.57	1.46
1	A	157	ALA	C-O	-8.87	1.12	1.24
1	A	156	ARG	CD-NE	8.86	1.58	1.46
1	A	375	ASP	CG-OD2	8.85	1.42	1.25
2	B	362	LEU	CA-C	-8.80	1.41	1.52
2	B	376	ALA	CA-C	8.79	1.63	1.52
2	B	33	LEU	N-CA	-8.77	1.34	1.45
2	B	380	VAL	CA-CB	8.72	1.65	1.54
2	B	28	HIS	CG-CD2	8.69	1.45	1.35
2	B	264	ALA	CA-C	-8.69	1.41	1.52
1	A	395	VAL	C-N	-8.58	1.22	1.33
2	B	143	ALA	CA-C	8.51	1.63	1.52
2	B	317	GLY	CA-C	8.50	1.63	1.51
2	B	349	LEU	CA-C	-8.44	1.42	1.52
2	B	115	ALA	C-O	8.42	1.33	1.24
1	A	360	VAL	C-N	8.38	1.44	1.33
2	B	61	ASP	CA-C	8.37	1.63	1.52
1	A	328	PRO	CA-C	-8.34	1.39	1.52
2	B	254	ALA	CA-C	-8.33	1.40	1.52
1	A	27	GLN	N-CA	-8.32	1.35	1.46
1	A	127	MET	C-O	-8.20	1.13	1.24
1	A	148	LEU	C-N	-8.19	1.22	1.33
1	A	198	SER	C-O	8.16	1.32	1.23
1	A	324	ARG	N-CA	-8.11	1.38	1.46
2	B	363	GLU	CD-OE2	8.08	1.40	1.25
2	B	43	GLY	C-N	8.07	1.41	1.33
2	B	125	VAL	CA-CB	-8.07	1.45	1.54
1	A	225	THR	C-O	-8.01	1.13	1.24
2	B	412	SER	CA-CB	-7.99	1.40	1.53
1	A	395	VAL	C-O	-7.97	1.13	1.24
2	B	268	GLY	CA-C	7.88	1.62	1.51
1	A	47	GLY	CA-C	7.86	1.61	1.51
2	B	320	HIS	CG-ND1	7.86	1.46	1.38
2	B	62	GLU	N-CA	-7.85	1.35	1.46
2	B	227	LEU	N-CA	7.79	1.55	1.46
2	B	177	ASP	CA-C	-7.75	1.42	1.52
2	B	20	ARG	CZ-NH1	7.71	1.43	1.32
2	B	425	MET	CA-C	7.68	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	413	ARG	C-O	-7.66	1.14	1.24
2	B	401	ARG	NE-CZ	-7.65	1.24	1.33
2	B	315	VAL	N-CA	7.63	1.55	1.46
2	B	208	ASP	CG-OD2	7.62	1.39	1.25
2	B	264	ALA	C-O	-7.60	1.14	1.24
2	B	136	HIS	CA-C	-7.57	1.43	1.52
2	B	304	TYR	C-O	7.57	1.33	1.24
2	B	373	ASN	C-O	-7.56	1.14	1.24
2	B	164	ARG	C-N	-7.56	1.23	1.33
1	A	4	THR	C-N	7.52	1.44	1.33
2	B	377	HIS	CB-CG	-7.50	1.39	1.50
2	B	376	ALA	C-O	7.50	1.32	1.24
2	B	28	HIS	C-N	7.47	1.45	1.33
1	A	212	ASN	N-CA	-7.46	1.36	1.46
2	B	34	GLY	N-CA	7.45	1.54	1.45
2	B	125	VAL	CA-C	-7.44	1.43	1.52
1	A	123	HIS	CE1-NE2	7.39	1.40	1.32
2	B	204	ASP	N-CA	-7.38	1.37	1.46
2	B	170	MET	CA-C	-7.33	1.43	1.52
2	B	62	GLU	C-O	7.29	1.33	1.24
1	A	414	ALA	C-O	7.28	1.32	1.24
1	A	13	LEU	C-N	7.26	1.41	1.33
2	B	424	SER	N-CA	-7.26	1.37	1.45
2	B	322	VAL	CA-CB	-7.25	1.46	1.54
1	A	284	TRP	CA-CB	7.24	1.65	1.53
1	A	420	GLU	C-O	7.21	1.32	1.23
2	B	126	THR	C-O	-7.21	1.15	1.24
1	A	332	CYS	C-O	-7.18	1.15	1.24
1	A	193	LEU	CA-C	-7.17	1.43	1.52
1	A	349	LEU	CA-C	-7.09	1.43	1.52
1	A	389	GLU	CA-C	-7.09	1.44	1.53
2	B	269	LEU	CA-C	-7.09	1.43	1.52
2	B	400	SER	C-O	-7.07	1.15	1.24
2	B	145	ILE	CA-C	-7.04	1.43	1.52
1	A	66	PHE	CA-C	7.03	1.62	1.52
1	A	334	ARG	NE-CZ	7.00	1.40	1.33
2	B	238	HIS	CB-CG	-7.00	1.40	1.50
1	A	365	GLY	C-N	-6.99	1.25	1.33
1	A	364	GLN	C-N	6.98	1.43	1.33
2	B	367	ALA	CA-C	-6.97	1.43	1.52
2	B	183	PRO	N-CA	-6.97	1.38	1.47
1	A	222	ALA	C-N	6.96	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	HIS	CE1-NE2	6.96	1.39	1.32
1	A	81	GLY	C-N	6.95	1.43	1.33
1	A	419	LEU	CA-C	-6.92	1.43	1.52
2	B	71	ILE	C-O	6.91	1.30	1.24
1	A	254	ALA	CA-C	-6.91	1.43	1.52
2	B	166	LYS	CA-C	6.89	1.62	1.52
1	A	6	LEU	CA-C	-6.87	1.43	1.52
1	A	129	ASP	C-O	-6.85	1.16	1.24
2	B	358	PRO	CA-C	-6.78	1.42	1.52
2	B	428	ASP	CG-OD2	6.77	1.38	1.25
1	A	86	GLU	CA-C	6.77	1.60	1.52
2	B	342	PRO	C-N	6.76	1.43	1.33
2	B	410	ILE	N-CA	-6.75	1.39	1.46
2	B	147	ALA	N-CA	-6.74	1.37	1.46
2	B	337	ALA	C-O	-6.74	1.16	1.24
1	A	10	LEU	C-O	-6.66	1.16	1.24
2	B	202	ALA	C-O	-6.64	1.15	1.24
2	B	77	LEU	CA-C	-6.63	1.44	1.52
2	B	127	MET	C-O	-6.62	1.15	1.24
2	B	343	GLY	C-N	6.62	1.43	1.33
2	B	89	PRO	CA-C	6.61	1.61	1.52
2	B	225	THR	N-CA	6.61	1.54	1.46
1	A	232	LEU	N-CA	-6.59	1.37	1.46
2	B	376	ALA	N-CA	6.59	1.54	1.46
2	B	274	HIS	CA-C	6.58	1.59	1.52
2	B	29	GLY	CA-C	6.57	1.59	1.51
1	A	221	ASP	C-O	6.54	1.32	1.23
1	A	296	GLY	N-CA	-6.54	1.38	1.45
1	A	235	HIS	CA-C	-6.53	1.43	1.52
1	A	137	PRO	CA-C	6.51	1.61	1.52
2	B	321	ALA	N-CA	-6.50	1.38	1.46
1	A	116	LYS	CA-C	-6.49	1.44	1.52
2	B	227	LEU	C-O	-6.49	1.16	1.24
1	A	33	LEU	CA-C	6.48	1.61	1.52
2	B	103	THR	CB-OG1	6.48	1.54	1.43
2	B	360	VAL	N-CA	-6.48	1.39	1.46
1	A	279	GLN	C-N	6.47	1.42	1.33
1	A	306	TRP	C-N	-6.47	1.25	1.34
2	B	196	ALA	CA-C	-6.44	1.45	1.53
2	B	206	LYS	N-CA	-6.44	1.38	1.46
1	A	335	GLU	C-N	6.44	1.41	1.33
1	A	186	ALA	N-CA	-6.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	297	ALA	CA-C	-6.37	1.45	1.52
2	B	101	ILE	CA-C	6.37	1.59	1.52
1	A	358	PRO	N-CD	6.34	1.56	1.47
1	A	324	ARG	NE-CZ	6.33	1.40	1.33
1	A	77	LEU	C-O	-6.33	1.18	1.23
1	A	255	LEU	CA-CB	6.33	1.63	1.53
2	B	390	MET	CA-C	-6.31	1.44	1.52
2	B	286	ALA	N-CA	6.30	1.54	1.46
2	B	48	MET	N-CA	-6.29	1.38	1.46
2	B	373	ASN	C-N	-6.28	1.26	1.33
1	A	239	GLU	CD-OE2	6.26	1.37	1.25
2	B	116	LYS	C-O	-6.26	1.16	1.24
1	A	364	GLN	N-CA	6.26	1.53	1.46
1	A	69	PHE	N-CA	-6.25	1.38	1.46
2	B	67	ARG	CA-C	-6.24	1.44	1.52
2	B	256	SER	CA-C	-6.23	1.45	1.52
1	A	5	ASN	C-N	6.22	1.42	1.33
1	A	357	VAL	CA-C	6.22	1.59	1.52
2	B	408	GLN	CA-C	-6.21	1.44	1.52
1	A	304	TYR	C-N	6.21	1.41	1.33
1	A	39	ASP	C-N	6.20	1.42	1.33
2	B	69	PHE	CA-C	-6.19	1.44	1.52
2	B	303	ASP	CG-OD2	6.19	1.37	1.25
1	A	89	PRO	N-CD	6.19	1.56	1.47
2	B	133	THR	CA-C	-6.18	1.44	1.52
1	A	285	LEU	CA-C	-6.18	1.45	1.52
1	A	154	PHE	C-O	-6.16	1.16	1.24
1	A	6	LEU	C-O	-6.13	1.16	1.24
1	A	258	PRO	C-N	6.10	1.41	1.33
1	A	21	ILE	C-O	-6.10	1.16	1.24
2	B	323	LEU	CA-C	-6.10	1.45	1.52
2	B	65	ARG	NE-CZ	6.09	1.39	1.33
2	B	211	HIS	CB-CG	6.09	1.58	1.50
2	B	237	ASP	N-CA	6.09	1.53	1.45
2	B	306	TRP	NE1-CE2	6.09	1.44	1.37
2	B	385	TYR	N-CA	-6.09	1.38	1.46
1	A	402	ALA	N-CA	6.09	1.53	1.46
1	A	207	LEU	N-CA	6.09	1.53	1.45
1	A	217	LEU	CA-C	6.08	1.61	1.52
1	A	413	ARG	N-CA	-6.08	1.39	1.46
2	B	349	LEU	C-O	-6.06	1.17	1.24
2	B	222	ALA	C-O	-6.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	LEU	CA-CB	6.03	1.62	1.53
1	A	123	HIS	C-N	6.01	1.41	1.33
2	B	395	VAL	N-CA	-6.01	1.39	1.46
1	A	17	GLU	C-O	-6.00	1.16	1.24
1	A	432	ALA	CA-CB	-6.00	1.44	1.53
2	B	424	SER	CA-C	-5.99	1.44	1.53
1	A	149	ASN	N-CA	-5.99	1.38	1.46
2	B	340	HIS	CD2-NE2	5.97	1.44	1.37
1	A	287	GLN	C-O	-5.97	1.17	1.24
2	B	103	THR	N-CA	5.97	1.53	1.45
1	A	247	THR	C-O	-5.96	1.16	1.24
1	A	229	ARG	C-O	-5.95	1.17	1.24
1	A	366	ALA	CA-C	5.95	1.60	1.53
1	A	16	LYS	N-CA	-5.94	1.39	1.46
1	A	408	GLN	CA-CB	5.93	1.63	1.53
2	B	170	MET	C-O	-5.93	1.16	1.24
1	A	129	ASP	C-N	-5.91	1.25	1.33
2	B	109	TRP	CA-CB	5.91	1.62	1.53
1	A	238	HIS	CB-CG	-5.91	1.41	1.50
2	B	173	GLU	CD-OE2	5.90	1.36	1.25
2	B	74	CYS	C-N	5.89	1.42	1.33
1	A	257	ASP	C-O	-5.88	1.16	1.24
1	A	150	SER	N-CA	5.87	1.53	1.46
1	A	368	ALA	CA-C	5.87	1.61	1.52
2	B	332	CYS	C-N	-5.85	1.26	1.33
1	A	132	PRO	C-O	5.84	1.30	1.23
1	A	226	GLU	CD-OE2	5.84	1.36	1.25
2	B	15	PRO	N-CD	5.84	1.55	1.47
2	B	114	TRP	C-N	5.83	1.41	1.33
2	B	178	LEU	C-N	-5.83	1.27	1.34
1	A	318	TYR	CA-C	-5.80	1.45	1.52
1	A	195	ARG	CZ-NH2	5.79	1.41	1.33
2	B	177	ASP	CG-OD2	5.78	1.36	1.25
2	B	247	THR	CA-CB	5.78	1.62	1.53
2	B	202	ALA	C-N	-5.78	1.26	1.33
1	A	170	MET	CA-C	-5.77	1.45	1.52
1	A	199	SER	CA-CB	-5.77	1.44	1.53
2	B	236	SER	CA-C	-5.76	1.45	1.52
1	A	86	GLU	C-O	5.76	1.31	1.24
1	A	152	SER	C-N	5.76	1.42	1.34
2	B	117	ARG	N-CA	-5.76	1.38	1.46
2	B	421	ARG	NE-CZ	5.76	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	401	ARG	C-N	5.75	1.41	1.33
1	A	337	ALA	C-N	-5.75	1.26	1.33
2	B	131	PHE	C-O	5.75	1.31	1.24
2	B	169	GLU	N-CA	-5.74	1.38	1.46
1	A	73	GLU	CD-OE2	5.74	1.36	1.25
2	B	30	GLY	CA-C	5.73	1.59	1.51
2	B	5	ASN	C-O	-5.73	1.16	1.24
1	A	408	GLN	C-N	-5.73	1.26	1.33
2	B	211	HIS	CG-ND1	5.73	1.44	1.38
2	B	17	GLU	CD-OE2	5.71	1.36	1.25
2	B	67	ARG	CZ-NH1	5.71	1.40	1.32
1	A	247	THR	C-N	-5.68	1.26	1.33
1	A	103	THR	CB-OG1	5.68	1.52	1.43
2	B	24	PHE	CA-C	5.65	1.60	1.52
2	B	426	SER	C-N	-5.64	1.26	1.33
1	A	71	ILE	N-CA	5.63	1.53	1.46
1	A	100	GLN	N-CA	-5.62	1.38	1.45
1	A	353	LEU	C-O	-5.61	1.17	1.24
1	A	171	VAL	C-O	-5.61	1.17	1.24
1	A	376	ALA	C-O	-5.60	1.16	1.24
2	B	325	LYS	C-O	-5.60	1.17	1.23
1	A	29	GLY	CA-C	5.60	1.59	1.51
2	B	8	ASP	N-CA	-5.60	1.39	1.46
2	B	421	ARG	N-CA	-5.59	1.41	1.46
2	B	428	ASP	C-O	-5.58	1.16	1.24
2	B	184	CYS	CA-C	5.57	1.60	1.52
1	A	162	ILE	C-O	5.57	1.30	1.24
2	B	180	ALA	C-N	5.57	1.41	1.33
1	A	342	PRO	C-O	-5.57	1.16	1.24
1	A	35	GLN	CA-C	5.56	1.59	1.52
2	B	195	ARG	CZ-NH1	5.56	1.40	1.32
2	B	239	GLU	C-O	5.56	1.30	1.24
1	A	428	ASP	CG-OD2	5.56	1.35	1.25
2	B	395	VAL	CA-CB	-5.56	1.47	1.54
1	A	52	VAL	CA-CB	5.55	1.62	1.54
1	A	24	PHE	N-CA	-5.54	1.39	1.46
1	A	211	HIS	CE1-NE2	5.54	1.38	1.32
2	B	175	ALA	N-CA	-5.54	1.39	1.46
2	B	340	HIS	CG-ND1	5.54	1.44	1.38
2	B	239	GLU	CD-OE2	5.53	1.35	1.25
2	B	105	ALA	C-O	5.52	1.31	1.24
1	A	192	ASN	N-CA	5.51	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	66	PHE	CA-C	5.51	1.60	1.52
2	B	142	SER	N-CA	-5.51	1.39	1.46
1	A	274	HIS	CA-C	5.50	1.60	1.52
1	A	214	THR	CB-OG1	-5.50	1.34	1.43
1	A	107	VAL	CA-CB	-5.49	1.47	1.54
1	A	373	ASN	C-O	-5.49	1.17	1.24
2	B	178	LEU	CA-CB	5.49	1.62	1.53
2	B	364	GLN	C-O	5.48	1.33	1.24
2	B	285	LEU	C-N	5.47	1.41	1.33
1	A	156	ARG	NE-CZ	5.47	1.39	1.33
2	B	320	HIS	CG-CD2	5.47	1.41	1.35
1	A	206	LYS	C-O	5.46	1.30	1.24
2	B	239	GLU	C-N	5.45	1.41	1.33
1	A	298	ASP	C-O	-5.44	1.17	1.24
2	B	279	GLN	N-CA	5.44	1.52	1.46
1	A	131	PHE	CA-CB	-5.44	1.44	1.53
2	B	9	VAL	C-N	-5.42	1.27	1.33
1	A	393	TYR	C-O	-5.41	1.17	1.24
2	B	189	ILE	N-CA	-5.41	1.40	1.46
1	A	147	ALA	N-CA	-5.39	1.39	1.46
2	B	300	SER	C-N	5.39	1.41	1.33
1	A	21	ILE	N-CA	-5.39	1.39	1.46
2	B	224	PHE	C-N	5.38	1.41	1.33
2	B	346	MET	C-O	-5.38	1.17	1.24
2	B	362	LEU	C-O	-5.38	1.17	1.24
1	A	4	THR	C-O	5.38	1.30	1.23
1	A	143	ALA	N-CA	5.37	1.52	1.46
2	B	258	PRO	N-CD	5.37	1.55	1.47
1	A	65	ARG	C-N	5.36	1.39	1.33
1	A	338	LEU	N-CA	5.36	1.52	1.46
1	A	51	LEU	CA-C	-5.35	1.45	1.52
2	B	230	LEU	CA-CB	5.35	1.61	1.53
1	A	340	HIS	ND1-CE1	5.35	1.37	1.32
2	B	173	GLU	C-O	-5.35	1.18	1.24
2	B	335	GLU	CD-OE2	5.34	1.35	1.25
2	B	107	VAL	N-CA	-5.34	1.39	1.46
2	B	118	ALA	C-N	5.33	1.41	1.33
2	B	88	LEU	CA-C	5.33	1.59	1.52
2	B	344	ASP	CG-OD2	5.33	1.35	1.25
2	B	392	TYR	CA-C	5.33	1.60	1.52
1	A	401	ARG	CA-C	5.32	1.59	1.52
1	A	132	PRO	CA-C	5.32	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	ASP	C-O	-5.32	1.17	1.23
2	B	211	HIS	C-N	-5.30	1.26	1.34
1	A	206	LYS	C-N	5.30	1.40	1.33
2	B	25	ARG	CZ-NH2	5.30	1.40	1.33
2	B	185	VAL	C-N	5.29	1.41	1.33
2	B	321	ALA	CA-C	-5.29	1.46	1.52
2	B	271	GLY	N-CA	-5.28	1.37	1.44
2	B	364	GLN	C-N	5.28	1.41	1.33
2	B	25	ARG	CA-C	-5.28	1.45	1.52
1	A	422	PRO	N-CA	-5.27	1.40	1.47
1	A	142	SER	CA-C	-5.27	1.45	1.52
2	B	114	TRP	N-CA	-5.26	1.40	1.46
2	B	123	HIS	C-N	-5.26	1.27	1.33
2	B	9	VAL	CA-CB	-5.25	1.47	1.54
1	A	146	THR	CA-C	5.25	1.59	1.52
1	A	233	THR	CA-CB	5.23	1.61	1.53
2	B	53	TYR	CA-CB	-5.22	1.45	1.53
1	A	183	PRO	N-CA	-5.21	1.40	1.47
1	A	208	ASP	CA-C	-5.21	1.46	1.52
2	B	413	ARG	CA-C	-5.21	1.45	1.52
2	B	9	VAL	C-O	-5.21	1.17	1.24
2	B	401	ARG	CD-NE	-5.20	1.39	1.46
1	A	92	LEU	CA-C	-5.20	1.46	1.52
2	B	128	LEU	C-O	5.20	1.30	1.24
2	B	230	LEU	CA-C	5.20	1.59	1.52
1	A	15	PRO	N-CA	5.20	1.53	1.47
1	A	291	ALA	CA-C	-5.20	1.42	1.52
2	B	151	GLU	CD-OE2	5.19	1.35	1.25
2	B	268	GLY	C-O	-5.19	1.17	1.23
1	A	123	HIS	CG-ND1	5.18	1.44	1.38
2	B	51	LEU	C-O	-5.18	1.17	1.24
1	A	359	ASN	CA-C	-5.17	1.46	1.52
2	B	421	ARG	CZ-NH1	5.17	1.40	1.32
2	B	272	PRO	N-CA	-5.16	1.41	1.47
2	B	192	ASN	CA-C	-5.16	1.46	1.52
2	B	253	SER	C-N	5.16	1.40	1.33
2	B	78	LEU	CA-C	5.15	1.59	1.52
1	A	105	ALA	C-N	5.14	1.41	1.33
1	A	264	ALA	C-O	-5.13	1.16	1.23
1	A	280	GLU	CD-OE2	5.13	1.35	1.25
1	A	304	TYR	CA-C	5.13	1.59	1.52
1	A	249	HIS	C-O	5.12	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	189	ILE	C-O	5.12	1.29	1.24
2	B	261	SER	C-N	5.11	1.41	1.33
2	B	248	SER	C-O	5.11	1.30	1.24
1	A	225	THR	C-N	-5.11	1.27	1.34
2	B	257	ASP	C-N	-5.10	1.28	1.34
2	B	354	TYR	CA-C	-5.10	1.45	1.52
2	B	156	ARG	CA-C	5.09	1.59	1.52
2	B	178	LEU	CA-C	-5.09	1.46	1.52
1	A	36	ILE	N-CA	-5.09	1.40	1.46
1	A	107	VAL	N-CA	-5.08	1.40	1.46
2	B	301	LEU	N-CA	-5.07	1.40	1.46
1	A	390	MET	C-O	-5.07	1.18	1.24
1	A	98	THR	CB-OG1	-5.05	1.35	1.43
2	B	207	LEU	CA-C	-5.05	1.46	1.53
1	A	356	ILE	CA-CB	5.05	1.61	1.54
1	A	141	LEU	CA-C	-5.04	1.46	1.52
2	B	281	VAL	CA-CB	-5.03	1.48	1.54
1	A	117	ARG	N-CA	-5.03	1.39	1.46
1	A	343	GLY	CA-C	5.03	1.58	1.51
1	A	120	LEU	CA-C	5.03	1.58	1.52
1	A	322	VAL	N-CA	5.02	1.50	1.46
2	B	25	ARG	CZ-NH1	5.02	1.39	1.32
1	A	3	SER	CA-CB	-5.02	1.45	1.53
1	A	112	LYS	C-N	5.01	1.40	1.33
2	B	379	GLY	C-O	-5.01	1.17	1.23
1	A	411	TRP	CE2-CZ2	5.01	1.50	1.39
1	A	309	LEU	CA-C	5.01	1.60	1.52
2	B	247	THR	N-CA	5.00	1.52	1.46

