



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:51 AM UTC

PDB ID : 2ATC / pdb_00002atc
Title : CRYSTAL AND MOLECULAR STRUCTURES OF NATIVE AND CTP-LIGANDED ASPARTATE CARBAMOYLTRANSFERASE FROM ES-CHERICHIA COLI
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Deposited on : 1982-03-24
Resolution : 3.00 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

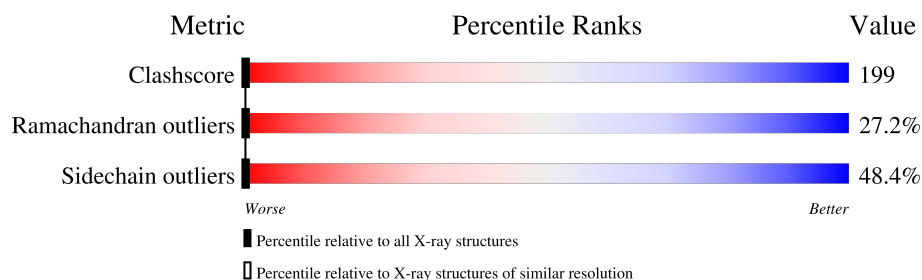
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	305	
2	B	152	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	B	153	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3511 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 ASPARTATE CARBAMOYLTRANSFERASE, CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	X	0	0	0
			2362	1491	420	441	8	2			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	SER	LYS	conflict	UNP P0A786
A	60	GLN	GLU	conflict	UNP P0A786
A	86	GLN	GLU	conflict	UNP P0A786
A	90	ASN	ASP	conflict	UNP P0A786
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLU	GLN	conflict	UNP P0A786
A	153	ASN	ASP	conflict	UNP P0A786
A	196	GLU	GLN	conflict	UNP P0A786
A	?	-	MET	deletion	UNP P0A786
A	?	-	ALA	deletion	UNP P0A786
A	?	-	GLU	deletion	UNP P0A786
A	?	-	VAL	deletion	UNP P0A786
A	?	-	ASP	deletion	UNP P0A786
A	?	-	ILE	deletion	UNP P0A786
A	?	-	LEU	deletion	UNP P0A786
A	?	-	TYR	deletion	UNP P0A786
A	234	ASX	ASN	conflict	UNP P0A786
A	240	LEU	VAL	conflict	UNP P0A786
A	241	VAL	LEU	conflict	UNP P0A786
A	244	ASN	-	insertion	UNP P0A786
A	246	LEU	-	insertion	UNP P0A786
A	247	GLY	-	insertion	UNP P0A786
A	248	GLY	ASP	conflict	UNP P0A786
A	254	MET	ALA	conflict	UNP P0A786
A	256	ALA	MET	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	152	Total	C	N	O	S	0	0	0
			1148	714	202	227	5			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ASN	ASP	conflict	UNP P0A7F3
B	5	ASP	ASN	conflict	UNP P0A7F3
B	10	ALA	GLU	conflict	UNP P0A7F3
B	11	GLU	ALA	conflict	UNP P0A7F3
B	19	ASN	ASP	conflict	UNP P0A7F3
B	24	GLU	GLN	conflict	UNP P0A7F3
B	39	GLN	ASP	conflict	UNP P0A7F3
B	40	ASP	GLN	conflict	UNP P0A7F3
B	70	GLU	GLN	conflict	UNP P0A7F3
B	73	GLU	GLN	conflict	UNP P0A7F3
B	87	ASN	ASP	conflict	UNP P0A7F3
B	88	ASP	ASN	conflict	UNP P0A7F3
B	103	ASN	-	insertion	UNP P0A7F3
B	?	-	ASN	deletion	UNP P0A7F3
B	111	ASP	ASN	conflict	UNP P0A7F3
B	?	-	LYS	deletion	UNP P0A7F3
B	131	ASP	ASN	conflict	UNP P0A7F3

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

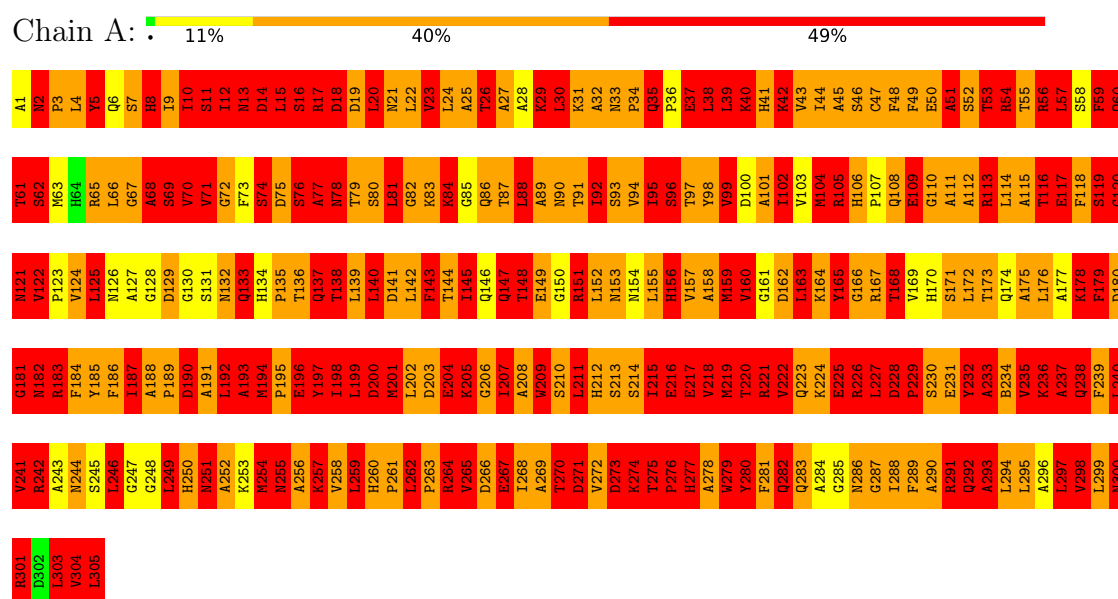
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

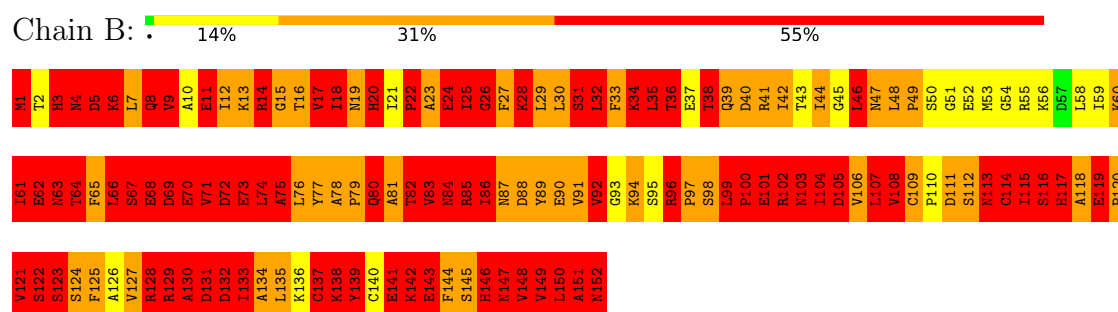
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE, REGULATORY CHAIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	131.70Å 131.70Å 199.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.270 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3511	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2.28	96/2399 (4.0%)	4.51	719/3256 (22.1%)
2	B	2.38	48/1165 (4.1%)	4.50	375/1575 (23.8%)
All	All	2.31	144/3564 (4.0%)	4.50	1094/4831 (22.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
2	B	0	4
All	All	0	19

All (144) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	15	GLY	N-CA	13.98	1.65	1.45
1	A	230	SER	N-CA	12.34	1.62	1.46
1	A	230	SER	C-O	12.21	1.39	1.24
1	A	231	GLU	N-CA	9.65	1.57	1.46
1	A	239	PHE	CA-CB	-8.73	1.40	1.53
2	B	64	THR	C-O	8.57	1.34	1.24
1	A	79	THR	N-CA	8.53	1.55	1.45
2	B	104	ILE	CA-C	-8.43	1.42	1.52
1	A	9	ILE	CA-CB	8.38	1.64	1.54
1	A	251	ASN	N-CA	8.24	1.56	1.46
2	B	56	LYS	N-CA	8.24	1.56	1.46
1	A	224	LYS	N-CA	8.21	1.55	1.46
1	A	26	THR	N-CA	8.15	1.56	1.46
2	B	81	ALA	N-CA	8.15	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	THR	CA-CB	7.91	1.64	1.53
2	B	50	SER	CA-C	7.86	1.62	1.52
2	B	38	THR	CA-CB	7.79	1.66	1.53
1	A	33	ASN	CA-CB	7.69	1.65	1.53
1	A	234	ASX	C-N	-7.56	1.35	1.43
1	A	71	VAL	N-CA	7.54	1.55	1.46
1	A	277	HIS	CE1-NE2	-7.53	1.25	1.32
2	B	116	SER	C-O	7.36	1.32	1.23
2	B	2	THR	CA-CB	7.28	1.62	1.53
2	B	62	GLU	N-CA	-7.24	1.36	1.45
1	A	296	ALA	CA-CB	-7.18	1.41	1.53
2	B	129	ARG	CZ-NH2	7.13	1.42	1.33
2	B	91	VAL	CA-CB	7.01	1.63	1.54
1	A	61	THR	CA-CB	6.94	1.65	1.53
1	A	277	HIS	C-O	6.94	1.32	1.24
2	B	89	TYR	C-O	6.91	1.32	1.24
1	A	217	GLU	C-N	-6.89	1.24	1.33
1	A	5	TYR	CA-CB	6.75	1.64	1.53
1	A	102	ILE	CA-C	-6.74	1.44	1.52
2	B	118	ALA	N-CA	6.73	1.54	1.46
1	A	246	LEU	CA-C	6.70	1.61	1.52
1	A	207	ILE	CA-CB	6.70	1.63	1.54
1	A	291	ARG	NE-CZ	-6.68	1.25	1.33
1	A	286	ASN	C-N	-6.68	1.25	1.34
1	A	158	ALA	N-CA	6.66	1.53	1.46
1	A	264	ARG	CD-NE	-6.65	1.36	1.46
1	A	17	ARG	C-O	6.63	1.32	1.24
2	B	71	VAL	CA-CB	6.53	1.63	1.54
1	A	214	SER	CA-CB	-6.47	1.44	1.53
1	A	242	ARG	CA-C	6.46	1.61	1.53
1	A	79	THR	CB-OG1	6.42	1.54	1.43
1	A	169	VAL	C-N	-6.38	1.25	1.33
1	A	122	VAL	CA-CB	-6.31	1.46	1.54
1	A	112	ALA	CA-CB	-6.24	1.43	1.53
1	A	291	ARG	CD-NE	-6.24	1.37	1.46
1	A	54	ARG	C-N	-6.20	1.25	1.34
1	A	43	VAL	C-N	-6.20	1.25	1.33
1	A	250	HIS	C-O	6.20	1.31	1.24
2	B	143	GLU	CA-CB	6.18	1.62	1.53
1	A	93	SER	C-N	-6.18	1.26	1.33
1	A	29	LYS	C-O	-6.13	1.17	1.24
2	B	105	ASP	N-CA	6.09	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	VAL	N-CA	6.07	1.53	1.46
1	A	196	GLU	C-N	-6.05	1.26	1.33
2	B	53	MET	C-O	6.02	1.31	1.24
1	A	214	SER	C-N	-6.02	1.25	1.33
1	A	61	THR	C-O	-6.00	1.16	1.24
2	B	131	ASP	CA-C	5.92	1.60	1.52
1	A	106	HIS	CE1-NE2	-5.90	1.26	1.32
2	B	78	ALA	N-CA	5.88	1.53	1.46
2	B	15	GLY	C-N	-5.87	1.26	1.33
1	A	172	LEU	N-CA	-5.86	1.39	1.46
1	A	65	ARG	CD-NE	5.84	1.54	1.46
1	A	238	GLN	N-CA	5.84	1.53	1.46
1	A	219	MET	CA-C	-5.83	1.46	1.53
2	B	104	ILE	N-CA	-5.82	1.39	1.46
1	A	181	GLY	C-O	5.82	1.31	1.23
2	B	54	GLY	N-CA	5.78	1.53	1.45
2	B	93	GLY	C-O	5.77	1.31	1.23
1	A	52	SER	N-CA	5.77	1.53	1.46
1	A	262	LEU	C-O	-5.77	1.16	1.24
1	A	296	ALA	N-CA	5.75	1.53	1.46
2	B	65	PHE	N-CA	5.75	1.53	1.46
1	A	147	GLN	CA-CB	-5.72	1.43	1.53
1	A	301	ARG	CZ-NH1	5.71	1.40	1.32
1	A	226	ARG	N-CA	5.69	1.54	1.46
1	A	301	ARG	CZ-NH2	5.64	1.40	1.33
1	A	175	ALA	CA-CB	-5.63	1.45	1.53
2	B	124	SER	N-CA	5.62	1.52	1.46
1	A	62	SER	C-O	-5.60	1.17	1.24
1	A	238	GLN	CA-CB	-5.60	1.44	1.53
1	A	120	GLY	C-N	-5.59	1.25	1.33
1	A	45	ALA	C-N	-5.58	1.26	1.33
1	A	39	LEU	C-O	5.58	1.30	1.23
2	B	129	ARG	CA-CB	5.57	1.62	1.53
2	B	136	LYS	N-CA	5.56	1.52	1.46
2	B	98	SER	C-O	5.53	1.30	1.23
2	B	113	ASN	C-N	-5.52	1.25	1.33
1	A	122	VAL	N-CA	5.52	1.53	1.46
1	A	97	THR	CA-CB	5.51	1.62	1.53
2	B	130	ALA	C-N	-5.51	1.25	1.33
2	B	18	ILE	C-N	-5.50	1.26	1.33
1	A	292	GLN	N-CA	5.49	1.53	1.46
2	B	123	SER	N-CA	5.49	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	144	PHE	C-O	5.49	1.30	1.24
1	A	67	GLY	N-CA	5.49	1.53	1.45
2	B	73	GLU	N-CA	-5.48	1.39	1.46
1	A	248	GLY	N-CA	-5.46	1.37	1.45
1	A	247	GLY	N-CA	-5.45	1.39	1.45
1	A	87	THR	CA-C	-5.44	1.46	1.52
2	B	94	LYS	C-N	5.44	1.41	1.33
1	A	10	ILE	CA-CB	5.42	1.61	1.54
1	A	212	HIS	CA-CB	5.41	1.63	1.53
1	A	35	GLN	C-O	5.40	1.30	1.24
1	A	189	PRO	C-N	-5.40	1.26	1.33
2	B	65	PHE	C-O	5.39	1.30	1.24
1	A	153	ASN	C-N	-5.38	1.26	1.33
1	A	35	GLN	CD-NE2	5.38	1.44	1.33
1	A	79	THR	C-O	5.37	1.30	1.23
1	A	45	ALA	N-CA	5.35	1.52	1.46
1	A	249	LEU	CA-C	5.34	1.59	1.52
1	A	197	TYR	N-CA	5.29	1.53	1.46
1	A	273	ASP	C-N	-5.29	1.26	1.33
1	A	242	ARG	CZ-NH2	5.28	1.40	1.33
1	A	263	PRO	N-CD	-5.26	1.40	1.47
1	A	267	GLU	C-N	-5.25	1.26	1.33
2	B	87	ASN	N-CA	5.25	1.52	1.46
2	B	104	ILE	C-N	-5.25	1.26	1.33
2	B	42	ILE	CA-CB	5.24	1.63	1.54
2	B	92	VAL	C-O	5.23	1.30	1.24
1	A	89	ALA	C-O	-5.23	1.17	1.24
1	A	239	PHE	C-N	-5.23	1.26	1.33
1	A	10	ILE	C-N	-5.22	1.26	1.33
2	B	19	ASN	C-O	5.22	1.30	1.23
2	B	126	ALA	N-CA	5.21	1.52	1.46
1	A	49	PHE	CA-CB	-5.17	1.45	1.53
2	B	117	HIS	CB-CG	-5.16	1.43	1.50
1	A	4	LEU	C-N	-5.16	1.26	1.33
2	B	138	LYS	N-CA	5.16	1.52	1.46
1	A	12	ILE	N-CA	-5.15	1.40	1.46
1	A	16	SER	N-CA	-5.15	1.39	1.46
2	B	18	ILE	CA-C	5.14	1.59	1.52
1	A	113	ARG	N-CA	5.14	1.52	1.46
2	B	3	HIS	ND1-CE1	5.13	1.37	1.32
1	A	43	VAL	N-CA	5.13	1.51	1.46
1	A	54	ARG	C-O	-5.12	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	ALA	N-CA	5.10	1.52	1.46
1	A	89	ALA	C-N	-5.07	1.26	1.33
1	A	69	SER	C-O	5.03	1.28	1.24
2	B	16	THR	CA-C	5.01	1.59	1.52

