



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:05 AM UTC

PDB ID : 1R24 / pdb_00001r24
Title : FAB FROM MURINE IGG3 KAPPA
Authors : Evans, S.V.
Deposited on : 1998-11-05
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

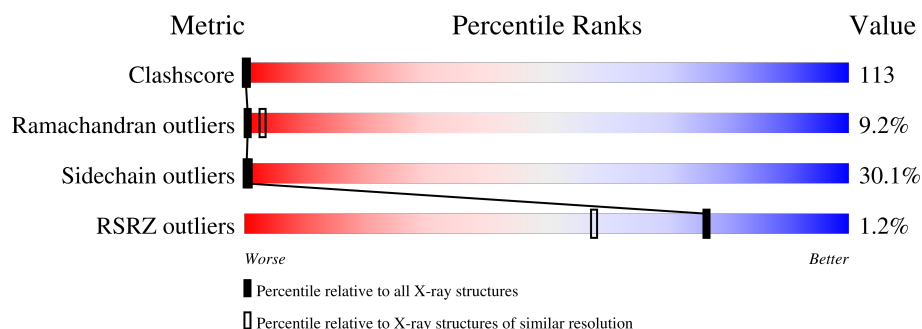
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	206	
1	C	206	
2	B	217	
2	D	217	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6458 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 PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1605	1004	266	329	6			
1	C	206	Total	C	N	O	S	0	0	0
			1605	1004	266	329	6			

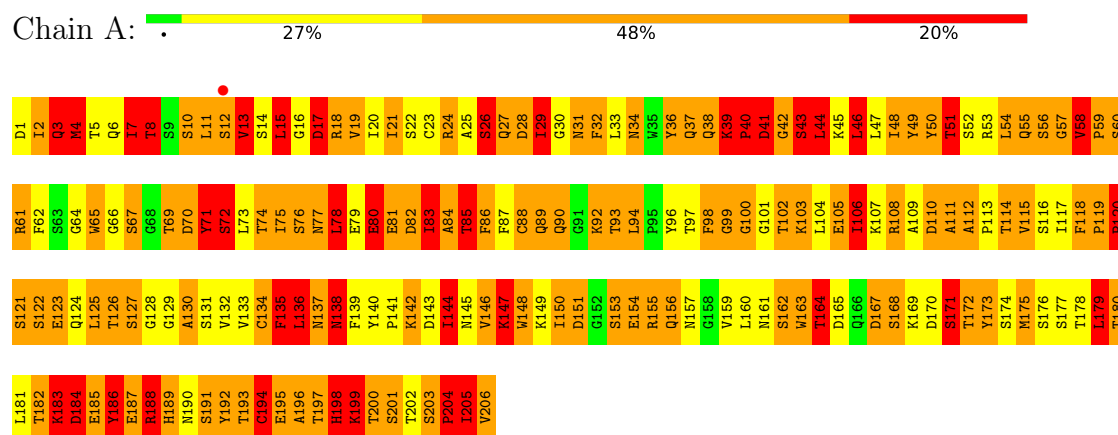
- Molecule 2 is a protein called PROTEIN (IGG3-KAPPA ANTIBODY (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1624	1029	271	317	7			
2	D	217	Total	C	N	O	S	0	0	0
			1624	1029	271	317	7			

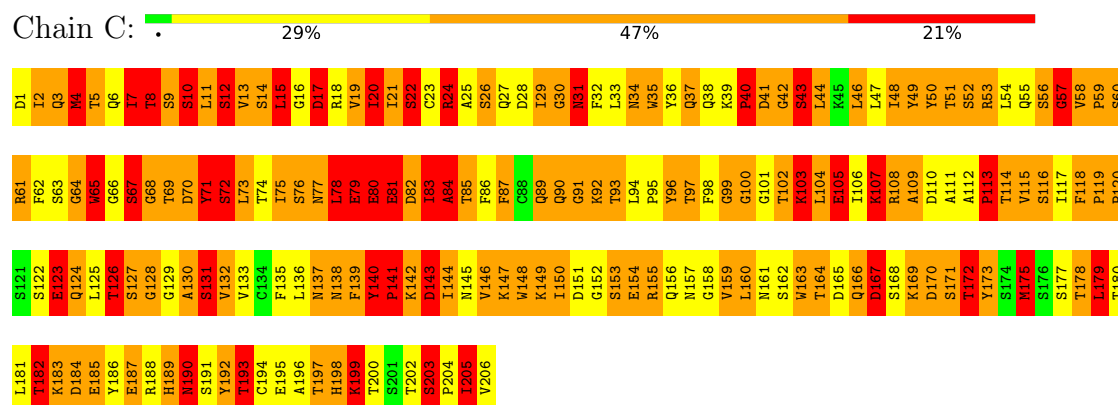
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

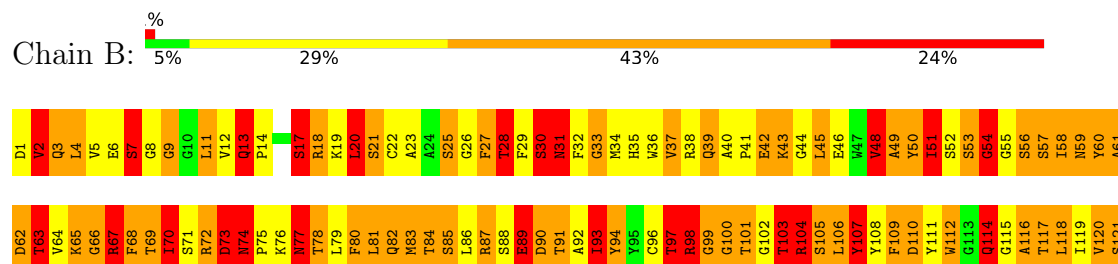
• Molecule 1: PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN))

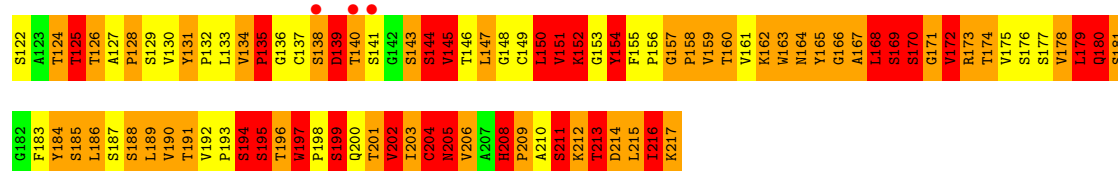


• Molecule 1: PROTEIN (IGG3-KAPPA ANTIBODY (LIGHT CHAIN))

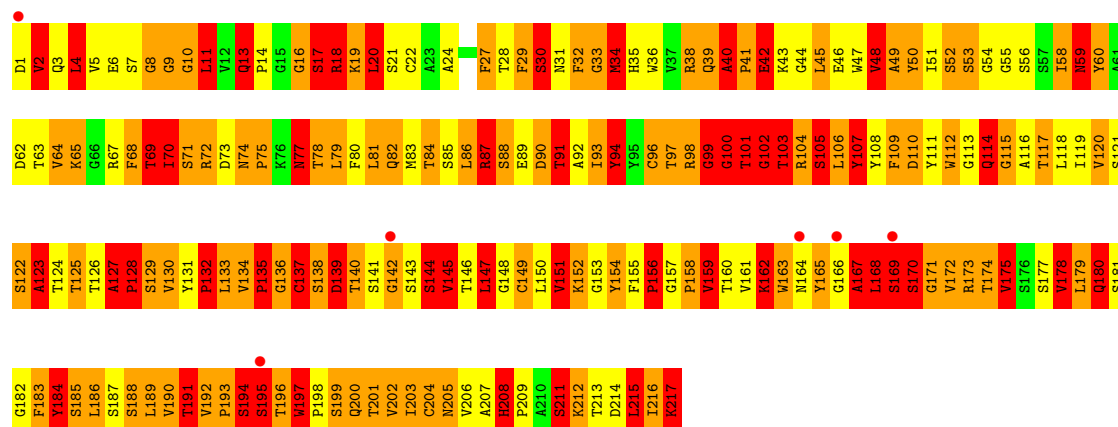


• Molecule 2: PROTEIN (IGG3-KAPPA ANTIBODY (HEAVY CHAIN))