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	374	VAL	CB-CA-C	-15.51	97.41	111.06
1	A	276	LEU	CB-CA-C	-12.83	95.31	111.22
2	B	340	HIS	CA-CB-CG	-12.02	101.78	113.80
2	B	267	ASN	CA-CB-CG	-11.70	100.90	112.60
2	B	377	HIS	N-CA-C	11.64	123.97	111.28
2	B	213	PHE	CA-CB-CG	-11.43	102.37	113.80
1	A	204	ASP	CA-CB-CG	10.89	123.49	112.60
1	A	215	ASN	CA-CB-CG	10.84	123.44	112.60
1	A	267	ASN	CA-CB-CG	-10.71	101.89	112.60
1	A	59	ASP	CA-CB-CG	10.10	122.70	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	171	VAL	N-CA-C	-10.08	98.49	111.09
2	B	390	MET	N-CA-C	10.07	123.29	111.71
2	B	377	HIS	CA-CB-CG	-9.95	103.85	113.80
1	A	128	LEU	CA-C-N	9.74	133.33	120.28
1	A	128	LEU	C-N-CA	9.74	133.33	120.28
2	B	51	LEU	N-CA-C	9.65	131.36	110.80
1	A	285	LEU	N-CA-C	-9.63	100.47	110.97
2	B	374	VAL	N-CA-C	-9.63	103.33	112.96
1	A	360	VAL	CA-C-N	9.56	134.07	120.79
1	A	360	VAL	C-N-CA	9.56	134.07	120.79
1	A	234	ILE	N-CA-C	9.47	122.89	111.05
1	A	417	PHE	CA-CB-CG	9.44	123.24	113.80
1	A	208	ASP	CA-C-O	-9.39	110.20	121.28
2	B	235	HIS	CA-CB-CG	-9.38	104.42	113.80
1	A	324	ARG	CB-CA-C	9.26	130.50	110.41
1	A	33	LEU	N-CA-C	9.06	122.30	111.33
1	A	248	SER	CA-C-N	9.05	132.41	120.28
1	A	248	SER	C-N-CA	9.05	132.41	120.28
2	B	276	LEU	N-CA-C	8.87	123.71	113.15
2	B	26	GLN	N-CA-C	8.85	121.82	111.02
2	B	373	ASN	CA-CB-CG	-8.84	103.76	112.60
2	B	33	LEU	CB-CA-C	8.82	123.89	109.07
2	B	301	LEU	N-CA-CB	8.80	123.27	110.06
1	A	267	ASN	CA-C-N	8.69	129.41	119.94
1	A	267	ASN	C-N-CA	8.69	129.41	119.94
1	A	163	LEU	N-CA-C	8.65	123.15	108.02
1	A	167	TYR	N-CA-C	8.64	120.77	111.36
1	A	7	LYS	N-CA-C	-8.62	101.89	111.28
2	B	264	ALA	N-CA-C	-8.58	100.52	112.45
2	B	28	HIS	CA-C-N	8.58	130.94	120.13
2	B	28	HIS	C-N-CA	8.58	130.94	120.13
1	A	364	GLN	CA-C-N	8.58	138.22	121.41
1	A	364	GLN	C-N-CA	8.58	138.22	121.41
2	B	204	ASP	CB-CA-C	8.55	124.04	110.19
2	B	324	ARG	N-CA-C	8.50	123.46	113.18
2	B	344	ASP	CA-C-N	8.35	130.27	119.84
2	B	344	ASP	C-N-CA	8.35	130.27	119.84
2	B	180	ALA	CA-C-N	8.34	132.14	120.29
2	B	180	ALA	C-N-CA	8.34	132.14	120.29
1	A	327	ASP	N-CA-C	-8.32	97.50	109.48
2	B	234	ILE	N-CA-C	8.30	119.09	110.62
1	A	4	THR	N-CA-CB	8.28	125.23	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ASP	CA-CB-CG	8.16	120.76	112.60
1	A	298	ASP	N-CA-C	-8.15	102.33	111.71
1	A	257	ASP	CA-CB-CG	-8.13	104.47	112.60
1	A	306	TRP	CA-C-O	8.10	129.04	120.70
2	B	167	TYR	N-CA-CB	8.07	122.93	109.78
1	A	264	ALA	N-CA-C	-8.05	103.05	113.12
1	A	228	MET	CA-C-N	8.04	131.06	120.28
1	A	228	MET	C-N-CA	8.04	131.06	120.28
2	B	36	ILE	N-CA-C	8.04	120.52	108.23
2	B	179	ILE	CA-C-O	7.97	129.73	119.85
2	B	222	ALA	N-CA-C	-7.97	102.68	111.36
1	A	326	THR	N-CA-CB	7.91	121.78	109.69
1	A	278	ASN	CA-CB-CG	7.87	120.47	112.60
1	A	46	ARG	N-CA-CB	-7.85	97.22	110.49
2	B	199	SER	N-CA-C	7.84	121.51	108.73
2	B	418	PRO	CA-C-N	7.83	133.70	121.26
2	B	418	PRO	C-N-CA	7.83	133.70	121.26
2	B	338	LEU	N-CA-CB	7.82	121.79	110.06
1	A	315	VAL	N-CA-CB	-7.80	102.54	111.20
2	B	361	LEU	N-CA-C	7.77	119.83	111.36
2	B	93	PHE	CA-CB-CG	-7.77	106.03	113.80
2	B	7	LYS	N-CA-C	-7.71	102.57	110.97
2	B	164	ARG	CA-C-O	7.69	131.51	120.51
2	B	28	HIS	ND1-CE1-NE2	7.66	116.06	108.40
1	A	177	ASP	CA-CB-CG	7.66	120.26	112.60
1	A	5	ASN	N-CA-C	7.65	121.87	112.54
2	B	177	ASP	CB-CA-C	-7.64	96.49	110.63
2	B	5	ASN	CA-CB-CG	-7.63	104.97	112.60
1	A	6	LEU	N-CA-CB	7.61	123.35	110.49
1	A	53	TYR	N-CA-C	-7.61	96.50	108.90
1	A	112	LYS	CA-C-N	7.60	130.79	120.54
1	A	112	LYS	C-N-CA	7.60	130.79	120.54
2	B	120	LEU	CB-CA-C	-7.56	101.23	109.85
2	B	274	HIS	N-CA-C	7.50	122.32	112.72
1	A	130	ASN	N-CA-CB	7.50	121.50	110.56
1	A	408	GLN	N-CA-C	-7.50	105.30	114.75
2	B	102	PRO	CB-CA-C	-7.49	102.05	111.56
2	B	182	LEU	CA-C-O	7.47	125.23	117.98
1	A	10	LEU	CA-C-N	7.44	131.00	120.28
1	A	10	LEU	C-N-CA	7.44	131.00	120.28
1	A	66	PHE	CA-C-N	7.43	135.73	121.54
1	A	66	PHE	C-N-CA	7.43	135.73	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	ILE	CB-CA-C	-7.40	100.69	112.16
1	A	204	ASP	CB-CA-C	7.40	122.58	110.22
2	B	133	THR	N-CA-CB	7.38	122.63	110.39
2	B	242	ASN	CA-CB-CG	7.37	119.97	112.60
1	A	51	LEU	N-CA-C	7.36	126.48	110.80
1	A	328	PRO	O-C-N	7.36	132.60	122.38
2	B	2	SER	N-CA-C	7.35	118.24	107.88
2	B	36	ILE	N-CA-CB	7.34	119.37	111.00
2	B	202	ALA	CA-C-N	-7.32	110.61	122.33
2	B	202	ALA	C-N-CA	-7.32	110.61	122.33
1	A	136	HIS	CB-CA-C	-7.30	95.79	110.17
2	B	278	ASN	CA-C-N	7.29	132.69	120.88
2	B	278	ASN	C-N-CA	7.29	132.69	120.88
2	B	391	ASN	CA-C-N	7.27	131.00	120.38
2	B	391	ASN	C-N-CA	7.27	131.00	120.38
2	B	326	THR	N-CA-C	7.27	120.37	109.25
2	B	375	ASP	CA-CB-CG	7.27	119.87	112.60
1	A	86	GLU	CA-C-N	7.24	127.67	119.92
1	A	86	GLU	C-N-CA	7.24	127.67	119.92
1	A	78	LEU	O-C-N	7.23	129.64	121.32
2	B	371	TRP	CB-CA-C	7.23	119.67	108.61
1	A	107	VAL	CA-CB-CG2	-7.20	98.16	110.40
1	A	227	LEU	N-CA-C	-7.20	103.17	112.23
2	B	173	GLU	N-CA-C	7.17	118.74	111.07
2	B	362	LEU	O-C-N	7.16	130.31	122.15
1	A	249	HIS	N-CA-C	7.16	119.08	111.28
1	A	45	MET	CB-CA-C	-7.12	101.40	111.80
2	B	117	ARG	NE-CZ-NH1	7.07	128.57	121.50
2	B	40	MET	N-CA-CB	7.07	121.24	110.28
2	B	8	ASP	CA-CB-CG	-7.05	105.55	112.60
2	B	264	ALA	N-CA-CB	7.05	120.76	110.26
1	A	258	PRO	N-CA-CB	7.04	110.64	103.25
1	A	419	LEU	CB-CA-C	-7.02	100.06	110.16
2	B	25	ARG	N-CA-CB	7.00	122.23	110.32
1	A	366	ALA	CA-C-N	7.00	131.40	122.16
1	A	366	ALA	C-N-CA	7.00	131.40	122.16
1	A	367	ALA	O-C-N	7.00	134.58	121.70
1	A	35	GLN	CA-C-O	6.99	129.01	121.11
2	B	189	ILE	N-CA-C	-6.97	103.98	110.53
2	B	109	TRP	O-C-N	6.96	129.24	122.07
2	B	271	GLY	CA-C-N	6.95	126.20	118.97
2	B	271	GLY	C-N-CA	6.95	126.20	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	304	TYR	CA-C-N	6.95	131.45	120.47
2	B	304	TYR	C-N-CA	6.95	131.45	120.47
2	B	177	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	318	TYR	CA-C-O	-6.92	113.29	121.11
1	A	276	LEU	N-CA-C	6.92	122.61	113.20
2	B	298	ASP	CA-C-N	6.90	129.82	120.44
2	B	298	ASP	C-N-CA	6.90	129.82	120.44
1	A	288	LEU	O-C-N	6.87	129.43	122.08
1	A	424	SER	CA-C-N	6.84	132.55	121.74
1	A	424	SER	C-N-CA	6.84	132.55	121.74
1	A	228	MET	O-C-N	6.84	129.11	122.07
1	A	374	VAL	CB-CA-C	-6.83	103.33	111.94
2	B	376	ALA	CA-C-O	6.83	128.17	121.00
1	A	99	GLY	N-CA-C	-6.81	104.85	116.01
2	B	215	ASN	CA-CB-CG	6.76	119.36	112.60
1	A	216	MET	CA-C-N	6.76	131.52	120.63
1	A	216	MET	C-N-CA	6.76	131.52	120.63
2	B	213	PHE	CA-C-N	6.76	129.23	120.44
2	B	213	PHE	C-N-CA	6.76	129.23	120.44
1	A	127	MET	CA-C-O	-6.76	110.84	120.51
1	A	164	ARG	CA-C-N	6.74	131.39	120.60
1	A	164	ARG	C-N-CA	6.74	131.39	120.60
2	B	242	ASN	N-CA-CB	6.71	120.65	110.45
2	B	3	SER	CB-CA-C	-6.70	97.08	110.42
2	B	16	LYS	O-C-N	6.70	129.78	122.15
1	A	390	MET	N-CA-C	6.69	118.58	111.28
2	B	410	ILE	CA-C-N	6.68	129.53	120.44
2	B	410	ILE	C-N-CA	6.68	129.53	120.44
1	A	4	THR	CB-CA-C	6.66	122.44	109.33
1	A	372	PRO	CA-C-N	6.64	134.22	121.54
1	A	372	PRO	C-N-CA	6.64	134.22	121.54
2	B	251	VAL	N-CA-CB	-6.64	101.51	110.54
2	B	332	CYS	CB-CA-C	6.64	121.30	110.88
1	A	302	ARG	CA-C-N	6.62	129.69	120.29
1	A	302	ARG	C-N-CA	6.62	129.69	120.29
2	B	25	ARG	CA-C-N	6.61	129.98	120.79
2	B	25	ARG	C-N-CA	6.61	129.98	120.79
1	A	73	GLU	N-CA-CB	6.59	120.50	110.28
2	B	341	LEU	CA-C-N	6.59	126.03	118.85
2	B	341	LEU	C-N-CA	6.59	126.03	118.85
2	B	349	LEU	N-CA-CB	6.59	119.84	109.82
2	B	410	ILE	CB-CA-C	-6.59	103.44	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	334	ARG	NE-CZ-NH1	6.58	128.09	121.50
2	B	324	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	A	369	ASN	CA-C-N	6.57	128.05	119.84
1	A	369	ASN	C-N-CA	6.57	128.05	119.84
1	A	127	MET	CA-C-N	6.57	129.62	120.29
1	A	127	MET	C-N-CA	6.57	129.62	120.29
1	A	310	ASN	CB-CA-C	6.56	121.68	110.79
2	B	333	GLN	OE1-CD-NE2	6.54	129.14	122.60
2	B	26	GLN	CB-CA-C	6.51	121.28	110.92
2	B	278	ASN	O-C-N	6.51	129.02	122.12
1	A	387	MET	CB-CA-C	6.50	123.36	110.42
1	A	316	PRO	CB-CA-C	-6.49	100.85	111.56
1	A	327	ASP	CA-CB-CG	6.49	119.09	112.60
2	B	360	VAL	O-C-N	6.47	128.23	121.89
1	A	323	LEU	N-CA-CB	6.45	120.21	109.56
1	A	377	HIS	CA-CB-CG	-6.45	107.35	113.80
1	A	78	LEU	CA-C-N	6.45	126.79	119.83
1	A	78	LEU	C-N-CA	6.45	126.79	119.83
1	A	304	TYR	CA-C-N	6.45	130.87	120.30
1	A	304	TYR	C-N-CA	6.45	130.87	120.30
1	A	142	SER	CA-C-O	-6.44	113.68	120.63
2	B	126	THR	CA-C-N	6.43	130.09	120.31
2	B	126	THR	C-N-CA	6.43	130.09	120.31
1	A	212	ASN	CB-CA-C	-6.43	97.99	110.46
1	A	295	ALA	N-CA-CB	6.42	120.03	110.40
2	B	267	ASN	N-CA-C	-6.42	103.97	110.97
2	B	390	MET	N-CA-CB	6.40	120.07	110.22
1	A	344	ASP	CA-C-N	6.39	127.83	119.84
1	A	344	ASP	C-N-CA	6.39	127.83	119.84
2	B	360	VAL	CA-C-N	6.38	129.35	120.29
2	B	360	VAL	C-N-CA	6.38	129.35	120.29
1	A	3	SER	CB-CA-C	-6.37	97.75	110.42
2	B	385	TYR	CA-CB-CG	-6.36	102.46	113.90
2	B	225	THR	N-CA-CB	6.33	119.54	110.16
2	B	412	SER	CA-CB-OG	-6.33	98.43	111.10
2	B	79	PRO	N-CA-CB	6.32	109.89	103.25
2	B	413	ARG	NE-CZ-NH2	-6.31	113.52	119.20
2	B	389	GLU	CA-C-N	6.31	129.36	120.28
2	B	389	GLU	C-N-CA	6.31	129.36	120.28
1	A	364	GLN	O-C-N	6.30	130.48	121.97
1	A	169	GLU	N-CA-CB	6.28	121.11	110.49
2	B	166	LYS	N-CA-C	6.27	119.09	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	367	ALA	N-CA-C	6.27	124.15	110.80
2	B	431	ILE	O-C-N	-6.26	115.79	121.87
1	A	18	GLN	N-CA-CB	-6.26	100.67	110.44
1	A	369	ASN	OD1-CG-ND2	-6.25	116.35	122.60
2	B	277	ALA	N-CA-C	6.25	119.38	111.69
1	A	290	LYS	CA-C-O	6.25	126.56	119.18
1	A	291	ALA	CA-C-O	-6.25	110.17	120.80
1	A	317	GLY	CA-C-N	-6.25	113.00	122.81
1	A	317	GLY	C-N-CA	-6.25	113.00	122.81
2	B	149	ASN	OD1-CG-ND2	-6.25	116.35	122.60
2	B	315	VAL	C-N-CD	-6.24	99.41	125.00
2	B	387	MET	N-CA-CB	6.24	119.67	110.49
2	B	204	ASP	N-CA-C	6.24	118.90	108.73
2	B	187	ALA	N-CA-C	-6.24	104.56	111.36
2	B	116	LYS	CA-C-N	-6.22	110.65	120.60
2	B	116	LYS	C-N-CA	-6.22	110.65	120.60
2	B	234	ILE	CB-CA-C	6.21	120.52	112.14
1	A	210	SER	CA-C-N	6.20	130.92	120.88
1	A	210	SER	C-N-CA	6.20	130.92	120.88
2	B	136	HIS	O-C-N	6.20	128.45	121.32
1	A	390	MET	CB-CA-C	6.20	121.08	110.79
2	B	55	THR	N-CA-C	6.19	119.00	111.82
2	B	25	ARG	O-C-N	6.19	130.43	122.39
2	B	109	TRP	N-CA-CB	6.18	118.98	110.01
1	A	369	ASN	N-CA-C	-6.16	96.19	109.81
2	B	244	SER	N-CA-C	6.16	118.97	111.82
2	B	88	LEU	O-C-N	-6.15	111.51	121.59
1	A	111	SER	N-CA-CB	6.14	118.97	110.07
2	B	17	GLU	O-C-N	6.14	128.63	122.12
2	B	212	ASN	OD1-CG-ND2	6.14	128.74	122.60
1	A	141	LEU	O-C-N	6.14	128.66	122.03
2	B	413	ARG	CD-NE-CZ	6.13	132.98	124.40
1	A	373	ASN	CA-CB-CG	-6.12	106.48	112.60
2	B	345	PRO	CA-C-N	6.12	128.80	120.54
2	B	345	PRO	C-N-CA	6.12	128.80	120.54
1	A	199	SER	CA-CB-OG	-6.12	98.86	111.10
2	B	175	ALA	CA-C-N	6.11	128.46	120.28
2	B	175	ALA	C-N-CA	6.11	128.46	120.28
1	A	187	ALA	CA-C-O	6.10	126.89	120.42
1	A	143	ALA	CA-C-N	6.10	128.70	120.65
1	A	143	ALA	C-N-CA	6.10	128.70	120.65
2	B	304	TYR	O-C-N	6.10	130.70	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	156	ARG	CD-NE-CZ	6.09	132.93	124.40
1	A	171	VAL	N-CA-C	-6.06	104.76	113.07
2	B	291	ALA	N-CA-CB	6.06	119.49	110.40
2	B	421	ARG	NE-CZ-NH1	6.05	127.55	121.50
1	A	326	THR	CA-CB-OG1	6.05	118.68	109.60
1	A	300	SER	CA-C-N	-6.05	110.39	120.68
1	A	300	SER	C-N-CA	-6.05	110.39	120.68
1	A	256	SER	CA-C-O	-6.04	113.90	120.36
2	B	190	TYR	CA-C-N	6.04	133.07	121.54
2	B	190	TYR	C-N-CA	6.04	133.07	121.54
2	B	320	HIS	CA-CB-CG	-6.04	107.76	113.80
1	A	334	ARG	NE-CZ-NH2	-6.02	113.78	119.20
1	A	40	MET	CA-C-N	6.01	128.83	120.29
1	A	40	MET	C-N-CA	6.01	128.83	120.29
1	A	277	ALA	CA-C-O	5.99	127.31	120.00
2	B	152	SER	N-CA-CB	5.99	118.50	109.34
1	A	367	ALA	CB-CA-C	-5.97	99.53	114.11
2	B	425	MET	CB-CA-C	5.97	125.27	113.45
2	B	412	SER	N-CA-CB	-5.97	101.10	110.06
2	B	281	VAL	CA-CB-CG2	-5.97	100.25	110.40
2	B	114	TRP	N-CA-CB	5.97	118.66	110.01
1	A	51	LEU	N-CA-CB	5.96	120.57	110.49
2	B	95	LEU	N-CA-CB	5.96	119.49	109.78
1	A	382	LEU	CA-C-N	5.95	128.85	120.28
1	A	382	LEU	C-N-CA	5.95	128.85	120.28
1	A	139	SER	O-C-N	5.95	131.06	122.13
1	A	332	CYS	N-CA-CB	5.95	119.55	110.14
2	B	367	ALA	O-C-N	5.95	130.51	122.59
1	A	385	TYR	CA-CB-CG	-5.95	103.19	113.90
2	B	114	TRP	CA-C-O	-5.95	114.58	120.82
2	B	357	VAL	N-CA-C	5.94	121.71	108.88
1	A	308	THR	CB-CA-C	5.93	122.23	110.42
2	B	29	GLY	N-CA-C	5.93	121.16	113.27
1	A	297	ALA	N-CA-C	5.92	119.28	110.52
1	A	390	MET	N-CA-CB	5.92	118.82	110.12
1	A	109	TRP	O-C-N	5.90	128.23	122.09
1	A	86	GLU	O-C-N	5.90	127.18	121.28
1	A	331	THR	CA-C-O	5.90	127.00	120.63
1	A	54	GLU	N-CA-C	5.89	121.38	113.72
1	A	277	ALA	N-CA-C	5.89	120.64	112.45
2	B	80	LYS	CA-C-N	5.89	132.96	121.41
2	B	80	LYS	C-N-CA	5.89	132.96	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	LEU	N-CA-C	-5.89	106.06	113.18
2	B	146	THR	N-CA-CB	-5.88	101.17	110.28
2	B	196	ALA	CB-CA-C	-5.87	103.05	112.09
1	A	28	HIS	CE1-NE2-CD2	-5.87	103.13	109.00
2	B	362	LEU	CB-CA-C	-5.87	100.87	110.85
2	B	229	ARG	CA-C-N	5.87	128.42	120.44
2	B	229	ARG	C-N-CA	5.87	128.42	120.44
1	A	80	LYS	N-CA-C	5.86	118.77	110.50
2	B	28	HIS	CE1-NE2-CD2	-5.86	103.14	109.00
2	B	300	SER	O-C-N	5.85	128.90	122.11
2	B	216	MET	N-CA-C	-5.85	105.98	113.23
2	B	13	LEU	N-CA-CB	-5.84	101.30	110.30
2	B	120	LEU	N-CA-C	5.84	117.91	109.04
1	A	409	LEU	CA-C-N	5.82	129.67	120.47
1	A	409	LEU	C-N-CA	5.82	129.67	120.47
1	A	413	ARG	N-CA-C	-5.82	104.56	111.03
2	B	126	THR	O-C-N	5.82	128.07	122.07
2	B	69	PHE	CA-CB-CG	5.81	119.61	113.80
2	B	254	ALA	O-C-N	5.81	129.31	122.34
1	A	121	PRO	N-CA-CB	5.80	109.34	103.25
2	B	77	LEU	CA-C-O	-5.80	114.71	120.80
1	A	355	LYS	CA-C-N	5.79	132.40	121.97
1	A	355	LYS	C-N-CA	5.79	132.40	121.97
1	A	45	MET	CA-C-N	5.78	132.57	121.54
1	A	45	MET	C-N-CA	5.78	132.57	121.54
1	A	173	GLU	CA-C-N	5.78	128.49	120.29
1	A	173	GLU	C-N-CA	5.78	128.49	120.29
1	A	321	ALA	N-CA-C	5.77	118.31	111.33
1	A	274	HIS	CA-CB-CG	-5.76	108.03	113.80
2	B	146	THR	OG1-CB-CG2	5.76	120.82	109.30
1	A	139	SER	CB-CA-C	5.75	118.26	109.34
1	A	208	ASP	N-CA-C	-5.73	100.95	110.17
2	B	233	THR	N-CA-C	-5.71	104.43	111.40
1	A	340	HIS	N-CA-C	5.71	122.96	110.80
1	A	99	GLY	CA-C-O	5.70	124.13	118.77
1	A	424	SER	O-C-N	5.68	129.45	123.03
2	B	328	PRO	CA-C-O	5.68	125.39	118.92
2	B	413	ARG	NE-CZ-NH1	5.67	127.17	121.50
2	B	129	ASP	CA-CB-CG	5.65	118.25	112.60
2	B	307	ASN	CA-C-O	5.65	126.41	120.42
2	B	341	LEU	N-CA-C	5.65	122.29	109.81
2	B	314	VAL	CA-C-O	-5.65	116.04	121.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	LYS	CA-C-N	5.64	127.84	120.28
2	B	16	LYS	C-N-CA	5.64	127.84	120.28
1	A	140	GLN	N-CA-CB	5.62	119.56	110.40
2	B	69	PHE	O-C-N	5.62	130.06	122.59
2	B	408	GLN	CB-CG-CD	5.62	122.15	112.60
2	B	176	MET	CA-C-N	5.62	128.37	120.28
2	B	176	MET	C-N-CA	5.62	128.37	120.28
1	A	352	GLN	N-CA-CB	5.61	118.44	110.13
2	B	324	ARG	CD-NE-CZ	-5.61	116.55	124.40
2	B	7	LYS	CB-CA-C	-5.61	102.33	110.96
2	B	135	LEU	CB-CA-C	-5.59	101.58	110.81
2	B	128	LEU	CA-C-N	5.59	130.92	121.14
2	B	128	LEU	C-N-CA	5.59	130.92	121.14
2	B	67	ARG	N-CA-C	-5.59	98.89	110.80
1	A	296	GLY	O-C-N	5.58	129.92	123.44
2	B	431	ILE	N-CA-C	-5.58	104.93	110.62
1	A	109	TRP	N-CA-CB	5.57	118.25	109.94
1	A	226	GLU	N-CA-CB	-5.57	101.64	110.22
1	A	432	ALA	CB-CA-C	-5.57	98.47	109.67
1	A	251	VAL	CB-CA-C	-5.57	104.78	112.24
1	A	324	ARG	CA-C-O	5.57	125.30	119.51
2	B	157	ALA	O-C-N	-5.57	115.15	122.39
1	A	173	GLU	CA-CB-CG	-5.57	102.97	114.10
1	A	340	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	345	PRO	CB-CA-C	-5.55	102.40	111.56
1	A	377	HIS	N-CA-C	5.55	121.07	113.97
1	A	158	TYR	N-CA-CB	5.55	118.11	110.07
2	B	235	HIS	O-C-N	5.54	130.11	122.46
1	A	278	ASN	N-CA-C	-5.54	104.46	111.11
2	B	31	THR	CA-C-N	5.54	130.30	121.66
2	B	31	THR	C-N-CA	5.54	130.30	121.66
1	A	339	LYS	N-CA-C	-5.54	104.93	110.97
1	A	350	VAL	CB-CA-C	5.54	120.37	111.29
1	A	359	ASN	CA-CB-CG	-5.54	107.06	112.60
2	B	68	GLY	CA-C-N	5.54	132.12	121.54
2	B	68	GLY	C-N-CA	5.54	132.12	121.54
2	B	274	HIS	CB-CA-C	5.53	119.44	110.37
1	A	310	ASN	CA-CB-CG	5.53	118.13	112.60
2	B	365	GLY	CA-C-N	-5.53	114.25	123.04
2	B	365	GLY	C-N-CA	-5.53	114.25	123.04
2	B	145	ILE	N-CA-CB	5.53	117.38	110.47
2	B	54	GLU	N-CA-C	5.52	120.08	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	367	ALA	CB-CA-C	-5.52	99.44	110.42
1	A	106	GLN	CA-C-O	5.51	126.29	119.79
2	B	171	VAL	O-C-N	5.50	128.01	121.80
1	A	150	SER	CA-C-N	5.50	132.30	121.58
1	A	150	SER	C-N-CA	5.50	132.30	121.58
2	B	358	PRO	O-C-N	5.50	128.83	122.23
1	A	301	LEU	N-CA-CB	5.50	118.76	110.30
2	B	116	LYS	N-CA-CB	5.49	118.04	110.07
2	B	430	LEU	CA-C-N	-5.49	112.94	120.46
2	B	430	LEU	C-N-CA	-5.49	112.94	120.46
2	B	156	ARG	N-CA-C	5.49	116.94	111.07
1	A	350	VAL	CA-C-O	5.48	127.63	120.78
1	A	302	ARG	O-C-N	5.48	128.63	122.22
2	B	212	ASN	CA-CB-CG	-5.48	107.12	112.60
2	B	375	ASP	N-CA-CB	5.48	118.66	110.22
1	A	194	TYR	O-C-N	-5.47	115.25	122.42
2	B	140	GLN	CG-CD-NE2	-5.47	108.19	116.40
2	B	408	GLN	N-CA-C	-5.47	107.15	113.88
1	A	271	GLY	CA-C-N	5.47	126.68	119.84
1	A	271	GLY	C-N-CA	5.47	126.68	119.84
2	B	196	ALA	CA-C-O	-5.47	115.36	122.14
1	A	333	GLN	CA-C-N	5.47	129.93	120.58
1	A	333	GLN	C-N-CA	5.47	129.93	120.58
2	B	5	ASN	N-CA-C	5.47	122.44	110.80
2	B	259	TYR	CA-C-O	5.46	125.99	119.60
2	B	261	SER	N-CA-C	-5.45	106.47	113.23
1	A	210	SER	N-CA-C	5.45	118.72	111.75
2	B	236	SER	CA-C-O	-5.45	114.64	121.02
1	A	248	SER	O-C-N	5.44	127.89	122.12
1	A	194	TYR	CA-C-O	5.44	125.35	119.15
2	B	215	ASN	N-CA-CB	-5.44	101.36	110.39
2	B	279	GLN	N-CA-C	5.44	118.26	111.24
2	B	65	ARG	N-CA-CB	-5.43	102.42	110.90
2	B	315	VAL	CB-CA-C	-5.43	101.47	111.36
2	B	332	CYS	O-C-N	-5.43	116.48	122.07
1	A	145	ILE	N-CA-CB	-5.42	104.49	110.51
1	A	422	PRO	N-CA-CB	5.42	108.95	103.25
2	B	342	PRO	CA-N-CD	-5.42	104.41	112.00
2	B	207	LEU	O-C-N	5.40	129.01	122.85
2	B	349	LEU	CB-CA-C	-5.40	102.33	110.92
2	B	61	ASP	O-C-N	-5.39	115.84	122.20
2	B	113	GLU	CA-C-N	-5.39	113.43	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	GLU	C-N-CA	-5.39	113.43	120.44
1	A	314	VAL	CB-CA-C	-5.39	102.07	110.69
2	B	316	PRO	CB-CA-C	-5.39	102.67	111.56
2	B	177	ASP	CA-C-O	-5.39	114.01	120.10
2	B	236	SER	CA-CB-OG	-5.38	100.34	111.10
2	B	36	ILE	CB-CA-C	5.36	117.45	110.96
1	A	401	ARG	CA-C-N	5.36	127.41	120.44
1	A	401	ARG	C-N-CA	5.36	127.41	120.44
1	A	13	LEU	O-C-N	5.36	127.60	122.03
1	A	288	LEU	CA-C-N	5.36	131.78	121.54
1	A	288	LEU	C-N-CA	5.36	131.78	121.54
1	A	383	GLN	CA-C-N	5.35	127.45	120.28
1	A	383	GLN	C-N-CA	5.35	127.45	120.28
2	B	158	TYR	N-CA-C	-5.35	105.10	111.03
1	A	334	ARG	CB-CA-C	-5.34	100.92	110.70
2	B	123	HIS	N-CA-CB	5.34	117.75	110.01
2	B	32	ALA	N-CA-CB	5.33	118.35	109.60
2	B	107	VAL	CA-CB-CG1	5.33	119.47	110.40
1	A	229	ARG	CA-C-N	5.29	131.25	121.52
1	A	229	ARG	C-N-CA	5.29	131.25	121.52
2	B	373	ASN	OD1-CG-ND2	5.29	127.89	122.60
2	B	143	ALA	CA-C-O	5.29	126.55	121.00
1	A	71	ILE	N-CA-CB	5.28	118.61	111.21
2	B	106	GLN	N-CA-C	-5.28	105.44	111.14
2	B	148	LEU	CA-C-N	5.27	131.61	121.54
2	B	148	LEU	C-N-CA	5.27	131.61	121.54
2	B	123	HIS	CA-C-N	-5.27	114.11	120.70
2	B	123	HIS	C-N-CA	-5.27	114.11	120.70
1	A	56	SER	N-CA-C	5.27	117.26	108.99
1	A	171	VAL	CA-C-O	5.26	125.57	119.36
2	B	322	VAL	CA-C-N	-5.26	114.09	121.72
2	B	322	VAL	C-N-CA	-5.26	114.09	121.72
2	B	31	THR	CB-CA-C	5.25	118.90	110.29
2	B	220	THR	CB-CA-C	5.25	120.04	110.11
1	A	32	ALA	N-CA-C	5.25	121.98	110.80
1	A	45	MET	N-CA-CB	-5.24	104.03	111.84
1	A	279	GLN	CA-C-O	-5.24	115.50	120.90
2	B	424	SER	O-C-N	5.24	128.81	122.94
1	A	28	HIS	ND1-CE1-NE2	5.24	113.64	108.40
1	A	371	TRP	CA-C-N	5.23	125.21	120.03
1	A	371	TRP	C-N-CA	5.23	125.21	120.03
1	A	66	PHE	CA-CB-CG	5.22	119.02	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	MET	N-CA-C	5.22	117.58	109.60
2	B	109	TRP	N-CA-C	-5.21	105.49	111.07
1	A	31	THR	CA-CB-OG1	5.21	117.41	109.60
2	B	195	ARG	CD-NE-CZ	-5.21	117.11	124.40
1	A	180	ALA	CB-CA-C	5.20	119.12	110.90
2	B	368	ALA	CB-CA-C	5.20	120.77	110.42
2	B	398	GLY	CA-C-N	5.20	128.83	120.30
2	B	398	GLY	C-N-CA	5.20	128.83	120.30
1	A	22	LYS	CA-C-N	-5.20	113.52	120.54
1	A	22	LYS	C-N-CA	-5.20	113.52	120.54
2	B	34	GLY	O-C-N	-5.20	118.92	123.76
2	B	201	GLY	N-CA-C	5.20	117.61	111.63
1	A	164	ARG	CA-CB-CG	5.20	124.49	114.10
2	B	189	ILE	O-C-N	5.19	127.30	121.90
2	B	111	SER	N-CA-CB	5.19	117.67	109.94
2	B	165	THR	CB-CA-C	5.19	119.67	110.85
1	A	215	ASN	CB-CA-C	5.19	120.08	109.55
1	A	85	GLY	CA-C-N	5.19	127.62	120.67
1	A	85	GLY	C-N-CA	5.19	127.62	120.67
1	A	235	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	278	ASN	CA-C-N	5.18	127.67	120.63
1	A	278	ASN	C-N-CA	5.18	127.67	120.63
1	A	194	TYR	CA-C-N	-5.17	111.66	121.54
1	A	194	TYR	C-N-CA	-5.17	111.66	121.54
1	A	417	PHE	CB-CA-C	-5.17	101.30	109.42
2	B	86	GLU	CA-C-O	5.17	122.65	119.29
2	B	25	ARG	NE-CZ-NH1	-5.17	116.33	121.50
2	B	300	SER	CA-C-O	-5.17	115.37	120.80
1	A	332	CYS	CB-CA-C	5.17	120.49	110.46
2	B	403	LEU	CA-C-O	-5.17	113.12	120.51
1	A	70	SER	CB-CA-C	-5.15	100.78	110.51
1	A	126	THR	CA-C-N	5.15	131.37	121.54
1	A	126	THR	C-N-CA	5.15	131.37	121.54
2	B	167	TYR	N-CA-C	5.15	119.86	111.37
1	A	134	ASN	OD1-CG-ND2	5.15	127.75	122.60
1	A	112	LYS	CA-C-O	-5.14	115.10	120.55
1	A	229	ARG	N-CA-C	5.14	116.89	111.28
2	B	385	TYR	CB-CA-C	5.14	120.18	109.95
2	B	238	HIS	O-C-N	-5.14	115.75	122.59
1	A	366	ALA	N-CA-CB	-5.14	103.64	111.19
1	A	149	ASN	CA-C-N	5.14	127.17	120.28
1	A	149	ASN	C-N-CA	5.14	127.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	325	LYS	N-CA-CB	5.14	119.17	110.49
2	B	362	LEU	CA-C-N	5.12	127.41	120.65
2	B	362	LEU	C-N-CA	5.12	127.41	120.65
2	B	323	LEU	N-CA-CB	5.12	118.22	109.87
2	B	224	PHE	CA-C-N	5.11	127.55	120.29
2	B	224	PHE	C-N-CA	5.11	127.55	120.29
2	B	330	TYR	CA-C-N	5.11	127.38	120.38
2	B	330	TYR	C-N-CA	5.11	127.38	120.38
1	A	192	ASN	CB-CA-C	-5.11	102.64	110.81
2	B	430	LEU	N-CA-CB	5.11	117.81	110.20
1	A	5	ASN	O-C-N	5.11	129.27	122.43
1	A	413	ARG	NE-CZ-NH2	-5.11	114.61	119.20
2	B	51	LEU	N-CA-CB	5.11	119.12	110.49
1	A	12	ALA	CA-C-N	5.10	127.39	120.65
1	A	12	ALA	C-N-CA	5.10	127.39	120.65
2	B	299	ALA	N-CA-C	5.10	116.64	111.14
1	A	288	LEU	N-CA-C	-5.10	104.80	111.02
2	B	407	ALA	N-CA-CB	5.10	118.97	110.41
1	A	315	VAL	N-CA-C	5.09	112.20	107.56
1	A	49	LYS	CA-CB-CG	-5.09	103.93	114.10
2	B	146	THR	CA-C-O	5.09	125.82	119.97
2	B	95	LEU	CA-C-N	5.08	127.60	120.28
2	B	95	LEU	C-N-CA	5.08	127.60	120.28
2	B	432	ALA	N-CA-C	5.08	117.72	111.82
1	A	199	SER	CA-C-N	5.08	128.97	120.64
1	A	199	SER	C-N-CA	5.08	128.97	120.64
2	B	151	GLU	N-CA-CB	-5.08	102.19	110.42
2	B	200	ILE	CA-C-N	-5.08	114.49	122.92
2	B	200	ILE	C-N-CA	-5.08	114.49	122.92
1	A	241	GLY	CA-C-N	-5.07	111.88	122.07
1	A	241	GLY	C-N-CA	-5.07	111.88	122.07
2	B	134	ASN	N-CA-C	5.07	119.31	113.18
2	B	233	THR	CA-CB-CG2	5.07	119.11	110.50
2	B	157	ALA	CA-C-O	5.06	125.61	119.49
1	A	237	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	364	GLN	CA-C-O	-5.05	114.91	121.17
1	A	418	PRO	N-CA-C	5.05	118.53	110.40
2	B	118	ALA	N-CA-C	5.05	121.55	110.80
1	A	320	HIS	ND1-CG-CD2	5.04	111.14	106.10
2	B	361	LEU	CA-C-O	5.04	125.77	120.42
2	B	116	LYS	O-C-N	-5.04	116.65	122.09
1	A	132	PRO	CA-C-O	5.04	126.77	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	155	ALA	O-C-N	5.03	127.47	122.08
1	A	153	ASN	CA-CB-CG	5.03	117.63	112.60
2	B	117	ARG	NE-CZ-NH2	-5.03	114.67	119.20
2	B	368	ALA	CA-C-O	5.02	127.69	120.51
1	A	110	LEU	CA-C-N	-5.02	113.62	120.44
1	A	110	LEU	C-N-CA	-5.02	113.62	120.44
1	A	383	GLN	N-CA-C	5.01	117.48	111.71
2	B	238	HIS	N-CA-CB	-5.01	102.02	110.49
1	A	357	VAL	N-CA-C	5.01	119.70	108.88
2	B	122	SER	CA-C-N	5.01	126.95	120.44
2	B	122	SER	C-N-CA	5.01	126.95	120.44
1	A	112	LYS	O-C-N	5.00	127.42	122.12