All (1094) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	ASP	CA-CB-CG	36.36	148.96	112.60
1	A	301	ARG	CD-NE-CZ	25.46	160.05	124.40
1	A	271	ASP	CA-CB-CG	24.21	136.81	112.60
2	B	103	ASN	CA-CB-CG	-22.09	90.51	112.60
1	A	212	HIS	CA-CB-CG	-21.96	91.84	113.80
2	B	117	HIS	CA-CB-CG	21.93	135.73	113.80
1	A	292	GLN	OE1-CD-NE2	-21.53	101.07	122.60
1	A	204	GLU	CB-CG-CD	21.46	149.08	112.60
1	A	242	ARG	CD-NE-CZ	21.11	153.95	124.40
1	A	147	GLN	CA-CB-CG	20.34	154.79	114.10
2	B	16	THR	N-CA-CB	19.31	142.82	110.77
1	A	43	VAL	CA-C-O	-18.83	101.90	121.67
1	A	292	GLN	CB-CG-CD	18.79	144.53	112.60
1	A	21	ASN	CA-CB-CG	18.45	131.05	112.60
1	A	152	LEU	CA-C-N	18.36	149.56	122.39
1	A	152	LEU	C-N-CA	18.36	149.56	122.39
1	A	227	LEU	CA-C-O	-18.27	101.11	121.58
1	A	291	ARG	CD-NE-CZ	18.07	149.70	124.40
1	A	149	GLU	CA-C-N	17.94	153.19	121.07
1	A	149	GLU	C-N-CA	17.94	153.19	121.07
2	B	143	GLU	CB-CG-CD	17.76	142.78	112.60
1	A	38	LEU	O-C-N	17.54	142.75	122.22
1	A	102	ILE	CA-C-O	-17.38	99.06	120.78
1	A	54	ARG	CD-NE-CZ	17.12	148.37	124.40
1	A	292	GLN	CA-CB-CG	16.80	147.69	114.10
1	A	121	ASN	CA-CB-CG	16.42	129.02	112.60
2	B	84	ASN	CA-CB-CG	16.03	128.63	112.60
1	A	238	GLN	N-CA-C	-15.99	93.72	113.38
2	B	72	ASP	CA-C-N	15.89	142.86	120.29
2	B	72	ASP	C-N-CA	15.89	142.86	120.29
2	B	149	VAL	O-C-N	15.83	142.36	122.57
1	A	143	PHE	CA-CB-CG	15.75	129.55	113.80
1	A	249	LEU	N-CA-CB	15.36	133.23	110.35
2	B	27	PHE	N-CA-C	-15.27	94.08	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ILE	CA-C-N	15.09	146.16	122.62
2	B	61	ILE	C-N-CA	15.09	146.16	122.62
1	A	8	HIS	CA-CB-CG	-14.94	98.86	113.80
1	A	167	ARG	CD-NE-CZ	14.91	145.27	124.40
2	B	72	ASP	CA-CB-CG	-14.89	97.71	112.60
1	A	45	ALA	CA-C-O	-14.88	104.29	120.36
1	A	143	PHE	CA-C-O	14.21	140.84	120.51
1	A	251	ASN	CA-C-O	-14.14	100.29	120.51
1	A	26	THR	CA-CB-OG1	-14.09	88.47	109.60
1	A	19	ASP	CA-CB-CG	13.97	126.57	112.60
1	A	15	LEU	CA-C-N	13.92	142.69	122.09
1	A	15	LEU	C-N-CA	13.92	142.69	122.09
1	A	33	ASN	CA-CB-CG	-13.74	98.86	112.60
1	A	223	GLN	OE1-CD-NE2	13.68	136.28	122.60
2	B	97	PRO	CA-C-O	-13.45	107.15	121.27
1	A	169	VAL	CA-C-N	13.36	138.61	120.44
1	A	169	VAL	C-N-CA	13.36	138.61	120.44
1	A	94	VAL	CA-C-O	13.33	134.69	120.69
1	A	9	ILE	N-CA-CB	-13.14	96.39	110.72
1	A	125	LEU	CB-CA-C	13.11	133.30	109.71
2	B	5	ASP	CA-C-O	12.99	136.08	121.40
2	B	16	THR	O-C-N	12.99	137.81	123.52
1	A	108	GLN	CA-C-O	-12.93	105.38	121.67
1	A	220	THR	O-C-N	12.89	139.74	122.59
1	A	305	LEU	CA-CB-CG	12.81	161.14	116.30
1	A	250	HIS	CB-CA-C	12.77	135.84	110.42
1	A	226	ARG	N-CA-CB	-12.76	88.89	110.46
2	B	127	VAL	N-CA-C	12.71	126.55	107.99
1	A	200	ASP	CA-CB-CG	-12.65	99.95	112.60
1	A	95	ILE	N-CA-CB	-12.62	97.37	110.62
1	A	23	VAL	N-CA-C	-12.60	97.77	110.62
1	A	258	VAL	CA-C-O	-12.56	105.98	120.67
1	A	230	SER	CA-C-O	-12.38	102.81	120.51
2	B	50	SER	N-CA-C	-12.37	96.72	113.30
1	A	299	LEU	N-CA-C	12.37	128.22	112.89
1	A	204	GLU	CA-CB-CG	12.34	138.79	114.10
1	A	264	ARG	CD-NE-CZ	12.32	141.65	124.40
1	A	13	ASN	N-CA-C	-12.27	97.59	110.97
2	B	70	GLU	N-CA-C	-12.25	98.32	113.02
1	A	168	THR	CA-CB-OG1	-12.18	91.33	109.60
1	A	204	GLU	CA-C-N	12.17	144.78	121.54
1	A	204	GLU	C-N-CA	12.17	144.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	60	GLN	OE1-CD-NE2	-12.16	110.44	122.60
2	B	144	PHE	CA-CB-CG	12.14	125.94	113.80
1	A	73	PHE	CA-C-O	-12.06	107.67	121.06
1	A	144	THR	OG1-CB-CG2	11.92	133.15	109.30
2	B	37	GLU	CA-C-O	-11.89	108.07	121.39
1	A	243	ALA	N-CA-CB	-11.88	95.29	110.98
1	A	106	HIS	CA-CB-CG	11.88	125.68	113.80
2	B	84	ASN	OD1-CG-ND2	-11.88	110.72	122.60
1	A	217	GLU	N-CA-CB	11.87	129.22	109.87
1	A	235	VAL	N-CA-CB	11.87	131.67	111.50
1	A	56	ARG	CD-NE-CZ	-11.82	107.85	124.40
2	B	16	THR	CA-C-O	-11.79	106.98	120.31
1	A	108	GLN	O-C-N	11.78	137.17	121.74
2	B	125	PHE	CA-C-O	-11.77	107.64	120.36
1	A	167	ARG	NE-CZ-NH2	11.76	129.79	119.20
1	A	226	ARG	CB-CA-C	11.70	131.34	111.22
2	B	75	ALA	CA-C-N	11.68	136.32	120.44
2	B	75	ALA	C-N-CA	11.68	136.32	120.44
1	A	220	THR	N-CA-CB	11.61	130.11	110.49
1	A	25	ALA	CA-C-O	-11.52	105.94	120.00
1	A	247	GLY	CA-C-N	11.47	143.89	121.41
1	A	247	GLY	C-N-CA	11.47	143.89	121.41
2	B	103	ASN	CA-C-N	-11.46	101.34	121.97
2	B	103	ASN	C-N-CA	-11.46	101.34	121.97
1	A	212	HIS	O-C-N	11.45	134.79	123.46
2	B	18	ILE	CA-C-N	11.45	139.64	122.47
2	B	18	ILE	C-N-CA	11.45	139.64	122.47
1	A	266	ASP	CA-CB-CG	-11.42	101.18	112.60
2	B	105	ASP	CA-CB-CG	-11.41	101.19	112.60
1	A	129	ASP	CA-CB-CG	11.40	124.00	112.60
1	A	175	ALA	N-CA-C	-11.36	95.95	111.96
2	B	91	VAL	N-CA-C	11.27	124.44	107.77
1	A	239	PHE	CA-C-N	11.25	143.26	121.66
1	A	239	PHE	C-N-CA	11.25	143.26	121.66
1	A	225	GLU	CB-CG-CD	-11.25	93.48	112.60
1	A	160	VAL	N-CA-CB	-11.22	97.32	111.46
1	A	270	THR	CA-CB-OG1	-11.21	92.79	109.60
1	A	192	LEU	CA-C-O	11.19	134.42	120.65
2	B	70	GLU	CA-C-O	11.18	132.96	119.43
1	A	269	ALA	N-CA-C	11.14	127.41	109.24
1	A	116	THR	N-CA-CB	11.03	129.12	110.49
2	B	2	THR	CA-C-O	-11.02	108.79	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	ASN	OD1-CG-ND2	10.97	133.57	122.60
2	B	4	ASN	CA-C-N	10.96	139.97	122.21
2	B	4	ASN	C-N-CA	10.96	139.97	122.21
1	A	126	ASN	CA-C-O	-10.93	108.61	120.30
2	B	70	GLU	CA-C-N	10.90	141.59	121.97
2	B	70	GLU	C-N-CA	10.90	141.59	121.97
1	A	106	HIS	N-CA-CB	-10.89	95.90	111.25
2	B	31	SER	N-CA-C	-10.88	100.13	113.41
1	A	57	LEU	CB-CA-C	10.88	128.85	110.79
1	A	155	LEU	CA-C-O	10.86	134.91	121.66
1	A	69	SER	CA-C-O	10.79	132.37	121.05
1	A	231	GLU	CA-C-O	-10.75	109.53	121.25
1	A	73	PHE	O-C-N	10.73	133.07	123.41
1	A	180	ASP	N-CA-C	10.72	125.20	108.79
1	A	207	ILE	N-CA-C	10.69	131.57	109.34
1	A	242	ARG	NE-CZ-NH1	10.69	132.19	121.50
1	A	33	ASN	N-CA-CB	-10.68	91.35	110.37
1	A	8	HIS	O-C-N	10.67	135.54	123.16
2	B	117	HIS	O-C-N	10.66	136.77	122.59
1	A	71	VAL	N-CA-CB	-10.60	93.74	111.23
1	A	219	MET	CA-C-O	-10.59	110.17	122.13
2	B	22	PRO	N-CA-C	-10.57	90.69	112.47
2	B	137	CYS	O-C-N	10.57	136.65	122.59
1	A	212	HIS	CB-CA-C	-10.56	92.69	110.43
1	A	11	SER	CA-C-N	10.49	140.85	121.97
1	A	11	SER	C-N-CA	10.49	140.85	121.97
1	A	89	ALA	O-C-N	10.47	136.52	122.59
2	B	137	CYS	CA-C-O	-10.46	105.55	120.51
1	A	33	ASN	OD1-CG-ND2	10.46	133.06	122.60
1	A	196	GLU	O-C-N	10.36	139.10	122.42
1	A	212	HIS	CA-C-O	-10.35	109.71	121.10
1	A	288	ILE	N-CA-CB	10.30	132.69	111.05
1	A	205	LYS	CA-CB-CG	10.30	134.69	114.10
1	A	188	ALA	CA-C-O	10.28	129.73	119.86
1	A	288	ILE	O-C-N	10.24	135.46	122.05
1	A	141	ASP	CA-CB-CG	-10.22	102.38	112.60
2	B	36	THR	N-CA-CB	10.19	127.72	110.49
1	A	16	SER	O-C-N	10.16	134.95	123.16
2	B	47	ASN	O-C-N	10.14	135.57	122.39
1	A	197	TYR	O-C-N	-10.12	110.25	122.19
1	A	242	ARG	N-CA-CB	10.09	129.33	110.56
1	A	203	ASP	CA-CB-CG	10.07	122.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ASP	CA-CB-CG	-10.05	102.55	112.60
2	B	68	GLU	N-CA-CB	9.95	127.31	110.49
1	A	225	GLU	CA-C-O	9.94	131.10	120.36
1	A	197	TYR	CB-CA-C	9.93	128.46	110.88
1	A	144	THR	N-CA-CB	-9.92	93.72	110.49
2	B	68	GLU	N-CA-C	-9.91	89.68	110.80
2	B	24	GLU	N-CA-CB	-9.91	95.75	113.10
1	A	153	ASN	CB-CG-ND2	-9.91	101.53	116.40
1	A	54	ARG	NE-CZ-NH2	-9.90	110.29	119.20
1	A	240	LEU	N-CA-C	-9.86	96.74	110.35
1	A	246	LEU	CA-C-N	9.84	141.59	121.22
1	A	246	LEU	C-N-CA	9.84	141.59	121.22
1	A	121	ASN	OD1-CG-ND2	-9.84	112.76	122.60
1	A	134	HIS	CA-C-N	9.82	130.86	119.47
1	A	134	HIS	C-N-CA	9.82	130.86	119.47
1	A	158	ALA	CA-C-O	-9.82	109.22	120.31
1	A	18	ASP	N-CA-CB	-9.80	93.93	110.49
1	A	144	THR	CB-CA-C	9.79	129.90	110.42
1	A	270	THR	CA-CB-CG2	9.77	127.10	110.50
2	B	16	THR	N-CA-C	-9.74	93.75	108.46
2	B	118	ALA	CB-CA-C	9.74	129.80	110.42
1	A	165	TYR	N-CA-C	-9.72	101.58	113.15
2	B	150	LEU	CB-CA-C	9.71	127.45	111.05
1	A	225	GLU	CG-CD-OE2	-9.70	96.08	118.40
1	A	303	LEU	CA-C-O	9.70	131.81	121.33
1	A	10	ILE	CA-C-O	-9.69	108.67	120.78
2	B	14	ARG	NE-CZ-NH2	9.68	127.91	119.20
1	A	217	GLU	O-C-N	9.65	134.90	123.02
2	B	152	ASN	CA-CB-CG	-9.64	102.95	112.60
1	A	237	ALA	N-CA-C	-9.64	90.26	110.80
1	A	21	ASN	OD1-CG-ND2	-9.64	112.96	122.60
1	A	38	LEU	CA-C-O	-9.63	109.22	120.10
1	A	5	TYR	CA-CB-CG	-9.62	96.58	113.90
1	A	77	ALA	O-C-N	9.60	135.36	122.59
2	B	39	GLN	N-CA-C	9.57	122.70	111.02
1	A	35	GLN	CA-CB-CG	9.55	133.21	114.10
1	A	238	GLN	CA-CB-CG	9.51	133.11	114.10
2	B	47	ASN	CA-CB-CG	9.50	122.10	112.60
1	A	86	GLN	N-CA-C	9.49	123.36	110.55
2	B	116	SER	CA-C-O	-9.49	111.46	120.95
1	A	16	SER	CA-C-O	-9.49	110.01	120.92
1	A	221	ARG	NE-CZ-NH2	9.48	127.74	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASN	OD1-CG-ND2	9.47	132.07	122.60
1	A	159	MET	CB-CA-C	9.46	124.43	110.62
1	A	225	GLU	CA-C-N	-9.44	109.17	123.14
1	A	225	GLU	C-N-CA	-9.44	109.17	123.14
1	A	34	PRO	CA-C-N	9.43	134.02	122.42
1	A	34	PRO	C-N-CA	9.43	134.02	122.42
1	A	109	GLU	CA-C-O	-9.43	111.22	121.78
1	A	125	LEU	N-CA-C	-9.40	95.56	110.14
1	A	210	SER	N-CA-CB	-9.38	95.37	111.69
1	A	90	ASN	N-CA-C	-9.37	90.84	110.80
1	A	127	ALA	N-CA-C	-9.36	101.99	113.50
1	A	214	SER	CA-C-O	-9.36	110.28	121.60
2	B	127	VAL	CB-CA-C	-9.36	98.16	110.98
1	A	183	ARG	CA-C-O	9.29	133.79	120.51
1	A	288	ILE	CA-C-O	-9.26	108.36	119.85
2	B	148	VAL	CA-C-O	-9.26	109.21	120.78
1	A	287	GLY	N-CA-C	-9.25	103.19	114.66
1	A	66	LEU	N-CA-C	-9.24	102.00	113.18
1	A	129	ASP	N-CA-CB	9.23	124.49	110.19
1	A	1	ALA	N-CA-CB	-9.22	96.57	110.40
1	A	238	GLN	N-CA-CB	9.21	124.25	110.53
1	A	269	ALA	CA-C-O	-9.18	110.42	120.43
1	A	69	SER	O-C-N	-9.15	112.20	122.72
2	B	124	SER	CB-CA-C	9.15	124.77	110.14
2	B	95	SER	CA-C-O	9.14	129.99	120.40
1	A	290	ALA	CA-C-O	-9.13	107.46	120.51
1	A	298	VAL	CA-C-N	9.12	137.10	121.14
1	A	298	VAL	C-N-CA	9.12	137.10	121.14
1	A	72	GLY	CA-C-O	-9.12	110.87	121.08
1	A	206	GLY	CA-C-N	9.11	138.38	121.97
1	A	206	GLY	C-N-CA	9.11	138.38	121.97
1	A	8	HIS	N-CA-CB	9.09	124.96	110.23
1	A	300	ASN	CA-CB-CG	-9.08	103.52	112.60
2	B	48	LEU	CA-C-N	-9.08	111.53	120.52
2	B	48	LEU	C-N-CA	-9.08	111.53	120.52
1	A	79	THR	CB-CA-C	9.05	124.80	109.50
1	A	29	LYS	O-C-N	9.05	132.73	122.32
2	B	67	SER	CA-CB-OG	9.03	129.16	111.10
1	A	67	GLY	O-C-N	-9.01	110.99	122.70
1	A	154	ASN	CA-CB-CG	-9.01	103.59	112.60
2	B	14	ARG	CA-C-N	-9.00	103.77	121.41
2	B	14	ARG	C-N-CA	-9.00	103.77	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	GLY	CA-C-O	-8.95	105.00	120.57
1	A	43	VAL	N-CA-CB	-8.94	97.42	112.44
1	A	52	SER	CA-C-N	8.94	138.61	121.54
1	A	52	SER	C-N-CA	8.94	138.61	121.54
1	A	190	ASP	CA-CB-CG	8.93	121.53	112.60
2	B	105	ASP	CB-CA-C	8.91	124.96	110.09
1	A	225	GLU	N-CA-C	8.90	123.41	108.90
1	A	25	ALA	N-CA-CB	8.89	123.50	110.26
1	A	129	ASP	N-CA-C	-8.88	99.25	112.04
1	A	178	LYS	CA-C-O	-8.85	107.85	120.51
1	A	136	THR	N-CA-CB	8.85	122.89	110.07
1	A	88	LEU	CA-C-O	-8.83	107.88	120.51
1	A	13	ASN	CB-CG-ND2	-8.83	103.16	116.40
1	A	283	GLN	OE1-CD-NE2	8.82	131.42	122.60
2	B	117	HIS	CA-C-N	-8.82	104.69	121.54
2	B	117	HIS	C-N-CA	-8.82	104.69	121.54
1	A	82	GLY	N-CA-C	-8.81	99.01	113.02
1	A	9	ILE	CA-C-O	-8.81	110.76	120.71
2	B	47	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	A	278	ALA	CA-C-O	-8.79	107.94	120.51
1	A	126	ASN	O-C-N	8.78	133.46	123.27
1	A	303	LEU	N-CA-C	8.78	122.41	109.07
1	A	223	GLN	N-CA-C	8.78	125.63	114.31
1	A	298	VAL	O-C-N	-8.78	111.60	122.57
2	B	23	ALA	CA-C-N	-8.77	110.43	123.93
2	B	23	ALA	C-N-CA	-8.77	110.43	123.93
1	A	186	PHE	N-CA-C	8.76	120.89	108.54
1	A	141	ASP	N-CA-C	8.74	120.89	111.36
1	A	121	ASN	CB-CG-ND2	8.74	129.50	116.40
2	B	18	ILE	N-CA-CB	-8.73	98.53	110.05
2	B	131	ASP	N-CA-CB	8.72	125.24	110.49
2	B	33	PHE	CA-CB-CG	-8.72	105.08	113.80
2	B	32	LEU	CB-CA-C	8.71	127.75	110.42
1	A	35	GLN	CB-CA-C	-8.71	97.70	111.02
1	A	106	HIS	N-CA-C	8.71	118.35	108.25
2	B	44	ILE	O-C-N	8.69	133.01	122.58
1	A	211	LEU	O-C-N	-8.67	111.92	123.19
1	A	40	LYS	CB-CA-C	-8.66	93.18	110.42
2	B	62	GLU	O-C-N	8.65	133.88	123.24
1	A	140	LEU	CA-C-N	8.65	132.57	120.29
1	A	140	LEU	C-N-CA	8.65	132.57	120.29
2	B	129	ARG	N-CA-C	8.63	129.18	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	68	GLU	O-C-N	8.63	134.07	122.59
1	A	41	HIS	N-CA-CB	-8.62	100.12	114.27
1	A	23	VAL	CB-CA-C	8.62	123.78	112.14
1	A	20	LEU	CB-CA-C	-8.62	96.03	110.68
1	A	173	THR	CA-CB-OG1	-8.61	96.68	109.60
1	A	72	GLY	O-C-N	8.61	133.31	123.58
1	A	75	ASP	CA-CB-CG	-8.61	103.99	112.60
1	A	198	ILE	CA-C-O	-8.60	110.03	120.78
1	A	97	THR	CA-C-O	-8.59	111.35	120.63
1	A	112	ALA	N-CA-CB	8.57	124.29	109.72
2	B	6	LYS	CA-C-O	8.57	132.76	120.51
1	A	207	ILE	N-CA-CB	-8.55	97.13	111.23
2	B	151	ALA	N-CA-C	-8.55	92.60	110.80
2	B	78	ALA	O-C-N	-8.53	114.97	121.19
1	A	133	GLN	CA-C-N	8.52	132.05	122.59
1	A	133	GLN	C-N-CA	8.52	132.05	122.59
1	A	238	GLN	CA-C-N	-8.51	109.82	122.24
1	A	238	GLN	C-N-CA	-8.51	109.82	122.24
1	A	255	ASN	CA-C-N	8.51	136.95	122.15
1	A	255	ASN	C-N-CA	8.51	136.95	122.15
2	B	143	GLU	CA-C-O	-8.50	111.48	120.40
2	B	24	GLU	CA-CB-CG	8.49	131.09	114.10
1	A	200	ASP	O-C-N	8.49	133.88	122.59
1	A	231	GLU	O-C-N	8.46	131.84	123.04
1	A	196	GLU	CA-C-O	-8.46	106.20	119.23
1	A	41	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	138	THR	CA-CB-OG1	-8.45	96.92	109.60
2	B	80	GLN	CA-CB-CG	8.45	131.00	114.10
2	B	94	LYS	CB-CG-CD	8.45	130.74	111.30
2	B	117	HIS	N-CA-CB	8.44	124.76	110.49
2	B	15	GLY	N-CA-C	-8.42	93.23	113.18
1	A	184	PHE	CA-CB-CG	8.41	122.21	113.80
1	A	131	SER	N-CA-C	-8.41	102.03	112.88
1	A	122	VAL	O-C-N	8.40	130.68	121.10
1	A	132	ASN	CA-CB-CG	8.39	120.99	112.60
1	A	29	LYS	CB-CA-C	-8.37	95.38	111.03
2	B	147	ASN	CA-CB-CG	-8.35	104.25	112.60
1	A	33	ASN	CB-CG-ND2	-8.35	103.88	116.40
2	B	121	VAL	O-C-N	8.33	132.98	122.57
1	A	156	HIS	CA-CB-CG	-8.31	105.49	113.80
1	A	153	ASN	N-CA-CB	-8.28	97.27	110.77
2	B	1	MET	CA-C-O	8.28	134.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	GLU	N-CA-CB	-8.27	96.51	110.49
1	A	135	PRO	CB-CA-C	-8.26	98.46	112.26
2	B	94	LYS	N-CA-CB	8.24	124.42	110.49
2	B	81	ALA	CB-CA-C	8.24	126.82	110.42
1	A	167	ARG	CA-C-N	8.24	136.17	121.92
1	A	167	ARG	C-N-CA	8.24	136.17	121.92
1	A	70	VAL	O-C-N	8.23	132.86	122.57
2	B	81	ALA	N-CA-CB	-8.23	96.58	110.49
2	B	122	SER	CA-C-O	-8.23	108.74	120.51
2	B	101	GLU	CB-CG-CD	8.22	126.58	112.60
1	A	95	ILE	N-CA-C	-8.18	101.72	110.23
2	B	61	ILE	CA-C-O	8.16	130.99	120.78
1	A	301	ARG	CG-CD-NE	8.16	129.95	112.00
1	A	209	TRP	CA-C-O	8.15	132.17	120.51
1	A	270	THR	N-CA-CB	-8.15	96.71	110.49
2	B	149	VAL	N-CA-C	-8.15	92.38	109.34
1	A	145	ILE	CA-CB-CG1	-8.15	96.55	110.40
2	B	97	PRO	N-CA-C	-8.15	97.75	110.95
1	A	13	ASN	O-C-N	8.14	130.49	122.03
1	A	174	GLN	CA-C-O	-8.14	108.69	119.11
1	A	203	ASP	CA-C-N	8.14	137.09	121.54
1	A	203	ASP	C-N-CA	8.14	137.09	121.54
1	A	93	SER	CA-C-O	-8.13	109.65	119.49
1	A	43	VAL	CA-CB-CG2	8.11	124.19	110.40
1	A	257	LYS	O-C-N	8.11	131.40	123.29
1	A	250	HIS	N-CA-CB	-8.11	96.79	110.49
1	A	185	TYR	CA-C-N	-8.09	112.03	123.20
1	A	185	TYR	C-N-CA	-8.09	112.03	123.20
1	A	75	ASP	N-CA-C	8.09	120.67	109.18
1	A	269	ALA	N-CA-CB	-8.08	97.26	110.43
2	B	126	ALA	CA-C-N	8.08	133.25	122.90
2	B	126	ALA	C-N-CA	8.08	133.25	122.90
1	A	240	LEU	CA-C-O	-8.07	112.76	121.88
1	A	49	PHE	CA-C-O	-8.06	112.27	120.90
1	A	141	ASP	CA-C-O	8.04	128.94	120.42
1	A	296	ALA	CB-CA-C	8.03	126.76	110.38
1	A	36	PRO	N-CA-C	-8.00	97.63	111.32
2	B	46	LEU	CB-CA-C	7.99	123.48	111.17
1	A	118	PHE	CA-CB-CG	-7.99	105.81	113.80
2	B	14	ARG	NH1-CZ-NH2	-7.99	108.92	119.30
2	B	141	GLU	CG-CD-OE2	-7.96	100.09	118.40
1	A	171	SER	CA-C-O	7.96	129.06	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASN	CA-CB-CG	7.95	120.55	112.60
1	A	128	GLY	O-C-N	-7.93	112.39	122.70
1	A	154	ASN	N-CA-C	7.93	122.54	111.92
1	A	113	ARG	NE-CZ-NH1	-7.92	113.58	121.50
2	B	83	VAL	CA-C-N	7.92	136.67	121.54
2	B	83	VAL	C-N-CA	7.92	136.67	121.54
1	A	32	ALA	N-CA-CB	-7.92	98.65	110.61
2	B	71	VAL	CB-CA-C	-7.91	98.31	111.29
1	A	3	PRO	O-C-N	-7.89	113.16	122.24
1	A	226	ARG	CD-NE-CZ	-7.89	113.36	124.40
1	A	114	LEU	N-CA-CB	7.88	123.12	109.72
1	A	304	VAL	CA-C-N	7.88	135.88	121.70
1	A	304	VAL	C-N-CA	7.88	135.88	121.70
2	B	35	LEU	O-C-N	-7.88	113.72	123.33
2	B	104	ILE	CA-C-O	-7.88	110.93	120.78
2	B	104	ILE	CA-C-N	-7.87	109.55	122.54
2	B	104	ILE	C-N-CA	-7.87	109.55	122.54
1	A	216	GLU	N-CA-CB	-7.87	97.19	110.49
2	B	68	GLU	CG-CD-OE1	7.86	136.47	118.40
1	A	267	GLU	CA-C-N	7.85	134.20	122.58
1	A	267	GLU	C-N-CA	7.85	134.20	122.58
1	A	269	ALA	CB-CA-C	-7.85	96.79	109.75
1	A	275	THR	N-CA-C	7.84	118.62	109.60
2	B	119	GLU	CG-CD-OE2	-7.83	100.38	118.40
1	A	197	TYR	N-CA-CB	-7.83	96.26	110.27
1	A	197	TYR	CB-CG-CD1	-7.82	109.07	120.80
1	A	273	ASP	O-C-N	7.81	132.98	122.59
2	B	37	GLU	N-CA-C	-7.81	92.42	107.57
1	A	145	ILE	N-CA-C	-7.80	102.93	110.42
1	A	185	TYR	O-C-N	7.79	132.57	123.30
2	B	15	GLY	O-C-N	7.79	132.83	122.70
1	A	303	LEU	CA-C-N	7.79	135.99	121.97
1	A	303	LEU	C-N-CA	7.79	135.99	121.97
1	A	148	THR	O-C-N	7.77	132.93	122.59
2	B	138	LYS	N-CA-C	-7.77	99.14	110.64
1	A	109	GLU	CB-CG-CD	7.76	125.80	112.60
2	B	2	THR	CA-CB-OG1	-7.76	97.96	109.60
1	A	38	LEU	CB-CA-C	-7.76	96.27	110.63
2	B	148	VAL	N-CA-CB	-7.76	98.43	111.23
1	A	49	PHE	CB-CA-C	7.73	123.18	110.81
1	A	238	GLN	CB-CA-C	7.73	123.11	109.65
1	A	299	LEU	N-CA-CB	-7.73	97.80	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	103	ASN	CB-CG-OD1	-7.73	105.34	120.80
2	B	94	LYS	CA-C-N	-7.72	111.79	123.07
2	B	94	LYS	C-N-CA	-7.72	111.79	123.07
2	B	71	VAL	N-CA-CB	-7.72	98.49	111.23
1	A	182	ASN	CB-CA-C	7.71	120.94	109.29
1	A	197	TYR	CB-CG-CD2	7.69	132.34	120.80
2	B	123	SER	CA-CB-OG	7.69	126.48	111.10
1	A	25	ALA	CA-C-N	-7.69	109.16	120.38
1	A	25	ALA	C-N-CA	-7.69	109.16	120.38
2	B	78	ALA	CB-CA-C	7.69	120.68	111.15
2	B	103	ASN	CA-C-O	7.68	131.49	120.51
1	A	98	TYR	N-CA-CB	7.67	121.53	110.40
1	A	226	ARG	CB-CG-CD	-7.67	93.66	111.30
1	A	195	PRO	CB-CA-C	7.64	121.01	111.23
2	B	50	SER	O-C-N	7.62	131.46	122.24
2	B	88	ASP	CB-CA-C	7.62	123.21	110.79
2	B	29	LEU	CA-C-O	7.61	129.44	120.92
2	B	55	ARG	N-CA-C	-7.58	96.54	108.90
2	B	46	LEU	O-C-N	-7.57	111.48	122.99
1	A	151	ARG	O-C-N	-7.56	115.97	123.46
2	B	142	LYS	CA-C-N	7.56	134.10	123.07
2	B	142	LYS	C-N-CA	7.56	134.10	123.07
1	A	144	THR	CA-C-N	-7.55	111.05	120.56
1	A	144	THR	C-N-CA	-7.55	111.05	120.56
1	A	275	THR	CA-C-O	-7.54	112.70	120.02
2	B	134	ALA	CA-C-N	7.54	133.37	122.44
2	B	134	ALA	C-N-CA	7.54	133.37	122.44
1	A	256	ALA	CB-CA-C	-7.53	96.76	114.16
2	B	87	ASN	CA-C-N	-7.53	112.42	123.11
2	B	87	ASN	C-N-CA	-7.53	112.42	123.11
2	B	52	GLU	CA-C-O	-7.52	112.34	121.06
1	A	109	GLU	CA-CB-CG	7.50	129.10	114.10
2	B	6	LYS	N-CA-CB	7.50	123.17	110.49
2	B	146	HIS	CB-CA-C	-7.50	95.50	110.42
1	A	172	LEU	O-C-N	7.49	131.26	122.20
2	B	117	HIS	CB-CA-C	-7.48	95.53	110.42
1	A	207	ILE	CA-C-N	-7.48	107.25	121.54
1	A	207	ILE	C-N-CA	-7.48	107.25	121.54
1	A	208	ALA	CA-C-O	7.48	131.21	120.51
1	A	218	VAL	N-CA-C	-7.48	93.79	109.34
2	B	22	PRO	CA-C-N	-7.46	111.34	122.39
2	B	22	PRO	C-N-CA	-7.46	111.34	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ILE	CB-CA-C	-7.46	99.06	111.29
2	B	126	ALA	CB-CA-C	7.46	122.01	109.48
1	A	231	GLU	N-CA-CB	-7.45	98.38	111.49
1	A	7	SER	CA-CB-OG	-7.43	96.23	111.10
1	A	243	ALA	CA-C-O	7.43	127.23	118.69
1	A	162	ASP	CA-CB-CG	-7.41	105.19	112.60
1	A	179	PHE	N-CA-CB	7.41	123.01	110.49
1	A	41	HIS	CA-C-O	7.41	130.94	118.94
1	A	105	ARG	NE-CZ-NH1	7.41	128.91	121.50
2	B	18	ILE	N-CA-C	-7.39	99.61	109.30
1	A	66	LEU	CA-C-O	-7.39	109.65	119.11
2	B	24	GLU	CA-C-O	7.39	130.75	119.96
2	B	81	ALA	CA-C-O	-7.39	109.94	120.51
1	A	185	TYR	CA-C-O	-7.39	112.38	120.36
1	A	224	LYS	CB-CA-C	7.38	124.30	109.68
1	A	255	ASN	CA-CB-CG	7.38	119.98	112.60
1	A	112	ALA	CA-C-N	-7.38	110.53	120.79
1	A	112	ALA	C-N-CA	-7.38	110.53	120.79
1	A	292	GLN	CG-CD-OE1	7.38	135.56	120.80
1	A	168	THR	N-CA-CB	-7.38	99.69	110.53
2	B	113	ASN	CA-C-O	-7.37	110.91	119.24
1	A	47	CYS	CA-C-N	-7.36	112.92	122.79
1	A	47	CYS	C-N-CA	-7.36	112.92	122.79
2	B	121	VAL	N-CA-C	7.36	124.65	109.34
1	A	4	LEU	CA-C-O	-7.35	111.52	119.97
2	B	119	GLU	CB-CG-CD	-7.35	100.11	112.60
1	A	54	ARG	N-CA-C	-7.33	102.98	110.97
1	A	56	ARG	CA-C-O	7.33	128.37	120.24
1	A	241	VAL	CB-CA-C	7.32	123.29	111.29
1	A	96	SER	CA-C-N	7.31	130.40	120.38
1	A	96	SER	C-N-CA	7.31	130.40	120.38
1	A	74	SER	N-CA-C	-7.31	98.03	109.72
2	B	79	PRO	O-C-N	7.30	132.23	122.30
2	B	62	GLU	CB-CA-C	-7.30	94.13	109.38
2	B	105	ASP	CA-C-N	-7.29	113.38	122.93
2	B	105	ASP	C-N-CA	-7.29	113.38	122.93
1	A	93	SER	N-CA-CB	7.27	122.68	110.32
1	A	273	ASP	N-CA-CB	7.26	122.77	110.49
1	A	52	SER	CB-CA-C	7.26	124.87	110.42
2	B	135	LEU	CA-C-O	-7.26	111.11	120.25
1	A	31	LYS	N-CA-CB	7.25	121.51	110.28
1	A	227	LEU	N-CA-CB	-7.24	99.78	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	LEU	N-CA-C	-7.24	93.81	109.81
2	B	123	SER	O-C-N	-7.22	113.86	122.96
2	B	133	ILE	CA-C-N	7.22	133.77	122.94
2	B	133	ILE	C-N-CA	7.22	133.77	122.94
2	B	151	ALA	N-CA-CB	-7.21	98.30	110.49
1	A	115	ALA	CA-C-O	-7.20	112.85	120.63
1	A	221	ARG	CG-CD-NE	7.16	127.75	112.00
2	B	80	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	A	257	LYS	CA-CB-CG	7.15	128.40	114.10
1	A	71	VAL	N-CA-C	-7.14	94.48	109.34
1	A	135	PRO	CA-C-N	-7.14	110.73	120.44
1	A	135	PRO	C-N-CA	-7.14	110.73	120.44
1	A	272	VAL	CB-CA-C	-7.14	99.58	111.29
2	B	36	THR	O-C-N	7.14	132.09	122.59
1	A	52	SER	CA-C-O	7.14	130.72	120.51
1	A	249	LEU	O-C-N	7.13	131.73	122.68
1	A	149	GLU	CG-CD-OE1	7.12	134.79	118.40
1	A	242	ARG	CA-C-O	7.12	129.86	121.11
2	B	97	PRO	CB-CA-C	7.11	120.96	111.71
1	A	140	LEU	O-C-N	7.11	129.66	122.12
1	A	32	ALA	CA-C-O	7.10	127.77	119.32
1	A	138	THR	N-CA-C	7.09	119.91	111.33
2	B	44	ILE	CA-C-N	7.09	130.43	120.57
2	B	44	ILE	C-N-CA	7.09	130.43	120.57
2	B	2	THR	N-CA-CB	-7.08	98.95	110.21
1	A	84	LYS	CA-C-N	7.08	135.29	121.41
1	A	84	LYS	C-N-CA	7.08	135.29	121.41
1	A	155	LEU	N-CA-C	7.06	121.36	110.42
1	A	54	ARG	NE-CZ-NH1	7.05	128.55	121.50
2	B	117	HIS	CA-C-O	-7.04	110.44	120.51
1	A	179	PHE	CA-C-O	-7.04	110.44	120.51
1	A	295	LEU	CA-C-N	-7.04	108.72	120.68
1	A	295	LEU	C-N-CA	-7.04	108.72	120.68
2	B	146	HIS	N-CA-CB	7.03	122.37	110.49
1	A	299	LEU	O-C-N	-7.02	112.77	122.46
1	A	280	TYR	CB-CA-C	7.02	124.39	110.42
2	B	129	ARG	CD-NE-CZ	7.02	134.23	124.40
2	B	73	GLU	CA-C-O	-7.01	112.99	120.42
2	B	61	ILE	CA-CB-CG2	6.99	122.39	110.50
1	A	153	ASN	OD1-CG-ND2	6.98	129.58	122.60
1	A	181	GLY	CA-C-N	-6.97	108.66	121.41
1	A	181	GLY	C-N-CA	-6.97	108.66	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	THR	CA-C-O	-6.97	113.53	120.70
1	A	92	ILE	N-CA-CB	-6.96	102.41	110.55
1	A	138	THR	OG1-CB-CG2	6.95	123.20	109.30
1	A	43	VAL	O-C-N	-6.95	115.33	123.04
1	A	65	ARG	N-CA-CB	6.93	121.02	110.28
1	A	246	LEU	N-CA-C	-6.93	99.25	110.20
2	B	103	ASN	O-C-N	6.92	131.80	122.59