● Molecule 2: PROTEIN (IGG3-KAPPA ANTIBODY (HEAVY CHAIN))



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.24Å 82.07Å 73.58Å 90.00° 94.13° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10 6.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	92.0 (6.00-3.10) 74.4 (6.00-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 3.10Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.245 , (Not available) 0.246 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	52.1	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.57 , 246.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	6458	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.72	25/1639 (1.5%)	3.57	288/2223 (13.0%)
1	C	1.73	29/1639 (1.8%)	3.52	295/2223 (13.3%)
2	B	1.81	25/1665 (1.5%)	3.35	291/2269 (12.8%)
2	D	1.74	26/1665 (1.6%)	3.51	303/2269 (13.4%)
All	All	1.75	105/6608 (1.6%)	3.49	1177/8984 (13.1%)

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	2
1	C	0	4
2	B	0	5
2	D	0	8
All	All	0	19

All (105) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	5	VAL	CA-CB	-12.70	1.38	1.54
2	B	202	VAL	CA-CB	10.14	1.68	1.54
1	A	114	THR	CA-CB	-9.89	1.40	1.52
2	D	140	THR	CA-CB	9.88	1.70	1.53
2	D	114	GLN	CA-CB	-9.31	1.40	1.53
2	D	78	THR	CA-CB	-8.99	1.39	1.53
2	B	91	THR	CA-CB	8.14	1.66	1.53
1	C	85	THR	CA-CB	7.44	1.65	1.53
2	D	86	LEU	CA-CB	7.29	1.62	1.52
2	D	208	HIS	CD2-NE2	-7.27	1.29	1.37
1	C	18	ARG	NE-CZ	7.19	1.41	1.33
2	D	174	THR	CA-CB	-7.15	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	137	CYS	CA-CB	7.08	1.65	1.53
2	B	54	GLY	CA-C	7.05	1.61	1.51
2	D	132	PRO	CA-CB	-7.02	1.46	1.54
1	A	12	SER	CA-CB	6.95	1.64	1.53
2	B	35	HIS	CD2-NE2	-6.93	1.30	1.37
1	C	19	VAL	CA-CB	6.89	1.63	1.53
2	D	35	HIS	CD2-NE2	-6.74	1.30	1.37
2	D	178	VAL	CA-CB	6.73	1.62	1.54
1	C	35	TRP	CA-CB	6.67	1.65	1.53
1	C	83	ILE	CA-CB	6.65	1.62	1.54
2	B	97	THR	CA-CB	-6.64	1.43	1.53
1	A	13	VAL	C-N	6.63	1.39	1.32
1	C	72	SER	CA-CB	-6.62	1.43	1.53
1	C	198	HIS	CD2-NE2	-6.62	1.30	1.37
2	B	215	LEU	CA-CB	-6.55	1.42	1.53
2	D	69	THR	CA-C	6.53	1.60	1.52
2	D	59	ASN	CA-CB	-6.50	1.43	1.53
2	D	69	THR	CA-CB	6.43	1.63	1.53
1	C	50	TYR	CA-CB	6.42	1.64	1.53
1	C	192	TYR	CA-CB	-6.35	1.43	1.53
1	C	2	ILE	CA-CB	6.33	1.61	1.54
2	B	199	SER	CA-C	6.30	1.61	1.52
2	B	18	ARG	C-O	6.25	1.31	1.23
1	A	186	TYR	CA-CB	6.24	1.63	1.53
2	B	157	GLY	CA-C	6.24	1.60	1.51
2	B	208	HIS	CD2-NE2	-6.18	1.31	1.37
1	C	70	ASP	CA-CB	6.15	1.64	1.53
1	A	189	HIS	CD2-NE2	-6.10	1.31	1.37
2	B	203	ILE	CA-CB	-6.07	1.49	1.55
1	C	205	ILE	CA-C	6.00	1.59	1.52
2	D	207	ALA	CA-C	-6.00	1.45	1.52
1	C	21	ILE	CA-CB	-5.95	1.47	1.54
1	A	71	TYR	C-O	5.94	1.31	1.23
1	A	198	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	120	PRO	CA-CB	-5.93	1.45	1.53
1	A	94	LEU	CA-C	-5.89	1.45	1.53
1	C	93	THR	CA-CB	-5.88	1.44	1.53
1	A	40	PRO	CA-CB	-5.86	1.45	1.53
1	A	51	THR	CA-CB	5.86	1.63	1.53
1	A	94	LEU	CA-CB	-5.85	1.43	1.53
1	A	198	HIS	CG-ND1	-5.85	1.31	1.38
2	B	128	PRO	CA-CB	-5.84	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	ARG	C-O	5.81	1.30	1.23
2	B	112	TRP	NE1-CE2	-5.76	1.31	1.37
1	A	83	ILE	CA-CB	5.75	1.60	1.53
1	A	200	THR	CA-CB	5.73	1.62	1.53
1	A	44	LEU	CA-CB	-5.72	1.44	1.53
1	C	56	SER	CA-CB	-5.71	1.44	1.53
2	D	156	PRO	CA-CB	-5.68	1.43	1.53
2	B	215	LEU	CA-C	-5.67	1.45	1.52
1	C	145	ASN	CA-CB	-5.64	1.44	1.53
2	B	174	THR	CA-CB	-5.63	1.45	1.53
2	D	91	THR	CA-CB	-5.63	1.45	1.53
1	A	117	ILE	CA-CB	-5.60	1.46	1.54
1	A	110	ASP	CA-C	-5.57	1.45	1.53
1	C	120	PRO	CA-CB	-5.55	1.46	1.53
2	B	184	TYR	CA-C	-5.50	1.46	1.52
1	C	119	PRO	CA-CB	-5.46	1.46	1.54
2	D	114	GLN	C-N	-5.46	1.28	1.33
1	C	153	SER	CA-CB	-5.46	1.42	1.53
2	B	5	VAL	N-CA	-5.46	1.39	1.46
2	B	78	THR	CA-CB	-5.46	1.43	1.53
1	C	44	LEU	CA-C	5.45	1.59	1.52
2	D	168	LEU	CB-CG	5.45	1.64	1.53
1	A	69	THR	CA-CB	5.44	1.62	1.54
1	A	39	LYS	CA-CB	-5.41	1.46	1.54
1	C	52	SER	CA-C	-5.41	1.46	1.52
2	B	167	ALA	CA-C	5.39	1.60	1.52
1	A	13	VAL	CA-C	-5.38	1.46	1.52
1	C	203	SER	CA-CB	-5.37	1.46	1.54
2	B	170	SER	C-N	-5.35	1.30	1.33
1	C	159	VAL	CA-CB	-5.35	1.47	1.53
2	D	190	VAL	CA-CB	5.33	1.62	1.54
1	C	170	ASP	CA-CB	5.30	1.61	1.53
2	B	216	ILE	C-O	5.26	1.30	1.24
2	B	195	SER	CA-CB	-5.23	1.45	1.53
2	D	52	SER	CA-C	-5.22	1.46	1.53
1	C	143	ASP	CA-CB	-5.20	1.44	1.53
1	C	53	ARG	CZ-NH2	5.19	1.40	1.33
1	A	148	TRP	CG-CD2	-5.18	1.34	1.43
2	B	161	VAL	CA-CB	-5.17	1.47	1.54
1	C	189	HIS	CA-CB	-5.11	1.45	1.53
1	C	20	ILE	CA-CB	5.11	1.61	1.54
2	D	86	LEU	CB-CG	5.11	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	LYS	CA-CB	-5.09	1.45	1.53
1	A	190	ASN	CA-CB	-5.07	1.45	1.53
1	A	119	PRO	CA-CB	-5.06	1.47	1.54
2	D	29	PHE	CA-CB	-5.06	1.45	1.53
2	D	151	VAL	CA-CB	5.05	1.60	1.53
2	D	13	GLN	CA-C	-5.05	1.46	1.53
2	D	32	PHE	CA-CB	-5.04	1.43	1.53
2	B	59	ASN	CA-CB	5.04	1.59	1.52
2	D	142	GLY	CA-C	5.02	1.58	1.51