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	A	5	ASN	CA
1	A	51	LEU	CA
1	A	289	GLN	CA
1	A	340	HIS	CA
1	A	390	MET	CA
1	A	425	MET	CA
2	B	26	GLN	CA
2	B	46	ARG	CA
2	B	51	LEU	CA
2	B	390	MET	CA
2	B	425	MET	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	215	ASN	Sidechain
1	A	337	ALA	Mainchain
1	A	339	LYS	Mainchain
1	A	348	LYS	Mainchain
1	A	385	TYR	Sidechain
2	B	149	ASN	Sidechain
2	B	231	TYR	Sidechain
2	B	354	TYR	Sidechain

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	3303	0	3288	505	26
2	B	3303	0	3288	557	26
All	All	6606	0	6576	1010	26

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 77.

All (1010) 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:46:ARG:HB2	1:A:46:ARG:NH1	1.52	1.22
1:A:33:LEU:HD11	2:B:433:LEU:HD21	1.16	1.13
2:B:86:GLU:HG3	2:B:230:LEU:HB2	1.31	1.12
2:B:79:PRO:HG2	2:B:107:VAL:HG21	1.33	1.11
2:B:341:LEU:HD22	2:B:384:TYR:CD2	1.85	1.10
1:A:178:LEU:HD23	1:A:406:LEU:HD11	1.28	1.09
1:A:323:LEU:HD22	1:A:324:ARG:H	1.18	1.08
1:A:25:ARG:HD2	2:B:42:TYR:CD2	1.89	1.07
1:A:424:SER:HB2	2:B:51:LEU:HB2	1.32	1.07
2:B:350:VAL:HG21	2:B:380:VAL:HG21	1.34	1.04
1:A:86:GLU:HG2	1:A:230:LEU:HB2	1.35	1.03
1:A:92:LEU:HG	1:A:233:THR:HG23	1.34	1.03
2:B:327:ASP:OD2	2:B:329:ARG:HG3	1.54	1.03
2:B:320:HIS:N	2:B:369:ASN:OD1	1.90	1.03
1:A:94:TRP:CE3	1:A:110:LEU:HD21	1.94	1.02
1:A:298:ASP:HA	1:A:356:ILE:HD11	1.40	1.02
2:B:329:ARG:HH21	2:B:374:VAL:HG21	1.24	1.02
2:B:329:ARG:HH21	2:B:374:VAL:CG2	1.73	1.00
2:B:323:LEU:O	2:B:369:ASN:ND2	1.93	0.99
2:B:124:VAL:HG21	2:B:148:LEU:CD2	1.91	0.99
2:B:33:LEU:C	2:B:33:LEU:HD12	1.87	0.99
2:B:281:VAL:CG2	2:B:316:PRO:HB2	1.92	0.99
2:B:125:VAL:CG1	2:B:188:LYS:HE2	1.94	0.96
1:A:33:LEU:HD11	2:B:433:LEU:CD2	1.95	0.96
2:B:339:LYS:HB3	2:B:340:HIS:CD2	2.00	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:VAL:HG21	2:B:148:LEU:HD21	1.46	0.95
2:B:362:LEU:HD11	2:B:370:PRO:HG3	1.48	0.95
1:A:109:TRP:CE3	1:A:110:LEU:HD23	2.01	0.95
2:B:412:SER:HA	2:B:417:PHE:CD2	2.01	0.95
1:A:340:HIS:O	1:A:342:PRO:HD3	1.67	0.94
1:A:350:VAL:HG21	1:A:380:VAL:HG21	1.50	0.94
2:B:269:LEU:HD11	2:B:397:PHE:CE2	2.02	0.94
2:B:136:HIS:CD2	2:B:137:PRO:HD2	2.03	0.94
1:A:266:MET:HA	1:A:266:MET:HE2	1.48	0.93
2:B:92:LEU:HD13	2:B:233:THR:HG23	1.50	0.93
1:A:326:THR:HG22	1:A:327:ASP:O	1.68	0.93
1:A:98:THR:HG22	1:A:100:GLN:HG3	1.48	0.93
2:B:281:VAL:HG22	2:B:316:PRO:HB2	1.50	0.93
1:A:34:GLY:O	2:B:36:ILE:N	2.03	0.92
2:B:329:ARG:NH2	2:B:374:VAL:HG21	1.85	0.91
1:A:425:MET:HA	2:B:52:VAL:H	1.36	0.91
1:A:33:LEU:CD1	2:B:433:LEU:HD21	2.01	0.90
2:B:141:LEU:HD22	2:B:395:VAL:HG13	1.50	0.90
1:A:273:LEU:HD13	2:B:255:LEU:HD12	1.54	0.90
2:B:125:VAL:HG13	2:B:188:LYS:HE2	1.51	0.90
2:B:271:GLY:O	2:B:275:GLY:N	2.03	0.90
2:B:22:LYS:O	2:B:26:GLN:HB2	1.71	0.90
2:B:362:LEU:HD12	2:B:367:ALA:HB2	1.54	0.90
2:B:174:SER:HB2	2:B:258:PRO:HG2	1.53	0.89
1:A:126:THR:O	1:A:129:ASP:HB2	1.70	0.89
2:B:424:SER:O	2:B:425:MET:HG3	1.71	0.89
2:B:251:VAL:HG11	2:B:261:SER:HA	1.53	0.89
2:B:64:ILE:HG13	2:B:65:ARG:H	1.37	0.88
1:A:46:ARG:HB2	1:A:46:ARG:CZ	2.04	0.88
2:B:342:PRO:HD2	2:B:343:GLY:H	1.38	0.88
1:A:273:LEU:CD1	2:B:255:LEU:HD12	2.04	0.88
2:B:64:ILE:HG13	2:B:65:ARG:N	1.86	0.88
1:A:30:GLY:HA2	2:B:37:THR:CG2	2.04	0.87
2:B:131:PHE:CD2	2:B:140:GLN:HB3	2.10	0.87
1:A:80:LYS:HG2	1:A:85:GLY:O	1.75	0.87
1:A:109:TRP:CH2	1:A:113:GLU:HG2	2.09	0.87
2:B:285:LEU:HG	2:B:346:MET:HE2	1.57	0.86
2:B:36:ILE:HG23	2:B:48:MET:HE2	1.57	0.86
1:A:135:LEU:HD11	1:A:139:SER:HB3	1.57	0.86
1:A:125:VAL:HG13	1:A:188:LYS:HE2	1.57	0.85
1:A:192:ASN:HA	1:A:197:GLY:HA2	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:NH2	1:A:374:VAL:HG21	1.92	0.85
1:A:243:VAL:HB	1:A:274:HIS:CD2	2.12	0.85
1:A:182:LEU:HD22	1:A:399:VAL:HG22	1.57	0.85
1:A:191:ARG:NH1	1:A:216:MET:O	2.09	0.84
2:B:412:SER:HB3	2:B:417:PHE:HD2	1.42	0.84
1:A:94:TRP:HE3	1:A:110:LEU:HD21	1.38	0.84
1:A:136:HIS:HD2	1:A:138:MET:H	1.23	0.84
2:B:305:ILE:HD13	2:B:357:VAL:HG22	1.60	0.84
2:B:311:SER:HB3	2:B:313:ARG:CZ	2.08	0.84
1:A:46:ARG:HB2	1:A:46:ARG:HH11	1.42	0.83
2:B:94:TRP:CD1	2:B:102:PRO:HB3	2.14	0.83
2:B:127:MET:HE2	2:B:131:PHE:CZ	2.13	0.83
2:B:301:LEU:CD1	2:B:356:ILE:HD13	2.08	0.83
1:A:279:GLN:HG2	1:A:390:MET:HG3	1.59	0.83
1:A:411:TRP:CE3	1:A:415:LEU:HD21	2.14	0.83
2:B:174:SER:CB	2:B:258:PRO:HG2	2.07	0.82
1:A:362:LEU:CD1	1:A:370:PRO:HG3	2.08	0.82
1:A:369:ASN:N	1:A:370:PRO:HD3	1.93	0.82
2:B:149:ASN:CG	2:B:149:ASN:O	2.21	0.82
2:B:301:LEU:HG	2:B:356:ILE:HD13	1.62	0.82
2:B:319:GLY:HA2	2:B:369:ASN:O	1.79	0.82
1:A:6:LEU:HB2	1:A:94:TRP:CZ3	2.14	0.82
2:B:340:HIS:O	2:B:342:PRO:HD3	1.78	0.82
2:B:357:VAL:HB	2:B:358:PRO:HD3	1.62	0.82
1:A:424:SER:HB2	2:B:51:LEU:CB	2.08	0.81
1:A:347:PHE:O	1:A:348:LYS:C	2.23	0.81
1:A:330:TYR:HB2	1:A:373:ASN:O	1.80	0.80
1:A:251:VAL:HG12	1:A:261:SER:HB3	1.61	0.80
1:A:109:TRP:CZ3	1:A:110:LEU:HD23	2.16	0.80
1:A:25:ARG:HD2	2:B:42:TYR:CG	2.16	0.80
2:B:301:LEU:CG	2:B:356:ILE:HD13	2.11	0.80
2:B:377:HIS:O	2:B:381:LEU:HD22	1.81	0.80
2:B:6:LEU:HD23	2:B:172:TYR:OH	1.81	0.80
1:A:281:VAL:HG22	1:A:316:PRO:O	1.82	0.80
2:B:131:PHE:CE2	2:B:140:GLN:HB3	2.16	0.80
2:B:192:ASN:HA	2:B:197:GLY:HA2	1.64	0.80
1:A:281:VAL:HG22	1:A:316:PRO:HB2	1.63	0.80
2:B:302:ARG:O	2:B:306:TRP:HB2	1.82	0.80
1:A:277:ALA:HB3	1:A:375:ASP:OD1	1.82	0.79
1:A:191:ARG:HA	1:A:195:ARG:HB2	1.65	0.79
2:B:311:SER:HB3	2:B:313:ARG:NH1	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ARG:HG3	2:B:68:GLY:O	1.81	0.79
1:A:341:LEU:HD22	1:A:384:TYR:CD2	2.16	0.79
2:B:33:LEU:C	2:B:33:LEU:CD1	2.56	0.79
1:A:109:TRP:HE3	1:A:110:LEU:HD23	1.47	0.79
1:A:236:SER:O	1:A:401:ARG:HA	1.82	0.79
1:A:431:ILE:HD12	2:B:20:ARG:NH2	1.98	0.79
1:A:362:LEU:HD12	1:A:367:ALA:HB2	1.63	0.79
2:B:350:VAL:CG2	2:B:380:VAL:HG21	2.12	0.79
1:A:370:PRO:HD2	1:A:371:TRP:NE1	1.97	0.79
2:B:412:SER:HB3	2:B:417:PHE:CD2	2.17	0.79
2:B:145:ILE:HG22	2:B:263:ALA:HB2	1.63	0.78
1:A:204:ASP:OD2	1:A:206:LYS:HD3	1.83	0.78
1:A:323:LEU:HD22	1:A:324:ARG:N	1.96	0.78
2:B:157:ALA:HB1	2:B:162:ILE:HG21	1.65	0.78
2:B:300:SER:O	2:B:303:ASP:HB2	1.84	0.78
2:B:2:SER:O	2:B:3:SER:HB3	1.82	0.78
1:A:94:TRP:CD1	1:A:102:PRO:HB3	2.18	0.78
2:B:86:GLU:CG	2:B:230:LEU:HB2	2.10	0.78
1:A:329:ARG:HH21	1:A:374:VAL:CG2	1.96	0.78
2:B:330:TYR:HB2	2:B:373:ASN:O	1.83	0.78
1:A:136:HIS:CD2	1:A:138:MET:H	2.02	0.78
1:A:54:GLU:OE2	2:B:427:THR:OG1	2.02	0.77
2:B:276:LEU:HB3	2:B:280:GLU:OE2	1.85	0.77
1:A:223:GLN:NE2	1:A:340:HIS:CG	2.53	0.77
1:A:362:LEU:HD13	1:A:370:PRO:HG3	1.66	0.77
2:B:65:ARG:NH1	2:B:70:SER:HB3	2.00	0.77
1:A:178:LEU:CD2	1:A:406:LEU:HD11	2.11	0.77
2:B:307:ASN:O	2:B:311:SER:HB2	1.85	0.77
1:A:347:PHE:O	1:A:348:LYS:O	2.02	0.77
2:B:236:SER:O	2:B:401:ARG:HA	1.84	0.77
1:A:269:LEU:HD11	1:A:397:PHE:CD2	2.21	0.76
1:A:127:MET:HE2	1:A:131:PHE:CZ	2.20	0.76
2:B:154:PHE:HE1	2:B:167:TYR:HB3	1.46	0.76
1:A:340:HIS:C	1:A:342:PRO:HD3	2.09	0.76
1:A:323:LEU:CD2	1:A:324:ARG:H	1.98	0.76
2:B:81:GLY:HA2	2:B:88:LEU:HD11	1.67	0.76
2:B:415:LEU:HD12	2:B:417:PHE:CZ	2.21	0.76
2:B:157:ALA:HB1	2:B:162:ILE:CG2	2.15	0.75
1:A:94:TRP:CZ3	1:A:110:LEU:HD21	2.21	0.75
2:B:146:THR:O	2:B:149:ASN:HB3	1.86	0.75
2:B:182:LEU:N	2:B:183:PRO:CD	2.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:GLN:NE2	2:B:340:HIS:ND1	2.33	0.75
1:A:184:CYS:SG	1:A:216:MET:HE1	2.26	0.75
1:A:411:TRP:HE3	1:A:415:LEU:HD21	1.48	0.75
2:B:411:TRP:O	2:B:415:LEU:N	2.18	0.75
2:B:181:LYS:C	2:B:183:PRO:HD2	2.11	0.75
1:A:119:ALA:O	1:A:181:LYS:HE3	1.87	0.74
1:A:223:GLN:NE2	1:A:340:HIS:ND1	2.34	0.74
1:A:207:LEU:N	1:A:207:LEU:HD23	2.00	0.74
2:B:362:LEU:HD12	2:B:367:ALA:CB	2.17	0.74
1:A:311:SER:O	1:A:313:ARG:NH1	2.20	0.74
2:B:79:PRO:CG	2:B:107:VAL:HG21	2.13	0.74
1:A:424:SER:CB	2:B:51:LEU:HB2	2.15	0.74
1:A:5:ASN:HA	1:A:8:ASP:HB2	1.68	0.74
1:A:79:PRO:HG2	1:A:107:VAL:HG21	1.69	0.74
1:A:168:TRP:CE2	1:A:169:GLU:HG3	2.23	0.74
1:A:329:ARG:HH21	1:A:374:VAL:HG21	1.53	0.74
1:A:172:TYR:O	1:A:175:ALA:HB3	1.87	0.73
1:A:157:ALA:HB1	1:A:162:ILE:CG2	2.19	0.73
2:B:107:VAL:O	2:B:110:LEU:N	2.21	0.73
2:B:124:VAL:HG21	2:B:148:LEU:HD23	1.70	0.73
2:B:301:LEU:HD21	2:B:352:GLN:HB3	1.69	0.73
1:A:131:PHE:CE2	1:A:140:GLN:HB3	2.24	0.73
2:B:288:LEU:HD23	2:B:349:LEU:HD21	1.70	0.73
1:A:121:PRO:O	1:A:125:VAL:HG23	1.90	0.72
1:A:51:LEU:HB2	2:B:424:SER:HA	1.71	0.72
1:A:174:SER:HB2	1:A:258:PRO:HG2	1.72	0.72
2:B:65:ARG:NH1	2:B:68:GLY:O	2.22	0.72
1:A:305:ILE:CD1	1:A:357:VAL:HG22	2.18	0.72
1:A:42:TYR:CG	2:B:25:ARG:HD2	2.25	0.72
2:B:333:GLN:NE2	2:B:377:HIS:HB3	2.05	0.72
2:B:56:SER:HB2	2:B:64:ILE:HD11	1.72	0.72
1:A:390:MET:HB2	1:A:393:TYR:CE2	2.24	0.72
2:B:207:LEU:N	2:B:207:LEU:HD23	2.04	0.72
1:A:102:PRO:HB2	1:A:107:VAL:HG23	1.72	0.71
2:B:324:ARG:CZ	2:B:324:ARG:CB	2.67	0.71
2:B:94:TRP:CE3	2:B:110:LEU:HD11	2.25	0.71
2:B:115:ALA:O	2:B:118:ALA:HB3	1.88	0.71
1:A:348:LYS:O	1:A:351:ALA:HB3	1.90	0.71
2:B:109:TRP:CE3	2:B:110:LEU:HD23	2.24	0.71
2:B:339:LYS:HB3	2:B:340:HIS:NE2	2.05	0.71
1:A:95:LEU:HA	1:A:100:GLN:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:27:GLN:HE21	2:B:28:HIS:CE1	2.09	0.71
2:B:384:TYR:HD2	2:B:385:TYR:CE2	2.09	0.71
2:B:269:LEU:HD11	2:B:397:PHE:CD2	2.25	0.71
2:B:357:VAL:O	2:B:361:LEU:HB2	1.89	0.71
2:B:349:LEU:O	2:B:353:LEU:HD22	1.91	0.71
1:A:168:TRP:O	1:A:170:MET:N	2.24	0.70
1:A:30:GLY:HA2	2:B:37:THR:HG22	1.72	0.70
2:B:412:SER:CA	2:B:417:PHE:CD2	2.74	0.70
1:A:285:LEU:HG	1:A:346:MET:CE	2.21	0.70
2:B:46:ARG:HH11	2:B:46:ARG:HA	1.56	0.70
2:B:93:PHE:O	2:B:97:VAL:HG23	1.90	0.70
2:B:184:CYS:O	2:B:188:LYS:HB2	1.91	0.70
2:B:94:TRP:HE3	2:B:110:LEU:HD11	1.55	0.70
2:B:40:MET:HB2	2:B:48:MET:HE3	1.73	0.70
2:B:18:GLN:O	2:B:22:LYS:HG2	1.92	0.70
1:A:311:SER:HB2	1:A:313:ARG:CZ	2.21	0.70
2:B:322:VAL:HG12	2:B:322:VAL:O	1.91	0.70
2:B:282:LEU:HD23	2:B:390:MET:HE2	1.74	0.69
2:B:315:VAL:CG1	2:B:316:PRO:HD2	2.20	0.69
2:B:349:LEU:HG	2:B:353:LEU:HD22	1.74	0.69
1:A:178:LEU:HD23	1:A:406:LEU:CD1	2.17	0.69
2:B:281:VAL:HG23	2:B:316:PRO:HB2	1.74	0.69
1:A:162:ILE:HD12	1:A:167:TYR:HD1	1.57	0.69
2:B:46:ARG:HH11	2:B:46:ARG:CA	2.06	0.69
2:B:214:THR:HG22	2:B:215:ASN:N	2.08	0.69
2:B:350:VAL:O	2:B:353:LEU:HB2	1.92	0.69
1:A:94:TRP:CG	1:A:102:PRO:HB3	2.27	0.69
1:A:320:HIS:HB3	1:A:369:ASN:OD1	1.92	0.69
2:B:125:VAL:HG12	2:B:188:LYS:HE2	1.72	0.69
2:B:320:HIS:H	2:B:369:ASN:CG	2.01	0.69
1:A:131:PHE:CD2	1:A:140:GLN:HB3	2.28	0.69
1:A:86:GLU:HG2	1:A:230:LEU:CB	2.19	0.69
1:A:297:ALA:HB1	1:A:299:ALA:H	1.57	0.68
1:A:384:TYR:HD2	1:A:385:TYR:CE2	2.12	0.68
2:B:320:HIS:O	2:B:369:ASN:HB3	1.93	0.68
1:A:86:GLU:CG	1:A:230:LEU:HB2	2.20	0.68
1:A:98:THR:HG21	1:A:100:GLN:HB2	1.74	0.68
1:A:245:ALA:HA	1:A:405:VAL:CG2	2.23	0.68
2:B:102:PRO:HB2	2:B:107:VAL:HG23	1.76	0.68
2:B:301:LEU:HD11	2:B:356:ILE:HD13	1.75	0.68
1:A:190:TYR:O	1:A:193:LEU:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HB3	1:A:417:PHE:CD2	2.29	0.68
1:A:377:HIS:O	1:A:377:HIS:ND1	2.24	0.68
2:B:279:GLN:HG2	2:B:390:MET:HG3	1.75	0.68
1:A:162:ILE:HD12	1:A:167:TYR:CD1	2.29	0.68
2:B:109:TRP:CZ3	2:B:110:LEU:HD23	2.28	0.68
2:B:92:LEU:HD22	2:B:233:THR:HA	1.76	0.68
2:B:93:PHE:CZ	2:B:97:VAL:HG21	2.28	0.68