2	B	152	ASN	OD1-CG-ND2	6.92	129.52	122.60
1	A	132	ASN	OD1-CG-ND2	6.91	129.51	122.60
1	A	211	LEU	N-CA-C	6.91	120.78	109.72
2	B	151	ALA	O-C-N	6.90	131.76	122.59
2	B	27	PHE	O-C-N	6.90	129.48	122.03
1	A	244	ASN	N-CA-C	-6.89	103.35	112.72
1	A	99	VAL	O-C-N	6.88	131.17	122.57
2	B	108	VAL	N-CA-CB	-6.88	99.88	111.23
1	A	221	ARG	N-CA-C	-6.87	96.17	110.80
2	B	72	ASP	CB-CG-OD1	-6.87	102.59	118.40
1	A	122	VAL	CB-CA-C	6.86	123.85	111.36
2	B	55	ARG	O-C-N	6.86	131.46	123.30
2	B	114	CYS	CA-C-O	-6.85	110.71	120.51
2	B	139	TYR	O-C-N	6.85	131.70	122.59
2	B	73	GLU	N-CA-CB	6.85	120.29	110.16
1	A	275	THR	CA-C-N	6.82	128.36	119.84
1	A	275	THR	C-N-CA	6.82	128.36	119.84
1	A	288	ILE	CA-CB-CG2	6.81	122.07	110.50
1	A	93	SER	CA-CB-OG	6.80	124.69	111.10
2	B	98	SER	CA-CB-OG	-6.79	97.52	111.10
1	A	50	GLU	CB-CG-CD	6.79	124.13	112.60
2	B	76	LEU	N-CA-C	6.78	118.46	111.14
2	B	23	ALA	N-CA-C	6.77	119.49	108.26
1	A	44	ILE	CA-C-N	-6.75	113.47	122.99
1	A	44	ILE	C-N-CA	-6.75	113.47	122.99
1	A	202	LEU	N-CA-C	-6.75	102.79	111.02
1	A	42	LYS	N-CA-CB	-6.74	100.04	110.56
1	A	141	ASP	CB-CA-C	-6.74	99.39	110.85
2	B	115	ILE	N-CA-C	-6.74	102.66	111.09
1	A	189	PRO	CB-CA-C	-6.74	100.44	111.56
2	B	65	PHE	CA-CB-CG	6.73	120.53	113.80
1	A	223	GLN	CA-CB-CG	-6.73	100.64	114.10
2	B	94	LYS	O-C-N	6.72	131.53	122.59
1	A	155	LEU	CA-C-N	6.72	132.62	122.95
1	A	155	LEU	C-N-CA	6.72	132.62	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	GLU	OE1-CD-OE2	6.71	139.02	122.90
1	A	97	THR	N-CA-C	6.71	119.45	111.33
1	A	140	LEU	N-CA-CB	6.70	119.97	110.12
2	B	91	VAL	N-CA-CB	-6.69	102.72	111.82
1	A	148	THR	N-CA-CB	6.69	121.79	110.49
2	B	129	ARG	CB-CA-C	-6.69	97.11	110.42
1	A	233	ALA	CB-CA-C	-6.68	100.48	110.50
2	B	34	LYS	CB-CA-C	-6.67	97.14	110.42
1	A	5	TYR	CB-CA-C	-6.66	97.17	110.42
1	A	216	GLU	CB-CA-C	-6.66	97.17	110.42
1	A	241	VAL	CA-C-O	6.66	129.10	120.78
1	A	112	ALA	CA-C-O	-6.65	113.24	121.02
1	A	52	SER	N-CA-CB	-6.65	99.26	110.49
1	A	163	LEU	CA-C-O	-6.65	111.01	120.51
1	A	221	ARG	CD-NE-CZ	6.64	133.69	124.40
1	A	200	ASP	N-CA-C	-6.62	96.70	110.80
1	A	31	LYS	CA-C-O	-6.62	112.36	119.97
1	A	274	LYS	CA-C-N	6.61	130.09	120.51
1	A	274	LYS	C-N-CA	6.61	130.09	120.51
1	A	106	HIS	CA-C-N	6.60	128.09	119.84
1	A	106	HIS	C-N-CA	6.60	128.09	119.84
1	A	153	ASN	N-CA-C	6.60	119.22	108.26
1	A	230	SER	N-CA-CB	-6.60	99.33	110.49
2	B	103	ASN	CB-CA-C	-6.60	97.28	110.42
1	A	89	ALA	N-CA-C	-6.60	96.74	110.80
2	B	59	ILE	N-CA-C	6.60	115.75	107.70
2	B	31	SER	CA-C-O	6.59	126.86	119.41
1	A	207	ILE	O-C-N	-6.58	114.34	122.57
1	A	35	GLN	CA-C-O	-6.58	113.56	121.00
1	A	273	ASP	N-CA-C	-6.58	96.78	110.80
1	A	201	MET	CA-C-O	-6.58	113.51	120.55
2	B	80	GLN	CA-C-N	-6.58	108.97	121.54
2	B	80	GLN	C-N-CA	-6.58	108.97	121.54
2	B	130	ALA	CA-C-O	-6.57	111.11	120.51
1	A	242	ARG	NH1-CZ-NH2	-6.57	110.76	119.30
2	B	98	SER	CA-C-O	-6.56	111.40	120.52
1	A	95	ILE	CA-C-O	6.56	128.24	121.41
1	A	167	ARG	NH1-CZ-NH2	-6.55	110.78	119.30
1	A	256	ALA	O-C-N	6.55	130.36	121.78
1	A	87	THR	CA-CB-OG1	-6.54	99.79	109.60
2	B	136	LYS	CG-CD-CE	6.54	126.34	111.30
2	B	16	THR	CA-C-N	-6.54	110.20	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	16	THR	C-N-CA	-6.54	110.20	121.97
2	B	17	VAL	CA-C-O	6.54	128.95	120.78
2	B	55	ARG	CA-C-O	-6.53	113.31	120.36
2	B	28	LYS	CA-C-N	6.53	130.61	120.82
2	B	28	LYS	C-N-CA	6.53	130.61	120.82
2	B	6	LYS	CA-C-N	-6.52	112.56	122.21
2	B	6	LYS	C-N-CA	-6.52	112.56	122.21
2	B	135	LEU	O-C-N	6.52	131.62	123.14
1	A	119	SER	CA-C-O	-6.51	111.75	120.15
2	B	6	LYS	O-C-N	6.51	131.25	122.59
1	A	78	ASN	OD1-CG-ND2	-6.51	116.09	122.60
1	A	248	GLY	CA-C-O	-6.49	109.27	120.57
1	A	242	ARG	N-CA-C	-6.49	94.31	107.41
1	A	18	ASP	CA-C-O	6.48	129.78	120.51
1	A	145	ILE	CA-CB-CG2	6.47	121.50	110.50
1	A	141	ASP	CA-C-N	6.46	129.18	120.65
1	A	141	ASP	C-N-CA	6.46	129.18	120.65
1	A	105	ARG	CD-NE-CZ	6.46	133.44	124.40
2	B	83	VAL	CA-C-O	6.45	128.84	120.78
2	B	142	LYS	N-CA-CB	6.45	123.53	111.53
1	A	84	LYS	CA-C-O	6.45	129.73	120.51
2	B	34	LYS	N-CA-CB	-6.45	99.59	110.49
1	A	130	GLY	O-C-N	6.43	131.06	122.70
1	A	137	GLN	CA-C-N	6.43	129.19	120.38
1	A	137	GLN	C-N-CA	6.43	129.19	120.38
2	B	115	ILE	N-CA-CB	6.43	122.41	110.77
1	A	230	SER	CA-C-N	-6.42	111.02	122.45
1	A	230	SER	C-N-CA	-6.42	111.02	122.45
1	A	71	VAL	CA-C-O	-6.42	112.76	120.78
1	A	48	PHE	O-C-N	6.42	130.61	122.65
2	B	73	GLU	O-C-N	6.42	129.46	122.15
2	B	110	PRO	N-CD-CG	-6.40	93.60	103.20
2	B	150	LEU	N-CA-C	-6.40	97.23	108.23
1	A	97	THR	N-CA-CB	6.39	119.64	110.06
2	B	18	ILE	CA-C-O	6.37	129.02	120.99
1	A	175	ALA	CA-C-N	-6.36	109.39	121.54
1	A	175	ALA	C-N-CA	-6.36	109.39	121.54
2	B	29	LEU	N-CA-CB	-6.36	99.41	109.78
1	A	138	THR	CA-C-O	-6.36	113.77	120.63
1	A	67	GLY	CA-C-O	-6.35	109.52	120.57
1	A	65	ARG	N-CA-C	-6.34	104.46	111.82
2	B	37	GLU	CB-CG-CD	6.34	123.38	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	ARG	NH1-CZ-NH2	-6.33	111.06	119.30
1	A	149	GLU	CG-CD-OE2	-6.33	103.84	118.40
1	A	267	GLU	CB-CG-CD	-6.33	101.84	112.60
1	A	60	GLN	CA-CB-CG	6.32	126.74	114.10
2	B	68	GLU	CA-C-O	-6.32	111.48	120.51
1	A	289	PHE	CA-CB-CG	6.31	120.11	113.80
2	B	35	LEU	CB-CA-C	6.31	123.31	112.27
2	B	61	ILE	O-C-N	-6.31	114.69	122.57
2	B	127	VAL	CA-C-N	6.30	132.69	122.29
2	B	127	VAL	C-N-CA	6.30	132.69	122.29
1	A	235	VAL	CA-C-N	6.30	133.90	123.25
1	A	235	VAL	C-N-CA	6.30	133.90	123.25
1	A	59	PHE	N-CA-CB	6.29	121.13	110.49
2	B	34	LYS	CA-C-O	6.29	129.51	120.51
2	B	49	PRO	CA-C-O	6.29	130.45	122.15
1	A	135	PRO	O-C-N	6.29	129.78	122.17
2	B	53	MET	N-CA-C	6.29	124.19	110.80
1	A	262	LEU	O-C-N	6.28	128.54	121.32
2	B	128	ARG	O-C-N	6.28	130.56	123.27
1	A	52	SER	O-C-N	-6.27	114.25	122.59
1	A	136	THR	O-C-N	6.27	128.86	122.09
1	A	1	ALA	CA-C-O	6.27	131.45	120.80
1	A	119	SER	CB-CA-C	-6.26	101.35	111.06
2	B	64	THR	CA-C-N	-6.26	109.58	121.54
2	B	64	THR	C-N-CA	-6.26	109.58	121.54
2	B	103	ASN	N-CA-CB	6.26	121.07	110.49
1	A	123	PRO	CA-C-O	-6.26	114.30	121.56
1	A	139	LEU	N-CA-C	-6.26	104.56	111.82
1	A	166	GLY	O-C-N	-6.26	114.57	122.70
1	A	281	PHE	N-CA-CB	6.26	121.06	110.49
1	A	232	TYR	CB-CA-C	-6.25	97.98	110.42
1	A	102	ILE	N-CA-C	6.24	122.33	109.34
1	A	145	ILE	CB-CG1-CD1	-6.24	100.69	113.80
2	B	80	GLN	CB-CG-CD	6.24	123.20	112.60
2	B	41	ARG	N-CA-CB	6.23	119.91	110.45
2	B	89	TYR	CB-CA-C	6.23	122.81	110.42
1	A	236	LYS	N-CA-C	-6.22	102.41	111.30
1	A	157	VAL	N-CA-CB	-6.21	105.26	112.34
2	B	147	ASN	CA-C-O	6.21	129.39	120.51
1	A	194	MET	CB-CA-C	6.21	116.80	109.47
1	A	226	ARG	NE-CZ-NH1	6.21	127.71	121.50
2	B	139	TYR	CA-CB-CG	-6.20	102.73	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	67	SER	O-C-N	6.17	130.79	122.59
1	A	230	SER	N-CA-C	-6.16	97.67	110.80
2	B	48	LEU	CA-CB-CG	6.16	137.86	116.30
1	A	4	LEU	N-CA-C	6.16	118.96	111.82
1	A	229	PRO	CA-N-CD	-6.14	103.40	112.00
1	A	281	PHE	CA-C-O	-6.13	111.74	120.51
1	A	108	GLN	N-CA-CB	6.13	119.28	110.45
2	B	122	SER	CA-C-N	-6.13	112.41	121.24
2	B	122	SER	C-N-CA	-6.13	112.41	121.24
1	A	273	ASP	CA-C-O	-6.11	111.77	120.51
2	B	126	ALA	N-CA-CB	-6.11	100.44	110.52
1	A	93	SER	O-C-N	6.10	130.32	122.39
1	A	131	SER	O-C-N	6.10	129.50	122.25
1	A	148	THR	OG1-CB-CG2	6.09	121.49	109.30
2	B	92	VAL	CA-C-O	-6.09	113.16	120.78
1	A	164	LYS	N-CA-CB	6.09	118.75	110.10
2	B	6	LYS	N-CA-C	-6.09	97.84	110.80
1	A	11	SER	O-C-N	6.08	130.68	122.59
2	B	70	GLU	CG-CD-OE2	-6.08	104.41	118.40
2	B	84	ASN	CA-C-N	6.08	133.16	121.54
2	B	84	ASN	C-N-CA	6.08	133.16	121.54
1	A	140	LEU	N-CA-C	-6.08	104.65	111.28
1	A	217	GLU	N-CA-C	-6.08	99.95	109.25
1	A	215	ILE	CA-C-O	6.07	128.36	120.78
1	A	105	ARG	CA-C-N	-6.06	111.89	122.38
1	A	105	ARG	C-N-CA	-6.06	111.89	122.38
1	A	219	MET	CA-CB-CG	6.06	126.22	114.10
1	A	84	LYS	CA-CB-CG	6.05	126.20	114.10
2	B	147	ASN	CB-CG-ND2	-6.05	107.32	116.40
1	A	137	GLN	CA-C-O	-6.05	111.86	120.51
2	B	33	PHE	CA-C-O	-6.05	114.37	121.44
1	A	153	ASN	O-C-N	-6.04	115.54	123.28
1	A	30	LEU	N-CA-C	-6.04	97.93	110.80
1	A	97	THR	CB-CA-C	-6.04	100.41	110.68
1	A	65	ARG	CD-NE-CZ	-6.04	115.95	124.40
1	A	61	THR	CB-CA-C	-6.03	98.41	110.42
1	A	267	GLU	OE1-CD-OE2	6.03	137.38	122.90
2	B	136	LYS	CA-C-O	-6.03	112.82	120.84
1	A	71	VAL	O-C-N	6.03	130.11	122.57
2	B	82	THR	CA-CB-OG1	-6.03	100.56	109.60
1	A	101	ALA	CA-C-N	-6.02	111.13	121.97
1	A	101	ALA	C-N-CA	-6.02	111.13	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	LEU	O-C-N	6.01	128.49	122.12
1	A	174	GLN	O-C-N	6.00	131.20	122.43
1	A	259	LEU	CB-CA-C	-6.00	97.48	109.79
1	A	122	VAL	N-CA-C	-5.99	95.93	108.88
1	A	290	ALA	N-CA-CB	5.99	120.62	110.49
2	B	46	LEU	CA-C-O	5.99	128.85	120.52
2	B	112	SER	O-C-N	5.99	130.92	122.41
2	B	104	ILE	CA-CB-CG1	-5.99	100.22	110.40
1	A	283	GLN	CA-C-N	5.99	130.58	120.88
1	A	283	GLN	C-N-CA	5.99	130.58	120.88
1	A	193	ALA	O-C-N	5.98	130.55	122.59
2	B	37	GLU	CG-CD-OE1	5.98	132.15	118.40
2	B	71	VAL	CG1-CB-CG2	5.98	123.95	110.80
1	A	59	PHE	CA-C-N	5.96	132.93	121.54
1	A	59	PHE	C-N-CA	5.96	132.93	121.54
2	B	25	ILE	O-C-N	5.95	130.00	122.57
1	A	185	TYR	N-CA-CB	-5.94	100.69	110.68
2	B	64	THR	OG1-CB-CG2	5.94	121.19	109.30
1	A	223	GLN	CA-C-O	-5.94	112.18	118.77
2	B	9	VAL	CB-CA-C	5.93	121.02	111.29
1	A	26	THR	N-CA-CB	-5.93	100.77	110.14
1	A	57	LEU	CA-C-O	-5.93	114.27	120.55
2	B	111	ASP	N-CA-C	-5.92	101.89	110.24
1	A	105	ARG	NE-CZ-NH2	-5.92	113.87	119.20
2	B	94	LYS	CA-C-O	-5.91	112.05	120.51
2	B	152	ASN	CA-C-O	-5.91	110.75	120.80
2	B	31	SER	O-C-N	5.91	130.75	122.36
2	B	59	ILE	O-C-N	5.90	129.13	122.94
2	B	28	LYS	CA-C-O	5.89	128.94	120.51
1	A	42	LYS	CB-CA-C	5.89	119.52	109.80
2	B	151	ALA	CA-C-O	-5.89	112.09	120.51
1	A	195	PRO	N-CA-CB	5.88	108.47	103.35
1	A	77	ALA	CB-CA-C	5.88	122.13	110.42
1	A	57	LEU	N-CA-C	-5.88	104.87	111.28
1	A	87	THR	N-CA-C	5.88	118.54	109.07
1	A	106	HIS	O-C-N	5.88	125.94	121.65
2	B	118	ALA	N-CA-C	-5.88	98.28	110.80
1	A	40	LYS	O-C-N	5.88	130.40	122.59
1	A	90	ASN	O-C-N	5.88	130.40	122.59
1	A	189	PRO	N-CD-CG	-5.87	94.39	103.20
2	B	138	LYS	CA-C-O	-5.87	115.36	120.88
1	A	145	ILE	N-CA-CB	5.87	117.42	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	GLN	N-CA-C	-5.87	99.63	108.96
1	A	182	ASN	N-CA-CB	-5.86	101.75	111.06
1	A	205	LYS	CB-CG-CD	5.86	124.77	111.30
2	B	128	ARG	CA-C-O	-5.85	114.27	121.06
1	A	81	LEU	CA-C-N	5.85	129.02	121.13
1	A	81	LEU	C-N-CA	5.85	129.02	121.13
1	A	237	ALA	CA-C-N	-5.84	112.15	122.26
1	A	237	ALA	C-N-CA	-5.84	112.15	122.26
1	A	117	GLU	CA-CB-CG	5.84	125.78	114.10
1	A	126	ASN	N-CA-C	-5.84	98.89	108.41
1	A	156	HIS	N-CA-CB	-5.84	101.35	110.87
1	A	211	LEU	N-CA-CB	-5.84	101.09	111.08
1	A	48	PHE	N-CA-CB	5.83	119.27	110.11
2	B	46	LEU	CA-C-N	5.83	129.93	120.60
2	B	46	LEU	C-N-CA	5.83	129.93	120.60
2	B	42	ILE	N-CA-CB	-5.83	102.65	112.44
2	B	105	ASP	N-CA-CB	-5.83	101.87	110.49
1	A	44	ILE	CA-C-O	-5.82	113.50	120.78
2	B	86	ILE	CA-C-O	-5.82	114.36	120.76
1	A	217	GLU	CA-C-N	5.82	132.44	121.97
1	A	217	GLU	C-N-CA	5.82	132.44	121.97
2	B	7	LEU	O-C-N	5.82	130.29	122.61
1	A	71	VAL	CA-C-N	-5.82	113.41	120.51
1	A	71	VAL	C-N-CA	-5.82	113.41	120.51
2	B	90	GLU	N-CA-C	5.82	117.38	108.42
1	A	258	VAL	O-C-N	5.81	129.46	123.18
1	A	2	ASN	CA-CB-CG	-5.81	106.79	112.60
2	B	111	ASP	CA-CB-CG	5.80	118.41	112.60
2	B	48	LEU	O-C-N	5.79	127.98	121.32
2	B	107	LEU	CA-C-N	-5.79	111.55	121.97
2	B	107	LEU	C-N-CA	-5.79	111.55	121.97
1	A	300	ASN	CA-C-O	-5.79	114.82	121.82
2	B	131	ASP	N-CA-C	-5.78	98.48	110.80
2	B	17	VAL	CB-CA-C	5.78	120.77	111.29
2	B	62	GLU	CB-CG-CD	-5.77	102.79	112.60
1	A	27	ALA	CB-CA-C	5.77	122.14	110.38
1	A	125	LEU	O-C-N	-5.76	115.67	123.10
1	A	281	PHE	O-C-N	5.76	130.25	122.59
1	A	56	ARG	CA-C-N	-5.76	112.57	120.28
1	A	56	ARG	C-N-CA	-5.76	112.57	120.28
1	A	91	THR	N-CA-C	-5.75	104.70	110.97
1	A	250	HIS	CA-C-N	-5.75	110.55	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	HIS	C-N-CA	-5.75	110.55	121.54
1	A	117	GLU	CB-CA-C	-5.75	98.97	110.42
2	B	31	SER	CA-C-N	-5.75	110.56	121.54
2	B	31	SER	C-N-CA	-5.75	110.56	121.54
2	B	149	VAL	CA-CB-CG2	5.74	120.16	110.40
1	A	105	ARG	CA-C-O	5.74	127.83	121.11
2	B	142	LYS	CB-CG-CD	5.74	124.50	111.30
1	A	90	ASN	CB-CA-C	5.74	121.83	110.42
2	B	144	PHE	CB-CA-C	5.73	121.82	110.42
1	A	3	PRO	CA-C-O	5.73	129.52	119.84
1	A	129	ASP	O-C-N	5.72	130.03	122.30
1	A	193	ALA	CA-C-O	-5.71	112.34	120.51
1	A	49	PHE	N-CA-C	-5.71	104.26	111.11
2	B	22	PRO	CA-C-O	-5.71	110.22	120.60
1	A	90	ASN	CA-C-N	-5.71	113.12	120.65
1	A	90	ASN	C-N-CA	-5.71	113.12	120.65
2	B	9	VAL	CA-CB-CG1	5.70	120.09	110.40
1	A	33	ASN	CA-C-N	5.69	125.89	120.31
1	A	33	ASN	C-N-CA	5.69	125.89	120.31
1	A	54	ARG	N-CA-CB	5.69	118.21	109.91
1	A	222	VAL	N-CA-C	5.68	115.84	108.35
2	B	64	THR	O-C-N	5.68	130.14	122.59
1	A	19	ASP	CB-CA-C	5.67	121.71	110.42
1	A	261	PRO	N-CD-CG	-5.67	94.69	103.20
1	A	54	ARG	CA-C-N	5.67	128.66	120.38
1	A	54	ARG	C-N-CA	5.67	128.66	120.38
1	A	223	GLN	CG-CD-OE1	-5.67	109.46	120.80
2	B	110	PRO	CB-CA-C	5.67	119.96	111.68
1	A	104	MET	CA-CB-CG	5.67	125.43	114.10
1	A	199	LEU	CA-C-O	5.67	128.61	120.51
2	B	104	ILE	N-CA-C	5.65	121.10	109.34
2	B	119	GLU	CG-CD-OE1	5.65	131.40	118.40
1	A	42	LYS	O-C-N	-5.64	116.65	123.03
1	A	224	LYS	CA-C-N	-5.64	115.03	122.99
1	A	224	LYS	C-N-CA	-5.64	115.03	122.99
2	B	78	ALA	CA-C-O	5.64	126.64	121.34
1	A	113	ARG	CA-C-O	-5.64	114.87	121.07
2	B	68	GLU	CG-CD-OE2	-5.64	105.43	118.40
1	A	113	ARG	CD-NE-CZ	-5.63	116.52	124.40
1	A	28	ALA	CA-C-O	-5.61	114.57	120.63
1	A	202	LEU	O-C-N	5.61	128.09	122.08
2	B	143	GLU	N-CA-C	5.61	117.84	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	VAL	CA-C-O	-5.61	113.77	120.78
2	B	8	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	A	114	LEU	CA-C-N	-5.59	112.72	120.38
1	A	114	LEU	C-N-CA	-5.59	112.72	120.38
2	B	20	HIS	CA-CB-CG	-5.59	108.20	113.80
1	A	221	ARG	CB-CG-CD	5.59	124.16	111.30
1	A	25	ALA	N-CA-C	-5.59	104.68	112.45
2	B	38	THR	CB-CA-C	-5.59	99.31	110.42
1	A	187	ILE	CA-C-O	5.58	127.75	120.78
1	A	274	LYS	CB-CA-C	-5.58	99.32	110.42
1	A	221	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	61	THR	CA-C-O	5.56	128.46	120.51
1	A	218	VAL	CB-CA-C	5.55	120.39	111.29
1	A	249	LEU	CB-CA-C	-5.55	101.87	111.30
1	A	262	LEU	C-N-CD	5.55	132.80	120.60
1	A	91	THR	CA-C-N	5.54	127.54	120.56
1	A	91	THR	C-N-CA	5.54	127.54	120.56
2	B	131	ASP	O-C-N	5.54	129.96	122.59
1	A	8	HIS	CB-CA-C	-5.54	100.39	109.53
1	A	119	SER	N-CA-C	5.53	118.82	112.57
2	B	74	LEU	N-CA-C	-5.53	106.03	112.89
1	A	17	ARG	NH1-CZ-NH2	5.53	126.49	119.30
2	B	36	THR	CA-CB-OG1	-5.53	101.31	109.60
1	A	231	GLU	CB-CG-CD	-5.52	103.21	112.60
1	A	100	ASP	N-CA-C	-5.52	107.19	114.31
2	B	71	VAL	O-C-N	5.51	129.46	122.57
1	A	69	SER	N-CA-CB	-5.51	102.38	110.97
1	A	201	MET	N-CA-CB	5.50	118.27	110.13
1	A	135	PRO	N-CD-CG	-5.50	94.95	103.20
1	A	237	ALA	CA-C-O	5.50	128.37	120.51
1	A	209	TRP	N-CA-CB	-5.50	101.20	110.49
2	B	35	LEU	CA-C-O	5.50	129.69	122.44
1	A	215	ILE	N-CA-C	-5.49	97.92	109.34
2	B	125	PHE	CB-CA-C	-5.49	99.67	109.71
1	A	8	HIS	CA-C-N	-5.49	115.29	122.37
1	A	8	HIS	C-N-CA	-5.49	115.29	122.37
1	A	42	LYS	CA-C-O	5.48	128.34	121.66
2	B	26	GLY	N-CA-C	-5.48	100.20	113.18
1	A	14	ASP	CA-CB-CG	-5.47	107.12	112.60
1	A	61	THR	OG1-CB-CG2	5.47	120.24	109.30
2	B	30	LEU	N-CA-CB	-5.47	101.85	110.06
1	A	77	ALA	N-CA-CB	5.47	119.73	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	THR	OG1-CB-CG2	5.46	120.22	109.30
1	A	17	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	A	50	GLU	CA-CB-CG	5.46	125.01	114.10
2	B	138	LYS	CA-C-N	5.46	131.96	121.54
2	B	138	LYS	C-N-CA	5.46	131.96	121.54
1	A	51	ALA	CA-C-N	-5.45	111.12	121.54
1	A	51	ALA	C-N-CA	-5.45	111.12	121.54
2	B	96	ARG	CB-CA-C	5.45	116.22	108.76
1	A	273	ASP	CA-C-N	5.44	131.94	121.54
1	A	273	ASP	C-N-CA	5.44	131.94	121.54
1	A	213	SER	N-CA-C	-5.44	105.08	112.26
2	B	96	ARG	CA-C-O	5.44	126.30	120.05
1	A	45	ALA	O-C-N	5.43	129.77	123.30
1	A	200	ASP	OD1-CG-OD2	5.43	135.94	122.90
1	A	39	LEU	N-CA-C	5.43	120.92	113.97
1	A	134	HIS	O-C-N	-5.43	116.64	121.20
1	A	80	SER	O-C-N	5.43	129.81	122.59
1	A	150	GLY	N-CA-C	5.43	123.44	115.08
2	B	144	PHE	CA-C-N	-5.42	113.23	122.33
2	B	144	PHE	C-N-CA	-5.42	113.23	122.33
2	B	18	ILE	CA-CB-CG1	-5.42	101.19	110.40
2	B	5	ASP	N-CA-C	5.41	117.41	109.24
1	A	297	LEU	N-CA-C	-5.41	99.28	110.80
1	A	271	ASP	CB-CA-C	5.41	121.18	110.42
1	A	242	ARG	O-C-N	5.39	129.31	122.84
2	B	143	GLU	O-C-N	5.39	130.23	123.12
1	A	36	PRO	CB-CA-C	5.38	118.43	110.85
1	A	60	GLN	CG-CD-NE2	5.38	124.47	116.40
1	A	108	GLN	CA-CB-CG	-5.38	103.35	114.10
2	B	106	VAL	CA-CB-CG2	-5.38	101.26	110.40
2	B	116	SER	CB-CA-C	-5.38	102.24	109.71
1	A	73	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	281	PHE	CA-CB-CG	5.37	119.17	113.80
2	B	29	LEU	CB-CA-C	5.36	119.64	110.74
1	A	45	ALA	N-CA-CB	-5.36	101.68	110.68
1	A	115	ALA	CA-C-N	-5.36	111.31	121.54
1	A	115	ALA	C-N-CA	-5.36	111.31	121.54
1	A	30	LEU	O-C-N	5.35	129.71	122.59
1	A	48	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	228	ASP	CB-CA-C	5.35	120.71	110.17
1	A	296	ALA	CA-C-O	-5.35	113.48	119.79
1	A	220	THR	CA-C-O	-5.35	112.87	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	ARG	NH1-CZ-NH2	-5.34	112.35	119.30
1	A	195	PRO	CA-C-O	5.34	127.75	121.56
1	A	37	GLU	CB-CG-CD	5.33	121.67	112.60
1	A	158	ALA	N-CA-C	-5.33	100.41	108.46
1	A	242	ARG	CG-CD-NE	5.33	123.73	112.00
1	A	215	ILE	CB-CG1-CD1	-5.33	102.60	113.80
1	A	293	ALA	CA-C-O	-5.33	112.89	120.51
1	A	251	ASN	CB-CG-ND2	5.33	124.39	116.40
1	A	3	PRO	CA-C-N	5.33	128.41	120.31
1	A	3	PRO	C-N-CA	5.33	128.41	120.31
1	A	261	PRO	CA-C-O	-5.32	110.91	120.60
2	B	66	LEU	CA-C-N	5.32	131.69	121.54
2	B	66	LEU	C-N-CA	5.32	131.69	121.54
2	B	128	ARG	NE-CZ-NH1	5.32	126.81	121.50
1	A	158	ALA	N-CA-CB	-5.31	101.95	110.77
2	B	11	GLU	CA-C-O	-5.31	112.91	120.51
2	B	47	ASN	N-CA-CB	5.31	119.34	110.32
2	B	67	SER	N-CA-C	-5.30	99.50	110.80
1	A	30	LEU	CB-CA-C	5.30	120.97	110.42
1	A	69	SER	N-CA-C	5.30	115.23	108.24
1	A	250	HIS	ND1-CE1-NE2	-5.29	103.11	108.40
2	B	99	LEU	CA-C-N	5.29	126.45	119.84
2	B	99	LEU	C-N-CA	5.29	126.45	119.84
2	B	145	SER	CA-C-O	-5.28	113.78	120.28
1	A	300	ASN	OD1-CG-ND2	5.27	127.87	122.60
2	B	55	ARG	CA-C-N	-5.27	115.57	123.00
2	B	55	ARG	C-N-CA	-5.27	115.57	123.00
2	B	51	GLY	CA-C-N	5.27	130.98	122.29
2	B	51	GLY	C-N-CA	5.27	130.98	122.29
2	B	108	VAL	CG1-CB-CG2	5.27	122.39	110.80
1	A	129	ASP	CB-CA-C	-5.26	100.92	110.56
1	A	99	VAL	CA-C-N	5.26	130.50	122.24
1	A	99	VAL	C-N-CA	5.26	130.50	122.24
1	A	287	GLY	CA-C-O	-5.26	113.24	119.45
2	B	95	SER	N-CA-C	5.26	117.23	108.02
1	A	255	ASN	CA-C-O	5.26	128.03	120.51
2	B	141	GLU	CA-C-N	5.25	130.95	122.29
2	B	141	GLU	C-N-CA	5.25	130.95	122.29
1	A	160	VAL	CB-CA-C	5.24	118.62	110.96
1	A	301	ARG	NH1-CZ-NH2	-5.24	112.49	119.30
2	B	48	LEU	CD1-CG-CD2	-5.24	99.27	110.80
1	A	53	THR	CA-C-N	-5.24	113.74	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	THR	C-N-CA	-5.24	113.74	120.65
2	B	102	ARG	N-CA-CB	-5.24	101.64	110.49
2	B	124	SER	CA-C-O	5.24	125.79	120.24
1	A	251	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	54	ARG	CB-CG-CD	-5.23	99.26	111.30
1	A	133	GLN	CB-CG-CD	5.23	121.49	112.60
1	A	100	ASP	CB-CA-C	5.23	117.80	109.02
2	B	73	GLU	N-CA-C	-5.22	105.67	111.36
1	A	260	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	147	GLN	CB-CG-CD	5.21	121.46	112.60
2	B	132	ASP	CB-CG-OD1	5.20	130.37	118.40
1	A	59	PHE	O-C-N	5.20	129.51	122.59
2	B	146	HIS	CA-CB-CG	5.20	119.00	113.80
1	A	11	SER	CA-CB-OG	5.20	121.50	111.10
1	A	155	LEU	O-C-N	-5.19	117.17	123.03
1	A	209	TRP	CA-CB-CG	-5.19	103.74	113.60
2	B	106	VAL	N-CA-CB	-5.19	104.93	111.41
2	B	100	PRO	O-C-N	5.19	129.64	122.64
1	A	217	GLU	CG-CD-OE2	-5.18	106.47	118.40
1	A	246	LEU	CA-C-O	5.18	126.95	121.05
1	A	248	GLY	N-CA-C	5.18	125.45	113.18
2	B	31	SER	N-CA-CB	-5.18	102.91	110.47
2	B	60	LYS	N-CA-C	5.18	115.07	108.24
2	B	137	CYS	CA-C-N	-5.17	113.03	121.97
2	B	137	CYS	C-N-CA	-5.17	113.03	121.97
1	A	147	GLN	OE1-CD-NE2	-5.17	117.43	122.60
2	B	5	ASP	O-C-N	-5.17	116.92	123.17
1	A	21	ASN	N-CA-C	-5.17	107.04	113.19
2	B	142	LYS	CA-CB-CG	5.17	124.43	114.10
1	A	148	THR	CA-C-O	-5.16	113.13	120.51
1	A	16	SER	CB-CA-C	-5.16	101.02	109.53
1	A	121	ASN	O-C-N	-5.16	115.73	122.59
1	A	123	PRO	N-CA-CB	-5.16	98.86	103.35
1	A	149	GLU	O-C-N	-5.16	115.73	122.59
1	A	203	ASP	CB-CG-OD1	5.16	130.26	118.40
2	B	85	ARG	CA-CB-CG	5.15	124.40	114.10
2	B	120	PRO	CA-C-O	5.15	129.98	120.60
1	A	97	THR	CA-CB-CG2	5.15	119.25	110.50
2	B	74	LEU	CB-CA-C	5.15	120.76	109.99
2	B	92	VAL	O-C-N	5.14	129.00	122.57
2	B	32	LEU	O-C-N	5.14	129.43	122.59
1	A	118	PHE	CA-C-O	-5.13	112.95	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	ASN	OD1-CG-ND2	-5.13	117.47	122.60
2	B	40	ASP	O-C-N	5.12	129.37	122.82
1	A	42	LYS	CB-CG-CD	5.11	123.06	111.30
1	A	276	PRO	N-CA-C	5.11	123.00	112.47
1	A	31	LYS	O-C-N	5.11	128.55	122.27
1	A	167	ARG	CG-CD-NE	5.10	123.23	112.00
1	A	266	ASP	N-CA-C	-5.10	105.89	112.68
2	B	115	ILE	O-C-N	5.09	127.55	121.80
1	A	250	HIS	CA-CB-CG	-5.08	108.72	113.80
2	B	147	ASN	CB-CG-OD1	5.08	130.97	120.80
1	A	257	LYS	CB-CG-CD	5.08	122.99	111.30
2	B	82	THR	N-CA-CB	-5.08	101.91	110.49
2	B	147	ASN	O-C-N	5.08	129.34	122.59
1	A	39	LEU	O-C-N	-5.07	116.34	122.48
1	A	279	TRP	CB-CA-C	5.07	120.51	110.42
2	B	63	ASN	N-CA-CB	-5.07	102.23	110.59
1	A	94	VAL	N-CA-C	-5.06	106.86	111.67
1	A	134	HIS	N-CA-CB	-5.06	103.66	110.74
1	A	258	VAL	CA-C-N	5.06	130.54	122.59
1	A	258	VAL	C-N-CA	5.06	130.54	122.59
1	A	140	LEU	CA-C-O	-5.06	115.19	120.55
1	A	226	ARG	CA-C-O	-5.06	114.94	120.70
2	B	47	ASN	CA-C-O	-5.06	113.37	119.49
1	A	20	LEU	CA-C-N	-5.05	109.69	121.52
1	A	20	LEU	C-N-CA	-5.05	109.69	121.52
1	A	291	ARG	N-CA-CB	5.05	119.03	110.49
2	B	149	VAL	CB-CA-C	-5.05	103.00	111.29
1	A	259	LEU	N-CA-C	5.05	117.35	109.52
1	A	12	ILE	CA-C-N	-5.05	113.98	120.65
1	A	12	ILE	C-N-CA	-5.05	113.98	120.65
2	B	31	SER	CA-CB-OG	-5.05	101.00	111.10
1	A	36	PRO	CA-C-N	5.04	131.18	121.54
1	A	36	PRO	C-N-CA	5.04	131.18	121.54
1	A	208	ALA	O-C-N	-5.04	115.89	122.59
2	B	18	ILE	O-C-N	-5.04	117.90	122.79
1	A	163	LEU	CB-CA-C	-5.04	100.40	110.42
1	A	85	GLY	N-CA-C	5.03	125.11	113.18
1	A	144	THR	CA-CB-CG2	-5.03	101.94	110.50
2	B	70	GLU	CB-CA-C	-5.03	101.41	110.37
1	A	300	ASN	CB-CG-ND2	-5.02	108.86	116.40
1	A	237	ALA	CB-CA-C	5.02	120.42	110.42
2	B	119	GLU	CA-C-N	5.02	126.12	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	119	GLU	C-N-CA	5.02	126.12	119.84
1	A	240	LEU	CA-CB-CG	5.02	133.87	116.30
1	A	194	MET	CA-C-N	5.02	124.95	119.78
1	A	194	MET	C-N-CA	5.02	124.95	119.78
1	A	44	ILE	O-C-N	5.01	128.83	122.57
1	A	164	LYS	CG-CD-CE	5.00	122.81	111.30
2	B	3	HIS	N-CA-C	5.00	121.46	110.80
1	A	60	GLN	CA-C-N	5.00	131.09	121.54
1	A	60	GLN	C-N-CA	5.00	131.09	121.54
1	A	112	ALA	N-CA-C	-5.00	103.17	111.37