All (1177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	116	ALA	N-CA-C	-27.35	66.84	109.23
1	A	13	VAL	N-CA-C	-26.91	66.74	108.44
1	A	114	THR	N-CA-CB	-23.10	76.30	110.49
1	C	65	TRP	N-CA-C	-23.06	76.92	108.74
1	A	13	VAL	CA-C-O	-20.21	101.24	121.45
2	B	115	GLY	N-CA-C	-19.78	93.16	111.95
2	D	18	ARG	N-CA-C	-19.02	81.06	107.88
1	C	1	ASP	CA-CB-CG	-17.96	94.64	112.60
1	A	88	CYS	N-CA-C	-17.68	81.83	109.23
1	A	12	SER	N-CA-C	-17.64	82.28	110.32
1	C	198	HIS	CA-CB-CG	-17.53	96.27	113.80
1	C	150	ILE	N-CA-C	-16.88	83.23	108.89
1	A	186	TYR	N-CA-C	-16.85	90.85	111.40
2	D	169	SER	N-CA-C	-16.75	75.13	110.80
1	A	144	ILE	N-CA-C	-16.74	86.26	108.35
1	C	1	ASP	N-CA-C	-16.17	65.71	111.00
1	A	13	VAL	O-C-N	16.15	140.42	122.82
2	D	192	VAL	CA-C-O	15.28	128.98	119.51
2	B	54	GLY	O-C-N	-14.95	103.26	122.70
1	C	15	LEU	N-CA-C	-14.77	91.48	110.53
1	A	145	ASN	O-C-N	-14.56	106.82	123.27
2	D	116	ALA	CA-C-O	-14.52	104.22	121.06
2	D	33	GLY	O-C-N	-14.24	108.17	122.84
2	B	48	VAL	N-CA-CB	-13.72	97.11	112.21
1	A	96	TYR	N-CA-C	-13.63	90.31	110.48
2	D	30	SER	CA-C-N	-13.55	100.57	122.66
2	D	30	SER	C-N-CA	-13.55	100.57	122.66
1	C	4	MET	CA-C-N	-13.45	104.03	123.00
1	C	4	MET	C-N-CA	-13.45	104.03	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	ILE	N-CA-C	-13.41	88.48	108.87
1	C	19	VAL	CA-C-N	-13.09	104.19	122.91
1	C	19	VAL	C-N-CA	-13.09	104.19	122.91
1	C	84	ALA	N-CA-C	-13.01	83.09	110.80
1	A	179	LEU	N-CA-C	-12.96	88.50	109.76
2	B	199	SER	O-C-N	-12.83	105.53	122.59
1	A	190	ASN	O-C-N	-12.72	105.67	122.59
1	C	64	GLY	O-C-N	-12.70	111.86	123.42
1	A	184	ASP	N-CA-C	12.68	126.68	111.33
2	D	8	GLY	CA-C-N	-12.60	107.60	122.85
2	D	8	GLY	C-N-CA	-12.60	107.60	122.85
2	B	115	GLY	CA-C-O	-12.59	114.04	122.22
2	B	201	THR	CA-C-O	-12.54	108.41	120.95
1	A	190	ASN	CA-C-N	-12.52	100.88	122.92
1	A	190	ASN	C-N-CA	-12.52	100.88	122.92
1	A	135	PHE	CA-CB-CG	12.49	126.29	113.80
1	C	31	ASN	CA-CB-CG	-12.46	100.14	112.60
2	B	48	VAL	O-C-N	-12.42	109.71	122.25
1	C	18	ARG	NE-CZ-NH2	12.34	130.31	119.20
2	B	160	THR	O-C-N	-12.32	108.98	123.27
1	A	156	GLN	N-CA-C	-12.28	92.36	111.02
2	D	19	LYS	N-CA-C	-12.26	87.79	108.75
2	D	72	ARG	O-C-N	-12.18	109.06	123.31
2	D	107	TYR	CA-CB-CG	-12.07	92.17	113.90
1	C	44	LEU	O-C-N	-12.05	109.09	123.19
2	D	171	GLY	O-C-N	-12.02	110.98	123.48
1	C	1	ASP	CA-C-O	-12.00	100.40	120.80
1	C	153	SER	O-C-N	-11.98	112.00	123.26
2	B	73	ASP	CA-CB-CG	-11.94	100.66	112.60
1	A	38	GLN	O-C-N	-11.86	109.30	123.29
2	D	122	SER	CA-C-N	-11.77	99.07	121.54
2	D	122	SER	C-N-CA	-11.77	99.07	121.54
2	D	168	LEU	CA-C-O	11.71	134.10	119.11
1	A	128	GLY	CA-C-N	-11.61	110.34	122.30
1	A	128	GLY	C-N-CA	-11.61	110.34	122.30
2	B	11	LEU	N-CA-C	-11.60	89.01	108.26
2	B	72	ARG	N-CA-C	-11.59	91.75	109.94
2	B	159	VAL	N-CA-C	-11.53	91.36	108.89
1	A	58	VAL	N-CA-C	-11.51	96.29	108.96
1	C	83	ILE	O-C-N	-11.42	110.13	122.81
2	D	144	SER	N-CA-C	-11.40	86.52	110.80
2	D	172	VAL	N-CA-C	-11.37	91.61	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	74	ASN	OD1-CG-ND2	-11.35	111.25	122.60
2	D	8	GLY	O-C-N	-11.33	107.97	122.70
1	A	74	THR	O-C-N	-11.28	108.23	123.12
1	C	72	SER	CA-CB-OG	-11.27	88.57	111.10
1	C	10	SER	N-CA-C	-11.23	92.09	109.95
2	D	139	ASP	N-CA-C	11.21	128.15	110.32
1	A	12	SER	CA-C-N	-11.20	107.84	122.51
1	A	12	SER	C-N-CA	-11.20	107.84	122.51
2	D	49	ALA	O-C-N	-11.17	110.75	123.48
2	B	153	GLY	O-C-N	-11.15	110.91	122.51
2	B	137	CYS	N-CA-C	-11.13	91.60	108.52
2	B	21	SER	CA-C-N	-11.08	106.32	122.94
2	B	21	SER	C-N-CA	-11.08	106.32	122.94
2	D	120	VAL	N-CA-CB	-11.07	99.95	111.90
1	C	161	ASN	O-C-N	-11.04	110.17	123.30
2	B	35	HIS	CB-CG-CD2	-10.99	116.91	131.20
1	A	206	VAL	N-CA-C	-10.99	80.24	111.00
2	B	70	ILE	N-CA-CB	-10.97	101.42	112.06
1	A	184	ASP	CA-CB-CG	-10.94	101.66	112.60
2	B	13	GLN	OE1-CD-NE2	-10.94	111.66	122.60
2	D	78	THR	N-CA-C	10.93	126.53	109.81
1	C	85	THR	N-CA-C	-10.89	93.26	110.14
1	A	84	ALA	N-CA-C	-10.87	93.70	108.38
1	A	20	ILE	N-CA-C	-10.83	92.19	108.97
1	C	194	CYS	O-C-N	-10.78	111.09	123.27
2	D	103	THR	N-CA-C	10.76	127.32	109.46
1	A	184	ASP	O-C-N	-10.71	110.77	122.12
2	B	80	PHE	CA-CB-CG	10.70	124.50	113.80
1	A	88	CYS	CA-C-O	-10.69	108.66	121.06
2	B	165	TYR	N-CA-C	-10.67	93.36	110.32
1	A	10	SER	N-CA-C	-10.62	90.58	108.75
1	C	177	SER	N-CA-C	-10.62	91.93	109.24
2	D	124	THR	N-CA-C	-10.59	94.79	110.46
1	A	29	ILE	O-C-N	-10.56	109.19	122.17
1	C	115	VAL	O-C-N	-10.55	111.17	122.67
2	B	44	GLY	CA-C-O	10.48	132.63	121.53
1	A	43	SER	N-CA-C	10.46	125.44	112.47
1	C	21	ILE	O-C-N	-10.44	111.44	123.03
1	C	53	ARG	NE-CZ-NH1	-10.43	111.07	121.50
1	A	98	PHE	N-CA-C	10.42	125.88	108.90
1	C	112	ALA	N-CA-C	-10.40	94.80	110.39