1:A:98:THR:CG2	1:A:100:GLN:HG3	2.21	0.68
2:B:301:LEU:HD23	2:B:352:GLN:NE2	2.09	0.68
2:B:326:THR:HG22	2:B:327:ASP:O	1.94	0.68
1:A:69:PHE:HA	1:A:73:GLU:OE1	1.93	0.67
2:B:212:ASN:O	2:B:216:MET:HG3	1.94	0.67
2:B:204:ASP:OD2	2:B:206:LYS:N	2.28	0.67
2:B:362:LEU:CD1	2:B:370:PRO:HG3	2.22	0.67
2:B:245:ALA:HA	2:B:405:VAL:CG2	2.24	0.67
2:B:251:VAL:CG1	2:B:261:SER:HA	2.24	0.67
1:A:80:LYS:HE2	1:A:85:GLY:O	1.94	0.67
1:A:184:CYS:O	1:A:188:LYS:HB2	1.94	0.67
2:B:46:ARG:HA	2:B:46:ARG:NH1	2.09	0.67
2:B:298:ASP:O	2:B:302:ARG:HB2	1.95	0.67
2:B:326:THR:O	2:B:327:ASP:C	2.38	0.67
1:A:339:LYS:HB3	1:A:340:HIS:CD2	2.29	0.67
1:A:14:ILE:O	1:A:17:GLU:N	2.27	0.67
1:A:157:ALA:HB1	1:A:162:ILE:HG23	1.77	0.67
1:A:274:HIS:O	1:A:274:HIS:ND1	2.27	0.67
2:B:178:LEU:HD23	2:B:406:LEU:HD11	1.76	0.67
2:B:327:ASP:OD1	2:B:374:VAL:HG22	1.95	0.67
1:A:271:GLY:O	1:A:275:GLY:N	2.23	0.66
1:A:136:HIS:HB3	1:A:139:SER:HB2	1.77	0.66
2:B:211:HIS:O	2:B:215:ASN:HB3	1.95	0.66
2:B:221:ASP:OD2	2:B:223:GLN:N	2.27	0.66
2:B:257:ASP:HB2	2:B:258:PRO:HD2	1.75	0.66
1:A:65:ARG:HH11	1:A:70:SER:HB3	1.59	0.66
1:A:213:PHE:O	1:A:217:LEU:HB2	1.95	0.66
2:B:311:SER:O	2:B:313:ARG:NH1	2.28	0.66
2:B:163:LEU:HD12	2:B:164:ARG:N	2.10	0.66
2:B:306:TRP:CZ3	2:B:364:GLN:NE2	2.64	0.66
1:A:10:LEU:O	1:A:14:ILE:HG13	1.95	0.66
2:B:107:VAL:O	2:B:109:TRP:N	2.28	0.66
1:A:13:LEU:O	1:A:16:LYS:HB2	1.96	0.66
1:A:27:GLN:HG2	1:A:28:HIS:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:TYR:CE2	1:A:385:TYR:CZ	2.83	0.66
2:B:46:ARG:HH11	2:B:46:ARG:C	2.04	0.66
2:B:109:TRP:CH2	2:B:113:GLU:HG2	2.31	0.66
2:B:193:LEU:HB3	2:B:194:TYR:CD2	2.31	0.66
1:A:243:VAL:HB	1:A:274:HIS:HD2	1.59	0.65
1:A:311:SER:HB3	1:A:313:ARG:HH12	1.62	0.65
2:B:412:SER:HA	2:B:417:PHE:CE2	2.30	0.65
1:A:50:GLY:O	1:A:51:LEU:HG	1.96	0.65
1:A:334:ARG:O	1:A:334:ARG:HG3	1.76	0.65
2:B:6:LEU:HD13	2:B:94:TRP:CE3	2.32	0.65
2:B:36:ILE:CG2	2:B:48:MET:HE2	2.26	0.65
1:A:127:MET:HE2	1:A:131:PHE:HZ	1.61	0.65
1:A:433:LEU:CD2	2:B:33:LEU:HD22	2.27	0.65
1:A:352:GLN:O	1:A:355:LYS:N	2.29	0.65
1:A:421:ARG:N	2:B:44:GLY:O	2.29	0.65
2:B:369:ASN:N	2:B:370:PRO:HD3	2.10	0.65
2:B:148:LEU:C	2:B:150:SER:H	2.04	0.64
1:A:128:LEU:HD23	1:A:131:PHE:CE2	2.32	0.64
1:A:362:LEU:HD12	1:A:367:ALA:CB	2.27	0.64
1:A:371:TRP:H	1:A:371:TRP:CD1	2.14	0.64
2:B:97:VAL:HG12	2:B:97:VAL:O	1.97	0.64
2:B:235:HIS:O	2:B:401:ARG:NH2	2.27	0.64
1:A:301:LEU:HD12	1:A:356:ILE:HG21	1.80	0.64
1:A:177:ASP:O	1:A:181:LYS:HG3	1.97	0.64
1:A:305:ILE:HD13	1:A:357:VAL:HG22	1.77	0.64
2:B:121:PRO:HB2	2:B:123:HIS:CD2	2.32	0.64
1:A:162:ILE:CD1	1:A:167:TYR:CD1	2.81	0.64
1:A:362:LEU:HD11	1:A:370:PRO:HG3	1.79	0.64
1:A:301:LEU:HD21	1:A:352:GLN:HB3	1.78	0.64
2:B:288:LEU:O	2:B:291:ALA:N	2.29	0.63
1:A:53:TYR:CD2	1:A:240:GLY:HA3	2.33	0.63
1:A:336:PHE:O	1:A:337:ALA:C	2.40	0.63
1:A:149:ASN:ND2	2:B:139:SER:OG	2.31	0.63
2:B:323:LEU:O	2:B:369:ASN:HB2	1.98	0.63
1:A:48:MET:O	1:A:49:LYS:C	2.40	0.63
1:A:411:TRP:HA	1:A:414:ALA:HB3	1.81	0.63
2:B:223:GLN:NE2	2:B:340:HIS:CG	2.66	0.63
2:B:311:SER:O	2:B:313:ARG:HD3	1.99	0.63
2:B:2:SER:O	2:B:3:SER:CB	2.47	0.63
1:A:44:GLY:O	1:A:45:MET:HB2	1.99	0.63
2:B:266:MET:HE2	2:B:266:MET:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:LEU:HG	2:B:353:LEU:CD2	2.29	0.63
1:A:203:ILE:HG13	1:A:216:MET:HE2	1.81	0.63
1:A:306:TRP:CD1	1:A:360:VAL:HG13	2.33	0.63
2:B:92:LEU:HG	2:B:92:LEU:O	1.97	0.63
2:B:106:GLN:O	2:B:109:TRP:HB3	1.99	0.63
1:A:52:VAL:H	2:B:425:MET:HA	1.63	0.62
1:A:53:TYR:CG	1:A:240:GLY:HA3	2.34	0.62
1:A:306:TRP:CE2	1:A:364:GLN:NE2	2.67	0.62
2:B:232:LEU:HD23	2:B:400:SER:HB2	1.82	0.62
2:B:305:ILE:HD11	2:B:353:LEU:HD12	1.81	0.62
1:A:284:TRP:CG	1:A:316:PRO:HG3	2.34	0.62
2:B:193:LEU:HD23	2:B:194:TYR:CE2	2.34	0.62
2:B:412:SER:CB	2:B:417:PHE:CD2	2.82	0.62
1:A:167:TYR:CE2	1:A:255:LEU:HD11	2.35	0.62
1:A:231:TYR:CD1	1:A:231:TYR:C	2.78	0.62
1:A:323:LEU:HD13	1:A:325:LYS:O	2.00	0.62
2:B:88:LEU:O	2:B:89:PRO:C	2.38	0.62
2:B:131:PHE:HD2	2:B:140:GLN:NE2	1.97	0.62
1:A:64:ILE:HG13	1:A:65:ARG:H	1.65	0.62
2:B:7:LYS:NZ	2:B:173:GLU:OE1	2.33	0.62
2:B:65:ARG:HH11	2:B:70:SER:HB3	1.64	0.62
2:B:149:ASN:O	2:B:149:ASN:OD1	2.17	0.62
1:A:114:TRP:O	1:A:115:ALA:C	2.40	0.62
1:A:425:MET:HA	2:B:52:VAL:N	2.11	0.62
2:B:163:LEU:O	2:B:165:THR:N	2.32	0.62
1:A:311:SER:CB	1:A:313:ARG:NH1	2.63	0.61
2:B:223:GLN:HE22	2:B:340:HIS:CE1	2.18	0.61
2:B:60:PRO:O	2:B:324:ARG:HB2	2.00	0.61
1:A:39:ASP:HB2	2:B:29:GLY:O	2.01	0.61
1:A:92:LEU:HD11	1:A:236:SER:OG	1.99	0.61
2:B:307:ASN:O	2:B:308:THR:O	2.18	0.61
1:A:223:GLN:HE22	1:A:340:HIS:CE1	2.18	0.61
1:A:285:LEU:HD21	1:A:350:VAL:CG2	2.30	0.61
2:B:334:ARG:O	2:B:334:ARG:HG3	1.91	0.61
2:B:384:TYR:HD2	2:B:385:TYR:CD2	2.18	0.61
1:A:206:LYS:C	1:A:207:LEU:HD23	2.24	0.61
2:B:94:TRP:CD1	2:B:102:PRO:CB	2.84	0.61
1:A:121:PRO:HD2	1:A:148:LEU:CD2	2.31	0.61
1:A:123:HIS:CG	2:B:132:PRO:HG3	2.35	0.61
1:A:29:GLY:O	2:B:39:ASP:N	2.33	0.61
1:A:269:LEU:HD11	1:A:397:PHE:CE2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:LEU:N	2:B:183:PRO:HD2	2.15	0.61
2:B:310:ASN:ND2	2:B:364:GLN:OE1	2.34	0.61
1:A:264:ALA:HB1	2:B:264:ALA:HB1	1.82	0.61
1:A:325:LYS:HD2	1:A:326:THR:O	2.00	0.61
2:B:350:VAL:HA	2:B:353:LEU:HD23	1.82	0.61
1:A:18:GLN:O	1:A:22:LYS:HG2	2.01	0.61
2:B:45:MET:O	2:B:48:MET:HB2	2.01	0.61
2:B:109:TRP:CE3	2:B:110:LEU:CD2	2.83	0.61
2:B:320:HIS:ND1	2:B:321:ALA:N	2.49	0.61
1:A:6:LEU:HD13	1:A:94:TRP:CE3	2.35	0.60
2:B:204:ASP:OD2	2:B:204:ASP:C	2.44	0.60
2:B:353:LEU:O	2:B:357:VAL:HB	2.01	0.60
1:A:298:ASP:HA	1:A:356:ILE:CD1	2.26	0.60
1:A:311:SER:HB3	1:A:313:ARG:NH1	2.17	0.60
1:A:384:TYR:HE2	1:A:385:TYR:CZ	2.18	0.60
2:B:190:TYR:O	2:B:193:LEU:N	2.34	0.60
1:A:78:LEU:HD11	1:A:92:LEU:HD23	1.84	0.60
1:A:125:VAL:CG1	1:A:188:LYS:HE2	2.31	0.60
2:B:131:PHE:CD2	2:B:140:GLN:NE2	2.69	0.60
2:B:349:LEU:O	2:B:350:VAL:C	2.44	0.60
1:A:46:ARG:NH1	1:A:46:ARG:CB	2.48	0.60
2:B:163:LEU:O	2:B:166:LYS:N	2.29	0.60
1:A:13:LEU:O	1:A:16:LYS:CB	2.49	0.60
2:B:136:HIS:HD2	2:B:138:MET:H	1.50	0.60
2:B:191:ARG:HA	2:B:195:ARG:HB2	1.83	0.60
1:A:311:SER:HB2	1:A:313:ARG:NH2	2.18	0.59
1:A:384:TYR:CE2	1:A:385:TYR:CE1	2.90	0.59
2:B:315:VAL:HG12	2:B:316:PRO:HD2	1.84	0.59
1:A:135:LEU:CD1	1:A:139:SER:HB3	2.30	0.59
2:B:127:MET:CE	2:B:131:PHE:CZ	2.85	0.59
2:B:269:LEU:HA	2:B:274:HIS:CD2	2.37	0.59
2:B:181:LYS:O	2:B:185:VAL:HG23	2.03	0.59
2:B:333:GLN:O	2:B:336:PHE:HB3	2.02	0.59
1:A:266:MET:HA	1:A:266:MET:CE	2.28	0.59
1:A:301:LEU:HD12	1:A:301:LEU:C	2.28	0.59
1:A:390:MET:HB2	1:A:393:TYR:CZ	2.37	0.59
1:A:67:ARG:HB3	1:A:69:PHE:HD2	1.68	0.59
1:A:191:ARG:HD3	1:A:200:ILE:HA	1.85	0.59
1:A:299:ALA:O	1:A:303:ASP:HB2	2.03	0.59
1:A:27:GLN:NE2	1:A:28:HIS:CE1	2.71	0.59
1:A:90:GLU:HG3	1:A:114:TRP:CZ3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HD12	2:B:20:ARG:HH21	1.68	0.59
2:B:70:SER:OG	2:B:72:PRO:HD2	2.02	0.59
2:B:136:HIS:CG	2:B:137:PRO:HD2	2.37	0.59
2:B:162:ILE:HD11	2:B:167:TYR:HD1	1.68	0.59
2:B:281:VAL:HG22	2:B:316:PRO:CB	2.30	0.59
2:B:397:PHE:HE1	2:B:401:ARG:NH2	2.01	0.59
1:A:420:GLU:O	1:A:421:ARG:HB2	2.03	0.58
2:B:323:LEU:C	2:B:369:ASN:HD22	2.06	0.58
1:A:164:ARG:O	1:A:167:TYR:HB2	2.03	0.58
2:B:91:GLY:CA	2:B:102:PRO:HG3	2.33	0.58
2:B:144:ALA:O	2:B:147:ALA:N	2.36	0.58
1:A:144:ALA:O	1:A:148:LEU:N	2.34	0.58
1:A:384:TYR:HE2	1:A:385:TYR:CE1	2.22	0.58
2:B:174:SER:HB3	2:B:258:PRO:HG2	1.85	0.58
1:A:326:THR:O	1:A:328:PRO:HD3	2.04	0.58
2:B:301:LEU:HD11	2:B:356:ILE:CD1	2.33	0.58
1:A:327:ASP:OD1	1:A:374:VAL:HG22	2.04	0.58
2:B:6:LEU:HB2	2:B:94:TRP:CZ3	2.39	0.58
2:B:145:ILE:HD11	2:B:182:LEU:HD21	1.85	0.58
1:A:413:ARG:HA	1:A:413:ARG:NE	2.19	0.58
2:B:341:LEU:HD22	2:B:384:TYR:CE2	2.36	0.58
1:A:59:ASP:OD2	1:A:61:ASP:N	2.32	0.58
1:A:149:ASN:HD21	2:B:139:SER:CB	2.16	0.58
2:B:334:ARG:O	2:B:338:LEU:HG	2.04	0.58
2:B:356:ILE:O	2:B:360:VAL:HG23	2.04	0.58
1:A:168:TRP:CZ2	1:A:169:GLU:HG3	2.38	0.58
2:B:107:VAL:C	2:B:109:TRP:N	2.59	0.58
2:B:284:TRP:CZ2	2:B:315:VAL:HG13	2.39	0.58
2:B:288:LEU:HD13	2:B:304:TYR:CE2	2.39	0.58
1:A:71:ILE:HG12	1:A:329:ARG:HG2	1.84	0.57
1:A:284:TRP:CZ3	1:A:285:LEU:CD1	2.87	0.57
1:A:302:ARG:HB2	1:A:356:ILE:HG12	1.84	0.57
1:A:13:LEU:O	1:A:16:LYS:HG3	2.05	0.57
1:A:91:GLY:CA	1:A:102:PRO:HG3	2.33	0.57
1:A:285:LEU:HD21	1:A:350:VAL:HG22	1.86	0.57
2:B:342:PRO:HD2	2:B:343:GLY:N	2.16	0.57
2:B:107:VAL:O	2:B:108:SER:C	2.47	0.57
2:B:328:PRO:O	2:B:332:CYS:HB2	2.05	0.57
2:B:92:LEU:CD1	2:B:233:THR:HG23	2.32	0.57
2:B:301:LEU:HG	2:B:356:ILE:CD1	2.32	0.57
2:B:357:VAL:CB	2:B:358:PRO:HD3	2.32	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:LEU:HD13	2:B:381:LEU:N	2.20	0.57
1:A:323:LEU:O	1:A:369:ASN:HB2	2.05	0.56
2:B:142:SER:O	2:B:146:THR:OG1	2.22	0.56
1:A:337:ALA:HB3	1:A:347:PHE:CZ	2.41	0.56
2:B:136:HIS:O	2:B:140:GLN:HG3	2.05	0.56
2:B:223:GLN:CD	2:B:340:HIS:ND1	2.63	0.56
2:B:288:LEU:HD13	2:B:304:TYR:CD2	2.39	0.56
1:A:48:MET:O	1:A:49:LYS:O	2.23	0.56
1:A:233:THR:O	1:A:236:SER:OG	2.14	0.56
1:A:267:ASN:O	1:A:270:ALA:HB3	2.05	0.56
1:A:333:GLN:OE1	1:A:378:SER:HA	2.05	0.56
2:B:42:TYR:OH	2:B:427:THR:HG23	2.04	0.56
2:B:103:THR:OG1	2:B:106:GLN:HG3	2.05	0.56
2:B:149:ASN:O	2:B:149:ASN:ND2	2.38	0.56
2:B:282:LEU:HD23	2:B:390:MET:CE	2.35	0.56
2:B:337:ALA:CB	2:B:347:PHE:CE2	2.88	0.56
1:A:305:ILE:HD11	1:A:357:VAL:HG22	1.87	0.56
1:A:352:GLN:O	1:A:353:LEU:C	2.48	0.56
2:B:59:ASP:HB3	2:B:63:GLY:O	2.04	0.56
1:A:214:THR:HA	1:A:217:LEU:HB2	1.86	0.56
2:B:342:PRO:CD	2:B:343:GLY:H	2.14	0.56
1:A:168:TRP:C	1:A:170:MET:H	2.14	0.56
1:A:253:SER:C	1:A:255:LEU:H	2.14	0.56
1:A:284:TRP:HZ3	1:A:285:LEU:CD1	2.17	0.56
1:A:320:HIS:N	1:A:369:ASN:OD1	2.39	0.56
1:A:322:VAL:O	1:A:323:LEU:C	2.49	0.56
1:A:157:ALA:HB1	1:A:162:ILE:HG21	1.85	0.56
1:A:430:LEU:CD2	2:B:33:LEU:CD2	2.83	0.56
2:B:138:MET:HE1	2:B:269:LEU:HD23	1.87	0.56
2:B:174:SER:HB2	2:B:258:PRO:CG	2.33	0.56
2:B:269:LEU:HD11	2:B:397:PHE:HE2	1.66	0.56
2:B:340:HIS:O	2:B:342:PRO:CD	2.51	0.56
2:B:401:ARG:HG2	2:B:401:ARG:NH1	2.21	0.56
1:A:42:TYR:CD2	2:B:25:ARG:HD2	2.40	0.56
2:B:46:ARG:NH1	2:B:46:ARG:C	2.64	0.56
1:A:287:GLN:O	1:A:288:LEU:C	2.49	0.56
1:A:425:MET:CA	2:B:52:VAL:H	2.14	0.56
2:B:65:ARG:CG	2:B:68:GLY:O	2.54	0.56
1:A:6:LEU:HB2	1:A:94:TRP:HZ3	1.66	0.55
1:A:109:TRP:HE3	1:A:110:LEU:CD2	2.18	0.55
1:A:136:HIS:CD2	1:A:137:PRO:HD2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:PHE:O	2:B:337:ALA:C	2.48	0.55
1:A:230:LEU:HD12	1:A:230:LEU:O	2.05	0.55
2:B:190:TYR:CD2	2:B:217:LEU:HD22	2.40	0.55
2:B:223:GLN:NE2	2:B:340:HIS:CE1	2.74	0.55
2:B:318:TYR:CE1	2:B:372:PRO:HG3	2.42	0.55
1:A:221:ASP:OD2	1:A:223:GLN:HB2	2.07	0.55
1:A:234:ILE:HG13	1:A:235:HIS:CE1	2.41	0.55
2:B:305:ILE:HD13	2:B:357:VAL:CG2	2.35	0.55
2:B:369:ASN:N	2:B:370:PRO:CD	2.69	0.55
2:B:408:GLN:O	2:B:412:SER:OG	2.24	0.55
2:B:86:GLU:CD	2:B:230:LEU:HD22	2.32	0.55
1:A:6:LEU:HD13	1:A:94:TRP:CZ3	2.41	0.55
1:A:306:TRP:HD1	1:A:360:VAL:HG13	1.72	0.55
2:B:163:LEU:HD12	2:B:164:ARG:H	1.72	0.55
2:B:305:ILE:HA	2:B:308:THR:HB	1.88	0.55
1:A:27:GLN:CG	1:A:28:HIS:N	2.66	0.55
1:A:163:LEU:O	1:A:165:THR:N	2.40	0.55
1:A:250:LEU:HD13	1:A:420:GLU:CD	2.32	0.55