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	113	ARG	Sidechain
1	A	151	ARG	Sidechain
1	A	17	ARG	Sidechain
1	A	183	ARG	Sidechain
1	A	221	ARG	Sidechain
1	A	226	ARG	Sidechain
1	A	242	ARG	Sidechain
1	A	264	ARG	Sidechain
1	A	291	ARG	Sidechain
1	A	301	ARG	Sidechain
1	A	35	GLN	Sidechain
1	A	54	ARG	Sidechain
1	A	56	ARG	Sidechain
1	A	65	ARG	Sidechain
2	B	129	ARG	Sidechain
2	B	14	ARG	Sidechain
2	B	85	ARG	Sidechain
2	B	96	ARG	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	2362	0	2370	866	6
2	B	1148	0	1117	532	10
3	B	1	0	0	2	0
All	All	3511	0	3487	1388	16

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 199.

All (1388) 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)
2:B:66:LEU:H	2:B:66:LEU:CD1	1.34	1.38
2:B:9:VAL:CG1	2:B:14:ARG:HA	1.56	1.32
1:A:282:GLN:HE21	1:A:282:GLN:N	1.23	1.32
2:B:128:ARG:NH1	2:B:143:GLU:OE1	1.60	1.32
1:A:294:LEU:O	1:A:298:VAL:HG23	1.25	1.32
1:A:251:ASN:O	1:A:253:LYS:N	1.60	1.31
1:A:282:GLN:H	1:A:282:GLN:NE2	1.29	1.31
1:A:69:SER:O	1:A:70:VAL:HG13	1.33	1.29
2:B:114:CYS:HB3	2:B:116:SER:OG	1.24	1.26
1:A:231:GLU:HB2	1:A:232:TYR:CE2	1.68	1.26
1:A:210:SER:C	1:A:211:LEU:HD23	1.60	1.25
1:A:157:VAL:O	1:A:185:TYR:HD1	1.14	1.24
2:B:18:ILE:HG23	2:B:62:GLU:OE2	1.37	1.24
1:A:108:GLN:O	1:A:129:ASP:O	1.56	1.24
1:A:140:LEU:HD13	1:A:287:GLY:CA	1.69	1.23
1:A:157:VAL:O	1:A:185:TYR:CD1	1.93	1.22
1:A:294:LEU:C	1:A:298:VAL:HG23	1.62	1.22
1:A:20:LEU:O	1:A:24:LEU:HB2	1.40	1.21
2:B:25:ILE:O	2:B:25:ILE:HD12	1.42	1.19
2:B:66:LEU:N	2:B:66:LEU:HD13	1.46	1.19
2:B:4:ASN:OD1	2:B:5:ASP:N	1.75	1.18
1:A:119:SER:O	1:A:120:GLY:O	1.59	1.18
2:B:145:SER:O	2:B:147:ASN:N	1.77	1.18
1:A:145:ILE:O	1:A:145:ILE:HD12	1.40	1.18
1:A:274:LYS:HD3	1:A:274:LYS:C	1.69	1.17
2:B:27:PHE:CA	2:B:30:LEU:HD12	1.73	1.17
1:A:59:PHE:O	1:A:62:SER:HB2	1.44	1.17
2:B:22:PRO:HG2	2:B:25:ILE:HG23	1.22	1.16
1:A:157:VAL:HG11	1:A:184:PHE:CD2	1.80	1.16
1:A:232:TYR:O	1:A:234:ASX:XD1	1.95	1.15
1:A:254:MET:O	1:A:255:ASN:OD1	1.63	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ILE:CG2	2:B:62:GLU:H	1.45	1.15
1:A:187:ILE:HD13	1:A:187:ILE:H	1.10	1.14
1:A:201:MET:HA	1:A:204:GLU:HB3	1.20	1.14
2:B:100:PRO:O	2:B:101:GLU:HG2	1.47	1.14
2:B:104:ILE:O	2:B:123:SER:O	1.64	1.14
1:A:264:ARG:NH2	1:A:273:ASP:OD1	1.81	1.14
2:B:71:VAL:C	2:B:73:GLU:H	1.50	1.14
1:A:303:LEU:HD11	1:A:305:LEU:HA	1.23	1.13
2:B:9:VAL:HG13	2:B:14:ARG:CA	1.79	1.13
2:B:71:VAL:HA	2:B:74:LEU:HD11	1.26	1.13
1:A:197:TYR:CD1	1:A:198:ILE:N	2.15	1.13
1:A:278:ALA:O	1:A:279:TRP:CB	1.95	1.13
2:B:61:ILE:HG23	2:B:62:GLU:HG2	1.29	1.13
2:B:114:CYS:CB	2:B:116:SER:OG	1.96	1.13
2:B:101:GLU:O	2:B:102:ARG:CB	1.97	1.13
1:A:216:GLU:O	1:A:219:MET:HB3	1.47	1.12
1:A:272:VAL:O	1:A:273:ASP:C	1.89	1.12
1:A:303:LEU:HD21	1:A:305:LEU:HB3	1.31	1.12
1:A:140:LEU:HD13	1:A:287:GLY:HA2	1.23	1.12
1:A:257:LYS:HA	1:A:277:HIS:HA	1.16	1.12
1:A:56:ARG:CD	1:A:60:GLN:HE22	1.61	1.11
2:B:27:PHE:O	2:B:30:LEU:HB2	1.50	1.11
1:A:210:SER:O	1:A:211:LEU:HD23	1.46	1.11
2:B:20:HIS:HD2	2:B:22:PRO:O	1.32	1.11
1:A:29:LYS:CG	1:A:30:LEU:H	1.57	1.10
1:A:40:LYS:HD3	1:A:41:HIS:NE2	1.65	1.10
1:A:143:PHE:O	1:A:146:GLN:N	1.84	1.10
2:B:128:ARG:O	2:B:134:ALA:HB3	1.49	1.10
1:A:198:ILE:O	1:A:199:LEU:HD12	1.52	1.10
2:B:86:ILE:HG12	2:B:89:TYR:O	1.48	1.10
2:B:61:ILE:HB	2:B:82:THR:O	1.50	1.10
1:A:219:MET:HG3	1:A:219:MET:O	1.51	1.09
2:B:27:PHE:HA	2:B:30:LEU:HD12	1.28	1.09
2:B:32:LEU:HD21	2:B:77:TYR:HE2	1.14	1.09
2:B:70:GLU:N	2:B:71:VAL:HG23	1.66	1.09
2:B:71:VAL:HG12	2:B:72:ASP:H	1.06	1.09
1:A:116:THR:HG22	1:A:117:GLU:N	1.58	1.08
1:A:160:VAL:HG12	1:A:187:ILE:HB	1.09	1.08
1:A:87:THR:O	1:A:89:ALA:N	1.87	1.08
1:A:157:VAL:HG11	1:A:184:PHE:HD2	0.92	1.08
2:B:34:LYS:HG2	2:B:35:LEU:H	0.95	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:119:GLU:HB3	2:B:120:PRO:HD2	1.32	1.07
2:B:1:MET:HE1	2:B:41:ARG:HH22	1.20	1.07
2:B:64:THR:HG22	2:B:64:THR:O	1.45	1.07
1:A:162:ASP:N	1:A:228:ASP:OD2	1.87	1.07
2:B:16:THR:O	2:B:17:VAL:HG23	1.55	1.07
1:A:194:MET:HE3	1:A:198:ILE:HG13	1.37	1.06
2:B:66:LEU:HD22	2:B:67:SER:N	1.69	1.06
1:A:56:ARG:HG2	1:A:60:GLN:NE2	1.70	1.06
2:B:61:ILE:HG22	2:B:62:GLU:H	0.91	1.06
2:B:150:LEU:O	2:B:151:ALA:HB2	1.50	1.06
1:A:95:ILE:O	1:A:99:VAL:CG2	2.03	1.06
1:A:70:VAL:O	1:A:71:VAL:HG13	1.54	1.05
2:B:70:GLU:H	2:B:71:VAL:HG23	1.15	1.05
1:A:231:GLU:CB	1:A:232:TYR:CE2	2.38	1.05
1:A:276:PRO:O	1:A:278:ALA:N	1.90	1.05
2:B:71:VAL:HA	2:B:74:LEU:CD1	1.85	1.05
2:B:74:LEU:HD13	2:B:74:LEU:N	1.71	1.05
1:A:35:GLN:HG3	1:A:38:LEU:HD21	1.38	1.05
1:A:229:PRO:HA	1:A:267:GLU:OE2	1.57	1.05
2:B:67:SER:HB3	2:B:70:GLU:OE2	1.57	1.04
1:A:187:ILE:HD13	1:A:187:ILE:N	1.73	1.04
2:B:71:VAL:O	2:B:73:GLU:N	1.90	1.03
1:A:27:ALA:HB2	1:A:293:ALA:HB2	1.37	1.03
1:A:228:ASP:HB2	1:A:229:PRO:HD3	1.07	1.03
2:B:27:PHE:HA	2:B:30:LEU:CD1	1.87	1.03
2:B:61:ILE:CG1	2:B:82:THR:H	1.72	1.03
2:B:128:ARG:NH1	2:B:143:GLU:CD	2.16	1.03
1:A:35:GLN:HE21	1:A:35:GLN:CA	1.62	1.03
1:A:249:LEU:O	1:A:250:HIS:ND1	1.92	1.03
1:A:274:LYS:CD	1:A:275:THR:N	2.22	1.03
1:A:187:ILE:N	1:A:187:ILE:CD1	2.21	1.02
1:A:145:ILE:HD12	1:A:145:ILE:C	1.76	1.02
1:A:142:LEU:O	1:A:145:ILE:HG23	1.58	1.02
2:B:61:ILE:HG13	2:B:82:THR:H	0.90	1.02
2:B:128:ARG:HB3	2:B:128:ARG:HH21	1.19	1.02
1:A:208:ALA:O	1:A:209:TRP:HB3	1.60	1.01
2:B:33:PHE:O	2:B:34:LYS:O	1.78	1.01
2:B:131:ASP:O	2:B:132:ASP:OD1	1.76	1.01
1:A:235:VAL:CG2	1:A:238:GLN:HB2	1.89	1.01
1:A:9:ILE:HB	1:A:125:LEU:CD1	1.90	1.01
1:A:260:HIS:H	1:A:283:GLN:HE22	1.05	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASN:O	2:B:64:THR:OG1	1.77	1.00
1:A:272:VAL:O	1:A:273:ASP:O	1.79	1.00
2:B:119:GLU:CB	2:B:120:PRO:HD2	1.85	1.00
2:B:15:GLY:O	2:B:64:THR:CG2	2.08	1.00
1:A:29:LYS:HG2	1:A:30:LEU:N	1.72	1.00
2:B:64:THR:N	2:B:84:ASN:HD22	1.60	1.00
2:B:66:LEU:HD22	2:B:67:SER:H	0.84	0.99
2:B:61:ILE:HG13	2:B:82:THR:N	1.74	0.99
1:A:29:LYS:HG2	1:A:30:LEU:H	0.87	0.99
1:A:31:LYS:HE2	1:A:289:PHE:CE2	1.97	0.99
2:B:34:LYS:CG	2:B:35:LEU:H	1.62	0.99
2:B:61:ILE:HG22	2:B:62:GLU:N	1.71	0.99
2:B:86:ILE:HG23	2:B:90:GLU:HB2	1.40	0.99
1:A:67:GLY:O	1:A:68:ALA:HB2	1.57	0.99
1:A:138:THR:HG21	1:A:171:SER:CB	1.91	0.99
1:A:16:SER:O	1:A:17:ARG:O	1.81	0.98
1:A:69:SER:O	1:A:70:VAL:CG1	2.11	0.98
1:A:194:MET:HG2	1:A:199:LEU:HD11	1.44	0.98
1:A:202:LEU:HD12	1:A:207:ILE:HG21	1.44	0.98
1:A:80:SER:O	1:A:81:LEU:HD12	1.63	0.98
1:A:228:ASP:HB2	1:A:229:PRO:CD	1.92	0.98
2:B:107:LEU:C	2:B:108:VAL:HG22	1.84	0.98
1:A:31:LYS:HE2	1:A:289:PHE:CD2	1.98	0.98
1:A:303:LEU:CD1	1:A:305:LEU:HA	1.94	0.98
1:A:8:HIS:HB2	1:A:10:ILE:HD11	1.43	0.97
1:A:10:ILE:O	1:A:10:ILE:HG22	1.60	0.97
2:B:28:LYS:O	2:B:32:LEU:N	1.96	0.97
2:B:34:LYS:HG2	2:B:35:LEU:N	1.80	0.97
1:A:191:ALA:O	1:A:192:LEU:HD13	1.63	0.97
2:B:32:LEU:CD2	2:B:77:TYR:HE2	1.77	0.97
1:A:81:LEU:HD22	1:A:82:GLY:N	1.78	0.97
1:A:231:GLU:HB2	1:A:232:TYR:CD2	1.99	0.97
2:B:66:LEU:CD2	2:B:67:SER:H	1.76	0.97
1:A:187:ILE:H	1:A:187:ILE:CD1	1.75	0.96
2:B:8:GLN:O	2:B:9:VAL:HG23	1.64	0.96
1:A:31:LYS:NZ	1:A:147:GLN:OE1	1.96	0.96
1:A:43:VAL:HA	1:A:69:SER:HB2	1.48	0.96
2:B:74:LEU:HD13	2:B:74:LEU:H	1.27	0.96
1:A:230:SER:C	1:A:231:GLU:HG2	1.91	0.96
1:A:164:LYS:HD3	1:A:165:TYR:CE2	1.99	0.96
1:A:5:TYR:HE2	1:A:300:ASN:O	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:LYS:O	2:B:35:LEU:HG	1.67	0.95
1:A:5:TYR:O	1:A:7:SER:N	1.98	0.95
1:A:56:ARG:CG	1:A:60:GLN:NE2	2.30	0.95
2:B:73:GLU:OE1	2:B:73:GLU:HA	1.66	0.95
1:A:14:ASP:OD1	1:A:14:ASP:O	1.85	0.95
2:B:4:ASN:CG	2:B:5:ASP:H	1.70	0.95
1:A:81:LEU:HD22	1:A:82:GLY:H	1.30	0.94
1:A:303:LEU:HD11	1:A:305:LEU:CA	1.96	0.94
1:A:145:ILE:C	1:A:145:ILE:CD1	2.38	0.94
1:A:40:LYS:HB3	1:A:41:HIS:CD2	2.03	0.94
1:A:261:PRO:O	1:A:262:LEU:O	1.85	0.94
1:A:88:LEU:O	1:A:88:LEU:HD22	1.68	0.94
1:A:262:LEU:HB3	1:A:263:PRO:HA	1.50	0.94
1:A:217:GLU:O	1:A:218:VAL:HG23	1.66	0.94
1:A:279:TRP:O	1:A:281:PHE:N	2.01	0.94
1:A:67:GLY:O	1:A:68:ALA:CB	2.14	0.93
2:B:128:ARG:HB3	2:B:128:ARG:NH2	1.83	0.93
1:A:92:ILE:O	1:A:96:SER:OG	1.85	0.93
1:A:303:LEU:HD21	1:A:305:LEU:CD2	1.98	0.93
2:B:23:ALA:O	2:B:24:GLU:CB	2.17	0.93
1:A:214:SER:HB3	1:A:216:GLU:HG3	1.50	0.93
2:B:105:ASP:C	2:B:105:ASP:OD2	2.07	0.93
1:A:202:LEU:CD1	1:A:207:ILE:HG21	1.97	0.93
2:B:114:CYS:HG	3:B:153:ZN:ZN	0.75	0.93
1:A:250:HIS:O	1:A:251:ASN:C	2.09	0.93
1:A:88:LEU:HD22	1:A:88:LEU:C	1.93	0.93
2:B:101:GLU:O	2:B:102:ARG:HB3	1.12	0.93
1:A:254:MET:C	1:A:255:ASN:OD1	2.10	0.93
1:A:8:HIS:HB2	1:A:10:ILE:CD1	1.97	0.92
1:A:44:ILE:O	1:A:71:VAL:CG2	2.17	0.92
1:A:251:ASN:O	1:A:253:LYS:CA	2.17	0.92
1:A:260:HIS:N	1:A:283:GLN:HE22	1.67	0.92
1:A:95:ILE:HG22	1:A:96:SER:N	1.82	0.92
1:A:294:LEU:C	1:A:298:VAL:CG2	2.43	0.92
1:A:138:THR:HG21	1:A:171:SER:HB3	1.52	0.92
2:B:20:HIS:CD2	2:B:22:PRO:O	2.21	0.92
1:A:201:MET:HA	1:A:204:GLU:CB	2.00	0.92
1:A:49:PHE:HB2	1:A:105:ARG:O	1.68	0.91
1:A:56:ARG:HG2	1:A:60:GLN:HE21	1.24	0.91
1:A:70:VAL:C	1:A:71:VAL:HG22	1.87	0.91
1:A:269:ALA:HB3	1:A:272:VAL:HG23	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ASP:OD1	2:B:98:SER:C	2.13	0.91
1:A:274:LYS:HD3	1:A:275:THR:N	1.82	0.91
1:A:94:VAL:O	1:A:97:THR:OG1	1.89	0.91
1:A:197:TYR:CD1	1:A:197:TYR:C	2.44	0.91
1:A:201:MET:CA	1:A:204:GLU:HB3	2.00	0.91
1:A:234:ASX:XD1	1:A:239:PHE:HE1	1.84	0.91
2:B:38:THR:HG22	2:B:38:THR:O	1.71	0.91
2:B:66:LEU:CD1	2:B:66:LEU:N	2.13	0.91
2:B:108:VAL:HG21	2:B:152:ASN:HB3	1.52	0.91
2:B:32:LEU:HD21	2:B:106:VAL:HG21	1.50	0.91
2:B:140:CYS:HG	3:B:153:ZN:ZN	0.77	0.91
2:B:9:VAL:HG21	2:B:14:ARG:C	1.96	0.90
2:B:32:LEU:CD2	2:B:106:VAL:HG21	2.00	0.90
1:A:2:ASN:OD1	1:A:2:ASN:C	2.12	0.90
1:A:235:VAL:HG23	1:A:238:GLN:HB2	1.52	0.90
1:A:24:LEU:HD21	1:A:142:LEU:HD23	1.52	0.90
1:A:110:GLY:HA2	2:B:139:TYR:O	1.70	0.90
2:B:32:LEU:HD21	2:B:77:TYR:CE2	2.06	0.90
2:B:25:ILE:O	2:B:25:ILE:CD1	2.18	0.90
1:A:197:TYR:O	1:A:199:LEU:N	2.04	0.90
2:B:71:VAL:O	2:B:73:GLU:HB2	1.72	0.90
1:A:95:ILE:O	1:A:99:VAL:HG23	1.72	0.89
2:B:18:ILE:CA	2:B:62:GLU:OE1	2.19	0.89
2:B:72:ASP:OD1	2:B:98:SER:N	2.05	0.89
1:A:9:ILE:C	1:A:10:ILE:HD12	1.97	0.89
1:A:159:MET:CE	1:A:172:LEU:HD23	2.01	0.89
2:B:22:PRO:HG2	2:B:25:ILE:CG2	2.01	0.89
2:B:86:ILE:HG23	2:B:90:GLU:CB	2.03	0.89
1:A:281:PHE:O	1:A:284:ALA:N	2.04	0.89
2:B:71:VAL:CG1	2:B:72:ASP:H	1.82	0.89
1:A:75:ASP:O	1:A:76:SER:HB2	1.72	0.89
2:B:64:THR:O	2:B:64:THR:CG2	2.21	0.89
1:A:303:LEU:O	1:A:303:LEU:HD23	1.73	0.89
2:B:17:VAL:HG22	2:B:43:THR:CB	2.01	0.89
2:B:23:ALA:O	2:B:24:GLU:HB2	1.65	0.88
2:B:15:GLY:O	2:B:64:THR:HG21	1.69	0.88
1:A:249:LEU:C	1:A:250:HIS:ND1	2.31	0.88
1:A:303:LEU:HG	1:A:305:LEU:N	1.88	0.88
2:B:17:VAL:HG13	2:B:43:THR:HB	1.55	0.88
1:A:216:GLU:O	1:A:219:MET:CB	2.21	0.88
2:B:111:ASP:O	2:B:117:HIS:HE1	1.57	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:HG23	1:A:238:GLN:N	1.88	0.88
1:A:293:ALA:O	1:A:297:LEU:HD12	1.74	0.88
1:A:35:GLN:CA	1:A:35:GLN:NE2	2.37	0.88
2:B:18:ILE:HA	2:B:62:GLU:OE1	1.73	0.88
2:B:91:VAL:O	2:B:92:VAL:HG23	1.73	0.88
2:B:1:MET:CE	2:B:41:ARG:HH22	1.85	0.87
1:A:29:LYS:H	1:A:29:LYS:HD2	1.37	0.87
1:A:211:LEU:C	1:A:212:HIS:ND1	2.32	0.87
1:A:231:GLU:CB	1:A:232:TYR:CD2	2.55	0.87
2:B:28:LYS:C	2:B:32:LEU:HB2	1.99	0.87
2:B:71:VAL:HG13	2:B:74:LEU:HD21	1.57	0.87
2:B:69:ASP:CG	2:B:69:ASP:O	2.16	0.87
1:A:50:GLU:O	1:A:51:ALA:O	1.92	0.87
1:A:56:ARG:HD2	1:A:60:GLN:HE22	1.40	0.87
2:B:9:VAL:CG1	2:B:14:ARG:CA	2.45	0.87
1:A:152:LEU:HD22	1:A:176:LEU:HD21	1.54	0.87
2:B:132:ASP:O	2:B:146:HIS:CE1	2.27	0.87
1:A:68:ALA:O	1:A:69:SER:OG	1.91	0.87
2:B:71:VAL:HG12	2:B:72:ASP:N	1.86	0.87
2:B:86:ILE:O	2:B:90:GLU:CG	2.22	0.87
2:B:9:VAL:CG2	2:B:14:ARG:C	2.48	0.87
2:B:9:VAL:HG12	2:B:10:ALA:H	1.40	0.87
2:B:107:LEU:O	2:B:108:VAL:HG13	1.74	0.87
1:A:116:THR:CG2	1:A:117:GLU:N	2.37	0.86
1:A:56:ARG:CD	1:A:60:GLN:NE2	2.38	0.86
1:A:115:ALA:O	1:A:116:THR:O	1.92	0.86
1:A:191:ALA:C	1:A:192:LEU:HD13	2.00	0.86
2:B:21:ILE:HB	2:B:22:PRO:HD3	1.58	0.86
2:B:145:SER:O	2:B:146:HIS:C	2.18	0.86
2:B:63:ASN:HA	2:B:84:ASN:HB2	1.57	0.86
1:A:145:ILE:O	1:A:145:ILE:CD1	2.22	0.86
1:A:235:VAL:HG23	1:A:238:GLN:CA	2.06	0.86
2:B:1:MET:HE1	2:B:41:ARG:NH2	1.90	0.86
1:A:35:GLN:HE21	1:A:35:GLN:HA	1.38	0.86
1:A:303:LEU:CD2	1:A:305:LEU:HB3	2.05	0.86
2:B:102:ARG:HD2	2:B:104:ILE:CD1	2.06	0.86
1:A:160:VAL:CG1	1:A:187:ILE:HB	2.03	0.86
1:A:278:ALA:O	1:A:279:TRP:HB2	1.07	0.86
2:B:106:VAL:O	2:B:107:LEU:HG	1.76	0.86
1:A:40:LYS:O	1:A:41:HIS:HB2	1.74	0.85
2:B:106:VAL:O	2:B:107:LEU:CB	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:O	1:A:198:ILE:HD12	1.75	0.85
1:A:136:THR:HB	1:A:291:ARG:HH21	1.41	0.85
1:A:214:SER:HB3	1:A:216:GLU:HB2	1.59	0.85
2:B:38:THR:O	2:B:38:THR:CG2	2.24	0.85
2:B:101:GLU:O	2:B:101:GLU:HG3	1.76	0.85
2:B:4:ASN:CG	2:B:5:ASP:N	2.23	0.84
1:A:211:LEU:C	1:A:212:HIS:CE1	2.55	0.84
1:A:234:ASX:XD2	1:A:234:ASX:H	1.88	0.84
2:B:18:ILE:HD13	2:B:44:ILE:CG1	2.07	0.84
1:A:75:ASP:CG	1:A:79:THR:HB	2.02	0.84
2:B:4:ASN:OD1	2:B:5:ASP:CA	2.26	0.84
1:A:91:THR:HG22	1:A:95:ILE:HD12	1.58	0.84
1:A:279:TRP:O	1:A:280:TYR:C	2.19	0.84
2:B:129:ARG:O	2:B:130:ALA:C	2.21	0.84
2:B:67:SER:OG	2:B:68:GLU:N	2.10	0.84
1:A:136:THR:HB	1:A:291:ARG:NH2	1.92	0.83
1:A:160:VAL:HG12	1:A:187:ILE:CB	2.03	0.83
1:A:235:VAL:HG22	1:A:238:GLN:HB2	1.60	0.83
2:B:128:ARG:HH21	2:B:128:ARG:CB	1.90	0.83
1:A:212:HIS:ND1	1:A:212:HIS:N	2.22	0.83
1:A:254:MET:O	1:A:255:ASN:CG	2.21	0.83
2:B:114:CYS:SG	2:B:116:SER:OG	2.31	0.83
2:B:106:VAL:O	2:B:107:LEU:CG	2.27	0.83
1:A:92:ILE:O	1:A:95:ILE:HG22	1.77	0.83
1:A:5:TYR:CE2	1:A:300:ASN:O	2.31	0.83
1:A:95:ILE:HG22	1:A:96:SER:H	1.39	0.83
1:A:197:TYR:C	1:A:197:TYR:HD1	1.84	0.83
2:B:106:VAL:O	2:B:107:LEU:HB2	1.78	0.83
2:B:119:GLU:CB	2:B:120:PRO:CD	2.55	0.83
1:A:279:TRP:HA	1:A:282:GLN:NE2	1.94	0.83
1:A:189:PRO:O	1:A:189:PRO:HG2	1.76	0.82
2:B:47:ASN:C	2:B:49:PRO:N	2.30	0.82
2:B:66:LEU:H	2:B:66:LEU:HD13	0.66	0.82
2:B:147:ASN:O	2:B:148:VAL:C	2.22	0.82
1:A:228:ASP:O	1:A:267:GLU:HG2	1.78	0.82
1:A:208:ALA:C	1:A:209:TRP:CD1	2.58	0.82
1:A:202:LEU:HD12	1:A:207:ILE:CG2	2.08	0.82
1:A:250:HIS:O	1:A:252:ALA:N	2.12	0.82
1:A:260:HIS:H	1:A:283:GLN:NE2	1.78	0.82
2:B:69:ASP:C	2:B:71:VAL:H	1.75	0.82
1:A:22:LEU:O	1:A:26:THR:N	2.13	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:LEU:HD23	2:B:33:PHE:HE1	1.45	0.82
1:A:262:LEU:CB	1:A:263:PRO:HA	2.07	0.82
1:A:162:ASP:HA	1:A:192:LEU:HB3	1.61	0.82
1:A:201:MET:HA	1:A:204:GLU:HG3	1.62	0.82
2:B:22:PRO:CG	2:B:25:ILE:HG23	2.09	0.81
1:A:228:ASP:CB	1:A:229:PRO:HD3	2.01	0.81
1:A:95:ILE:CG2	1:A:96:SER:N	2.42	0.81
1:A:208:ALA:O	1:A:209:TRP:CB	2.27	0.81
1:A:251:ASN:C	1:A:253:LYS:N	2.34	0.81
2:B:18:ILE:O	2:B:43:THR:O	1.99	0.81
1:A:187:ILE:HG21	1:A:214:SER:O	1.80	0.81
1:A:235:VAL:HG23	1:A:238:GLN:CB	2.11	0.81
2:B:18:ILE:HD13	2:B:44:ILE:HG12	1.63	0.81
2:B:29:LEU:O	2:B:33:PHE:N	2.13	0.81
2:B:71:VAL:C	2:B:73:GLU:N	2.28	0.81
2:B:34:LYS:C	2:B:35:LEU:HG	2.03	0.81
1:A:108:GLN:HG3	2:B:113:ASN:ND2	1.95	0.81
2:B:17:VAL:HA	2:B:18:ILE:HD12	1.62	0.81
2:B:72:ASP:CG	2:B:98:SER:O	2.24	0.81
2:B:86:ILE:O	2:B:90:GLU:OE2	1.97	0.81
1:A:111:ALA:O	1:A:112:ALA:C	2.22	0.80
1:A:159:MET:HE1	1:A:172:LEU:HD23	1.62	0.80
1:A:87:THR:C	1:A:89:ALA:H	1.90	0.80
1:A:208:ALA:HA	1:A:209:TRP:HD1	1.44	0.80
2:B:69:ASP:HB2	2:B:72:ASP:HB2	1.61	0.80
2:B:74:LEU:CD1	2:B:74:LEU:N	2.43	0.80
1:A:152:LEU:CD2	1:A:176:LEU:HD21	2.11	0.80
1:A:179:PHE:H	1:A:179:PHE:HD2	1.29	0.80
1:A:35:GLN:HE21	1:A:35:GLN:N	1.79	0.80
1:A:177:ALA:O	1:A:178:LYS:C	2.23	0.80
1:A:93:SER:C	1:A:96:SER:OG	2.25	0.80
1:A:257:LYS:HA	1:A:277:HIS:CA	2.08	0.80
1:A:31:LYS:NZ	1:A:286:ASN:OD1	2.13	0.79
2:B:83:VAL:HG23	2:B:92:VAL:HG11	1.61	0.79
2:B:9:VAL:HG13	2:B:14:ARG:HA	0.82	0.79
1:A:266:ASP:O	1:A:267:GLU:C	2.18	0.79
1:A:87:THR:C	1:A:89:ALA:N	2.39	0.79
1:A:230:SER:O	1:A:231:GLU:OE1	2.00	0.79
2:B:5:ASP:CG	2:B:6:LYS:N	2.40	0.79
2:B:26:GLY:O	2:B:30:LEU:CD1	2.29	0.79
2:B:100:PRO:O	2:B:101:GLU:CG	2.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLU:HG3	1:A:221:ARG:HH12	1.47	0.79
1:A:8:HIS:CB	1:A:10:ILE:HD11	2.12	0.79
1:A:10:ILE:O	1:A:10:ILE:CG2	2.21	0.79
1:A:29:LYS:O	1:A:33:ASN:N	2.15	0.79
1:A:212:HIS:CG	1:A:218:VAL:HG21	2.18	0.79
2:B:83:VAL:HG23	2:B:92:VAL:CG1	2.12	0.79
1:A:22:LEU:O	1:A:26:THR:OG1	2.01	0.78
1:A:211:LEU:HD23	1:A:211:LEU:N	1.89	0.78
1:A:253:LYS:C	1:A:254:MET:HG2	2.08	0.78
2:B:29:LEU:HA	2:B:32:LEU:HB3	1.65	0.78
2:B:61:ILE:CG2	2:B:62:GLU:N	2.30	0.78
2:B:102:ARG:HD2	2:B:104:ILE:HD11	1.63	0.78
2:B:150:LEU:O	2:B:151:ALA:CB	2.26	0.78
1:A:58:SER:O	1:A:59:PHE:O	2.02	0.78
1:A:232:TYR:O	1:A:234:ASX:CG	2.26	0.78
2:B:61:ILE:CG2	2:B:62:GLU:HG2	2.12	0.78
1:A:198:ILE:O	1:A:198:ILE:CG1	2.28	0.78
2:B:128:ARG:O	2:B:134:ALA:CB	2.32	0.78
1:A:66:LEU:CD1	1:A:292:GLN:HG3	2.14	0.78
2:B:16:THR:HG23	2:B:62:GLU:HB3	1.66	0.78
1:A:155:LEU:O	1:A:182:ASN:O	2.02	0.78
2:B:116:SER:O	2:B:117:HIS:CB	2.29	0.78
1:A:115:ALA:O	1:A:116:THR:C	2.19	0.78
1:A:132:ASN:HD21	2:B:141:GLU:HB2	1.46	0.78
1:A:214:SER:HB3	1:A:216:GLU:CG	2.14	0.78
1:A:274:LYS:HD2	1:A:275:THR:CA	2.14	0.78
2:B:28:LYS:O	2:B:32:LEU:HB2	1.82	0.78
2:B:61:ILE:HG23	2:B:62:GLU:CG	2.11	0.78
2:B:115:ILE:CG2	2:B:119:GLU:HG3	2.14	0.78
1:A:251:ASN:O	1:A:253:LYS:HG3	1.83	0.78
1:A:194:MET:HE3	1:A:198:ILE:CG1	2.13	0.77
2:B:18:ILE:CD1	2:B:18:ILE:N	2.45	0.77
1:A:207:ILE:HG23	1:A:208:ALA:N	1.98	0.77
1:A:303:LEU:HD11	1:A:305:LEU:CB	2.13	0.77
2:B:77:TYR:CD1	2:B:77:TYR:N	2.51	0.77
1:A:81:LEU:CD2	1:A:82:GLY:H	1.96	0.77
1:A:82:GLY:HA3	1:A:86:GLN:HB3	1.66	0.77
1:A:198:ILE:HD12	1:A:198:ILE:C	2.10	0.77
2:B:26:GLY:O	2:B:30:LEU:HD12	1.84	0.77
2:B:61:ILE:CB	2:B:82:THR:O	2.30	0.77
1:A:109:GLU:HA	1:A:129:ASP:HB3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:SER:O	1:A:119:SER:OG	1.94	0.77
1:A:210:SER:O	1:A:211:LEU:CD2	2.29	0.77
2:B:17:VAL:CG1	2:B:43:THR:HB	2.15	0.77
2:B:25:ILE:HD12	2:B:25:ILE:C	2.09	0.77
1:A:199:LEU:C	1:A:201:MET:N	2.36	0.77
2:B:115:ILE:HG22	2:B:119:GLU:HG3	1.66	0.77
2:B:137:CYS:SG	2:B:139:TYR:HB2	2.24	0.77
1:A:136:THR:CG2	1:A:291:ARG:NH2	2.48	0.77
1:A:141:ASP:O	1:A:145:ILE:HG22	1.85	0.77
2:B:86:ILE:O	2:B:90:GLU:HG3	1.84	0.77
2:B:27:PHE:O	2:B:30:LEU:CB	2.32	0.76
1:A:39:LEU:O	1:A:42:LYS:HB2	1.84	0.76
1:A:136:THR:CB	1:A:291:ARG:HH21	1.98	0.76
1:A:75:ASP:OD1	1:A:79:THR:HB	1.84	0.76
1:A:294:LEU:O	1:A:298:VAL:CG2	2.21	0.76
2:B:30:LEU:O	2:B:33:PHE:O	2.02	0.76
2:B:145:SER:C	2:B:147:ASN:N	2.44	0.76
1:A:119:SER:C	1:A:120:GLY:O	2.25	0.76
2:B:5:ASP:OD1	2:B:6:LYS:N	2.17	0.76
1:A:9:ILE:HD13	1:A:294:LEU:HD22	1.67	0.76
1:A:18:ASP:O	1:A:19:ASP:C	2.28	0.76
1:A:164:LYS:HD3	1:A:165:TYR:HE2	1.49	0.76
1:A:16:SER:HB3	1:A:19:ASP:OD1	1.85	0.76
1:A:175:ALA:O	1:A:176:LEU:C	2.24	0.76
2:B:18:ILE:HD12	2:B:18:ILE:N	1.99	0.76
1:A:52:SER:OG	1:A:55:THR:HG21	1.85	0.75
1:A:194:MET:HG3	1:A:195:PRO:HD2	1.68	0.75
2:B:67:SER:CB	2:B:70:GLU:OE2	2.33	0.75
1:A:214:SER:HB3	1:A:216:GLU:CB	2.15	0.75
1:A:234:ASX:XD1	1:A:239:PHE:CE1	2.69	0.75
1:A:152:LEU:HD22	1:A:176:LEU:CD2	2.15	0.75
1:A:198:ILE:O	1:A:198:ILE:CD1	2.34	0.75
1:A:276:PRO:C	1:A:278:ALA:H	1.95	0.75
1:A:110:GLY:O	1:A:113:ARG:N	2.20	0.75
1:A:140:LEU:CD1	1:A:287:GLY:CA	2.59	0.75
1:A:303:LEU:HG	1:A:305:LEU:H	1.51	0.75
2:B:28:LYS:O	2:B:31:SER:OG	2.04	0.75
2:B:16:THR:O	2:B:17:VAL:CG2	2.33	0.75
2:B:62:GLU:C	2:B:63:ASN:OD1	2.29	0.75
1:A:179:PHE:HD2	1:A:179:PHE:N	1.85	0.75
1:A:208:ALA:C	1:A:209:TRP:HD1	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:60:LYS:O	2:B:82:THR:O	2.04	0.74
1:A:116:THR:HG22	1:A:117:GLU:H	1.52	0.74
1:A:161:GLY:HA3	1:A:228:ASP:CG	2.11	0.74
2:B:146:HIS:O	2:B:150:LEU:HB2	1.87	0.74
1:A:29:LYS:CG	1:A:30:LEU:N	2.30	0.74
1:A:114:LEU:C	1:A:114:LEU:HD23	2.12	0.74
1:A:195:PRO:O	1:A:199:LEU:HD13	1.88	0.74
1:A:230:SER:H	1:A:231:GLU:HG2	1.50	0.74
2:B:72:ASP:OD1	2:B:98:SER:O	2.05	0.74