2	D	117	THR	N-CA-C	-10.39	93.43	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	204	CYS	CA-C-N	-10.39	108.36	123.11
2	B	204	CYS	C-N-CA	-10.39	108.36	123.11
2	B	168	LEU	N-CA-C	-10.38	88.69	110.80
2	D	31	ASN	OD1-CG-ND2	-10.36	112.24	122.60
2	B	23	ALA	N-CA-C	10.35	125.07	108.41
1	C	34	ASN	CA-CB-CG	10.33	122.93	112.60
1	A	114	THR	CB-CA-C	10.31	129.00	111.68
1	C	7	ILE	N-CA-C	-10.31	93.62	108.36
1	C	56	SER	CA-CB-OG	-10.29	90.53	111.10
2	D	122	SER	O-C-N	-10.28	108.42	122.30
1	C	153	SER	CA-C-N	-10.27	101.43	122.07
1	C	153	SER	C-N-CA	-10.27	101.43	122.07
2	D	40	ALA	N-CA-C	-10.24	98.35	110.13
1	A	114	THR	CA-CB-OG1	-10.24	94.25	109.60
1	C	165	ASP	CA-CB-CG	10.22	122.83	112.60
1	C	17	ASP	N-CA-C	10.21	125.60	110.48
1	C	198	HIS	CB-CG-CD2	-10.18	117.96	131.20
1	C	75	ILE	N-CA-C	-10.18	93.42	108.89
1	C	87	PHE	N-CA-C	-10.16	93.97	109.41
2	D	173	ARG	CB-CA-C	-10.14	94.20	111.23
2	D	171	GLY	N-CA-C	-10.13	93.12	111.25
2	D	81	LEU	N-CA-C	-10.04	89.41	110.80
1	C	44	LEU	N-CA-C	10.02	126.19	109.76
1	C	145	ASN	CB-CG-ND2	10.01	131.41	116.40
1	C	188	ARG	O-C-N	-10.01	111.51	122.12
2	D	140	THR	N-CA-C	-9.95	89.60	110.80
1	A	201	SER	CA-C-N	-9.95	102.62	121.63
1	A	201	SER	C-N-CA	-9.95	102.62	121.63
2	D	201	THR	N-CA-C	9.93	123.15	110.24
2	B	60	TYR	N-CA-C	9.92	126.09	110.32
1	A	14	SER	O-C-N	-9.91	113.42	121.65
2	B	159	VAL	CA-C-O	-9.90	108.82	121.40
2	D	165	TYR	N-CA-C	-9.90	91.20	108.23
2	D	191	THR	CA-C-N	-9.90	114.72	123.33
2	D	191	THR	C-N-CA	-9.90	114.72	123.33
1	A	80	GLU	O-C-N	-9.88	109.46	122.59
1	A	145	ASN	CA-C-N	-9.86	107.02	122.69
1	A	145	ASN	C-N-CA	-9.86	107.02	122.69
1	A	145	ASN	CA-CB-CG	-9.82	102.78	112.60
2	B	204	CYS	O-C-N	-9.81	111.72	123.19
1	C	128	GLY	CA-C-N	-9.80	113.75	122.47
1	C	128	GLY	C-N-CA	-9.80	113.75	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	131	TYR	O-C-N	-9.79	114.93	121.88
1	C	165	ASP	N-CA-C	-9.76	94.42	109.85
2	B	21	SER	O-C-N	-9.71	110.93	123.16
1	A	17	ASP	O-C-N	9.66	136.05	123.11
1	C	170	ASP	CA-CB-CG	9.63	122.23	112.60
2	D	62	ASP	CA-CB-CG	-9.62	102.98	112.60
1	C	166	GLN	O-C-N	-9.60	112.36	123.11
1	A	74	THR	CA-C-N	-9.59	110.38	122.37
1	A	74	THR	C-N-CA	-9.59	110.38	122.37
2	D	58	ILE	O-C-N	-9.58	112.97	123.03
1	C	22	SER	N-CA-C	9.56	124.11	108.52
1	C	26	SER	O-C-N	-9.56	111.25	122.15
2	B	116	ALA	N-CA-C	-9.55	90.47	110.80
1	A	205	ILE	N-CA-C	-9.55	94.73	108.48
1	C	127	SER	O-C-N	-9.53	109.94	122.33
1	C	197	THR	N-CA-C	-9.52	94.27	109.59
1	C	21	ILE	N-CA-C	9.51	121.96	108.36
1	A	85	THR	CA-CB-OG1	-9.50	95.36	109.60
2	B	205	ASN	OD1-CG-ND2	-9.48	113.12	122.60
1	C	91	GLY	O-C-N	9.47	135.01	122.70
2	D	122	SER	N-CA-CB	-9.46	95.52	110.19
2	D	186	LEU	O-C-N	-9.41	114.14	123.46
1	C	46	LEU	O-C-N	-9.39	112.06	123.04
1	C	3	GLN	CA-C-O	9.36	130.16	120.24
1	A	127	SER	CA-CB-OG	-9.35	92.41	111.10
2	D	77	ASN	N-CA-C	9.32	130.66	110.80
2	D	11	LEU	N-CA-C	-9.32	94.07	109.07
2	D	122	SER	CA-CB-OG	-9.31	92.47	111.10
1	C	19	VAL	O-C-N	-9.31	113.68	122.71
1	A	87	PHE	O-C-N	-9.26	110.70	123.11
1	A	51	THR	CA-C-N	-9.26	107.81	121.98
1	A	51	THR	C-N-CA	-9.26	107.81	121.98
1	C	116	SER	N-CA-C	-9.25	94.89	109.50
2	B	195	SER	N-CA-CB	-9.24	96.61	110.01
2	B	110	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	201	SER	CA-C-O	9.22	129.51	120.56
2	B	206	VAL	N-CA-C	9.22	121.24	107.51
1	A	82	ASP	N-CA-C	-9.13	100.54	112.41
1	A	151	ASP	CA-CB-CG	-9.12	103.48	112.60
2	D	159	VAL	N-CA-C	-9.10	95.33	107.88
1	A	2	ILE	N-CA-C	-9.09	97.86	109.58
2	D	53	SER	O-C-N	-9.08	111.65	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	154	TYR	N-CA-C	9.07	123.02	109.95
2	D	20	LEU	N-CA-C	-9.06	95.22	109.72
1	C	11	LEU	N-CA-C	-9.05	91.53	110.80
1	C	192	TYR	CA-CB-CG	-9.05	97.62	113.90
1	C	119	PRO	N-CA-C	9.04	121.73	110.70
2	D	62	ASP	N-CA-C	-9.03	101.41	111.07
1	A	48	ILE	CA-C-O	-9.03	111.89	121.19
2	B	216	ILE	O-C-N	9.00	133.81	122.57
1	A	187	GLU	O-C-N	-8.95	111.74	122.22
1	C	172	THR	N-CA-CB	-8.92	96.75	111.20
1	C	20	ILE	N-CA-C	-8.92	95.42	108.71
2	B	126	THR	CA-CB-OG1	-8.90	96.24	109.60
1	A	67	SER	N-CA-C	-8.89	95.04	108.46
1	C	2	ILE	N-CA-C	-8.85	98.03	109.80
2	B	203	ILE	CA-C-O	-8.83	113.55	120.96
2	B	30	SER	CA-C-N	-8.82	106.42	122.38
2	B	30	SER	C-N-CA	-8.82	106.42	122.38
2	B	196	THR	N-CA-C	-8.81	95.78	109.25
1	C	198	HIS	CB-CG-ND1	8.79	135.89	122.70
1	A	188	ARG	O-C-N	-8.77	110.92	122.59
1	C	99	GLY	O-C-N	-8.76	115.45	122.99
2	D	94	TYR	CA-C-O	-8.73	110.67	120.54
2	B	44	GLY	N-CA-C	8.73	125.12	112.55
2	B	208	HIS	CA-CB-CG	8.71	122.51	113.80
1	C	61	ARG	CA-C-O	8.67	130.07	119.31
1	C	24	ARG	NE-CZ-NH2	8.65	126.98	119.20
1	A	76	SER	CA-C-N	-8.64	109.20	123.37
1	A	76	SER	C-N-CA	-8.64	109.20	123.37
1	C	9	SER	CA-CB-OG	-8.62	93.86	111.10