1:A:384:TYR:CD2	1:A:385:TYR:CE2	2.93	0.55
2:B:390:MET:HB2	2:B:393:TYR:CE2	2.42	0.55
2:B:415:LEU:CD1	2:B:417:PHE:CZ	2.90	0.55
2:B:19:ALA:HA	2:B:22:LYS:HG2	1.88	0.55
2:B:54:GLU:N	2:B:408:GLN:OE1	2.29	0.55
2:B:272:PRO:C	2:B:274:HIS:H	2.14	0.55
2:B:13:LEU:HD11	2:B:100:GLN:NE2	2.22	0.54
2:B:138:MET:CE	2:B:269:LEU:HD23	2.37	0.54
2:B:179:ILE:O	2:B:209:TRP:NE1	2.36	0.54
1:A:77:LEU:O	1:A:78:LEU:C	2.50	0.54
1:A:327:ASP:HB3	1:A:373:ASN:HA	1.90	0.54
2:B:320:HIS:HB3	2:B:369:ASN:ND2	2.23	0.54
2:B:94:TRP:CG	2:B:102:PRO:HB3	2.41	0.54
2:B:415:LEU:HB2	2:B:417:PHE:CE1	2.43	0.54
1:A:88:LEU:CD1	1:A:229:ARG:HD3	2.37	0.54
2:B:28:HIS:O	2:B:31:THR:HB	2.06	0.54
1:A:14:ILE:HB	1:A:15:PRO:HD3	1.90	0.54
1:A:288:LEU:HD23	1:A:349:LEU:HD21	1.90	0.54
2:B:90:GLU:OE2	2:B:111:SER:OG	2.19	0.54
1:A:182:LEU:N	1:A:183:PRO:CD	2.70	0.54
2:B:33:LEU:HD12	2:B:34:GLY:N	2.23	0.54
2:B:109:TRP:CZ3	2:B:110:LEU:CD2	2.91	0.54
1:A:88:LEU:HD11	1:A:229:ARG:HD3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:HA2	1:A:102:PRO:HG3	1.90	0.53
1:A:370:PRO:HD2	1:A:371:TRP:CD1	2.44	0.53
2:B:130:ASN:O	2:B:131:PHE:C	2.50	0.53
2:B:214:THR:CG2	2:B:215:ASN:N	2.70	0.53
1:A:37:THR:HG21	2:B:30:GLY:HA2	1.90	0.53
1:A:251:VAL:HG11	1:A:261:SER:HA	1.88	0.53
2:B:337:ALA:HB3	2:B:347:PHE:CE2	2.43	0.53
1:A:251:VAL:CG1	1:A:261:SER:HB3	2.37	0.53
1:A:430:LEU:HD23	1:A:433:LEU:HD23	1.89	0.53
2:B:27:GLN:NE2	2:B:28:HIS:CE1	2.76	0.53
2:B:54:GLU:HB2	2:B:408:GLN:OE1	2.08	0.53
2:B:87:PRO:O	2:B:229:ARG:HB3	2.08	0.53
2:B:248:SER:OG	2:B:405:VAL:HG22	2.08	0.53
1:A:187:ALA:O	1:A:191:ARG:HB2	2.08	0.53
2:B:378:SER:O	2:B:381:LEU:N	2.39	0.53
2:B:384:TYR:CD2	2:B:385:TYR:CE2	2.92	0.53
1:A:310:ASN:C	1:A:312:GLY:H	2.16	0.53
1:A:411:TRP:O	1:A:415:LEU:HG	2.08	0.53
2:B:111:SER:OG	2:B:208:ASP:HA	2.09	0.52
1:A:45:MET:HA	1:A:48:MET:HE3	1.90	0.52
2:B:329:ARG:O	2:B:333:GLN:HG3	2.08	0.52
1:A:412:SER:HB3	1:A:417:PHE:HD2	1.74	0.52
2:B:101:ILE:O	2:B:102:PRO:C	2.51	0.52
2:B:168:TRP:CE2	2:B:169:GLU:HG2	2.45	0.52
2:B:324:ARG:CZ	2:B:324:ARG:HB3	2.33	0.52
1:A:306:TRP:CZ2	1:A:364:GLN:NE2	2.77	0.52
2:B:46:ARG:HH11	2:B:46:ARG:CG	2.22	0.52
1:A:86:GLU:HG3	1:A:87:PRO:HD2	1.91	0.52
1:A:305:ILE:O	1:A:309:LEU:HG	2.09	0.52
2:B:144:ALA:O	2:B:147:ALA:HB3	2.09	0.52
1:A:65:ARG:NH1	1:A:70:SER:HB3	2.25	0.52
1:A:399:VAL:HG12	1:A:399:VAL:O	2.09	0.52
1:A:162:ILE:CD1	1:A:167:TYR:CE1	2.93	0.52
1:A:162:ILE:CD1	1:A:167:TYR:HD1	2.18	0.52
1:A:405:VAL:O	1:A:405:VAL:HG13	2.09	0.52
1:A:427:THR:O	1:A:431:ILE:HG13	2.10	0.52
2:B:318:TYR:CE1	2:B:372:PRO:HB3	2.44	0.52
2:B:397:PHE:CE1	2:B:401:ARG:NH2	2.78	0.52
1:A:157:ALA:O	1:A:162:ILE:HG12	2.09	0.52
1:A:204:ASP:OD2	1:A:206:LYS:CD	2.55	0.52
1:A:347:PHE:O	1:A:350:VAL:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:LYS:C	2:B:82:GLY:H	2.18	0.52
2:B:95:LEU:HD12	2:B:95:LEU:O	2.10	0.52
2:B:272:PRO:C	2:B:274:HIS:N	2.67	0.52
1:A:38:VAL:O	1:A:38:VAL:CG1	2.58	0.52
1:A:337:ALA:HB3	1:A:347:PHE:CE2	2.45	0.51
2:B:61:ASP:O	2:B:62:GLU:OE2	2.28	0.51
1:A:33:LEU:N	2:B:36:ILE:O	2.43	0.51
2:B:36:ILE:CG2	2:B:48:MET:CE	2.87	0.51
1:A:428:ASP:OD2	1:A:428:ASP:N	2.43	0.51
2:B:230:LEU:O	2:B:234:ILE:HG23	2.10	0.51
2:B:371:TRP:HB3	2:B:372:PRO:CD	2.40	0.51
2:B:430:LEU:HD23	2:B:433:LEU:HD23	1.93	0.51
1:A:90:GLU:OE2	1:A:111:SER:OG	2.28	0.51
2:B:269:LEU:C	2:B:271:GLY:H	2.18	0.51
2:B:368:ALA:C	2:B:370:PRO:HD3	2.34	0.51
2:B:392:TYR:CE2	2:B:396:LEU:HD13	2.45	0.51
1:A:17:GLU:OE2	1:A:17:GLU:HA	2.11	0.51
1:A:168:TRP:C	1:A:170:MET:N	2.68	0.51
2:B:337:ALA:HB1	2:B:347:PHE:CD2	2.46	0.51
1:A:61:ASP:O	1:A:62:GLU:OE2	2.28	0.51
1:A:174:SER:CB	1:A:258:PRO:HG2	2.40	0.51
1:A:223:GLN:NE2	1:A:340:HIS:CE1	2.79	0.51
1:A:238:HIS:O	1:A:242:ASN:ND2	2.42	0.51
1:A:136:HIS:CD2	1:A:137:PRO:CD	2.93	0.51
1:A:171:VAL:HG21	1:A:413:ARG:HG2	1.93	0.51
1:A:273:LEU:HD11	2:B:255:LEU:HD12	1.91	0.51
1:A:285:LEU:HG	1:A:346:MET:HE2	1.93	0.51
2:B:40:MET:HB2	2:B:48:MET:CE	2.39	0.51
2:B:162:ILE:CD1	2:B:167:TYR:HD1	2.24	0.51
2:B:269:LEU:C	2:B:271:GLY:N	2.69	0.51
1:A:154:PHE:CD1	1:A:171:VAL:HG23	2.46	0.51
1:A:393:TYR:CD1	1:A:393:TYR:N	2.76	0.51
2:B:297:ALA:C	2:B:299:ALA:N	2.67	0.51
1:A:46:ARG:CZ	1:A:46:ARG:CB	2.81	0.50
1:A:423:LYS:NZ	2:B:239:GLU:OE1	2.38	0.50
1:A:433:LEU:HD23	2:B:33:LEU:HD22	1.92	0.50
2:B:92:LEU:HD13	2:B:233:THR:CG2	2.33	0.50
1:A:64:ILE:HG13	1:A:65:ARG:N	2.25	0.50
1:A:137:PRO:C	1:A:139:SER:H	2.19	0.50
1:A:157:ALA:CB	1:A:170:MET:SD	3.00	0.50
1:A:223:GLN:HE22	1:A:340:HIS:CG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:O	1:A:115:ALA:HB3	2.11	0.50
1:A:384:TYR:CD2	1:A:385:TYR:CZ	2.99	0.50
1:A:301:LEU:CD1	1:A:356:ILE:HG21	2.40	0.50
2:B:69:PHE:HA	2:B:73:GLU:OE1	2.10	0.50
2:B:145:ILE:CG2	2:B:263:ALA:HB2	2.36	0.50
2:B:236:SER:HA	2:B:400:SER:O	2.12	0.50
2:B:285:LEU:HG	2:B:346:MET:CE	2.35	0.50
2:B:357:VAL:N	2:B:358:PRO:CD	2.74	0.50
2:B:127:MET:HE2	2:B:131:PHE:HZ	1.72	0.50
2:B:203:ILE:HD11	2:B:216:MET:HE1	1.92	0.50
2:B:257:ASP:HB2	2:B:258:PRO:CD	2.40	0.50
2:B:305:ILE:CD1	2:B:357:VAL:HG22	2.39	0.50
2:B:377:HIS:O	2:B:377:HIS:ND1	2.45	0.50
1:A:92:LEU:HG	1:A:233:THR:CG2	2.24	0.50
2:B:41:SER:C	2:B:43:GLY:H	2.20	0.50
1:A:336:PHE:O	1:A:337:ALA:O	2.29	0.49
2:B:145:ILE:HG22	2:B:259:TYR:O	2.12	0.49
2:B:200:ILE:CG1	2:B:201:GLY:N	2.75	0.49
1:A:272:PRO:HG2	2:B:255:LEU:O	2.12	0.49
1:A:306:TRP:CD1	1:A:360:VAL:CG1	2.94	0.49
2:B:88:LEU:O	2:B:90:GLU:N	2.45	0.49
2:B:138:MET:HG2	2:B:395:VAL:HG22	1.94	0.49
1:A:223:GLN:CD	1:A:340:HIS:ND1	2.70	0.49
2:B:97:VAL:O	2:B:97:VAL:CG1	2.61	0.49
2:B:181:LYS:O	2:B:184:CYS:HB2	2.13	0.49
2:B:289:GLN:O	2:B:289:GLN:HG2	2.12	0.49
1:A:320:HIS:CB	1:A:369:ASN:OD1	2.60	0.49
2:B:149:ASN:ND2	2:B:149:ASN:C	2.67	0.49
2:B:269:LEU:CD1	2:B:397:PHE:CE2	2.85	0.49
2:B:306:TRP:CE3	2:B:364:GLN:NE2	2.80	0.49
2:B:388:THR:O	2:B:390:MET:N	2.44	0.49
1:A:281:VAL:CG2	1:A:316:PRO:HB2	2.37	0.49
2:B:37:THR:HB	2:B:40:MET:HG3	1.95	0.49
1:A:337:ALA:O	1:A:338:LEU:C	2.52	0.49
1:A:46:ARG:O	1:A:46:ARG:HG3	2.13	0.49
2:B:46:ARG:NH1	2:B:46:ARG:HG3	2.26	0.49
2:B:285:LEU:HB3	2:B:346:MET:HE1	1.93	0.49
2:B:320:HIS:HB3	2:B:369:ASN:CG	2.37	0.49
2:B:392:TYR:O	2:B:395:VAL:N	2.42	0.49
2:B:392:TYR:O	2:B:393:TYR:C	2.54	0.49
1:A:64:ILE:HG22	1:A:71:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LEU:CD2	2:B:352:GLN:NE2	2.76	0.49
2:B:346:MET:CG	2:B:380:VAL:HG13	2.42	0.49
2:B:390:MET:HE3	2:B:390:MET:HB3	1.75	0.49
2:B:408:GLN:HE22	2:B:417:PHE:HE2	1.59	0.49
1:A:37:THR:CG2	2:B:30:GLY:HA2	2.42	0.49
1:A:210:SER:CB	1:A:229:ARG:HG2	2.43	0.49
1:A:235:HIS:HB3	1:A:397:PHE:HD1	1.77	0.49
1:A:350:VAL:O	1:A:353:LEU:HB2	2.13	0.49
2:B:247:THR:O	2:B:251:VAL:HB	2.13	0.49
1:A:163:LEU:HD12	1:A:164:ARG:N	2.27	0.48
1:A:337:ALA:O	1:A:340:HIS:N	2.46	0.48
1:A:128:LEU:HD23	1:A:131:PHE:CD2	2.48	0.48
1:A:250:LEU:HD12	1:A:420:GLU:HB3	1.94	0.48
1:A:305:ILE:HD12	1:A:356:ILE:HG22	1.94	0.48
1:A:390:MET:HA	1:A:393:TYR:CE1	2.48	0.48
2:B:285:LEU:O	2:B:288:LEU:HB3	2.13	0.48
1:A:98:THR:HG22	1:A:100:GLN:CG	2.34	0.48
1:A:101:ILE:HG23	1:A:101:ILE:HD13	1.48	0.48
1:A:162:ILE:HD11	1:A:167:TYR:CD1	2.48	0.48
1:A:211:HIS:O	1:A:215:ASN:HB3	2.13	0.48
1:A:323:LEU:CD2	1:A:324:ARG:N	2.65	0.48
1:A:285:LEU:O	1:A:288:LEU:N	2.47	0.48
1:A:362:LEU:HD13	1:A:370:PRO:CG	2.40	0.48
2:B:127:MET:CE	2:B:131:PHE:HZ	2.26	0.48
2:B:162:ILE:HD11	2:B:167:TYR:CD1	2.49	0.48
2:B:206:LYS:C	2:B:207:LEU:HD23	2.38	0.48
2:B:324:ARG:CG	2:B:324:ARG:NH1	2.73	0.48
1:A:162:ILE:HD11	1:A:167:TYR:CE1	2.48	0.48
1:A:322:VAL:O	1:A:323:LEU:O	2.32	0.48
1:A:53:TYR:CD2	1:A:240:GLY:CA	2.96	0.48
1:A:340:HIS:CD2	1:A:340:HIS:N	2.82	0.48
2:B:43:GLY:O	2:B:46:ARG:HG2	2.14	0.48
1:A:53:TYR:CG	1:A:240:GLY:CA	2.97	0.48
1:A:284:TRP:CZ3	1:A:285:LEU:HD12	2.49	0.48
1:A:27:GLN:HG2	1:A:28:HIS:H	1.76	0.48
2:B:257:ASP:O	2:B:261:SER:OG	2.31	0.47
2:B:301:LEU:CG	2:B:356:ILE:CD1	2.88	0.47
2:B:353:LEU:O	2:B:357:VAL:CG2	2.62	0.47
1:A:213:PHE:O	1:A:213:PHE:CD1	2.68	0.47
1:A:245:ALA:HA	1:A:405:VAL:HG21	1.95	0.47
1:A:246:HIS:O	1:A:249:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:PHE:C	2:B:26:GLN:N	2.72	0.47
2:B:81:GLY:HA2	2:B:88:LEU:CD1	2.41	0.47
1:A:88:LEU:CD1	1:A:229:ARG:CD	2.93	0.47
1:A:136:HIS:HD2	1:A:138:MET:N	2.03	0.47
1:A:427:THR:O	1:A:427:THR:HG22	2.13	0.47
2:B:405:VAL:O	2:B:409:LEU:HB2	2.13	0.47
1:A:20:ARG:HG3	1:A:20:ARG:HH11	1.79	0.47
1:A:103:THR:OG1	1:A:106:GLN:HG3	2.14	0.47
1:A:111:SER:HB3	1:A:208:ASP:HA	1.96	0.47
1:A:132:PRO:HG3	2:B:123:HIS:CB	2.45	0.47
2:B:59:ASP:OD2	2:B:62:GLU:N	2.48	0.47
1:A:21:ILE:O	1:A:25:ARG:HG3	2.15	0.47
1:A:157:ALA:HB3	1:A:170:MET:SD	2.55	0.47
1:A:433:LEU:HD21	2:B:33:LEU:HD22	1.96	0.47
1:A:33:LEU:HD13	1:A:33:LEU:O	2.14	0.47
1:A:55:THR:HB	1:A:96:LEU:HD22	1.95	0.47
2:B:70:SER:O	2:B:71:ILE:C	2.55	0.47
2:B:333:GLN:O	2:B:336:PHE:N	2.41	0.47
1:A:231:TYR:CD1	1:A:231:TYR:O	2.67	0.47
1:A:331:THR:O	1:A:335:GLU:HB2	2.14	0.47
1:A:338:LEU:O	1:A:339:LYS:O	2.32	0.47
1:A:349:LEU:O	1:A:350:VAL:C	2.57	0.47
2:B:248:SER:HB3	2:B:265:ALA:HB2	1.97	0.47
2:B:346:MET:HG2	2:B:380:VAL:HG13	1.97	0.47
1:A:262:PHE:O	1:A:266:MET:HG2	2.15	0.47
2:B:200:ILE:HG13	2:B:201:GLY:N	2.30	0.47
2:B:217:LEU:HD23	2:B:217:LEU:HA	1.64	0.47
1:A:89:PRO:HG3	1:A:232:LEU:HB2	1.96	0.47
1:A:121:PRO:HD2	1:A:148:LEU:HD21	1.96	0.47
1:A:248:SER:HA	1:A:261:SER:O	2.14	0.47
1:A:430:LEU:HD21	2:B:33:LEU:HD21	1.97	0.47
2:B:91:GLY:O	2:B:102:PRO:HG3	2.15	0.47
1:A:4:THR:C	1:A:5:ASN:CG	2.83	0.47
1:A:311:SER:CB	1:A:313:ARG:CZ	2.91	0.47
1:A:323:LEU:O	1:A:324:ARG:HB2	2.15	0.47
1:A:389:GLU:OE2	1:A:389:GLU:N	2.39	0.47
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.60	0.47
2:B:149:ASN:HB2	2:B:260:LEU:HD13	1.98	0.47
2:B:157:ALA:HB1	2:B:162:ILE:HG23	1.91	0.47
2:B:323:LEU:HD23	2:B:324:ARG:H	1.80	0.47
1:A:91:GLY:O	1:A:102:PRO:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HB1	1:A:368:ALA:H	1.11	0.46
2:B:238:HIS:O	2:B:239:GLU:HB2	2.14	0.46
2:B:323:LEU:HB3	2:B:369:ASN:ND2	2.30	0.46
2:B:360:VAL:O	2:B:363:GLU:HB3	2.15	0.46
1:A:24:PHE:HD2	1:A:28:HIS:HD2	1.64	0.46
2:B:94:TRP:CD1	2:B:102:PRO:CA	2.98	0.46
1:A:58:LEU:HD23	1:A:322:VAL:HG11	1.97	0.46
1:A:59:ASP:OD2	1:A:61:ASP:HB2	2.15	0.46
1:A:168:TRP:CZ2	1:A:169:GLU:CG	2.99	0.46
1:A:226:GLU:O	1:A:229:ARG:HB2	2.14	0.46
1:A:209:TRP:CZ3	1:A:232:LEU:HD22	2.50	0.46
1:A:127:MET:HE1	1:A:143:ALA:HB1	1.97	0.46
1:A:285:LEU:CG	1:A:346:MET:HE2	2.45	0.46
1:A:306:TRP:CD2	1:A:364:GLN:NE2	2.83	0.46
2:B:6:LEU:HB2	2:B:94:TRP:HZ3	1.81	0.46
2:B:38:VAL:HG22	2:B:430:LEU:HD22	1.96	0.46
2:B:86:GLU:HG3	2:B:230:LEU:CB	2.23	0.46
2:B:408:GLN:NE2	2:B:417:PHE:HE2	2.14	0.46
1:A:98:THR:CG2	1:A:100:GLN:HB2	2.45	0.46
1:A:362:LEU:HD12	1:A:362:LEU:HA	1.59	0.46
1:A:38:VAL:HG12	2:B:29:GLY:HA2	1.98	0.46
2:B:71:ILE:HG22	2:B:72:PRO:HD3	1.97	0.46
2:B:110:LEU:O	2:B:114:TRP:N	2.42	0.46
2:B:331:THR:O	2:B:335:GLU:HB2	2.15	0.46
2:B:148:LEU:O	2:B:150:SER:N	2.44	0.46
2:B:306:TRP:CH2	2:B:364:GLN:NE2	2.83	0.46
1:A:112:LYS:HE3	1:A:112:LYS:HB2	1.55	0.46
1:A:149:ASN:ND2	2:B:139:SER:CB	2.79	0.46
2:B:141:LEU:HD22	2:B:395:VAL:CG1	2.35	0.46
2:B:324:ARG:CG	2:B:324:ARG:HH11	2.27	0.46
1:A:70:SER:OG	1:A:72:PRO:HD2	2.16	0.45