1:A:272:VAL:C	1:A:273:ASP:O	2.29	0.74
2:B:137:CYS:SG	2:B:137:CYS:O	2.45	0.74
1:A:29:LYS:C	1:A:31:LYS:N	2.40	0.74
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.68	0.74
1:A:132:ASN:ND2	2:B:141:GLU:HB2	2.02	0.74
1:A:194:MET:CE	1:A:198:ILE:HG13	2.16	0.74
1:A:297:LEU:O	1:A:298:VAL:C	2.30	0.74
2:B:16:THR:CG2	2:B:62:GLU:HB3	2.18	0.74
1:A:29:LYS:HD2	1:A:29:LYS:N	2.02	0.73
1:A:246:LEU:O	1:A:268:ILE:HA	1.88	0.73
1:A:83:LYS:O	1:A:84:LYS:C	2.31	0.73
2:B:18:ILE:HD12	2:B:43:THR:O	1.87	0.73
1:A:80:SER:O	1:A:81:LEU:CD1	2.35	0.73
1:A:175:ALA:O	1:A:177:ALA:N	2.22	0.73
1:A:294:LEU:O	1:A:298:VAL:N	2.20	0.73
1:A:41:HIS:CD2	1:A:41:HIS:N	2.53	0.73
2:B:32:LEU:CD2	2:B:77:TYR:CE2	2.65	0.73
2:B:147:ASN:O	2:B:149:VAL:HB	1.89	0.73
1:A:17:ARG:O	1:A:18:ASP:C	2.27	0.73
1:A:59:PHE:O	1:A:62:SER:CB	2.31	0.73
1:A:42:LYS:O	1:A:69:SER:OG	2.02	0.73
1:A:81:LEU:HD13	1:A:82:GLY:O	1.89	0.73
1:A:88:LEU:C	1:A:88:LEU:CD2	2.62	0.73
1:A:232:TYR:CD2	1:A:232:TYR:N	2.57	0.73
1:A:68:ALA:C	1:A:69:SER:OG	2.28	0.72
2:B:61:ILE:HG22	2:B:62:GLU:CA	2.19	0.72
1:A:80:SER:O	1:A:81:LEU:HB3	1.88	0.72
1:A:259:LEU:CD1	1:A:259:LEU:N	2.52	0.72
1:A:95:ILE:O	1:A:99:VAL:HG22	1.89	0.72
1:A:257:LYS:CA	1:A:277:HIS:HA	2.10	0.72
1:A:303:LEU:HD21	1:A:305:LEU:HD22	1.71	0.72
1:A:77:ALA:C	1:A:79:THR:H	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD22	1:A:241:VAL:HG22	1.72	0.72
2:B:74:LEU:O	2:B:76:LEU:N	2.22	0.72
1:A:17:ARG:O	1:A:19:ASP:N	2.23	0.72
1:A:56:ARG:NE	1:A:60:GLN:HE22	1.86	0.72
1:A:274:LYS:HD2	1:A:275:THR:HA	1.72	0.72
1:A:276:PRO:C	1:A:278:ALA:N	2.48	0.72
2:B:9:VAL:CG1	2:B:10:ALA:H	2.02	0.72
1:A:148:THR:OG1	1:A:149:GLU:HG2	1.89	0.72
1:A:184:PHE:CE1	1:A:202:LEU:HD11	2.25	0.72
2:B:64:THR:N	2:B:84:ASN:ND2	2.38	0.72
2:B:71:VAL:O	2:B:73:GLU:CB	2.38	0.72
2:B:16:THR:HA	2:B:64:THR:OG1	1.90	0.72
2:B:18:ILE:O	2:B:44:ILE:HG12	1.89	0.72
2:B:79:PRO:HG2	2:B:80:GLN:N	2.05	0.72
1:A:303:LEU:HG	1:A:304:VAL:N	2.05	0.71
1:A:274:LYS:HD2	1:A:275:THR:N	2.05	0.71
2:B:11:GLU:O	2:B:12:ILE:C	2.30	0.71
2:B:25:ILE:CD1	2:B:25:ILE:C	2.62	0.71
2:B:29:LEU:CD2	2:B:33:PHE:HE1	2.03	0.71
2:B:61:ILE:HG22	2:B:62:GLU:O	1.91	0.71
2:B:36:THR:O	2:B:36:THR:CG2	2.38	0.71
2:B:5:ASP:OD1	2:B:5:ASP:C	2.32	0.71
2:B:27:PHE:C	2:B:30:LEU:HD12	2.15	0.71
2:B:77:TYR:N	2:B:77:TYR:HD1	1.88	0.71
1:A:35:GLN:NE2	1:A:35:GLN:HA	2.02	0.70
2:B:29:LEU:HD23	2:B:33:PHE:CE1	2.26	0.70
2:B:46:LEU:HD23	2:B:46:LEU:O	1.91	0.70
1:A:35:GLN:HB3	1:A:38:LEU:CD2	2.20	0.70
1:A:273:ASP:HA	1:A:280:TYR:OH	1.92	0.70
1:A:293:ALA:O	1:A:297:LEU:CD1	2.39	0.70
2:B:69:ASP:O	2:B:69:ASP:OD1	2.09	0.70
2:B:128:ARG:HH11	2:B:143:GLU:CD	1.90	0.70
1:A:136:THR:CB	1:A:291:ARG:NH2	2.54	0.70
1:A:138:THR:HG21	1:A:171:SER:HB2	1.72	0.70
1:A:303:LEU:HD23	1:A:303:LEU:C	2.16	0.70
1:A:137:GLN:O	1:A:140:LEU:HB3	1.92	0.70
2:B:4:ASN:OD1	2:B:5:ASP:C	2.34	0.70
2:B:18:ILE:CD1	2:B:44:ILE:HG12	2.20	0.70
1:A:214:SER:CB	1:A:216:GLU:HG3	2.20	0.70
1:A:251:ASN:O	1:A:253:LYS:CB	2.40	0.70
1:A:38:LEU:C	1:A:39:LEU:HD23	2.17	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:SER:O	1:A:231:GLU:CG	2.40	0.70
1:A:249:LEU:O	1:A:250:HIS:CG	2.43	0.70
2:B:114:CYS:HG	2:B:140:CYS:HG	1.38	0.70
1:A:38:LEU:HB3	1:A:39:LEU:HD23	1.74	0.70
1:A:260:HIS:O	1:A:262:LEU:N	2.23	0.70
1:A:157:VAL:HG12	1:A:183:ARG:O	1.92	0.69
2:B:98:SER:O	2:B:99:LEU:O	2.10	0.69
2:B:134:ALA:O	2:B:135:LEU:HD12	1.91	0.69
1:A:76:SER:O	1:A:77:ALA:CB	2.38	0.69
2:B:108:VAL:CG2	2:B:152:ASN:HB3	2.21	0.69
1:A:35:GLN:CG	1:A:38:LEU:HD21	2.19	0.69
1:A:304:VAL:HG23	1:A:304:VAL:O	1.92	0.69
1:A:279:TRP:C	1:A:281:PHE:N	2.44	0.69
2:B:18:ILE:HG23	2:B:62:GLU:CD	2.17	0.69
2:B:107:LEU:HB3	2:B:125:PHE:CE1	2.26	0.69
2:B:75:ALA:HB1	2:B:99:LEU:HD22	1.74	0.69
1:A:81:LEU:HD22	1:A:82:GLY:O	1.92	0.69
1:A:88:LEU:O	1:A:88:LEU:CD2	2.41	0.69
1:A:60:GLN:O	1:A:63:MET:N	2.26	0.69
1:A:140:LEU:CD1	1:A:287:GLY:HA2	2.13	0.69
2:B:17:VAL:HG22	2:B:43:THR:OG1	1.92	0.69
2:B:86:ILE:CG2	2:B:90:GLU:HB2	2.20	0.69
1:A:211:LEU:O	1:A:212:HIS:CD2	2.46	0.69
2:B:31:SER:C	2:B:33:PHE:N	2.45	0.69
1:A:141:ASP:HA	1:A:144:THR:HG21	1.75	0.69
2:B:68:GLU:O	2:B:70:GLU:N	2.25	0.69
2:B:111:ASP:HB2	2:B:144:PHE:HZ	1.58	0.69
1:A:34:PRO:C	1:A:35:GLN:HE21	2.01	0.68
2:B:46:LEU:HD21	2:B:48:LEU:HG	1.75	0.68
2:B:86:ILE:O	2:B:90:GLU:CD	2.36	0.68
2:B:124:SER:HB3	2:B:138:LYS:HE3	1.73	0.68
1:A:158:ALA:HA	1:A:185:TYR:HB2	1.74	0.68
2:B:92:VAL:HG12	2:B:92:VAL:O	1.92	0.68
1:A:219:MET:O	1:A:219:MET:CG	2.24	0.68
2:B:15:GLY:O	2:B:64:THR:CB	2.40	0.68
1:A:58:SER:O	1:A:59:PHE:C	2.37	0.68
1:A:163:LEU:HD22	1:A:188:ALA:HB2	1.76	0.68
2:B:4:ASN:OD1	2:B:4:ASN:C	2.36	0.68
1:A:101:ALA:C	1:A:102:ILE:HG12	2.18	0.68
2:B:72:ASP:O	2:B:100:PRO:HG3	1.92	0.68
2:B:76:LEU:HB3	2:B:77:TYR:CD1	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CD1	1:A:202:LEU:HD11	2.29	0.68
2:B:107:LEU:HD21	2:B:150:LEU:HD22	1.75	0.68
1:A:280:TYR:O	1:A:283:GLN:HB3	1.92	0.67
2:B:106:VAL:O	2:B:106:VAL:HG13	1.95	0.67
1:A:249:LEU:C	1:A:250:HIS:CG	2.69	0.67
2:B:39:GLN:NE2	2:B:40:ASP:H	1.92	0.67
1:A:71:VAL:HG23	1:A:71:VAL:O	1.93	0.67
1:A:215:ILE:HG21	1:A:246:LEU:HD23	1.76	0.67
2:B:111:ASP:O	2:B:117:HIS:CE1	2.43	0.67
1:A:179:PHE:N	1:A:179:PHE:CD2	2.62	0.67
1:A:274:LYS:CD	1:A:275:THR:CA	2.72	0.67
1:A:44:ILE:HG22	1:A:45:ALA:H	1.59	0.67
1:A:272:VAL:O	1:A:275:THR:HG23	1.95	0.67
1:A:175:ALA:C	1:A:177:ALA:N	2.48	0.67
1:A:209:TRP:CD1	1:A:209:TRP:N	2.61	0.67
1:A:258:VAL:C	1:A:259:LEU:CD1	2.68	0.67
2:B:81:ALA:O	2:B:82:THR:HG23	1.95	0.67
2:B:20:HIS:CE1	2:B:47:ASN:HB2	2.30	0.67
1:A:230:SER:C	1:A:231:GLU:CG	2.63	0.67
1:A:2:ASN:OD1	1:A:4:LEU:N	2.28	0.66
1:A:113:ARG:O	1:A:116:THR:N	2.28	0.66
1:A:114:LEU:HD23	1:A:114:LEU:O	1.95	0.66
1:A:162:ASP:OD1	1:A:162:ASP:O	2.13	0.66
1:A:231:GLU:O	1:A:232:TYR:O	2.11	0.66
2:B:18:ILE:CG2	2:B:62:GLU:OE2	2.31	0.66
1:A:292:GLN:O	1:A:293:ALA:C	2.35	0.66
1:A:10:ILE:O	1:A:11:SER:CB	2.42	0.66
2:B:12:ILE:O	2:B:13:LYS:CG	2.43	0.66
1:A:35:GLN:HB3	1:A:38:LEU:HD23	1.78	0.66
1:A:39:LEU:O	1:A:40:LYS:C	2.37	0.66
1:A:162:ASP:OD1	1:A:162:ASP:C	2.37	0.66
1:A:303:LEU:HD11	1:A:305:LEU:HB2	1.77	0.66
1:A:231:GLU:CB	1:A:232:TYR:HE2	2.03	0.66
1:A:34:PRO:O	1:A:35:GLN:NE2	2.28	0.66
1:A:276:PRO:O	1:A:277:HIS:C	2.36	0.66
2:B:72:ASP:C	2:B:100:PRO:HG3	2.19	0.66
1:A:141:ASP:C	1:A:144:THR:CG2	2.69	0.66
1:A:189:PRO:O	1:A:189:PRO:CG	2.36	0.66
1:A:251:ASN:O	1:A:252:ALA:C	2.35	0.66
1:A:11:SER:HA	1:A:133:GLN:HG2	1.78	0.66
1:A:70:VAL:O	1:A:71:VAL:CG1	2.38	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:THR:HG21	1:A:291:ARG:NE	2.10	0.65
1:A:44:ILE:O	1:A:71:VAL:HG21	1.94	0.65
1:A:135:PRO:O	1:A:139:LEU:HG	1.95	0.65
1:A:249:LEU:O	1:A:250:HIS:CE1	2.49	0.65
2:B:39:GLN:CG	2:B:40:ASP:H	2.10	0.65
1:A:50:GLU:O	1:A:51:ALA:C	2.40	0.65
1:A:80:SER:O	1:A:81:LEU:CB	2.44	0.65
1:A:143:PHE:O	1:A:144:THR:C	2.37	0.65
2:B:10:ALA:O	2:B:11:GLU:CB	2.44	0.65
2:B:60:LYS:O	2:B:61:ILE:CB	2.45	0.65
2:B:100:PRO:C	2:B:101:GLU:HG2	2.21	0.65
2:B:116:SER:HA	2:B:121:VAL:HG11	1.79	0.65
1:A:40:LYS:CB	1:A:41:HIS:CD2	2.79	0.65
1:A:201:MET:HA	1:A:204:GLU:CG	2.26	0.65
1:A:230:SER:N	1:A:231:GLU:HG2	2.11	0.65
1:A:231:GLU:HB3	1:A:232:TYR:CD2	2.32	0.65
2:B:71:VAL:O	2:B:73:GLU:CA	2.44	0.65
2:B:28:LYS:HB3	2:B:32:LEU:HD12	1.79	0.65
2:B:69:ASP:HA	2:B:71:VAL:HB	1.77	0.65
1:A:18:ASP:O	1:A:21:ASN:N	2.30	0.64
1:A:49:PHE:CE1	1:A:104:MET:CE	2.79	0.64
2:B:17:VAL:CA	2:B:18:ILE:HD12	2.27	0.64
2:B:86:ILE:N	2:B:90:GLU:HB2	2.12	0.64
2:B:148:VAL:HG13	2:B:148:VAL:O	1.96	0.64
1:A:2:ASN:OD1	1:A:3:PRO:N	2.30	0.64
1:A:274:LYS:HD3	1:A:274:LYS:O	1.97	0.64
2:B:102:ARG:O	2:B:104:ILE:HD12	1.96	0.64
1:A:5:TYR:C	1:A:7:SER:H	2.05	0.64
2:B:4:ASN:O	2:B:43:THR:HG21	1.96	0.64
2:B:17:VAL:HG22	2:B:43:THR:HB	1.79	0.64
2:B:39:GLN:HG2	2:B:40:ASP:N	2.12	0.64
2:B:116:SER:O	2:B:117:HIS:CG	2.49	0.64
2:B:31:SER:O	2:B:32:LEU:C	2.38	0.64
1:A:9:ILE:HB	1:A:125:LEU:HD12	1.78	0.64
1:A:82:GLY:HA3	1:A:86:GLN:CB	2.27	0.64
1:A:110:GLY:O	1:A:111:ALA:C	2.40	0.64
1:A:77:ALA:O	1:A:79:THR:N	2.30	0.64
1:A:230:SER:O	1:A:231:GLU:HG2	1.98	0.64
2:B:17:VAL:HA	2:B:18:ILE:CD1	2.28	0.64
2:B:64:THR:H	2:B:84:ASN:HD22	1.44	0.64
2:B:147:ASN:O	2:B:148:VAL:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LYS:O	1:A:41:HIS:CB	2.44	0.64
1:A:159:MET:HE1	1:A:172:LEU:CD2	2.28	0.64
1:A:204:GLU:OE2	1:A:205:LYS:NZ	2.31	0.64
1:A:9:ILE:HD13	1:A:294:LEU:CD2	2.28	0.64
1:A:251:ASN:O	1:A:253:LYS:CG	2.46	0.64
1:A:275:THR:O	1:A:276:PRO:O	2.15	0.64
1:A:303:LEU:CD2	1:A:303:LEU:C	2.66	0.63
1:A:212:HIS:CG	1:A:218:VAL:CG2	2.82	0.63
2:B:66:LEU:HB2	2:B:70:GLU:HB2	1.80	0.63
2:B:84:ASN:O	2:B:92:VAL:HB	1.99	0.63
1:A:175:ALA:HA	1:A:178:LYS:HD2	1.80	0.63
2:B:20:HIS:O	2:B:20:HIS:CG	2.51	0.63
1:A:231:GLU:O	1:A:234:ASX:XD2	2.46	0.63
1:A:171:SER:O	1:A:172:LEU:C	2.38	0.63
1:A:140:LEU:CD1	1:A:287:GLY:N	2.61	0.63
1:A:196:GLU:O	1:A:200:ASP:OD2	2.16	0.63
1:A:253:LYS:HD3	1:A:277:HIS:NE2	2.14	0.63
2:B:18:ILE:HB	2:B:44:ILE:CD1	2.29	0.63
2:B:66:LEU:C	2:B:70:GLU:HG2	2.24	0.63
1:A:140:LEU:HD13	1:A:287:GLY:N	2.11	0.63
1:A:159:MET:CE	1:A:172:LEU:CD2	2.75	0.63
2:B:146:HIS:CD2	2:B:147:ASN:OD1	2.52	0.63
1:A:81:LEU:CD1	1:A:82:GLY:O	2.47	0.63
1:A:129:ASP:OD1	1:A:132:ASN:OD1	2.17	0.63
1:A:281:PHE:O	1:A:282:GLN:C	2.42	0.63
1:A:81:LEU:CD2	1:A:82:GLY:O	2.47	0.63
1:A:200:ASP:O	1:A:204:GLU:N	2.30	0.62
2:B:47:ASN:O	2:B:48:LEU:C	2.42	0.62
2:B:102:ARG:HD2	2:B:104:ILE:HD12	1.80	0.62
1:A:159:MET:HE2	1:A:172:LEU:HD23	1.80	0.62
1:A:218:VAL:O	1:A:222:VAL:CG2	2.47	0.62
1:A:251:ASN:C	1:A:253:LYS:H	2.03	0.62
2:B:18:ILE:N	2:B:62:GLU:OE1	2.32	0.62
2:B:146:HIS:CD2	2:B:147:ASN:N	2.68	0.62
1:A:25:ALA:O	1:A:26:THR:C	2.40	0.62
1:A:136:THR:HG21	1:A:291:ARG:CD	2.28	0.62
1:A:189:PRO:O	1:A:191:ALA:N	2.31	0.62
1:A:274:LYS:CD	1:A:275:THR:HA	2.29	0.62
2:B:102:ARG:O	2:B:103:ASN:C	2.40	0.62
1:A:8:HIS:CD2	1:A:8:HIS:H	2.18	0.62
1:A:201:MET:CG	1:A:204:GLU:HG3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:HG3	1:A:265:VAL:N	2.13	0.62
2:B:72:ASP:O	2:B:75:ALA:CB	2.46	0.62
1:A:230:SER:O	1:A:231:GLU:CD	2.42	0.62
1:A:149:GLU:OE2	1:A:149:GLU:HA	2.00	0.62
2:B:3:HIS:O	2:B:4:ASN:HB3	2.00	0.62
2:B:146:HIS:CD2	2:B:147:ASN:H	2.16	0.62
1:A:81:LEU:HD22	1:A:82:GLY:CA	2.30	0.62
1:A:303:LEU:O	1:A:303:LEU:CD2	2.46	0.62
2:B:39:GLN:CG	2:B:40:ASP:N	2.62	0.62
1:A:81:LEU:HD22	1:A:82:GLY:C	2.25	0.61
1:A:197:TYR:CE1	1:A:198:ILE:N	2.67	0.61
1:A:200:ASP:O	1:A:204:GLU:HB3	2.00	0.61
1:A:221:ARG:O	1:A:222:VAL:HG23	2.00	0.61
1:A:114:LEU:HD13	2:B:119:GLU:HG3	1.80	0.61
1:A:274:LYS:C	1:A:274:LYS:CD	2.45	0.61
1:A:40:LYS:HD3	1:A:41:HIS:CD2	2.33	0.61
1:A:258:VAL:N	1:A:277:HIS:O	2.30	0.61
1:A:269:ALA:O	1:A:270:THR:C	2.43	0.61
2:B:86:ILE:H	2:B:90:GLU:HG3	1.66	0.61
1:A:211:LEU:O	1:A:212:HIS:CE1	2.52	0.61
2:B:12:ILE:O	2:B:13:LYS:CB	2.48	0.61
2:B:60:LYS:O	2:B:61:ILE:HB	1.99	0.61
2:B:84:ASN:HB3	2:B:92:VAL:HG21	1.82	0.61
1:A:40:LYS:C	1:A:41:HIS:CD2	2.78	0.61
2:B:15:GLY:O	2:B:64:THR:OG1	2.17	0.61
2:B:79:PRO:O	2:B:97:PRO:HG2	2.01	0.61
1:A:61:THR:HG21	1:A:288:ILE:HG21	1.82	0.61
1:A:258:VAL:C	1:A:259:LEU:HD12	2.26	0.61
1:A:259:LEU:N	1:A:259:LEU:HD13	2.15	0.61
1:A:16:SER:O	1:A:17:ARG:C	2.44	0.61
1:A:111:ALA:O	1:A:115:ALA:N	2.33	0.61
1:A:184:PHE:CE1	1:A:202:LEU:CD1	2.82	0.61
2:B:39:GLN:HG2	2:B:40:ASP:H	1.65	0.61
2:B:133:ILE:HB	2:B:146:HIS:ND1	2.15	0.61
1:A:262:LEU:HB3	1:A:263:PRO:CA	2.26	0.61
1:A:274:LYS:HB3	1:A:275:THR:HG22	1.83	0.61
2:B:20:HIS:HB3	2:B:46:LEU:HA	1.81	0.61
1:A:45:ALA:HB2	1:A:99:VAL:CG1	2.30	0.61
1:A:144:THR:O	1:A:145:ILE:C	2.38	0.61
1:A:224:LYS:NZ	1:A:259:LEU:HD11	2.15	0.61
1:A:233:ALA:HB3	1:A:234:ASX:XD2	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:CG2	1:A:238:GLN:CB	2.72	0.61
2:B:33:PHE:O	2:B:34:LYS:C	2.42	0.61
2:B:115:ILE:CG2	2:B:119:GLU:CG	2.78	0.61
2:B:146:HIS:HD2	2:B:147:ASN:CG	2.09	0.61
1:A:11:SER:OG	1:A:133:GLN:CD	2.43	0.61
2:B:105:ASP:OD2	2:B:105:ASP:O	2.19	0.61
1:A:258:VAL:C	1:A:259:LEU:HD13	2.26	0.60
1:A:12:ILE:HG22	1:A:13:ASN:N	2.16	0.60
1:A:66:LEU:HD12	1:A:292:GLN:HG3	1.82	0.60
1:A:138:THR:O	1:A:142:LEU:HB2	2.01	0.60
1:A:161:GLY:HA3	1:A:228:ASP:OD1	2.00	0.60
1:A:16:SER:CB	1:A:19:ASP:OD1	2.48	0.60
1:A:16:SER:OG	1:A:18:ASP:HB2	2.00	0.60
1:A:224:LYS:HZ2	1:A:259:LEU:HD11	1.66	0.60
1:A:281:PHE:O	1:A:283:GLN:N	2.35	0.60
2:B:23:ALA:O	2:B:24:GLU:HB3	1.99	0.60
1:A:163:LEU:HB2	1:A:192:LEU:O	2.02	0.60
2:B:108:VAL:O	2:B:109:CYS:C	2.45	0.60
2:B:115:ILE:O	2:B:116:SER:C	2.43	0.60
1:A:20:LEU:O	1:A:24:LEU:CD2	2.49	0.60
1:A:187:ILE:HA	1:A:212:HIS:O	2.00	0.60
1:A:266:ASP:O	1:A:268:ILE:N	2.35	0.60
1:A:304:VAL:O	1:A:304:VAL:CG2	2.49	0.60
2:B:17:VAL:CG2	2:B:43:THR:CB	2.77	0.60
2:B:63:ASN:HB3	2:B:84:ASN:HA	1.83	0.60
1:A:49:PHE:CE1	1:A:104:MET:HE2	2.37	0.60
2:B:74:LEU:O	2:B:75:ALA:C	2.45	0.60
1:A:164:LYS:HB2	1:A:192:LEU:HA	1.84	0.60
2:B:17:VAL:CG2	2:B:43:THR:HB	2.31	0.60
1:A:217:GLU:HG3	1:A:221:ARG:NH1	2.15	0.60
1:A:69:SER:C	1:A:70:VAL:HG13	2.24	0.60
1:A:232:TYR:O	1:A:234:ASX:XD2	2.50	0.60
2:B:118:ALA:C	2:B:119:GLU:HG2	2.27	0.60
2:B:10:ALA:O	2:B:11:GLU:HB3	2.02	0.60
1:A:272:VAL:O	1:A:274:LYS:N	2.34	0.59
2:B:14:ARG:HG2	2:B:64:THR:CG2	2.31	0.59
2:B:66:LEU:HB2	2:B:70:GLU:CB	2.32	0.59
1:A:198:ILE:HD11	1:A:202:LEU:HD21	1.82	0.59
2:B:69:ASP:HB2	2:B:72:ASP:CB	2.32	0.59
2:B:140:CYS:O	2:B:140:CYS:SG	2.60	0.59
1:A:44:ILE:O	1:A:71:VAL:HG23	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:MET:HG3	1:A:195:PRO:CD	2.31	0.59
1:A:31:LYS:HE3	1:A:143:PHE:HZ	1.66	0.59
1:A:75:ASP:OD2	1:A:79:THR:HB	2.03	0.59
1:A:136:THR:HG21	1:A:291:ARG:CZ	2.32	0.59
1:A:12:ILE:HD13	1:A:175:ALA:HB2	1.84	0.59
1:A:29:LYS:H	1:A:29:LYS:CD	1.95	0.59
1:A:199:LEU:O	1:A:200:ASP:C	2.44	0.59
1:A:303:LEU:HD21	1:A:305:LEU:HD23	1.82	0.59
1:A:189:PRO:HD3	1:A:244:ASN:ND2	2.17	0.59
1:A:192:LEU:C	1:A:193:ALA:O	2.44	0.59
1:A:39:LEU:O	1:A:40:LYS:O	2.21	0.59
1:A:77:ALA:C	1:A:79:THR:N	2.61	0.59
1:A:155:LEU:HD23	1:A:223:GLN:OE1	2.02	0.59
2:B:85:ARG:HG2	2:B:90:GLU:HG2	1.84	0.59
1:A:178:LYS:O	1:A:179:PHE:O	2.21	0.59
2:B:18:ILE:HB	2:B:44:ILE:HD13	1.85	0.59
2:B:81:ALA:C	2:B:82:THR:OG1	2.46	0.59
1:A:157:VAL:CG1	1:A:184:PHE:HA	2.33	0.58
1:A:208:ALA:HA	1:A:209:TRP:CD1	2.33	0.58
1:A:303:LEU:CG	1:A:305:LEU:HB3	2.32	0.58
2:B:44:ILE:HG22	2:B:45:GLY:H	1.66	0.58
1:A:180:ASP:CG	1:A:181:GLY:N	2.62	0.58
1:A:232:TYR:O	1:A:234:ASX:N	2.35	0.58
1:A:143:PHE:O	1:A:146:GLN:CA	2.50	0.58
1:A:204:GLU:CD	1:A:205:LYS:NZ	2.61	0.58
2:B:116:SER:O	2:B:117:HIS:HB2	2.00	0.58
2:B:145:SER:O	2:B:147:ASN:CA	2.50	0.58
1:A:184:PHE:HE1	1:A:202:LEU:CD1	2.17	0.58
1:A:198:ILE:O	1:A:198:ILE:HG13	2.03	0.58
1:A:8:HIS:CD2	1:A:8:HIS:N	2.69	0.58
1:A:91:THR:O	1:A:95:ILE:HB	2.02	0.58
1:A:138:THR:CG2	1:A:171:SER:HB2	2.34	0.58
1:A:26:THR:HG21	1:A:297:LEU:HD11	1.84	0.58
1:A:226:ARG:HH11	1:A:261:PRO:HD3	1.69	0.58
2:B:72:ASP:OD2	2:B:98:SER:O	2.22	0.58
1:A:187:ILE:HD11	1:A:218:VAL:HG11	1.85	0.58
1:A:201:MET:CB	1:A:204:GLU:HG3	2.34	0.58
2:B:61:ILE:HG22	2:B:62:GLU:C	2.29	0.58
1:A:146:GLN:O	1:A:147:GLN:C	2.47	0.58
1:A:180:ASP:OD1	1:A:181:GLY:N	2.37	0.58
2:B:25:ILE:O	2:B:25:ILE:CG1	2.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:ASN:C	2:B:64:THR:OG1	2.47	0.58
1:A:156:HIS:O	1:A:223:GLN:HB2	2.03	0.58
1:A:226:ARG:NH1	1:A:261:PRO:HD3	2.19	0.58
1:A:182:ASN:N	1:A:182:ASN:OD1	2.37	0.57
1:A:282:GLN:N	1:A:282:GLN:NE2	2.09	0.57
2:B:12:ILE:O	2:B:13:LYS:HG3	2.04	0.57
2:B:39:GLN:HE21	2:B:40:ASP:H	1.50	0.57
1:A:49:PHE:CB	1:A:105:ARG:O	2.48	0.57
2:B:76:LEU:HB3	2:B:77:TYR:CE1	2.38	0.57
2:B:84:ASN:C	2:B:92:VAL:HG21	2.28	0.57
2:B:129:ARG:O	2:B:130:ALA:O	2.22	0.57
1:A:9:ILE:HB	1:A:125:LEU:HD11	1.80	0.57
1:A:200:ASP:O	1:A:204:GLU:CB	2.53	0.57
1:A:256:ALA:O	1:A:257:LYS:HD2	2.05	0.57
2:B:31:SER:HG	2:B:32:LEU:N	2.02	0.57
1:A:157:VAL:HG21	1:A:159:MET:HE3	1.86	0.57
2:B:137:CYS:O	2:B:138:LYS:C	2.47	0.57
1:A:192:LEU:O	1:A:193:ALA:O	2.22	0.57
1:A:49:PHE:HE1	1:A:104:MET:CE	2.17	0.57
1:A:303:LEU:CD2	1:A:305:LEU:HD22	2.35	0.57
2:B:60:LYS:O	2:B:61:ILE:HG13	2.04	0.57
1:A:86:GLN:HG2	1:A:87:THR:H	1.69	0.57
2:B:72:ASP:O	2:B:75:ALA:HB3	2.04	0.57
2:B:131:ASP:O	2:B:132:ASP:CG	2.47	0.57
2:B:138:LYS:O	2:B:138:LYS:HG3	2.05	0.57
1:A:140:LEU:CD1	1:A:286:ASN:C	2.78	0.57
1:A:217:GLU:OE2	1:A:221:ARG:NH1	2.38	0.57
2:B:84:ASN:O	2:B:92:VAL:CB	2.53	0.57
1:A:41:HIS:N	1:A:41:HIS:HD2	2.00	0.56
1:A:119:SER:O	1:A:120:GLY:C	2.43	0.56
1:A:270:THR:O	1:A:273:ASP:HB2	2.05	0.56
2:B:39:GLN:CD	2:B:39:GLN:H	2.13	0.56
2:B:39:GLN:CD	2:B:39:GLN:N	2.62	0.56
1:A:138:THR:CG2	1:A:171:SER:CB	2.77	0.56
1:A:141:ASP:C	1:A:144:THR:HG22	2.30	0.56
1:A:234:ASX:HB1	1:A:238:GLN:HG2	1.87	0.56
2:B:20:HIS:CD2	2:B:20:HIS:O	2.58	0.56
2:B:29:LEU:CD2	2:B:33:PHE:CE1	2.86	0.56
2:B:29:LEU:CA	2:B:32:LEU:HB3	2.35	0.56
2:B:72:ASP:OD1	2:B:98:SER:CA	2.52	0.56
2:B:114:CYS:SG	2:B:137:CYS:SG	3.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ARG:HG2	2:B:64:THR:HG23	1.88	0.56
2:B:15:GLY:C	2:B:64:THR:OG1	2.49	0.56
1:A:94:VAL:O	1:A:95:ILE:C	2.45	0.56
2:B:32:LEU:HD23	2:B:106:VAL:HG21	1.84	0.56
2:B:17:VAL:C	2:B:18:ILE:HD12	2.30	0.56
1:A:31:LYS:HG3	1:A:289:PHE:CZ	2.41	0.56
1:A:281:PHE:C	1:A:283:GLN:N	2.56	0.56
2:B:14:ARG:HB2	2:B:40:ASP:CG	2.31	0.56
1:A:34:PRO:C	1:A:35:GLN:NE2	2.64	0.55
2:B:96:ARG:HB3	2:B:97:PRO:HD2	1.88	0.55
2:B:15:GLY:H	2:B:64:THR:HG23	1.70	0.55
2:B:31:SER:HG	2:B:32:LEU:H	1.54	0.55
1:A:95:ILE:O	1:A:96:SER:C	2.49	0.55
1:A:202:LEU:HB3	1:A:207:ILE:HG22	1.88	0.55
2:B:111:ASP:HB2	2:B:144:PHE:CZ	2.40	0.55
2:B:71:VAL:CA	2:B:74:LEU:HD11	2.18	0.55
2:B:146:HIS:CD2	2:B:147:ASN:CG	2.84	0.55
1:A:23:VAL:O	1:A:24:LEU:C	2.48	0.55
1:A:136:THR:CG2	1:A:291:ARG:CZ	2.85	0.55
1:A:219:MET:HE2	1:A:252:ALA:O	2.05	0.55
2:B:32:LEU:HD13	2:B:77:TYR:HD2	1.72	0.55
1:A:29:LYS:HA	1:A:32:ALA:HB3	1.88	0.55
1:A:262:LEU:CB	1:A:263:PRO:CA	2.83	0.55
1:A:160:VAL:O	1:A:227:LEU:HA	2.07	0.55
1:A:211:LEU:C	1:A:212:HIS:CG	2.84	0.55
1:A:291:ARG:O	1:A:292:GLN:C	2.49	0.55
2:B:34:LYS:HB3	2:B:35:LEU:HD23	1.89	0.55
1:A:49:PHE:CD1	1:A:104:MET:HE2	2.42	0.55
1:A:160:VAL:HG11	1:A:215:ILE:CD1	2.37	0.55
1:A:279:TRP:C	1:A:281:PHE:H	2.15	0.55
1:A:116:THR:O	1:A:118:PHE:N	2.40	0.54
1:A:148:THR:OG1	1:A:224:LYS:HE3	2.07	0.54
1:A:165:TYR:N	1:A:165:TYR:CD2	2.75	0.54
1:A:289:PHE:O	1:A:290:ALA:C	2.50	0.54
1:A:294:LEU:O	1:A:297:LEU:N	2.40	0.54
1:A:9:ILE:HD12	1:A:125:LEU:HD11	1.89	0.54
1:A:10:ILE:O	1:A:11:SER:HB2	2.07	0.54
1:A:12:ILE:O	1:A:13:ASN:C	2.47	0.54
1:A:14:ASP:OD2	1:A:113:ARG:NH2	2.40	0.54
1:A:141:ASP:OD1	1:A:226:ARG:NH1	2.38	0.54
1:A:231:GLU:C	1:A:232:TYR:CD2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:HIS:CD2	2:B:20:HIS:C	2.83	0.54
1:A:145:ILE:HG13	1:A:146:GLN:N	2.18	0.54
1:A:303:LEU:CD1	1:A:305:LEU:CA	2.68	0.54
2:B:71:VAL:HG12	2:B:97:PRO:HA	1.89	0.54
1:A:70:VAL:CA	1:A:71:VAL:HG22	2.38	0.54
1:A:11:SER:CB	1:A:133:GLN:CD	2.80	0.54
1:A:70:VAL:C	1:A:71:VAL:HG13	2.29	0.54
1:A:198:ILE:CD1	1:A:202:LEU:CD2	2.85	0.54
1:A:231:GLU:HB3	1:A:232:TYR:CE2	2.34	0.54
1:A:60:GLN:C	1:A:62:SER:N	2.63	0.54
1:A:148:THR:OG1	1:A:149:GLU:N	2.38	0.54
1:A:279:TRP:O	1:A:281:PHE:C	2.50	0.54
2:B:114:CYS:SG	2:B:140:CYS:SG	3.05	0.54
2:B:145:SER:O	2:B:147:ASN:C	2.50	0.54
1:A:11:SER:OG	1:A:133:GLN:NE2	2.41	0.54
1:A:92:ILE:HA	1:A:95:ILE:HG21	1.88	0.54
1:A:136:THR:HG21	1:A:291:ARG:NH2	2.22	0.54
2:B:21:ILE:HG22	2:B:78:ALA:HB1	1.90	0.54
2:B:28:LYS:O	2:B:31:SER:N	2.38	0.54
1:A:66:LEU:HG	1:A:292:GLN:HG3	1.91	0.54
1:A:211:LEU:O	1:A:212:HIS:CG	2.60	0.54
2:B:5:ASP:O	2:B:6:LYS:HB2	2.06	0.54
2:B:9:VAL:HG22	2:B:14:ARG:C	2.29	0.54
2:B:71:VAL:HA	2:B:74:LEU:HD13	1.84	0.54
1:A:138:THR:HA	1:A:141:ASP:HB2	1.90	0.53
2:B:9:VAL:CG2	2:B:14:ARG:O	2.56	0.53
2:B:74:LEU:CD2	2:B:97:PRO:HB3	2.37	0.53
1:A:68:ALA:O	1:A:69:SER:CB	2.54	0.53