2	B	87	ARG	NE-CZ-NH2	8.62	126.96	119.20
1	A	188	ARG	CA-CB-CG	-8.61	96.88	114.10
1	C	153	SER	CA-CB-OG	-8.60	93.90	111.10
1	A	34	ASN	CA-CB-CG	8.60	121.20	112.60
1	A	154	GLU	CB-CG-CD	8.59	127.20	112.60
1	A	169	LYS	CA-CB-CG	-8.58	96.94	114.10
1	C	53	ARG	NE-CZ-NH2	8.57	126.91	119.20
1	A	165	ASP	N-CA-C	-8.54	96.53	109.94
2	D	211	SER	N-CA-C	8.54	128.99	110.80
2	D	69	THR	O-C-N	-8.52	112.06	123.14
2	D	32	PHE	O-C-N	-8.48	113.06	123.33
1	A	76	SER	CA-CB-OG	8.47	128.03	111.10
1	A	75	ILE	N-CA-C	8.45	121.16	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	45	LYS	O-C-N	-8.44	112.49	123.21
2	B	155	PHE	O-C-N	-8.44	115.25	121.83
1	C	58	VAL	CA-C-N	8.44	129.08	120.14
1	C	58	VAL	C-N-CA	8.44	129.08	120.14
2	B	3	GLN	N-CA-C	8.39	122.58	109.07
2	B	17	SER	O-C-N	8.37	133.50	122.96
2	B	119	ILE	O-C-N	-8.34	113.44	122.95
1	C	189	HIS	O-C-N	-8.34	112.35	123.10
2	B	214	ASP	CA-CB-CG	-8.33	104.27	112.60
1	C	44	LEU	CA-C-N	-8.33	109.51	122.59
1	C	44	LEU	C-N-CA	-8.33	109.51	122.59
2	D	98	ARG	NE-CZ-NH1	-8.33	113.17	121.50
2	B	197	TRP	CG-CD2-CE3	8.32	142.22	133.90
2	B	160	THR	CA-C-N	-8.31	111.65	122.37
2	B	160	THR	C-N-CA	-8.31	111.65	122.37
2	B	91	THR	CB-CA-C	8.31	122.30	109.84
2	B	211	SER	N-CA-C	8.30	128.47	110.80
2	D	169	SER	O-C-N	8.29	133.62	122.59
2	D	134	VAL	CA-C-N	8.29	128.17	120.21
2	D	134	VAL	C-N-CA	8.29	128.17	120.21
1	A	106	ILE	CB-CA-C	-8.29	102.28	111.23
2	D	101	THR	CA-CB-OG1	-8.28	97.18	109.60
1	A	200	THR	O-C-N	-8.28	111.78	122.37
2	B	77	ASN	OD1-CG-ND2	-8.27	114.33	122.60
1	A	69	THR	CA-C-N	-8.27	111.59	123.00
1	A	69	THR	C-N-CA	-8.27	111.59	123.00
1	A	176	SER	CB-CA-C	-8.26	97.42	110.14
2	B	215	LEU	N-CA-C	-8.25	94.64	108.75
2	D	115	GLY	O-C-N	-8.21	116.45	123.43
2	D	129	SER	CB-CA-C	-8.21	96.21	109.75
2	B	181	SER	CA-C-N	-8.20	110.89	122.86
2	B	181	SER	C-N-CA	-8.20	110.89	122.86
2	D	185	SER	CA-C-O	-8.19	112.14	121.40
2	B	17	SER	CA-CB-OG	-8.19	94.72	111.10
1	C	105	GLU	O-C-N	8.18	132.50	123.10
1	A	57	GLY	O-C-N	-8.17	112.50	122.23
1	C	97	THR	N-CA-C	8.16	122.20	108.90
1	C	78	LEU	O-C-N	-8.16	111.74	122.59
2	B	39	GLN	OE1-CD-NE2	-8.14	114.46	122.60
2	D	113	GLY	O-C-N	-8.11	114.22	122.82
2	B	90	ASP	CA-C-O	8.11	127.97	119.05
1	A	69	THR	N-CA-C	-8.09	102.66	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	GLY	CA-C-N	8.08	134.94	122.42
1	C	91	GLY	C-N-CA	8.08	134.94	122.42
2	D	21	SER	N-CA-C	-8.08	96.71	109.23
1	C	167	ASP	O-C-N	8.08	132.97	122.95
2	D	109	PHE	CA-C-N	8.06	130.92	120.44
2	D	109	PHE	C-N-CA	8.06	130.92	120.44
2	D	7	SER	O-C-N	-8.06	113.39	121.93
2	D	204	CYS	N-CA-C	-8.05	96.10	109.07
1	C	102	THR	CA-CB-OG1	-8.05	97.53	109.60
1	C	71	TYR	N-CA-C	8.03	121.11	109.14
2	D	138	SER	N-CA-C	8.03	127.90	110.80
1	A	88	CYS	O-C-N	8.02	132.58	123.27
2	B	162	LYS	CB-CG-CD	-8.01	92.87	111.30
1	A	86	PHE	CA-CB-CG	8.01	121.81	113.80
1	C	147	LYS	O-C-N	-8.01	116.20	123.41
2	B	205	ASN	CB-CG-ND2	8.00	128.41	116.40
1	A	153	SER	O-C-N	8.00	133.55	123.15
1	C	34	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	C	146	VAL	O-C-N	-7.99	112.59	122.57
1	C	76	SER	CA-CB-OG	-7.98	95.14	111.10
1	A	164	THR	N-CA-C	-7.97	99.35	110.35
1	C	41	ASP	N-CA-C	-7.96	94.43	108.13
2	B	208	HIS	CB-CG-ND1	7.95	134.63	122.70
1	C	179	LEU	CA-C-N	-7.95	112.03	123.00
1	C	179	LEU	C-N-CA	-7.95	112.03	123.00
2	D	185	SER	O-C-N	7.94	132.78	123.17
1	C	3	GLN	CA-CB-CG	-7.93	98.24	114.10
1	C	205	ILE	O-C-N	-7.93	114.03	122.67
2	D	50	TYR	CA-C-O	-7.93	112.11	120.99
1	A	43	SER	O-C-N	-7.93	107.13	122.11
1	C	155	ARG	O-C-N	-7.92	114.19	123.22
1	A	96	TYR	CA-C-O	-7.91	112.38	121.47
1	A	145	ASN	CA-C-O	-7.88	111.84	120.43
1	A	1	ASP	CA-CB-CG	7.88	120.48	112.60
2	D	4	LEU	O-C-N	-7.87	112.73	123.12
2	B	5	VAL	CA-C-O	-7.85	112.15	120.39
1	A	26	SER	O-C-N	-7.84	112.17	122.59
2	B	184	TYR	O-C-N	7.84	133.21	123.10
2	B	168	LEU	CA-C-O	7.83	131.71	120.51
1	C	159	VAL	N-CA-CB	-7.82	102.04	111.90
2	B	152	LYS	CB-CG-CD	-7.82	93.32	111.30
2	D	30	SER	O-C-N	-7.81	113.08	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	25	SER	O-C-N	-7.81	113.83	123.36
2	D	173	ARG	N-CA-CB	7.80	123.56	110.69
2	B	140	THR	O-C-N	7.80	132.96	122.59
1	A	183	LYS	O-C-N	-7.79	113.27	122.15
1	A	75	ILE	O-C-N	-7.78	113.44	122.94
2	B	69	THR	N-CA-C	7.78	121.17	108.26
1	C	102	THR	CA-CB-CG2	7.78	123.72	110.50
2	B	184	TYR	N-CA-C	-7.77	98.09	110.14
2	D	208	HIS	CB-CG-CD2	-7.77	121.09	131.20
1	C	138	ASN	CA-C-N	-7.76	107.28	123.20
1	C	138	ASN	C-N-CA	-7.76	107.28	123.20
2	B	4	LEU	O-C-N	-7.75	114.38	123.22
1	A	82	ASP	CA-C-N	-7.74	113.35	122.95
1	A	82	ASP	C-N-CA	-7.74	113.35	122.95
1	A	167	ASP	N-CA-C	7.72	122.04	109.76
2	B	167	ALA	CA-C-O	7.71	129.53	120.58
1	A	146	VAL	CA-C-O	-7.71	112.33	121.28
1	C	167	ASP	N-CA-CB	7.71	121.48	109.69