1:A:70:SER:O	1:A:71:ILE:C	2.58	0.45
1:A:89:PRO:HD3	1:A:229:ARG:O	2.16	0.45
1:A:172:TYR:C	1:A:172:TYR:CD2	2.94	0.45
2:B:164:ARG:HA	2:B:167:TYR:CE2	2.51	0.45
1:A:171:VAL:O	1:A:175:ALA:HB2	2.17	0.45
1:A:173:GLU:HA	1:A:173:GLU:OE2	2.14	0.45
1:A:266:MET:HE2	1:A:269:LEU:HB3	1.97	0.45
1:A:392:TYR:HE2	1:A:396:LEU:HD13	1.82	0.45
1:A:393:TYR:N	1:A:393:TYR:HD1	2.14	0.45
2:B:89:PRO:HD3	2:B:229:ARG:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:PRO:O	2:B:125:VAL:HG23	2.16	0.45
2:B:267:ASN:HD22	2:B:267:ASN:HA	1.20	0.45
2:B:329:ARG:HE	2:B:374:VAL:HG22	1.81	0.45
1:A:221:ASP:OD2	1:A:223:GLN:N	2.49	0.45
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.66	0.45
1:A:314:VAL:O	1:A:314:VAL:CG1	2.58	0.45
2:B:271:GLY:HA2	2:B:272:PRO:HD2	1.58	0.45
2:B:353:LEU:O	2:B:357:VAL:CB	2.65	0.45
1:A:378:SER:O	1:A:381:LEU:N	2.41	0.45
1:A:392:TYR:CE2	1:A:396:LEU:HD13	2.52	0.45
2:B:350:VAL:O	2:B:353:LEU:N	2.49	0.45
1:A:19:ALA:HA	1:A:22:LYS:HG2	1.99	0.45
1:A:369:ASN:H	1:A:370:PRO:HD3	1.78	0.45
2:B:298:ASP:HA	2:B:356:ILE:HD11	1.99	0.45
2:B:323:LEU:HD23	2:B:324:ARG:N	2.31	0.45
2:B:326:THR:HA	2:B:371:TRP:HB2	1.99	0.45
2:B:326:THR:OG1	2:B:371:TRP:HB3	2.17	0.45
2:B:371:TRP:CB	2:B:372:PRO:CD	2.95	0.45
1:A:19:ALA:O	1:A:22:LYS:HG3	2.16	0.45
1:A:53:TYR:O	2:B:425:MET:O	2.35	0.45
1:A:64:ILE:CD1	1:A:238:HIS:HA	2.47	0.45
1:A:344:ASP:HA	1:A:345:PRO:HD2	1.66	0.45
2:B:93:PHE:CE2	2:B:97:VAL:HG21	2.51	0.45
2:B:168:TRP:CE2	2:B:169:GLU:CG	2.98	0.45
2:B:172:TYR:CD2	2:B:172:TYR:C	2.94	0.45
2:B:255:LEU:HD23	2:B:255:LEU:HA	1.61	0.45
2:B:323:LEU:O	2:B:369:ASN:CB	2.64	0.45
2:B:327:ASP:O	2:B:330:TYR:HB3	2.17	0.45
1:A:334:ARG:O	1:A:338:LEU:HG	2.17	0.45
1:A:371:TRP:HA	1:A:372:PRO:HD3	1.69	0.45
2:B:233:THR:O	2:B:236:SER:OG	2.26	0.45
1:A:138:MET:HE3	1:A:138:MET:HB3	1.78	0.45
2:B:14:ILE:O	2:B:15:PRO:C	2.57	0.45
1:A:338:LEU:O	1:A:339:LYS:C	2.59	0.45
1:A:251:VAL:O	1:A:256:SER:HB2	2.16	0.45
2:B:262:PHE:O	2:B:266:MET:HG2	2.17	0.45
2:B:36:ILE:HG23	2:B:48:MET:CE	2.38	0.44
2:B:43:GLY:O	2:B:46:ARG:CG	2.65	0.44
2:B:107:VAL:C	2:B:109:TRP:H	2.24	0.44
1:A:42:TYR:OH	1:A:427:THR:HG23	2.17	0.44
2:B:28:HIS:H	2:B:28:HIS:CD2	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ARG:NH1	2:B:46:ARG:CG	2.73	0.44
2:B:212:ASN:O	2:B:216:MET:HB2	2.18	0.44
2:B:342:PRO:CD	2:B:343:GLY:N	2.78	0.44
1:A:2:SER:O	1:A:3:SER:HB3	2.18	0.44
1:A:98:THR:CG2	1:A:100:GLN:CG	2.92	0.44
1:A:377:HIS:HD1	1:A:377:HIS:C	2.20	0.44
2:B:6:LEU:O	2:B:6:LEU:HG	2.17	0.44
2:B:80:LYS:HG2	2:B:85:GLY:C	2.42	0.44
2:B:172:TYR:O	2:B:175:ALA:HB3	2.18	0.44
2:B:192:ASN:HA	2:B:192:ASN:HD22	1.71	0.44
1:A:181:LYS:HG3	1:A:181:LYS:H	1.72	0.44
1:A:330:TYR:CD2	1:A:377:HIS:HB2	2.52	0.44
2:B:121:PRO:HB2	2:B:123:HIS:HD2	1.81	0.44
2:B:148:LEU:C	2:B:150:SER:N	2.75	0.44
2:B:269:LEU:O	2:B:271:GLY:N	2.50	0.44
2:B:347:PHE:O	2:B:348:LYS:C	2.59	0.44
1:A:17:GLU:O	1:A:21:ILE:HG13	2.18	0.44
1:A:33:LEU:HD12	1:A:49:LYS:HD2	1.99	0.44
1:A:38:VAL:O	1:A:42:TYR:HD2	2.00	0.44
1:A:269:LEU:O	1:A:269:LEU:HG	2.16	0.44
1:A:274:HIS:ND1	1:A:274:HIS:C	2.74	0.44
1:A:430:LEU:HD21	2:B:33:LEU:CD2	2.47	0.44
2:B:277:ALA:HB3	2:B:375:ASP:OD1	2.18	0.44
1:A:320:HIS:O	1:A:369:ASN:HB3	2.17	0.44
1:A:325:LYS:HD2	1:A:326:THR:N	2.33	0.44
2:B:71:ILE:N	2:B:72:PRO:CD	2.80	0.44
2:B:113:GLU:O	2:B:114:TRP:C	2.59	0.44
2:B:362:LEU:HD12	2:B:362:LEU:HA	1.62	0.44
2:B:193:LEU:HD12	2:B:193:LEU:HA	1.71	0.44
2:B:297:ALA:C	2:B:299:ALA:H	2.26	0.44
2:B:188:LYS:HG3	2:B:200:ILE:HG21	1.99	0.44
2:B:224:PHE:HB2	2:B:385:TYR:CD1	2.53	0.44
2:B:405:VAL:HG12	2:B:406:LEU:HD23	1.99	0.44
1:A:64:ILE:CG2	1:A:71:ILE:CD1	2.96	0.44
2:B:91:GLY:HA3	2:B:102:PRO:HG3	1.99	0.44
2:B:170:MET:C	2:B:172:TYR:N	2.74	0.44
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.82	0.43
1:A:285:LEU:O	1:A:288:LEU:CB	2.66	0.43
2:B:109:TRP:HE3	2:B:110:LEU:CD2	2.28	0.43
2:B:285:LEU:HB3	2:B:346:MET:CE	2.47	0.43
2:B:411:TRP:HA	2:B:414:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:CG	1:A:169:GLU:N	2.86	0.43
1:A:182:LEU:HD11	1:A:262:PHE:CE2	2.53	0.43
1:A:13:LEU:O	1:A:16:LYS:CG	2.65	0.43
1:A:310:ASN:O	1:A:312:GLY:N	2.51	0.43
2:B:46:ARG:HH11	2:B:46:ARG:CB	2.31	0.43
2:B:371:TRP:HB3	2:B:372:PRO:HD2	2.00	0.43
1:A:40:MET:HB3	1:A:46:ARG:HG3	2.01	0.43
1:A:106:GLN:O	1:A:110:LEU:HG	2.18	0.43
1:A:141:LEU:HD22	1:A:395:VAL:HG13	2.01	0.43
1:A:232:LEU:O	1:A:400:SER:OG	2.33	0.43
2:B:326:THR:HG22	2:B:326:THR:O	2.18	0.43
2:B:329:ARG:NH2	2:B:374:VAL:CG2	2.52	0.43
2:B:393:TYR:CD1	2:B:393:TYR:N	2.83	0.43
2:B:86:GLU:CG	2:B:230:LEU:HD22	2.48	0.43
1:A:411:TRP:CZ3	1:A:415:LEU:HD21	2.52	0.43
2:B:213:PHE:HD1	2:B:213:PHE:HA	1.52	0.43
2:B:282:LEU:HD12	2:B:282:LEU:HA	1.83	0.43
2:B:350:VAL:HG21	2:B:380:VAL:CG2	2.26	0.43
2:B:357:VAL:CB	2:B:358:PRO:CD	2.96	0.43
1:A:37:THR:OG1	1:A:40:MET:HE3	2.18	0.43
1:A:64:ILE:HD13	1:A:238:HIS:CD2	2.53	0.43
1:A:246:HIS:O	1:A:246:HIS:CD2	2.72	0.43
1:A:276:LEU:HB3	1:A:280:GLU:OE2	2.17	0.43
1:A:362:LEU:CD1	1:A:367:ALA:CB	2.96	0.43
2:B:125:VAL:HG23	2:B:125:VAL:H	1.47	0.43
2:B:313:ARG:HD3	2:B:313:ARG:N	2.34	0.43
2:B:318:TYR:HE1	2:B:372:PRO:HG3	1.83	0.43
2:B:361:LEU:HD23	2:B:361:LEU:HA	1.71	0.43
1:A:149:ASN:CG	1:A:260:LEU:HD13	2.44	0.43
1:A:176:MET:HE3	1:A:176:MET:HB3	1.71	0.43
1:A:35:GLN:HA	2:B:35:GLN:HA	2.00	0.43
2:B:102:PRO:HB2	2:B:107:VAL:CG2	2.46	0.43
2:B:310:ASN:C	2:B:312:GLY:H	2.26	0.43
1:A:24:PHE:CD2	1:A:28:HIS:HD2	2.37	0.43
1:A:28:HIS:O	1:A:31:THR:HB	2.19	0.43
1:A:284:TRP:CZ3	1:A:285:LEU:HD13	2.54	0.43
2:B:94:TRP:NE1	2:B:102:PRO:HA	2.34	0.43
2:B:340:HIS:CD2	2:B:340:HIS:N	2.82	0.42
1:A:4:THR:HG22	1:A:5:ASN:H	1.84	0.42
1:A:65:ARG:HG2	1:A:68:GLY:HA2	2.00	0.42
2:B:10:LEU:HD23	2:B:10:LEU:HA	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:LEU:HD12	2:B:163:LEU:HA	1.69	0.42
2:B:246:HIS:HE2	2:B:420:GLU:CD	2.26	0.42
2:B:430:LEU:O	2:B:431:ILE:C	2.62	0.42
1:A:427:THR:HG21	2:B:21:ILE:HG12	2.00	0.42
2:B:51:LEU:O	2:B:52:VAL:HB	2.19	0.42
2:B:367:ALA:HB1	2:B:368:ALA:H	1.00	0.42
1:A:285:LEU:O	1:A:288:LEU:HB3	2.20	0.42
1:A:315:VAL:HA	1:A:316:PRO:HD3	1.96	0.42
1:A:353:LEU:HD12	1:A:357:VAL:CG2	2.49	0.42
2:B:145:ILE:CG2	2:B:259:TYR:O	2.66	0.42
2:B:200:ILE:H	2:B:200:ILE:HG23	1.61	0.42
2:B:281:VAL:O	2:B:282:LEU:C	2.61	0.42
2:B:320:HIS:ND1	2:B:320:HIS:C	2.76	0.42
1:A:231:TYR:C	1:A:231:TYR:HD1	2.26	0.42
1:A:269:LEU:O	1:A:275:GLY:CA	2.68	0.42
1:A:288:LEU:HA	1:A:288:LEU:HD12	1.61	0.42
2:B:121:PRO:HG3	2:B:151:GLU:CD	2.44	0.42
2:B:168:TRP:CZ2	2:B:169:GLU:HG2	2.55	0.42
2:B:341:LEU:HB3	2:B:384:TYR:CE2	2.54	0.42
1:A:36:ILE:CD1	2:B:49:LYS:O	2.68	0.42
1:A:101:ILE:CG2	1:A:102:PRO:HD2	2.49	0.42
2:B:36:ILE:HG21	2:B:48:MET:HE1	2.01	0.42
2:B:88:LEU:HD12	2:B:229:ARG:HD2	2.01	0.42
2:B:207:LEU:HB2	2:B:212:ASN:OD1	2.20	0.42
2:B:409:LEU:O	2:B:410:ILE:C	2.63	0.42
1:A:142:SER:CB	1:A:267:ASN:HD21	2.32	0.42
1:A:269:LEU:O	1:A:275:GLY:HA3	2.20	0.42
2:B:71:ILE:HG22	2:B:328:PRO:HB2	2.02	0.42
2:B:322:VAL:O	2:B:322:VAL:CG1	2.64	0.42
1:A:329:ARG:HH21	1:A:374:VAL:HG22	1.79	0.42
1:A:390:MET:HA	1:A:393:TYR:CD1	2.55	0.42
2:B:177:ASP:O	2:B:181:LYS:HG3	2.19	0.42
2:B:308:THR:HG22	2:B:309:LEU:N	2.34	0.42
2:B:383:GLN:HE21	2:B:383:GLN:HB3	1.55	0.42
1:A:58:LEU:CD2	1:A:322:VAL:HG11	2.49	0.42
1:A:310:ASN:HD22	1:A:310:ASN:HA	1.78	0.42
1:A:425:MET:O	1:A:426:SER:HB3	2.20	0.42
2:B:86:GLU:HB2	2:B:226:GLU:OE1	2.20	0.42
2:B:136:HIS:CG	2:B:137:PRO:CD	3.01	0.42
2:B:324:ARG:CZ	2:B:324:ARG:HB2	2.49	0.42
1:A:269:LEU:CD1	1:A:397:PHE:CE2	3.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:PHE:CE1	2:B:167:TYR:HB3	2.38	0.41
2:B:180:ALA:O	2:B:183:PRO:HG2	2.20	0.41
2:B:236:SER:O	2:B:401:ARG:HD3	2.20	0.41
1:A:43:GLY:O	1:A:46:ARG:HB3	2.20	0.41
1:A:168:TRP:CH2	1:A:169:GLU:HG2	2.55	0.41
1:A:410:ILE:O	1:A:410:ILE:CG2	2.66	0.41
2:B:41:SER:C	2:B:43:GLY:N	2.78	0.41
2:B:349:LEU:O	2:B:350:VAL:O	2.37	0.41
1:A:116:LYS:C	1:A:118:ALA:N	2.77	0.41
1:A:137:PRO:C	1:A:139:SER:N	2.78	0.41
1:A:297:ALA:CB	1:A:299:ALA:H	2.29	0.41
1:A:306:TRP:CH2	1:A:364:GLN:NE2	2.88	0.41
2:B:281:VAL:O	2:B:284:TRP:HB3	2.19	0.41
1:A:49:LYS:HG2	2:B:425:MET:SD	2.60	0.41
1:A:305:ILE:HD11	1:A:357:VAL:CG2	2.50	0.41
1:A:116:LYS:C	1:A:118:ALA:H	2.28	0.41
2:B:285:LEU:HD12	2:B:285:LEU:HA	1.88	0.41
2:B:297:ALA:O	2:B:299:ALA:N	2.54	0.41
2:B:381:LEU:HD12	2:B:381:LEU:HA	1.75	0.41
2:B:390:MET:HB2	2:B:393:TYR:CD2	2.54	0.41
1:A:22:LYS:HE3	1:A:22:LYS:HB2	1.80	0.41
1:A:38:VAL:HG22	1:A:430:LEU:HD22	2.03	0.41
1:A:101:ILE:HD12	1:A:101:ILE:HG21	1.73	0.41
1:A:272:PRO:HA	1:A:276:LEU:HD22	2.02	0.41
2:B:182:LEU:N	2:B:183:PRO:HD3	2.33	0.41
2:B:189:ILE:O	2:B:190:TYR:C	2.63	0.41
2:B:315:VAL:HG13	2:B:316:PRO:HD2	1.98	0.41
2:B:424:SER:C	2:B:425:MET:HG3	2.44	0.41
2:B:431:ILE:HG21	2:B:431:ILE:HD13	1.73	0.41
1:A:396:LEU:HA	1:A:396:LEU:HD12	1.70	0.41
2:B:133:THR:O	2:B:133:THR:CG2	2.68	0.41
2:B:267:ASN:N	2:B:267:ASN:ND2	2.63	0.41
2:B:281:VAL:O	2:B:284:TRP:N	2.38	0.41
2:B:400:SER:C	2:B:402:ALA:N	2.78	0.41
1:A:30:GLY:HA2	2:B:37:THR:HG23	1.99	0.41
1:A:211:HIS:O	1:A:212:ASN:C	2.61	0.41
1:A:392:TYR:O	1:A:392:TYR:CG	2.74	0.41
2:B:109:TRP:CZ2	2:B:113:GLU:HG2	2.55	0.41
1:A:11:ALA:HB2	1:A:168:TRP:HH2	1.86	0.41
1:A:138:MET:HG3	1:A:394:THR:HB	2.01	0.41
1:A:357:VAL:C	1:A:360:VAL:HG23	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:VAL:O	1:A:364:GLN:N	2.54	0.41
2:B:19:ALA:HA	2:B:22:LYS:CG	2.48	0.41
2:B:71:ILE:N	2:B:72:PRO:HD2	2.35	0.41
2:B:116:LYS:O	2:B:117:ARG:C	2.54	0.41
2:B:120:LEU:HD22	2:B:184:CYS:HB3	2.02	0.41
2:B:124:VAL:CG2	2:B:148:LEU:HD23	2.47	0.41
2:B:212:ASN:O	2:B:216:MET:CG	2.64	0.41
2:B:371:TRP:CD1	2:B:371:TRP:N	2.88	0.41
1:A:88:LEU:C	1:A:90:GLU:N	2.79	0.41
1:A:305:ILE:HD13	1:A:305:ILE:HG21	1.76	0.41
2:B:250:LEU:HD12	2:B:420:GLU:HB3	2.03	0.41
2:B:323:LEU:HD22	2:B:325:LYS:H	1.86	0.41
2:B:357:VAL:N	2:B:358:PRO:HD2	2.36	0.41
1:A:14:ILE:O	1:A:16:LYS:N	2.54	0.40
1:A:357:VAL:HB	1:A:358:PRO:HD3	2.02	0.40
1:A:392:TYR:O	1:A:392:TYR:CD2	2.74	0.40
1:A:431:ILE:HD13	1:A:431:ILE:HG21	1.59	0.40
1:A:59:ASP:HA	1:A:60:PRO:HD2	1.70	0.40
1:A:214:THR:CA	1:A:217:LEU:HB2	2.50	0.40
1:A:328:PRO:O	1:A:331:THR:HB	2.21	0.40
2:B:25:ARG:HH11	2:B:25:ARG:HD3	1.51	0.40
2:B:36:ILE:HG21	2:B:48:MET:CE	2.51	0.40
2:B:356:ILE:HG22	2:B:357:VAL:N	2.36	0.40
1:A:33:LEU:HA	1:A:33:LEU:HD22	1.55	0.40
1:A:210:SER:HB2	1:A:229:ARG:HG2	2.03	0.40
1:A:212:ASN:O	1:A:216:MET:N	2.54	0.40
1:A:234:ILE:H	1:A:234:ILE:HG23	1.68	0.40
2:B:195:ARG:HH11	2:B:195:ARG:HD3	1.61	0.40
2:B:337:ALA:CB	2:B:347:PHE:CD2	3.04	0.40
2:B:344:ASP:HA	2:B:345:PRO:HD2	1.84	0.40
1:A:278:ASN:ND2	1:A:393:TYR:HB3	2.36	0.40
1:A:371:TRP:CB	1:A:372:PRO:CD	2.97	0.40
1:A:390:MET:O	1:A:391:ASN:C	2.59	0.40
1:A:93:PHE:CD2	1:A:114:TRP:HZ2	2.39	0.40
1:A:193:LEU:HB3	1:A:194:TYR:CD2	2.56	0.40
1:A:255:LEU:O	2:B:272:PRO:HG2	2.22	0.40
1:A:348:LYS:O	1:A:351:ALA:N	2.54	0.40
1:A:361:LEU:HA	1:A:361:LEU:HD23	1.75	0.40
2:B:55:THR:HB	2:B:96:LEU:HD22	2.02	0.40
2:B:71:ILE:HG21	2:B:328:PRO:O	2.21	0.40
2:B:307:ASN:O	2:B:308:THR:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:HIS:ND1	2:B:322:VAL:N	2.59	0.40