1:A:185:TYR:C	1:A:186:PHE:CD1	2.86	0.53
1:A:44:ILE:HG23	1:A:101:ALA:HB3	1.89	0.53
1:A:190:ASP:N	1:A:190:ASP:OD1	2.42	0.53
1:A:260:HIS:C	1:A:260:HIS:CD2	2.84	0.53
2:B:22:PRO:O	2:B:22:PRO:CD	2.51	0.53
2:B:47:ASN:O	2:B:49:PRO:N	2.41	0.53
1:A:11:SER:OG	1:A:133:GLN:OE1	2.27	0.53
1:A:88:LEU:O	1:A:88:LEU:CG	2.56	0.53
1:A:187:ILE:CG2	1:A:214:SER:O	2.55	0.53
1:A:198:ILE:C	1:A:199:LEU:HD12	2.31	0.53
1:A:136:THR:CG2	1:A:291:ARG:HH21	2.17	0.53
1:A:159:MET:HE2	1:A:172:LEU:CD2	2.38	0.53
1:A:160:VAL:HG11	1:A:215:ILE:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:THR:C	2:B:17:VAL:HG23	2.32	0.53
2:B:134:ALA:C	2:B:135:LEU:HD12	2.34	0.53
1:A:142:LEU:O	1:A:145:ILE:CG2	2.45	0.53
2:B:107:LEU:O	2:B:108:VAL:CG1	2.52	0.53
1:A:142:LEU:HD12	1:A:176:LEU:HD23	1.91	0.53
2:B:17:VAL:HG22	2:B:43:THR:N	2.23	0.52
2:B:18:ILE:HD11	2:B:42:ILE:HG23	1.91	0.52
2:B:79:PRO:CG	2:B:80:GLN:N	2.70	0.52
2:B:36:THR:O	2:B:36:THR:HG22	2.09	0.52
1:A:109:GLU:CA	1:A:129:ASP:HB3	2.37	0.52
1:A:186:PHE:O	1:A:188:ALA:N	2.43	0.52
2:B:34:LYS:CG	2:B:35:LEU:N	2.38	0.52
2:B:113:ASN:O	2:B:114:CYS:C	2.53	0.52
1:A:70:VAL:C	1:A:71:VAL:CG2	2.58	0.52
1:A:107:PRO:C	1:A:108:GLN:O	2.50	0.52
1:A:201:MET:O	1:A:202:LEU:C	2.53	0.52
2:B:119:GLU:HB2	2:B:120:PRO:CD	2.38	0.52
1:A:5:TYR:CE2	1:A:301:ARG:HA	2.45	0.52
1:A:29:LYS:O	1:A:30:LEU:C	2.52	0.52
1:A:132:ASN:HD21	2:B:141:GLU:CB	2.18	0.52
2:B:9:VAL:HG21	2:B:15:GLY:N	2.24	0.52
2:B:86:ILE:H	2:B:90:GLU:HB2	1.74	0.52
1:A:20:LEU:HD23	1:A:179:PHE:CE2	2.44	0.52
1:A:201:MET:CA	1:A:204:GLU:HG3	2.35	0.52
2:B:76:LEU:HB3	2:B:77:TYR:HD1	1.72	0.52
2:B:86:ILE:HG12	2:B:90:GLU:HB3	1.92	0.52
1:A:84:LYS:HD2	1:A:84:LYS:N	2.25	0.52
1:A:11:SER:OG	2:B:141:GLU:OE1	2.28	0.52
2:B:27:PHE:O	2:B:28:LYS:C	2.52	0.52
1:A:56:ARG:HG2	1:A:56:ARG:O	2.10	0.52
2:B:16:THR:HG22	2:B:17:VAL:H	1.73	0.52
2:B:18:ILE:O	2:B:44:ILE:HA	2.10	0.52
1:A:92:ILE:HA	1:A:95:ILE:CG2	2.40	0.51
1:A:197:TYR:HA	1:A:200:ASP:OD2	2.11	0.51
1:A:199:LEU:HA	1:A:202:LEU:HD23	1.91	0.51
1:A:231:GLU:HA	1:A:239:PHE:HZ	1.74	0.51
2:B:17:VAL:CG2	2:B:43:THR:OG1	2.58	0.51
2:B:26:GLY:C	2:B:30:LEU:HD12	2.35	0.51
1:A:141:ASP:O	1:A:144:THR:CG2	2.58	0.51
1:A:143:PHE:O	1:A:145:ILE:N	2.43	0.51
1:A:227:LEU:HD21	1:A:246:LEU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:ILE:HG22	2:B:45:GLY:N	2.25	0.51
2:B:76:LEU:C	2:B:77:TYR:HD1	2.19	0.51
1:A:50:GLU:C	1:A:51:ALA:O	2.51	0.51
2:B:109:CYS:N	2:B:125:PHE:HZ	2.09	0.51
1:A:112:ALA:O	1:A:113:ARG:C	2.52	0.51
1:A:251:ASN:CA	1:A:253:LYS:HG3	2.41	0.51
1:A:35:GLN:HG3	1:A:38:LEU:CD2	2.25	0.51
1:A:48:PHE:O	1:A:49:PHE:C	2.53	0.51
1:A:148:THR:OG1	1:A:224:LYS:CE	2.59	0.51
1:A:198:ILE:HD12	1:A:202:LEU:CD2	2.41	0.51
1:A:208:ALA:CA	1:A:209:TRP:HD1	2.20	0.51
2:B:128:ARG:CZ	2:B:143:GLU:OE1	2.52	0.51
1:A:214:SER:CB	1:A:216:GLU:HB2	2.37	0.51
1:A:124:VAL:HG23	1:A:125:LEU:O	2.12	0.51
1:A:198:ILE:O	1:A:199:LEU:CD1	2.42	0.51
1:A:258:VAL:HB	1:A:277:HIS:O	2.11	0.51
2:B:99:LEU:CD1	2:B:127:VAL:HG11	2.40	0.51
1:A:13:ASN:O	1:A:15:LEU:N	2.38	0.50
1:A:215:ILE:O	1:A:219:MET:HB3	2.12	0.50
1:A:261:PRO:C	1:A:262:LEU:O	2.54	0.50
1:A:93:SER:CA	1:A:96:SER:OG	2.58	0.50
1:A:157:VAL:O	1:A:185:TYR:CE1	2.58	0.50
1:A:211:LEU:O	1:A:212:HIS:NE2	2.44	0.50
1:A:242:ARG:O	1:A:242:ARG:HG3	2.12	0.50
2:B:29:LEU:O	2:B:33:PHE:HD1	1.95	0.50
1:A:143:PHE:C	1:A:145:ILE:N	2.61	0.50
1:A:187:ILE:N	1:A:187:ILE:HD12	2.22	0.50
1:A:199:LEU:C	1:A:201:MET:H	2.16	0.50
2:B:16:THR:HG22	2:B:17:VAL:N	2.27	0.50
2:B:67:SER:HB3	2:B:70:GLU:HG2	1.94	0.50
2:B:148:VAL:O	2:B:149:VAL:HG23	2.11	0.50
1:A:80:SER:OG	1:A:81:LEU:N	2.33	0.50
1:A:125:LEU:HD21	1:A:298:VAL:HG11	1.93	0.50
2:B:71:VAL:HG13	2:B:74:LEU:CD2	2.36	0.50
1:A:86:GLN:HG2	1:A:87:THR:N	2.26	0.50
1:A:136:THR:HG21	1:A:291:ARG:CG	2.42	0.50
1:A:194:MET:CG	1:A:195:PRO:HD2	2.39	0.50
1:A:196:GLU:O	1:A:200:ASP:CG	2.55	0.50
1:A:267:GLU:OE1	1:A:267:GLU:N	2.43	0.50
1:A:284:ALA:C	1:A:286:ASN:N	2.68	0.50
1:A:11:SER:HA	1:A:133:GLN:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:CA	1:A:144:THR:HG21	2.41	0.50
1:A:303:LEU:CD2	1:A:305:LEU:CD2	2.83	0.50
2:B:63:ASN:C	2:B:84:ASN:HD22	2.19	0.50
2:B:69:ASP:C	2:B:71:VAL:N	2.56	0.50
1:A:56:ARG:HD2	1:A:60:GLN:NE2	2.15	0.50
1:A:56:ARG:NE	1:A:60:GLN:NE2	2.56	0.50
1:A:136:THR:HG21	1:A:291:ARG:HG3	1.94	0.50
1:A:199:LEU:H	1:A:201:MET:H	1.60	0.50
1:A:227:LEU:HD13	1:A:268:ILE:CD1	2.41	0.50
1:A:232:TYR:N	1:A:232:TYR:HD2	2.08	0.50
1:A:288:ILE:HD12	1:A:288:ILE:C	2.36	0.50
1:A:159:MET:HA	1:A:226:ARG:O	2.12	0.50
2:B:84:ASN:O	2:B:92:VAL:CG1	2.60	0.50
1:A:76:SER:O	1:A:77:ALA:HB2	2.12	0.49
2:B:22:PRO:O	2:B:22:PRO:HD2	2.11	0.49
1:A:11:SER:HA	1:A:133:GLN:CD	2.37	0.49
1:A:141:ASP:CG	1:A:226:ARG:HH12	2.19	0.49
2:B:72:ASP:O	2:B:75:ALA:HB2	2.11	0.49
2:B:86:ILE:O	2:B:90:GLU:CB	2.59	0.49
2:B:91:VAL:O	2:B:92:VAL:CG2	2.54	0.49
2:B:36:THR:O	2:B:36:THR:HG23	2.12	0.49
2:B:62:GLU:C	2:B:63:ASN:CG	2.81	0.49
1:A:163:LEU:HD21	1:A:186:PHE:HB3	1.94	0.49
1:A:199:LEU:O	1:A:203:ASP:N	2.40	0.49
1:A:222:VAL:O	1:A:254:MET:SD	2.71	0.49
2:B:9:VAL:HG11	2:B:15:GLY:N	2.27	0.49
2:B:63:ASN:HB3	2:B:84:ASN:CB	2.43	0.49
2:B:63:ASN:C	2:B:64:THR:HG1	2.08	0.49
2:B:99:LEU:HD12	2:B:127:VAL:HG11	1.94	0.49
1:A:216:GLU:O	1:A:219:MET:N	2.46	0.49
1:A:95:ILE:C	1:A:99:VAL:CG2	2.82	0.49
1:A:116:THR:O	1:A:117:GLU:C	2.55	0.49
2:B:33:PHE:N	2:B:33:PHE:CD1	2.79	0.49
1:A:44:ILE:HG22	1:A:45:ALA:N	2.26	0.49
2:B:145:SER:O	2:B:147:ASN:O	2.30	0.49
1:A:24:LEU:HD12	1:A:24:LEU:HA	1.64	0.49
1:A:199:LEU:O	1:A:202:LEU:N	2.45	0.49
1:A:294:LEU:O	1:A:295:LEU:C	2.56	0.49
2:B:128:ARG:NH1	2:B:143:GLU:OE2	2.27	0.49
1:A:17:ARG:O	1:A:20:LEU:N	2.46	0.49
1:A:81:LEU:CD2	1:A:82:GLY:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:CG1	2:B:89:TYR:O	2.41	0.49
1:A:111:ALA:O	1:A:114:LEU:N	2.46	0.49
2:B:86:ILE:H	2:B:90:GLU:CG	2.25	0.49
2:B:128:ARG:HG3	2:B:129:ARG:N	2.27	0.49
1:A:43:VAL:O	1:A:43:VAL:HG13	2.13	0.48
1:A:60:GLN:O	1:A:62:SER:N	2.45	0.48
1:A:142:LEU:CD1	1:A:176:LEU:HD23	2.43	0.48
2:B:148:VAL:O	2:B:148:VAL:CG1	2.56	0.48
1:A:4:LEU:O	1:A:5:TYR:O	2.32	0.48
1:A:120:GLY:O	1:A:122:VAL:N	2.45	0.48
2:B:19:ASN:O	2:B:20:HIS:C	2.56	0.48
2:B:32:LEU:HD13	2:B:77:TYR:CD2	2.48	0.48
2:B:60:LYS:O	2:B:61:ILE:CG1	2.61	0.48
1:A:201:MET:O	1:A:201:MET:HG2	2.13	0.48
2:B:71:VAL:CG1	2:B:72:ASP:N	2.53	0.48
2:B:75:ALA:CB	2:B:99:LEU:N	2.77	0.48
2:B:138:LYS:O	2:B:139:TYR:CG	2.66	0.48
1:A:204:GLU:CD	1:A:205:LYS:HZ1	2.20	0.48
1:A:264:ARG:HD3	1:A:268:ILE:HB	1.95	0.48
2:B:33:PHE:HB3	2:B:35:LEU:HD21	1.96	0.48
2:B:85:ARG:HG2	2:B:90:GLU:CG	2.42	0.48
1:A:17:ARG:HG3	1:A:18:ASP:N	2.28	0.48
1:A:124:VAL:O	1:A:125:LEU:HD13	2.13	0.48
1:A:9:ILE:O	1:A:10:ILE:HD12	2.12	0.48
1:A:212:HIS:CD2	1:A:218:VAL:CG2	2.96	0.48
1:A:260:HIS:C	1:A:262:LEU:H	2.21	0.48
2:B:27:PHE:O	2:B:30:LEU:N	2.47	0.48
1:A:149:GLU:HG3	1:A:224:LYS:HG3	1.95	0.48
2:B:9:VAL:CG2	2:B:14:ARG:CA	2.92	0.48
2:B:14:ARG:HB3	2:B:64:THR:HG23	1.95	0.48
2:B:86:ILE:H	2:B:90:GLU:CB	2.26	0.48
1:A:20:LEU:O	1:A:24:LEU:CB	2.35	0.48
1:A:63:MET:HG3	1:A:295:LEU:HD21	1.95	0.48
1:A:158:ALA:C	1:A:159:MET:HG2	2.38	0.48
2:B:23:ALA:C	2:B:25:ILE:HG22	2.39	0.48
2:B:28:LYS:O	2:B:32:LEU:CB	2.59	0.48
2:B:146:HIS:HD2	2:B:147:ASN:N	2.12	0.48
2:B:84:ASN:O	2:B:92:VAL:HG11	2.13	0.47
1:A:11:SER:HA	1:A:133:GLN:CG	2.44	0.47
1:A:20:LEU:O	1:A:24:LEU:HD22	2.13	0.47
2:B:113:ASN:C	2:B:114:CYS:O	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:THR:HB	1:A:297:LEU:HD11	1.96	0.47
1:A:49:PHE:HE1	1:A:104:MET:HE1	1.78	0.47
1:A:114:LEU:C	1:A:114:LEU:CD2	2.86	0.47
1:A:198:ILE:CD1	1:A:202:LEU:HD21	2.44	0.47
1:A:231:GLU:HA	1:A:239:PHE:CZ	2.49	0.47
2:B:145:SER:C	2:B:147:ASN:H	2.21	0.47
1:A:175:ALA:C	1:A:177:ALA:H	2.20	0.47
1:A:227:LEU:HD11	1:A:246:LEU:HG	1.97	0.47
2:B:140:CYS:O	2:B:141:GLU:C	2.55	0.47
1:A:2:ASN:O	1:A:3:PRO:C	2.57	0.47
1:A:14:ASP:OD1	1:A:14:ASP:C	2.55	0.47
1:A:48:PHE:CE2	1:A:56:ARG:HB2	2.49	0.47
1:A:138:THR:OG1	1:A:139:LEU:N	2.45	0.47
1:A:31:LYS:O	1:A:31:LYS:HG2	2.14	0.47
1:A:60:GLN:O	1:A:63:MET:HB2	2.15	0.47
1:A:260:HIS:CD2	1:A:262:LEU:HA	2.49	0.47
1:A:132:ASN:ND2	2:B:141:GLU:CB	2.74	0.47
1:A:185:TYR:O	1:A:186:PHE:HD1	1.98	0.47
1:A:189:PRO:O	1:A:190:ASP:C	2.57	0.47
1:A:260:HIS:C	1:A:262:LEU:N	2.71	0.47
1:A:83:LYS:O	1:A:83:LYS:HG2	2.14	0.47
1:A:137:GLN:HG2	1:A:168:THR:CG2	2.44	0.47
1:A:135:PRO:O	1:A:139:LEU:CG	2.61	0.47
1:A:281:PHE:O	1:A:284:ALA:HB3	2.15	0.47
2:B:86:ILE:CG1	2:B:90:GLU:HB3	2.45	0.47
1:A:20:LEU:HD23	1:A:179:PHE:HE2	1.79	0.46
1:A:43:VAL:O	1:A:43:VAL:CG1	2.63	0.46
1:A:157:VAL:HG13	1:A:184:PHE:HA	1.97	0.46
1:A:251:ASN:HA	1:A:253:LYS:HE3	1.97	0.46
1:A:264:ARG:HD2	1:A:268:ILE:O	2.14	0.46
2:B:8:GLN:O	2:B:9:VAL:CG2	2.50	0.46
2:B:86:ILE:N	2:B:90:GLU:CB	2.78	0.46
1:A:51:ALA:HA	1:A:74:SER:OG	2.16	0.46
1:A:121:ASN:O	1:A:122:VAL:HG22	2.15	0.46
1:A:157:VAL:CG2	1:A:159:MET:HE3	2.45	0.46
1:A:230:SER:H	1:A:231:GLU:CG	2.24	0.46
1:A:279:TRP:HA	1:A:282:GLN:CD	2.39	0.46
2:B:9:VAL:HG22	2:B:14:ARG:O	2.14	0.46
1:A:163:LEU:HD22	1:A:188:ALA:CB	2.46	0.46
1:A:284:ALA:O	1:A:285:GLY:C	2.57	0.46
2:B:84:ASN:CB	2:B:92:VAL:HG21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ASP:O	1:A:204:GLU:CA	2.64	0.46
2:B:5:ASP:OD1	2:B:6:LYS:CA	2.63	0.46
2:B:66:LEU:HD23	2:B:70:GLU:HB2	1.98	0.46
2:B:100:PRO:O	2:B:101:GLU:CB	2.63	0.46
2:B:102:ARG:O	2:B:102:ARG:CG	2.64	0.46
1:A:10:ILE:O	1:A:11:SER:HB3	2.15	0.46
1:A:106:HIS:CD2	1:A:111:ALA:HB2	2.50	0.46
1:A:142:LEU:HA	1:A:145:ILE:CG2	2.45	0.46
1:A:60:GLN:C	1:A:62:SER:H	2.22	0.46
1:A:143:PHE:CE2	1:A:286:ASN:HB3	2.51	0.46
1:A:303:LEU:HD21	1:A:305:LEU:CB	2.23	0.46
2:B:32:LEU:CD1	2:B:77:TYR:CD2	2.99	0.46
2:B:75:ALA:HB1	2:B:99:LEU:H	1.81	0.46
2:B:140:CYS:O	2:B:142:LYS:N	2.48	0.46
1:A:16:SER:C	1:A:17:ARG:O	2.54	0.46
1:A:88:LEU:CD2	1:A:92:ILE:HG12	2.45	0.46
1:A:185:TYR:O	1:A:186:PHE:CD1	2.69	0.46
2:B:6:LYS:C	2:B:8:GLN:H	2.22	0.46
2:B:39:GLN:NE2	2:B:40:ASP:OD2	2.49	0.46
1:A:165:TYR:N	1:A:165:TYR:HD2	2.13	0.46
2:B:14:ARG:HG2	2:B:64:THR:HG22	1.98	0.46
2:B:99:LEU:HA	2:B:100:PRO:HD3	1.65	0.46
2:B:1:MET:CG	2:B:4:ASN:ND2	2.79	0.46
2:B:18:ILE:H	2:B:18:ILE:HG13	1.00	0.46
2:B:63:ASN:HB3	2:B:84:ASN:CA	2.47	0.46
1:A:17:ARG:CG	1:A:18:ASP:N	2.79	0.45
2:B:44:ILE:CG2	2:B:45:GLY:H	2.29	0.45
2:B:16:THR:HG22	2:B:18:ILE:HG13	1.98	0.45
2:B:23:ALA:O	2:B:25:ILE:HG22	2.16	0.45
1:A:9:ILE:HB	1:A:125:LEU:HD13	1.89	0.45
1:A:111:ALA:O	1:A:112:ALA:O	2.34	0.45
1:A:218:VAL:O	1:A:222:VAL:HG23	2.14	0.45
1:A:231:GLU:O	1:A:234:ASX:XD1	2.64	0.45
1:A:282:GLN:O	1:A:283:GLN:C	2.58	0.45
2:B:61:ILE:CD1	2:B:82:THR:H	2.26	0.45
2:B:86:ILE:CG2	2:B:90:GLU:CB	2.84	0.45
1:A:152:LEU:HD13	1:A:179:PHE:CZ	2.51	0.45
1:A:232:TYR:HB2	1:A:233:ALA:H	1.38	0.45
1:A:279:TRP:HA	1:A:282:GLN:HE22	1.77	0.45
2:B:140:CYS:O	2:B:142:LYS:HG2	2.16	0.45
1:A:227:LEU:O	1:A:228:ASP:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HG23	2:B:92:VAL:HG13	1.97	0.45
1:A:20:LEU:C	1:A:22:LEU:H	2.25	0.45
1:A:146:GLN:C	1:A:148:THR:N	2.74	0.45
1:A:172:LEU:O	1:A:176:LEU:N	2.40	0.45
1:A:202:LEU:HB3	1:A:207:ILE:CG2	2.46	0.45
1:A:231:GLU:C	1:A:232:TYR:O	2.58	0.45
1:A:29:LYS:HE2	1:A:29:LYS:HB3	1.63	0.45
1:A:51:ALA:O	1:A:52:SER:HB2	2.15	0.45
1:A:199:LEU:O	1:A:201:MET:N	2.50	0.45
1:A:205:LYS:HZ3	1:A:205:LYS:HG2	1.33	0.45
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.75	0.45
1:A:16:SER:O	1:A:16:SER:OG	2.35	0.45
1:A:121:ASN:ND2	1:A:121:ASN:H	2.15	0.45
2:B:62:GLU:OE1	2:B:62:GLU:CA	2.65	0.45
1:A:156:HIS:CB	1:A:223:GLN:HG3	2.47	0.45
1:A:240:LEU:O	1:A:241:VAL:C	2.60	0.45
2:B:113:ASN:HD22	2:B:113:ASN:HA	1.68	0.45
1:A:187:ILE:HG23	1:A:213:SER:HA	1.97	0.45
1:A:251:ASN:N	1:A:253:LYS:HG3	2.32	0.45
1:A:260:HIS:HD2	1:A:262:LEU:N	2.14	0.45
2:B:21:ILE:CG2	2:B:78:ALA:HB1	2.47	0.45
1:A:11:SER:HG	1:A:133:GLN:CD	2.23	0.44
1:A:109:GLU:O	2:B:139:TYR:O	2.35	0.44
1:A:254:MET:HB3	1:A:254:MET:HE3	1.43	0.44
2:B:14:ARG:CG	2:B:64:THR:HG23	2.47	0.44
2:B:32:LEU:HD22	2:B:77:TYR:CE2	2.52	0.44
2:B:63:ASN:C	2:B:84:ASN:ND2	2.74	0.44
2:B:107:LEU:HD21	2:B:150:LEU:CD2	2.47	0.44
1:A:218:VAL:O	1:A:222:VAL:HG21	2.17	0.44
1:A:142:LEU:C	1:A:145:ILE:HG23	2.36	0.44
2:B:9:VAL:CB	2:B:14:ARG:HA	2.40	0.44
1:A:44:ILE:CG2	1:A:45:ALA:H	2.27	0.44
2:B:21:ILE:HB	2:B:22:PRO:CD	2.39	0.44
2:B:104:ILE:HD11	2:B:124:SER:OG	2.17	0.44
1:A:35:GLN:HB3	1:A:38:LEU:HD21	1.99	0.44
1:A:66:LEU:CG	1:A:292:GLN:HG3	2.46	0.44
1:A:173:THR:O	1:A:177:ALA:N	2.51	0.44
1:A:225:GLU:O	1:A:259:LEU:HB2	2.17	0.44
1:A:240:LEU:O	1:A:242:ARG:N	2.51	0.44
2:B:15:GLY:O	2:B:64:THR:HG23	2.11	0.44
2:B:86:ILE:O	2:B:90:GLU:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:LEU:HA	2:B:107:LEU:HD23	1.53	0.44
1:A:46:SER:O	1:A:72:GLY:HA3	2.17	0.44
1:A:109:GLU:HG2	1:A:132:ASN:HB3	2.00	0.44
2:B:39:GLN:O	2:B:40:ASP:C	2.61	0.44
1:A:37:GLU:C	1:A:39:LEU:N	2.75	0.44
1:A:192:LEU:N	1:A:192:LEU:HD22	2.33	0.44
1:A:280:TYR:HA	1:A:283:GLN:HE21	1.82	0.44
1:A:295:LEU:O	1:A:299:LEU:HD12	2.18	0.44
2:B:74:LEU:C	2:B:76:LEU:N	2.72	0.44
1:A:135:PRO:O	1:A:139:LEU:CD1	2.65	0.44
1:A:211:LEU:CA	1:A:212:HIS:CE1	3.01	0.44
2:B:7:LEU:HD13	2:B:63:ASN:HD22	1.83	0.44
2:B:27:PHE:O	2:B:30:LEU:HD12	2.18	0.44
1:A:11:SER:CA	1:A:133:GLN:OE1	2.66	0.43
1:A:24:LEU:HD11	1:A:143:PHE:HA	2.01	0.43
1:A:71:VAL:CG2	1:A:71:VAL:O	2.64	0.43
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.73	0.43
1:A:235:VAL:N	1:A:238:GLN:HB3	2.32	0.43
1:A:129:ASP:CG	1:A:132:ASN:OD1	2.62	0.43
1:A:52:SER:HB2	1:A:105:ARG:HD3	2.01	0.43
1:A:143:PHE:O	1:A:146:GLN:HB3	2.18	0.43
1:A:235:VAL:HB	1:A:236:LYS:H	1.37	0.43
1:A:20:LEU:C	1:A:22:LEU:N	2.75	0.43
1:A:76:SER:O	1:A:77:ALA:HB3	2.15	0.43
1:A:166:GLY:O	1:A:170:HIS:ND1	2.51	0.43
1:A:231:GLU:CA	1:A:239:PHE:HZ	2.32	0.43
2:B:31:SER:O	2:B:33:PHE:N	2.50	0.43
2:B:71:VAL:CA	2:B:74:LEU:CD1	2.77	0.43
1:A:143:PHE:HE2	1:A:286:ASN:HB3	1.82	0.43
1:A:202:LEU:HD13	1:A:207:ILE:HG21	1.96	0.43
1:A:39:LEU:O	1:A:42:LYS:HD2	2.18	0.43
1:A:113:ARG:O	1:A:114:LEU:C	2.62	0.43
2:B:61:ILE:HG22	2:B:62:GLU:CB	2.48	0.43
2:B:106:VAL:O	2:B:106:VAL:CG1	2.66	0.43
1:A:31:LYS:HG3	1:A:289:PHE:CE2	2.54	0.43
1:A:157:VAL:HG22	1:A:158:ALA:N	2.33	0.43
1:A:279:TRP:O	1:A:282:GLN:N	2.52	0.43
2:B:17:VAL:HG22	2:B:43:THR:CA	2.48	0.43
2:B:17:VAL:CA	2:B:18:ILE:CD1	2.92	0.43
1:A:40:LYS:C	1:A:41:HIS:CG	2.88	0.43
1:A:303:LEU:CG	1:A:305:LEU:N	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ASN:ND2	2:B:5:ASP:O	2.52	0.43
2:B:12:ILE:O	2:B:13:LYS:HB2	2.17	0.43
2:B:74:LEU:O	2:B:77:TYR:N	2.51	0.43
2:B:138:LYS:O	2:B:139:TYR:CD2	2.72	0.43
1:A:12:ILE:CG2	1:A:13:ASN:N	2.76	0.43
1:A:15:LEU:HD12	1:A:15:LEU:HA	1.88	0.43
1:A:114:LEU:CD1	2:B:119:GLU:HG3	2.48	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.58	0.43
1:A:201:MET:HG3	1:A:204:GLU:OE1	2.18	0.43
1:A:216:GLU:HB3	1:A:217:GLU:H	1.10	0.43
2:B:39:GLN:CD	2:B:40:ASP:H	2.27	0.43
1:A:55:THR:H	1:A:55:THR:HG22	1.55	0.43
1:A:59:PHE:CD1	1:A:103:VAL:HG21	2.53	0.43
1:A:92:ILE:O	1:A:95:ILE:CG2	2.60	0.43
1:A:121:ASN:H	1:A:121:ASN:HD22	1.66	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.84	0.43
1:A:197:TYR:CE1	1:A:198:ILE:HG22	2.54	0.43
1:A:215:ILE:HG21	1:A:246:LEU:CD2	2.47	0.43
2:B:75:ALA:O	2:B:79:PRO:HB3	2.18	0.43
2:B:107:LEU:HB3	2:B:125:PHE:HE1	1.82	0.42
1:A:106:HIS:HA	1:A:107:PRO:HD3	1.64	0.42
1:A:180:ASP:CG	1:A:181:GLY:H	2.27	0.42
2:B:73:GLU:OE1	2:B:100:PRO:HG2	2.18	0.42
1:A:53:THR:O	1:A:54:ARG:C	2.61	0.42
1:A:80:SER:O	1:A:81:LEU:CG	2.67	0.42
1:A:112:ALA:O	1:A:116:THR:N	2.51	0.42
1:A:141:ASP:O	1:A:144:THR:HG23	2.18	0.42
1:A:192:LEU:HD13	1:A:192:LEU:N	2.26	0.42
1:A:270:THR:O	1:A:271:ASP:C	2.63	0.42
2:B:9:VAL:CG1	2:B:10:ALA:N	2.78	0.42
2:B:70:GLU:OE1	2:B:70:GLU:HA	2.16	0.42
2:B:102:ARG:O	2:B:102:ARG:HG3	2.18	0.42
1:A:240:LEU:HD22	1:A:241:VAL:H	1.84	0.42
1:A:279:TRP:CD1	1:A:282:GLN:HB2	2.53	0.42
2:B:14:ARG:CB	2:B:64:THR:HG23	2.49	0.42
2:B:61:ILE:HD11	2:B:81:ALA:CB	2.49	0.42
1:A:56:ARG:O	1:A:57:LEU:C	2.62	0.42
2:B:104:ILE:CG2	2:B:105:ASP:N	2.83	0.42
2:B:146:HIS:NE2	2:B:147:ASN:OD1	2.53	0.42
1:A:8:HIS:C	1:A:10:ILE:HD12	2.45	0.42
2:B:30:LEU:HD21	2:B:44:ILE:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:64:THR:O	2:B:65:PHE:HB3	2.20	0.42
1:A:151:ARG:HH11	1:A:151:ARG:CG	2.33	0.42
1:A:253:LYS:O	1:A:254:MET:HG2	2.20	0.42
1:A:274:LYS:HD3	1:A:275:THR:CA	2.43	0.42
2:B:147:ASN:O	2:B:149:VAL:CB	2.66	0.42
1:A:189:PRO:HD3	1:A:244:ASN:HD21	1.85	0.42
1:A:50:GLU:O	1:A:50:GLU:HG2	2.18	0.42
1:A:52:SER:OG	1:A:55:THR:CG2	2.64	0.42
1:A:217:GLU:OE1	1:A:217:GLU:HA	2.11	0.42
1:A:256:ALA:C	1:A:257:LYS:HD2	2.44	0.42
1:A:184:PHE:HB3	1:A:186:PHE:CE1	2.55	0.42
1:A:227:LEU:HD13	1:A:268:ILE:HD11	2.02	0.42
2:B:61:ILE:CG1	2:B:82:THR:N	2.57	0.42
2:B:66:LEU:HD22	2:B:67:SER:C	2.45	0.42
2:B:72:ASP:O	2:B:100:PRO:CG	2.65	0.42
1:A:149:GLU:CG	1:A:224:LYS:HG3	2.50	0.41
1:A:303:LEU:CD1	1:A:305:LEU:CB	2.94	0.41
2:B:61:ILE:CG2	2:B:62:GLU:CG	2.86	0.41
2:B:85:ARG:HB3	2:B:90:GLU:HG3	2.02	0.41
1:A:121:ASN:C	1:A:122:VAL:CG2	2.93	0.41
1:A:227:LEU:HD11	1:A:246:LEU:CG	2.50	0.41
2:B:15:GLY:N	2:B:64:THR:HG23	2.35	0.41
2:B:67:SER:HB3	2:B:70:GLU:CG	2.51	0.41
2:B:68:GLU:HB3	2:B:69:ASP:H	1.44	0.41
1:A:4:LEU:O	1:A:5:TYR:C	2.62	0.41
1:A:8:HIS:CB	1:A:10:ILE:CD1	2.80	0.41
2:B:43:THR:C	2:B:44:ILE:CG1	2.93	0.41
2:B:75:ALA:CB	2:B:99:LEU:H	2.33	0.41
1:A:75:ASP:OD1	1:A:79:THR:CB	2.62	0.41
1:A:258:VAL:O	1:A:259:LEU:HD12	2.19	0.41
1:A:267:GLU:H	1:A:267:GLU:CD	2.28	0.41
2:B:46:LEU:C	2:B:48:LEU:H	2.28	0.41
2:B:107:LEU:HA	2:B:108:VAL:HG22	2.01	0.41
1:A:38:LEU:O	1:A:39:LEU:HD23	2.20	0.41
1:A:140:LEU:HD11	1:A:287:GLY:N	2.36	0.41
1:A:260:HIS:HA	1:A:261:PRO:HD2	1.67	0.41
1:A:291:ARG:O	1:A:294:LEU:HB2	2.21	0.41
2:B:18:ILE:HD13	2:B:44:ILE:HG13	1.98	0.41
2:B:115:ILE:HG22	2:B:119:GLU:CG	2.44	0.41
1:A:44:ILE:CG2	1:A:63:MET:HE2	2.51	0.41
1:A:160:VAL:CG1	1:A:187:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:PHE:CD1	1:A:202:LEU:CD1	3.02	0.41
1:A:201:MET:C	1:A:204:GLU:HB3	2.45	0.41
1:A:238:GLN:C	1:A:240:LEU:H	2.28	0.41
2:B:46:LEU:C	2:B:48:LEU:N	2.78	0.41
2:B:107:LEU:CB	2:B:125:PHE:CE1	3.01	0.41
1:A:35:GLN:CB	1:A:38:LEU:CD2	2.96	0.41
1:A:156:HIS:CE1	1:A:185:TYR:OH	2.74	0.41
1:A:176:LEU:HA	1:A:176:LEU:HD22	1.48	0.41
2:B:79:PRO:HG2	2:B:80:GLN:H	1.84	0.41
2:B:11:GLU:O	2:B:12:ILE:O	2.38	0.41
2:B:14:ARG:HG2	2:B:64:THR:O	2.20	0.41
2:B:63:ASN:CA	2:B:84:ASN:HB2	2.41	0.41
2:B:69:ASP:CB	2:B:72:ASP:HB2	2.41	0.41
1:A:20:LEU:HA	1:A:20:LEU:HD12	1.85	0.41
1:A:38:LEU:HD23	1:A:38:LEU:N	2.35	0.41
1:A:88:LEU:HD22	1:A:92:ILE:HG12	2.02	0.41
2:B:75:ALA:CB	2:B:99:LEU:HA	2.50	0.41
2:B:115:ILE:O	2:B:118:ALA:N	2.54	0.41
1:A:29:LYS:O	1:A:31:LYS:N	2.49	0.40
2:B:41:ARG:C	2:B:42:ILE:HG13	2.46	0.40
2:B:92:VAL:CG1	2:B:92:VAL:O	2.62	0.40
1:A:12:ILE:HD11	1:A:138:THR:OG1	2.21	0.40
1:A:38:LEU:CB	1:A:39:LEU:HD23	2.45	0.40
1:A:47:CYS:O	1:A:104:MET:HA	2.21	0.40
1:A:212:HIS:CD2	1:A:218:VAL:HG22	2.56	0.40
1:A:235:VAL:HG23	1:A:237:ALA:C	2.45	0.40
2:B:26:GLY:O	2:B:30:LEU:HG	2.21	0.40
2:B:102:ARG:HH11	2:B:104:ILE:HD13	1.86	0.40
2:B:115:ILE:HD13	2:B:115:ILE:HG21	1.62	0.40
1:A:143:PHE:CG	1:A:144:THR:N	2.86	0.40
1:A:215:ILE:HD13	1:A:215:ILE:HA	1.79	0.40
1:A:228:ASP:OD1	1:A:228:ASP:N	2.42	0.40
2:B:9:VAL:HG22	2:B:14:ARG:CA	2.51	0.40
2:B:20:HIS:ND1	2:B:47:ASN:HB2	2.36	0.40
2:B:76:LEU:HD13	2:B:150:LEU:HD21	2.03	0.40
1:A:4:LEU:HA	1:A:4:LEU:HD23	1.70	0.40
1:A:56:ARG:HH11	1:A:56:ARG:HD3	1.51	0.40
1:A:75:ASP:CG	1:A:76:SER:H	2.26	0.40
1:A:87:THR:O	1:A:90:ASN:N	2.55	0.40
1:A:137:GLN:HG3	1:A:141:ASP:OD2	2.22	0.40
1:A:267:GLU:HB3	1:A:268:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HE2	1:A:104:MET:HB2	1.99	0.40
1:A:254:MET:O	1:A:255:ASN:CB	2.70	0.40
2:B:17:VAL:HA	2:B:43:THR:O	2.20	0.40
2:B:86:ILE:CA	2:B:90:GLU:CB	3.00	0.40