2	D	127	ALA	CA-C-O	-7.71	109.60	120.16
2	B	50	TYR	CA-C-O	-7.67	110.84	120.28
2	B	181	SER	O-C-N	-7.67	112.41	122.00
1	C	20	ILE	CB-CG1-CD1	7.67	129.90	113.80
1	C	173	TYR	CA-C-O	-7.67	112.45	121.11
1	A	106	ILE	N-CA-C	7.66	119.55	107.98
1	C	205	ILE	N-CA-CB	-7.66	100.89	110.31
1	C	51	THR	O-C-N	-7.66	112.41	122.59
1	A	196	ALA	N-CA-C	7.64	122.05	109.06
2	B	126	THR	N-CA-CB	-7.64	98.39	110.69
1	C	148	TRP	N-CA-C	-7.64	97.39	109.23
2	D	173	ARG	CA-C-O	-7.63	110.95	120.57
1	A	105	GLU	O-C-N	7.63	132.03	123.48
2	B	202	VAL	N-CA-CB	7.63	123.82	111.23
1	C	73	LEU	O-C-N	7.63	131.92	123.22
1	A	172	THR	N-CA-C	7.63	121.40	109.96
1	A	202	THR	N-CA-C	-7.62	105.94	114.62
2	B	9	GLY	CA-C-N	-7.60	110.61	120.72
2	B	9	GLY	C-N-CA	-7.60	110.61	120.72
1	A	201	SER	O-C-N	7.60	131.62	122.88
1	C	103	LYS	N-CA-C	-7.60	97.19	109.96
1	A	55	GLN	O-C-N	-7.59	113.31	122.65
2	D	74	ASN	N-CA-C	7.58	126.57	109.81
2	D	123	ALA	CA-C-O	7.57	131.33	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	THR	O-C-N	-7.56	113.63	122.93
2	B	68	PHE	CA-CB-CG	-7.56	106.24	113.80
2	D	112	TRP	CG-CD2-CE3	7.55	141.45	133.90
1	A	41	ASP	CA-CB-CG	-7.55	105.05	112.60
1	C	84	ALA	CA-C-O	-7.54	109.73	120.51
1	A	100	GLY	O-C-N	-7.54	112.90	122.70
1	C	70	ASP	CA-CB-CG	7.54	120.14	112.60
2	B	65	LYS	CA-CB-CG	-7.53	99.03	114.10
2	D	101	THR	CA-C-O	7.53	130.24	121.28
2	B	94	TYR	CA-C-O	-7.52	112.05	120.32
1	A	10	SER	CA-C-O	-7.51	111.30	120.54
2	D	157	GLY	O-C-N	-7.50	113.47	122.03
2	B	43	LYS	O-C-N	-7.49	111.92	121.74
2	D	121	SER	CA-C-O	-7.49	112.36	120.75
2	D	101	THR	N-CA-C	-7.48	101.64	111.74
1	C	18	ARG	N-CA-C	-7.48	100.18	110.35
1	C	51	THR	CA-C-N	-7.47	108.92	121.18
1	C	51	THR	C-N-CA	-7.47	108.92	121.18
1	C	100	GLY	O-C-N	-7.47	112.99	122.70
1	C	164	THR	N-CA-C	-7.46	98.23	109.94
1	C	1	ASP	CA-C-N	7.46	131.64	120.75
1	C	1	ASP	C-N-CA	7.46	131.64	120.75
2	B	106	LEU	O-C-N	-7.45	113.10	123.01
2	B	120	VAL	N-CA-C	-7.45	97.12	107.99
2	D	59	ASN	CA-CB-CG	-7.44	105.16	112.60
1	C	203	SER	CA-C-O	7.43	127.31	120.26
1	A	36	TYR	N-CA-C	-7.42	98.12	109.85
2	B	132	PRO	CA-C-O	-7.42	112.40	121.31
2	D	213	THR	CA-C-O	-7.41	112.62	120.40
2	D	4	LEU	CA-C-N	-7.41	112.83	123.06
2	D	4	LEU	C-N-CA	-7.41	112.83	123.06
2	B	208	HIS	CB-CG-CD2	-7.40	121.58	131.20
1	C	160	LEU	O-C-N	-7.40	114.77	123.06
2	D	113	GLY	CA-C-O	-7.38	114.38	121.90
2	D	9	GLY	N-CA-C	-7.37	103.95	112.79
1	C	141	PRO	N-CA-C	7.35	131.21	112.10
2	B	110	ASP	N-CA-CB	-7.35	98.89	110.28
1	A	103	LYS	N-CA-C	-7.34	100.83	110.53
1	C	61	ARG	O-C-N	7.34	132.59	122.46
2	B	160	THR	N-CA-C	7.34	120.37	108.41
1	A	42	GLY	CA-C-N	-7.33	111.18	122.61
1	A	42	GLY	C-N-CA	-7.33	111.18	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	CA-C-N	-7.33	110.57	121.05
1	A	43	SER	C-N-CA	-7.33	110.57	121.05
1	C	65	TRP	O-C-N	7.33	131.49	122.92
1	C	122	SER	O-C-N	7.33	129.71	122.09
1	A	98	PHE	O-C-N	-7.32	114.59	123.30
1	C	192	TYR	CA-C-N	-7.32	112.90	123.00
1	C	192	TYR	C-N-CA	-7.32	112.90	123.00
1	C	130	ALA	CA-C-N	-7.31	112.68	122.99
1	C	130	ALA	C-N-CA	-7.31	112.68	122.99
1	A	191	SER	N-CA-C	-7.30	98.83	110.14
1	C	1	ASP	O-C-N	7.29	134.66	123.00
2	B	189	LEU	O-C-N	-7.29	113.35	123.11
2	D	161	VAL	CA-C-N	-7.29	110.58	122.82
2	D	161	VAL	C-N-CA	-7.29	110.58	122.82
1	A	150	ILE	CB-CA-C	-7.27	101.54	110.99
1	A	193	THR	N-CA-C	-7.26	95.84	108.69
2	D	104	ARG	CA-C-N	-7.26	111.90	124.82
2	D	104	ARG	C-N-CA	-7.26	111.90	124.82
2	D	167	ALA	O-C-N	-7.25	112.94	122.59
1	A	14	SER	CA-C-O	-7.25	113.76	118.33
1	A	99	GLY	N-CA-C	-7.25	102.88	111.36
2	B	49	ALA	O-C-N	-7.25	112.95	122.59
2	D	47	TRP	N-CA-C	-7.25	101.50	110.41
1	C	145	ASN	CA-C-O	-7.24	112.79	121.05
2	D	35	HIS	CA-CB-CG	7.24	121.04	113.80
2	D	91	THR	O-C-N	-7.24	114.77	123.16
2	D	211	SER	O-C-N	-7.23	112.97	122.59
1	A	204	PRO	N-CA-C	-7.23	97.58	112.47
2	B	13	GLN	CG-CD-NE2	7.23	127.24	116.40
2	D	84	THR	O-C-N	-7.22	116.31	123.46
2	D	164	ASN	CB-CA-C	-7.21	99.73	110.62
1	A	76	SER	CB-CA-C	-7.20	99.53	110.90
2	B	93	ILE	N-CA-C	-7.18	98.11	108.17
1	A	19	VAL	CA-C-O	-7.18	112.87	120.48
2	B	159	VAL	CB-CA-C	-7.18	99.39	110.95
1	C	131	SER	N-CA-C	-7.17	97.22	108.90
2	D	78	THR	OG1-CB-CG2	7.17	123.64	109.30
1	A	109	ALA	O-C-N	7.16	131.08	123.06
2	D	22	CYS	CA-C-O	-7.16	111.23	120.25
2	B	28	THR	OG1-CB-CG2	7.14	123.58	109.30
2	B	2	VAL	N-CA-C	7.14	124.18	109.34
1	A	164	THR	CA-C-N	-7.13	109.04	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	THR	C-N-CA	-7.13	109.04	122.73
2	D	164	ASN	N-CA-CB	7.13	121.68	110.84
2	D	215	LEU	O-C-N	-7.13	114.97	123.31
2	B	98	ARG	CB-CG-CD	-7.13	94.91	111.30
2	D	183	PHE	N-CA-CB	-7.12	100.62	110.38
1	A	4	MET	N-CA-C	-7.12	98.13	109.59
1	C	190	ASN	CA-CB-CG	-7.12	105.48	112.60