All (26) 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:220:THR:CB	2:B:290:LYS:O[3_664]	1.26	0.94
1:A:195:ARG:NH2	2:B:300:SER:OG[3_664]	1.27	0.93
1:A:195:ARG:CZ	2:B:300:SER:OG[3_664]	1.47	0.73
1:A:195:ARG:CD	2:B:297:ALA:CB[3_664]	1.48	0.72
1:A:290:LYS:CA	2:B:220:THR:OG1[3_764]	1.49	0.71
1:A:191:ARG:NH2	2:B:295:ALA:CB[3_664]	1.52	0.68
1:A:220:THR:OG1	2:B:290:LYS:C[3_664]	1.52	0.68
1:A:290:LYS:O	2:B:221:ASP:N[3_764]	1.52	0.68
1:A:195:ARG:NH2	2:B:300:SER:CB[3_664]	1.53	0.67
1:A:295:ALA:O	2:B:195:ARG:NE[3_764]	1.55	0.65
1:A:220:THR:OG1	2:B:291:ALA:N[3_664]	1.67	0.53
1:A:289:GLN:O	2:B:220:THR:OG1[3_764]	1.67	0.53
1:A:220:THR:CB	2:B:290:LYS:C[3_664]	1.75	0.45
1:A:220:THR:OG1	2:B:290:LYS:O[3_664]	1.76	0.44
1:A:220:THR:CA	2:B:290:LYS:O[3_664]	1.84	0.36
1:A:388:THR:CG2	2:B:303:ASP:OD1[3_664]	1.90	0.30
1:A:290:LYS:O	2:B:221:ASP:CA[3_764]	1.92	0.28
1:A:220:THR:C	2:B:290:LYS:O[3_664]	1.96	0.24
1:A:290:LYS:N	2:B:220:THR:OG1[3_764]	1.97	0.23
1:A:194:TYR:O	2:B:297:ALA:CB[3_664]	1.99	0.21
1:A:156:ARG:NH2	2:B:23:THR:O[1_455]	2.00	0.20
1:A:195:ARG:CD	2:B:297:ALA:N[3_664]	2.04	0.16
1:A:195:ARG:CD	2:B:297:ALA:CA[3_664]	2.06	0.14
1:A:289:GLN:C	2:B:220:THR:OG1[3_764]	2.06	0.14
1:A:27:GLN:NE2	2:B:156:ARG:NH1[1_545]	2.07	0.13
1:A:295:ALA:O	2:B:195:ARG:CD[3_764]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/433 (98%)	319 (75%)	77 (18%)	27 (6%)	1	3
2	B	423/429 (99%)	325 (77%)	72 (17%)	26 (6%)	1	3
All	All	846/862 (98%)	644 (76%)	149 (18%)	53 (6%)	1	3