All (16) 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)
2:B:3:HIS:CB	2:B:4:ASN:O[6_555]	0.69	1.51
2:B:3:HIS:O	2:B:4:ASN:CB[6_555]	0.71	1.49
2:B:3:HIS:C	2:B:4:ASN:CA[6_555]	0.72	1.48
2:B:3:HIS:O	2:B:4:ASN:CA[6_555]	1.03	1.17
1:A:75:ASP:O	1:A:78:ASN:OD1[3_555]	1.46	0.74
2:B:4:ASN:N	2:B:4:ASN:N[6_555]	1.46	0.74
2:B:3:HIS:CB	2:B:4:ASN:C[6_555]	1.50	0.70
1:A:54:ARG:NH2	1:A:86:GLN:NE2[3_555]	1.67	0.53
2:B:3:HIS:CG	2:B:4:ASN:O[6_555]	1.76	0.44
2:B:3:HIS:C	2:B:4:ASN:N[6_555]	1.77	0.43
2:B:4:ASN:N	2:B:4:ASN:CA[6_555]	1.77	0.43
1:A:76:SER:C	1:A:78:ASN:ND2[3_555]	2.00	0.20
1:A:75:ASP:C	1:A:78:ASN:OD1[3_555]	2.06	0.14
1:A:76:SER:O	1:A:78:ASN:ND2[3_555]	2.11	0.09
1:A:76:SER:O	1:A:78:ASN:CG[3_555]	2.13	0.07
2:B:3:HIS:NE2	2:B:17:VAL:CG1[6_555]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	302/305 (99%)	159 (53%)	71 (24%)	72 (24%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	150/152 (99%)	66 (44%)	33 (22%)	51 (34%)	0	0
All	All	452/457 (99%)	225 (50%)	104 (23%)	123 (27%)	0	0