2	B	151	VAL	CA-C-O	7.11	128.31	120.48
2	B	106	LEU	CA-C-N	-7.10	113.61	122.84
2	B	106	LEU	C-N-CA	-7.10	113.61	122.84
1	C	154	GLU	N-CA-C	-7.09	100.02	110.52
2	D	147	LEU	CA-C-O	-7.08	113.45	121.81
1	C	165	ASP	CA-C-O	-7.08	113.18	121.46
1	C	167	ASP	CB-CA-C	-7.08	98.86	109.90
2	B	153	GLY	CA-C-N	-7.07	110.13	122.64
2	B	153	GLY	C-N-CA	-7.07	110.13	122.64
1	C	60	SER	O-C-N	-7.07	113.19	122.59
1	A	201	SER	CB-CA-C	-7.06	99.32	113.80
2	D	101	THR	CA-C-N	-7.06	107.57	121.41
2	D	101	THR	C-N-CA	-7.06	107.57	121.41
1	C	124	GLN	O-C-N	7.05	129.71	122.09
2	D	139	ASP	CA-CB-CG	-7.05	105.55	112.60
1	A	199	LYS	O-C-N	-7.05	113.22	122.59
1	C	20	ILE	CA-C-O	-7.04	112.67	120.84
1	C	140	TYR	O-C-N	-7.04	113.22	121.32
1	C	12	SER	O-C-N	7.04	131.54	123.31
2	B	201	THR	O-C-N	7.04	130.99	123.11
1	A	4	MET	CA-CB-CG	7.03	128.16	114.10
1	A	39	LYS	CA-C-N	7.02	128.62	119.84
1	A	39	LYS	C-N-CA	7.02	128.62	119.84
1	C	138	ASN	CA-CB-CG	-7.02	105.58	112.60
2	B	13	GLN	N-CA-C	-7.01	101.23	109.93
1	A	112	ALA	O-C-N	7.01	126.86	121.88
1	A	60	SER	N-CA-C	7.00	125.70	110.80
1	A	8	THR	N-CA-CB	6.99	122.31	110.49
1	C	112	ALA	CA-C-O	-6.99	113.06	120.88
2	D	114	GLN	O-C-N	-6.98	113.00	122.36
2	B	121	SER	O-C-N	6.98	130.75	122.72
2	B	48	VAL	CB-CA-C	6.97	119.56	110.84
2	B	110	ASP	O-C-N	-6.97	113.70	122.27
2	D	173	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	A	44	LEU	O-C-N	-6.97	114.70	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	138	ASN	O-C-N	-6.96	113.28	122.47
1	C	179	LEU	O-C-N	-6.95	115.07	123.27
1	C	192	TYR	O-C-N	-6.94	113.95	123.12
1	A	80	GLU	CB-CG-CD	6.93	124.38	112.60
2	D	31	ASN	O-C-N	-6.92	112.79	122.06
1	C	145	ASN	O-C-N	-6.92	114.85	123.01
1	A	41	ASP	N-CA-C	-6.91	96.08	110.80
1	C	53	ARG	CA-CB-CG	-6.91	100.29	114.10
2	B	65	LYS	CA-C-N	-6.90	107.88	121.41
2	B	65	LYS	C-N-CA	-6.90	107.88	121.41
2	B	138	SER	N-CA-C	6.90	125.49	110.80
1	C	145	ASN	CA-CB-CG	-6.90	105.70	112.60
1	A	48	ILE	N-CA-C	-6.90	98.56	108.42
1	A	102	THR	CA-C-O	-6.89	113.67	121.39
2	B	103	THR	N-CA-C	6.89	118.87	108.46
1	C	138	ASN	CA-C-O	-6.89	112.44	120.98
1	A	15	LEU	CA-C-O	-6.88	113.50	121.49
1	C	28	ASP	N-CA-C	-6.88	96.54	108.52
1	A	29	ILE	N-CA-C	6.88	121.58	112.98
1	A	76	SER	N-CA-C	6.88	118.57	111.14
2	D	54	GLY	O-C-N	-6.88	113.75	122.70
2	D	133	LEU	O-C-N	-6.88	115.38	123.22
2	D	171	GLY	CA-C-N	-6.87	112.37	122.68
2	D	171	GLY	C-N-CA	-6.87	112.37	122.68
1	A	18	ARG	N-CA-C	-6.86	98.43	109.96
2	D	122	SER	CA-C-O	6.86	128.89	120.31
2	B	2	VAL	O-C-N	-6.86	114.00	122.57
2	B	50	TYR	CA-C-N	-6.86	114.25	123.10
2	B	50	TYR	C-N-CA	-6.86	114.25	123.10
1	A	121	SER	CA-C-O	6.86	129.78	122.03
2	B	155	PHE	N-CA-C	-6.85	99.27	108.11
2	B	58	ILE	CA-C-O	-6.85	112.32	121.02
1	C	162	SER	CA-C-O	6.84	128.72	121.33
1	A	70	ASP	CA-CB-CG	6.84	119.44	112.60
2	D	194	SER	CA-C-O	6.84	127.71	119.10
1	C	166	GLN	N-CA-C	6.83	120.39	110.42
2	D	174	THR	O-C-N	-6.83	115.05	123.04
1	C	114	THR	N-CA-CB	-6.82	99.44	110.69
2	D	42	GLU	CA-C-N	-6.81	109.24	123.20
2	D	42	GLU	C-N-CA	-6.81	109.24	123.20
2	D	99	GLY	O-C-N	-6.80	113.86	122.70
1	A	191	SER	CA-C-O	-6.79	113.34	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	GLY	N-CA-C	-6.79	106.61	114.69
1	C	115	VAL	N-CA-C	6.78	117.78	109.30
1	A	165	ASP	CA-CB-CG	-6.78	105.82	112.60
2	B	53	SER	O-C-N	-6.77	114.48	122.81
2	B	45	LEU	N-CA-C	-6.77	98.19	108.96
2	B	169	SER	N-CA-C	-6.77	96.38	110.80
1	A	84	ALA	CA-C-O	-6.76	114.08	121.31
2	B	214	ASP	O-C-N	-6.74	113.30	122.94
1	C	21	ILE	CB-CA-C	-6.74	101.68	110.84
2	D	87	ARG	O-C-N	-6.74	114.47	122.96
1	A	177	SER	N-CA-C	-6.73	99.25	109.95
1	A	108	ARG	N-CA-CB	-6.73	100.26	111.57
2	B	72	ARG	O-C-N	6.72	130.75	122.14
1	C	79	GLU	CB-CG-CD	6.72	124.02	112.60
2	D	63	THR	N-CA-CB	-6.72	99.14	110.49
1	A	125	LEU	N-CA-C	-6.72	103.05	111.11
2	B	194	SER	N-CA-C	6.72	125.11	110.80
1	A	205	ILE	CB-CG1-CD1	-6.71	99.71	113.80
1	C	130	ALA	O-C-N	-6.71	114.69	123.28
2	B	177	SER	N-CA-C	6.71	119.19	110.53
2	D	63	THR	CA-CB-OG1	-6.71	99.54	109.60
2	D	100	GLY	CA-C-N	-6.71	112.73	122.19
2	D	100	GLY	C-N-CA	-6.71	112.73	122.19
1	C	126	THR	N-CA-C	-6.70	103.90	111.07
1	C	143	ASP	CA-CB-CG	-6.70	105.90	112.60
2	D	11	LEU	O-C-N	-6.70	115.38	123.29
2	B	70	ILE	N-CA-C	6.69	116.25	106.55
2	D	16	GLY	O-C-N	-6.68	114.01	122.70
2	D	31	ASN	CB-CG-ND2	6.68	126.42	116.40
1	C	184	ASP	O-C-N	-6.67	114.37	122.11
1	C	192	TYR	N-CA-CB	-6.67	100.12	110.65
2	D	195	SER	N-CA-C	-6.66	103.27	111.33
1	A	134	CYS	O-C-N	-6.64	114.78	123.28
2	B	18	ARG	CA-C-O	6.63	128.33	121.23
2	D	167	ALA	CA-C-N	-6.63	108.65	121.58
2	D	167	ALA	C-N-CA	-6.63	108.65	121.58
2	B	180	GLN	CA-C-N	-6.63	113.24	124.31
2	B	180	GLN	C-N-CA	-6.63	113.24	124.31
2	D	112	TRP	CB-CG-CD1	-6.62	116.97	126.90