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	14	ILE
1	A	67	ARG
1	A	164	ARG
2	B	3	SER
2	B	6	LEU
2	B	67	ARG
2	B	118	ALA
2	B	149	ASN
2	B	164	ARG
2	B	190	TYR
2	B	341	LEU
1	A	3	SER
1	A	169	GLU
1	A	190	TYR
1	A	236	SER
1	A	340	HIS
1	A	348	LYS
2	B	11	ALA
2	B	81	GLY
2	B	191	ARG
2	B	289	GLN
2	B	308	THR
1	A	29	GLY
1	A	238	HIS
1	A	407	ALA
1	A	426	SER
2	B	52	VAL
2	B	85	GLY
2	B	389	GLU
1	A	32	ALA
1	A	191	ARG
1	A	239	GLU

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Mol	Chain	Res	Type
1	A	289	GLN
2	B	304	TYR
2	B	403	LEU
1	A	280	GLU
1	A	341	LEU
1	A	345	PRO
2	B	51	LEU
2	B	90	GLU
2	B	345	PRO
2	B	426	SER
2	B	87	PRO
2	B	144	ALA
2	B	257	ASP
2	B	350	VAL
1	A	50	GLY
1	A	369	ASN
1	A	281	VAL
1	A	316	PRO
1	A	15	PRO
1	A	52	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	344/345 (100%)	230 (67%)	114 (33%)	0	1
2	B	344/345 (100%)	242 (70%)	102 (30%)	0	1
All	All	688/690 (100%)	472 (69%)	216 (31%)	0	1

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	5	ASN
1	A	10	LEU

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Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	LYS
1	A	17	GLU
1	A	20	ARG
1	A	23	THR
1	A	25	ARG
1	A	33	LEU
1	A	35	GLN
1	A	36	ILE
1	A	37	THR
1	A	38	VAL
1	A	39	ASP
1	A	41	SER
1	A	46	ARG
1	A	48	MET
1	A	49	LYS
1	A	57	VAL
1	A	58	LEU
1	A	62	GLU
1	A	64	ILE
1	A	65	ARG
1	A	73	GLU
1	A	76	LYS
1	A	80	LYS
1	A	86	GLU
1	A	88	LEU
1	A	92	LEU
1	A	101	ILE
1	A	103	THR
1	A	108	SER
1	A	110	LEU
1	A	111	SER
1	A	112	LYS
1	A	125	VAL
1	A	131	PHE
1	A	134	ASN
1	A	139	SER
1	A	140	GLN
1	A	149	ASN
1	A	156	ARG
1	A	166	LYS
1	A	171	VAL

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Mol	Chain	Res	Type
1	A	179	ILE
1	A	181	LYS
1	A	182	LEU
1	A	189	ILE
1	A	191	ARG
1	A	193	LEU
1	A	195	ARG
1	A	199	SER
1	A	200	ILE
1	A	203	ILE
1	A	206	LYS
1	A	207	LEU
1	A	212	ASN
1	A	214	THR
1	A	217	LEU
1	A	225	THR
1	A	228	MET
1	A	229	ARG
1	A	233	THR
1	A	244	SER
1	A	251	VAL
1	A	256	SER
1	A	261	SER
1	A	266	MET
1	A	276	LEU
1	A	284	TRP
1	A	285	LEU
1	A	287	GLN
1	A	289	GLN
1	A	290	LYS
1	A	300	SER
1	A	301	LEU
1	A	305	ILE
1	A	306	TRP
1	A	307	ASN
1	A	308	THR
1	A	310	ASN
1	A	314	VAL
1	A	323	LEU
1	A	324	ARG
1	A	325	LYS
1	A	331	THR

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Mol	Chain	Res	Type
1	A	334	ARG
1	A	335	GLU
1	A	338	LEU
1	A	340	HIS
1	A	341	LEU
1	A	348	LYS
1	A	353	LEU
1	A	356	ILE
1	A	360	VAL
1	A	362	LEU
1	A	363	GLU
1	A	371	TRP
1	A	374	VAL
1	A	381	LEU
1	A	383	GLN
1	A	387	MET
1	A	388	THR
1	A	390	MET
1	A	394	THR
1	A	396	LEU
1	A	405	VAL
1	A	409	LEU
1	A	412	SER
1	A	413	ARG
1	A	415	LEU
1	A	423	LYS
1	A	424	SER
2	B	4	THR
2	B	5	ASN
2	B	10	LEU
2	B	13	LEU
2	B	23	THR
2	B	25	ARG
2	B	26	GLN
2	B	27	GLN
2	B	28	HIS
2	B	33	LEU
2	B	36	ILE
2	B	38	VAL
2	B	39	ASP
2	B	40	MET
2	B	41	SER

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Mol	Chain	Res	Type
2	B	46	ARG
2	B	49	LYS
2	B	56	SER
2	B	61	ASP
2	B	62	GLU
2	B	64	ILE
2	B	65	ARG
2	B	71	ILE
2	B	73	GLU
2	B	76	LYS
2	B	80	LYS
2	B	86	GLU
2	B	101	ILE
2	B	112	LYS
2	B	116	LYS
2	B	120	LEU
2	B	125	VAL
2	B	127	MET
2	B	134	ASN
2	B	146	THR
2	B	149	ASN
2	B	166	LYS
2	B	171	VAL
2	B	184	CYS
2	B	188	LYS
2	B	189	ILE
2	B	191	ARG
2	B	192	ASN
2	B	193	LEU
2	B	199	SER
2	B	203	ILE
2	B	204	ASP
2	B	205	SER
2	B	206	LYS
2	B	207	LEU
2	B	210	SER
2	B	212	ASN
2	B	214	THR
2	B	228	MET
2	B	234	ILE
2	B	251	VAL
2	B	260	LEU

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Mol	Chain	Res	Type
2	B	261	SER
2	B	276	LEU
2	B	281	VAL
2	B	285	LEU
2	B	287	GLN
2	B	289	GLN
2	B	301	LEU
2	B	306	TRP
2	B	307	ASN
2	B	308	THR
2	B	310	ASN
2	B	314	VAL
2	B	323	LEU
2	B	324	ARG
2	B	325	LYS
2	B	332	CYS
2	B	335	GLU
2	B	338	LEU
2	B	341	LEU
2	B	352	GLN
2	B	353	LEU
2	B	360	VAL
2	B	362	LEU
2	B	364	GLN
2	B	371	TRP
2	B	374	VAL
2	B	377	HIS
2	B	381	LEU
2	B	382	LEU
2	B	383	GLN
2	B	388	THR
2	B	390	MET
2	B	391	ASN
2	B	394	THR
2	B	401	ARG
2	B	405	VAL
2	B	406	LEU
2	B	409	LEU
2	B	412	SER
2	B	413	ARG
2	B	415	LEU
2	B	423	LYS

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Mol	Chain	Res	Type
2	B	428	ASP
2	B	431	ILE
2	B	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	26	GLN
1	A	27	GLN
1	A	28	HIS
1	A	35	GLN
1	A	134	ASN
1	A	136	HIS
1	A	140	GLN
1	A	149	ASN
1	A	192	ASN
1	A	212	ASN
1	A	223	GLN
1	A	238	HIS
1	A	267	ASN
1	A	278	ASN
1	A	287	GLN
1	A	310	ASN
1	A	352	GLN
1	A	364	GLN
1	A	383	GLN
1	A	391	ASN
2	B	26	GLN
2	B	27	GLN
2	B	28	HIS
2	B	100	GLN
2	B	123	HIS
2	B	136	HIS
2	B	140	GLN
2	B	149	ASN
2	B	153	ASN
2	B	192	ASN
2	B	223	GLN
2	B	238	HIS
2	B	242	ASN
2	B	267	ASN

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Mol	Chain	Res	Type
2	B	278	ASN
2	B	287	GLN
2	B	310	ASN
2	B	352	GLN
2	B	383	GLN
2	B	391	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
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	291:ALA	C	295:ALA	N	9.25

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	82:GLY	C	84:GLY	N	3.42

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.