All (123) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	TYR
1	A	6	GLN
1	A	10	ILE
1	A	11	SER
1	A	17	ARG
1	A	18	ASP
1	A	40	LYS
1	A	51	ALA
1	A	59	PHE
1	A	68	ALA
1	A	76	SER
1	A	77	ALA
1	A	78	ASN
1	A	81	LEU
1	A	88	LEU
1	A	111	ALA
1	A	116	THR
1	A	117	GLU
1	A	120	GLY
1	A	121	ASN
1	A	179	PHE
1	A	183	ARG
1	A	190	ASP
1	A	191	ALA
1	A	193	ALA
1	A	198	ILE
1	A	216	GLU
1	A	218	VAL
1	A	220	THR
1	A	228	ASP
1	A	232	TYR
1	A	237	ALA
1	A	241	VAL
1	A	252	ALA
1	A	254	MET
1	A	255	ASN

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	265	VAL
1	A	273	ASP
1	A	274	LYS
1	A	276	PRO
1	A	277	HIS
1	A	298	VAL
2	B	3	HIS
2	B	4	ASN
2	B	6	LYS
2	B	9	VAL
2	B	13	LYS
2	B	20	HIS
2	B	34	LYS
2	B	36	THR
2	B	58	LEU
2	B	61	ILE
2	B	64	THR
2	B	69	ASP
2	B	72	ASP
2	B	75	ALA
2	B	84	ASN
2	B	85	ARG
2	B	92	VAL
2	B	99	LEU
2	B	101	GLU
2	B	102	ARG
2	B	107	LEU
2	B	108	VAL
2	B	117	HIS
2	B	121	VAL
2	B	130	ALA
2	B	131	ASP
2	B	132	ASP
2	B	139	TYR
2	B	141	GLU
2	B	146	HIS
2	B	147	ASN
2	B	148	VAL
2	B	149	VAL
2	B	151	ALA
1	A	14	ASP

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Mol	Chain	Res	Type
1	A	60	GLN
1	A	61	THR
1	A	181	GLY
1	A	187	ILE
1	A	209	TRP
1	A	229	PRO
1	A	264	ARG
1	A	279	TRP
1	A	280	TYR
1	A	292	GLN
1	A	294	LEU
2	B	11	GLU
2	B	12	ILE
2	B	17	VAL
2	B	22	PRO
2	B	67	SER
2	B	100	PRO
2	B	103	ASN
2	B	122	SER
1	A	37	GLU
1	A	233	ALA
1	A	235	VAL
1	A	267	GLU
1	A	291	ARG
1	A	293	ALA
2	B	26	GLY
2	B	28	LYS
2	B	38	THR
2	B	114	CYS
2	B	133	ILE
1	A	137	GLN
1	A	282	GLN
2	B	94	LYS
1	A	30	LEU
1	A	53	THR
1	A	71	VAL
1	A	143	PHE
1	A	148	THR
1	A	199	LEU
1	A	251	ASN
2	B	25	ILE
1	A	110	GLY

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Mol	Chain	Res	Type
1	A	206	GLY
2	B	71	VAL
2	B	83	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	254/254 (100%)	130 (51%)	124 (49%)	0	0
2	B	126/136 (93%)	66 (52%)	60 (48%)	0	0
All	All	380/390 (97%)	196 (52%)	184 (48%)	0	0

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	8	HIS
1	A	10	ILE
1	A	12	ILE
1	A	13	ASN
1	A	14	ASP
1	A	15	LEU
1	A	16	SER
1	A	17	ARG
1	A	20	LEU
1	A	22	LEU
1	A	23	VAL
1	A	24	LEU
1	A	26	THR
1	A	29	LYS
1	A	35	GLN
1	A	38	LEU
1	A	39	LEU
1	A	42	LYS
1	A	46	SER

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Mol	Chain	Res	Type
1	A	54	ARG
1	A	55	THR
1	A	57	LEU
1	A	59	PHE
1	A	60	GLN
1	A	62	SER
1	A	69	SER
1	A	70	VAL
1	A	71	VAL
1	A	74	SER
1	A	76	SER
1	A	81	LEU
1	A	83	LYS
1	A	84	LYS
1	A	88	LEU
1	A	92	ILE
1	A	95	ILE
1	A	96	SER
1	A	98	TYR
1	A	99	VAL
1	A	102	ILE
1	A	104	MET
1	A	109	GLU
1	A	116	THR
1	A	117	GLU
1	A	119	SER
1	A	121	ASN
1	A	122	VAL
1	A	124	VAL
1	A	125	LEU
1	A	133	GLN
1	A	138	THR
1	A	140	LEU
1	A	142	LEU
1	A	145	ILE
1	A	147	GLN
1	A	151	ARG
1	A	153	ASN
1	A	156	HIS
1	A	159	MET
1	A	160	VAL
1	A	163	LEU

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Mol	Chain	Res	Type
1	A	165	TYR
1	A	167	ARG
1	A	168	THR
1	A	176	LEU
1	A	178	LYS
1	A	179	PHE
1	A	182	ASN
1	A	187	ILE
1	A	190	ASP
1	A	192	LEU
1	A	194	MET
1	A	196	GLU
1	A	197	TYR
1	A	198	ILE
1	A	199	LEU
1	A	200	ASP
1	A	201	MET
1	A	204	GLU
1	A	205	LYS
1	A	207	ILE
1	A	211	LEU
1	A	215	ILE
1	A	217	GLU
1	A	219	MET
1	A	220	THR
1	A	221	ARG
1	A	222	VAL
1	A	225	GLU
1	A	226	ARG
1	A	227	LEU
1	A	228	ASP
1	A	232	TYR
1	A	235	VAL
1	A	236	LYS
1	A	238	GLN
1	A	240	LEU
1	A	241	VAL
1	A	245	SER
1	A	246	LEU
1	A	249	LEU
1	A	254	MET
1	A	255	ASN

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Mol	Chain	Res	Type
1	A	257	LYS
1	A	259	LEU
1	A	264	ARG
1	A	268	ILE
1	A	270	THR
1	A	271	ASP
1	A	274	LYS
1	A	275	THR
1	A	276	PRO
1	A	277	HIS
1	A	279	TRP
1	A	280	TYR
1	A	282	GLN
1	A	297	LEU
1	A	298	VAL
1	A	300	ASN
1	A	301	ARG
1	A	303	LEU
1	A	304	VAL
1	A	305	LEU
2	B	1	MET
2	B	5	ASP
2	B	6	LYS
2	B	8	GLN
2	B	9	VAL
2	B	14	ARG
2	B	18	ILE
2	B	20	HIS
2	B	22	PRO
2	B	24	GLU
2	B	25	ILE
2	B	31	SER
2	B	32	LEU
2	B	35	LEU
2	B	36	THR
2	B	38	THR
2	B	46	LEU
2	B	61	ILE
2	B	62	GLU
2	B	63	ASN
2	B	66	LEU
2	B	67	SER

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Mol	Chain	Res	Type
2	B	68	GLU
2	B	69	ASP
2	B	70	GLU
2	B	72	ASP
2	B	73	GLU
2	B	74	LEU
2	B	77	TYR
2	B	80	GLN
2	B	82	THR
2	B	85	ARG
2	B	86	ILE
2	B	87	ASN
2	B	88	ASP
2	B	102	ARG
2	B	104	ILE
2	B	105	ASP
2	B	108	VAL
2	B	109	CYS
2	B	112	SER
2	B	113	ASN
2	B	114	CYS
2	B	115	ILE
2	B	116	SER
2	B	119	GLU
2	B	122	SER
2	B	123	SER
2	B	128	ARG
2	B	129	ARG
2	B	132	ASP
2	B	137	CYS
2	B	138	LYS
2	B	141	GLU
2	B	142	LYS
2	B	143	GLU
2	B	146	HIS
2	B	149	VAL
2	B	150	LEU
2	B	152	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	HIS
1	A	33	ASN
1	A	35	GLN
1	A	41	HIS
1	A	60	GLN
1	A	64	HIS
1	A	78	ASN
1	A	121	ASN
1	A	132	ASN
1	A	137	GLN
1	A	156	HIS
1	A	174	GLN
1	A	260	HIS
1	A	282	GLN
1	A	283	GLN
1	A	292	GLN
2	B	20	HIS
2	B	47	ASN
2	B	80	GLN
2	B	84	ASN
2	B	113	ASN
2	B	117	HIS
2	B	146	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.