2	D	114	GLN	CA-C-N	-6.62	113.37	122.57
2	D	114	GLN	C-N-CA	-6.62	113.37	122.57
1	A	137	ASN	OD1-CG-ND2	-6.61	115.99	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	192	TYR	O-C-N	-6.61	114.63	123.23
2	D	74	ASN	CB-CG-ND2	6.61	126.32	116.40
2	D	170	SER	CA-C-N	-6.61	115.95	122.36
2	D	170	SER	C-N-CA	-6.61	115.95	122.36
2	B	50	TYR	O-C-N	-6.61	115.30	123.36
2	B	199	SER	N-CA-CB	-6.61	99.32	110.49
1	C	83	ILE	N-CA-CB	-6.61	103.32	110.53
2	D	9	GLY	O-C-N	6.61	129.26	122.79
1	A	43	SER	N-CA-CB	-6.60	102.44	112.28
1	C	65	TRP	CA-C-O	-6.60	114.36	121.36
2	B	127	ALA	N-CA-C	-6.60	100.49	110.39
1	A	51	THR	O-C-N	-6.58	113.83	122.59
1	C	60	SER	CA-C-N	-6.58	109.62	121.14
1	C	60	SER	C-N-CA	-6.58	109.62	121.14
2	D	82	GLN	N-CA-C	-6.58	97.69	108.41
2	B	74	ASN	CA-C-O	-6.58	111.15	120.16
2	B	174	THR	CA-C-N	-6.57	111.89	120.63
2	B	174	THR	C-N-CA	-6.57	111.89	120.63
1	C	183	LYS	CA-CB-CG	-6.57	100.97	114.10
1	C	161	ASN	CB-CA-C	-6.56	97.70	109.71
1	A	76	SER	N-CA-CB	6.56	119.58	110.07
2	D	18	ARG	CA-CB-CG	6.56	127.22	114.10
2	B	56	SER	N-CA-C	6.54	119.00	111.02
1	C	84	ALA	O-C-N	6.54	131.29	122.59
2	D	102	GLY	N-CA-C	-6.54	97.69	113.18
2	D	173	ARG	CA-CB-CG	6.54	127.17	114.10
2	B	196	THR	O-C-N	6.51	131.03	123.02
1	A	24	ARG	O-C-N	6.51	131.45	123.44
1	A	159	VAL	N-CA-CB	-6.51	100.49	111.23
2	D	198	PRO	N-CA-CB	6.51	109.76	102.60
1	A	28	ASP	CA-CB-CG	6.50	119.10	112.60
2	D	174	THR	CA-C-N	-6.50	110.28	121.97
2	D	174	THR	C-N-CA	-6.50	110.28	121.97
2	D	98	ARG	NE-CZ-NH2	6.50	125.05	119.20
1	C	182	THR	OG1-CB-CG2	6.48	122.27	109.30
2	D	36	TRP	CD2-CE2-CZ2	-6.48	115.92	122.40
1	C	157	ASN	CA-CB-CG	6.48	119.08	112.60
2	B	27	PHE	O-C-N	-6.48	113.97	122.59
1	C	69	THR	CA-C-N	-6.48	111.45	122.33
1	C	69	THR	C-N-CA	-6.48	111.45	122.33
2	D	45	LEU	N-CA-C	-6.48	100.38	110.42
2	B	20	LEU	CA-C-N	-6.47	112.45	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	LEU	C-N-CA	-6.47	112.45	122.87
2	D	110	ASP	O-C-N	-6.47	115.41	122.07
2	B	7	SER	O-C-N	-6.46	114.00	122.59
2	B	143	SER	CA-C-N	6.45	133.86	121.54
2	B	143	SER	C-N-CA	6.45	133.86	121.54
2	B	51	ILE	CB-CA-C	-6.45	101.01	110.81
1	C	49	TYR	N-CA-C	6.45	118.34	109.18
2	D	151	VAL	O-C-N	-6.43	114.45	122.88
1	A	111	ALA	O-C-N	-6.42	117.22	123.26
1	A	200	THR	N-CA-C	-6.42	105.74	112.93
1	A	98	PHE	CA-C-N	-6.41	113.77	119.92
1	A	98	PHE	C-N-CA	-6.41	113.77	119.92
2	B	163	TRP	CA-C-O	-6.41	116.12	119.77
1	A	156	GLN	CA-C-O	6.40	127.72	119.98
2	D	13	GLN	N-CA-C	-6.40	101.46	110.29
2	B	68	PHE	N-CA-C	6.39	119.94	110.48
2	D	197	TRP	CG-CD2-CE3	6.39	140.29	133.90
1	C	72	SER	N-CA-C	6.37	118.21	108.52
1	A	52	SER	N-CA-C	6.37	123.63	114.39
2	D	205	ASN	CB-CG-ND2	6.37	125.95	116.40
1	A	19	VAL	N-CA-C	-6.36	99.26	108.17
2	D	165	TYR	O-C-N	6.36	131.09	122.57
1	C	119	PRO	CA-C-N	6.36	126.38	119.89
1	C	119	PRO	C-N-CA	6.36	126.38	119.89
2	B	124	THR	N-CA-C	6.36	119.86	109.24
2	D	137	CYS	CA-CB-SG	6.36	129.01	114.40
1	C	43	SER	CA-C-N	-6.34	113.20	122.65
1	C	43	SER	C-N-CA	-6.34	113.20	122.65
2	D	151	VAL	CA-C-N	-6.34	111.46	122.37
2	D	151	VAL	C-N-CA	-6.34	111.46	122.37
2	D	178	VAL	N-CA-C	-6.33	98.50	107.75
1	A	186	TYR	CA-C-N	-6.33	111.16	120.28
1	A	186	TYR	C-N-CA	-6.33	111.16	120.28
2	B	4	LEU	CA-C-N	-6.33	114.85	123.14
2	B	4	LEU	C-N-CA	-6.33	114.85	123.14
1	A	203	SER	CA-CB-OG	-6.32	98.45	111.10
2	D	97	THR	N-CA-C	6.32	119.80	109.06
2	D	77	ASN	OD1-CG-ND2	-6.31	116.29	122.60
1	A	192	TYR	N-CA-C	-6.31	99.11	109.40
2	D	133	LEU	CA-C-N	-6.31	112.78	121.68
2	D	133	LEU	C-N-CA	-6.31	112.78	121.68
1	C	69	THR	CA-CB-OG1	-6.31	100.14	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	21	SER	CA-C-O	-6.31	113.74	121.06
1	A	94	LEU	CA-C-O	-6.30	113.56	120.87
2	D	70	ILE	CB-CG1-CD1	-6.30	100.58	113.80
2	D	144	SER	O-C-N	6.29	130.96	122.59
2	B	85	SER	N-CA-C	-6.29	102.80	111.28
1	A	85	THR	CA-CB-CG2	6.28	121.18	110.50
2	D	52	SER	CA-C-N	-6.28	111.27	120.75
2	D	52	SER	C-N-CA	-6.28	111.27	120.75
2	B	197	TRP	CB-CG-CD1	-6.27	117.49	126.90
2	B	66	GLY	CA-C-N	-6.26	110.50	122.53
2	B	66	GLY	C-N-CA	-6.26	110.50	122.53
1	C	5	THR	N-CA-C	6.26	118.62	108.41
2	B	164	ASN	CA-C-N	-6.26	111.36	122.07
2	B	164	ASN	C-N-CA	-6.26	111.36	122.07
1	A	10	SER	N-CA-CB	-6.26	99.80	111.13
2	B	159	VAL	CG1-CB-CG2	-6.26	97.03	110.80
2	D	188	SER	CA-C-O	-6.25	113.38	120.32
1	A	106	ILE	O-C-N	6.25	129.50	122.68
1	C	61	ARG	N-CA-C	-6.25	105.14	112.89
2	B	63	THR	CA-CB-OG1	-6.25	100.22	109.60
2	B	152	LYS	N-CA-C	6.25	118.60	108.41
1	C	44	LEU	CA-C-O	6.24	127.72	120.80
1	C	93	THR	N-CA-CB	-6.22	100.92	111.31
1	C	175	MET	CB-CG-SD	-6.22	94.03	112.70
2	D	188	SER	N-CA-C	-6.22	98.25	108.76
2	D	207	ALA	CB-CA-C	-6.22	100.19	110.14
1	C	25	ALA	O-C-N	-6.21	115.96	123.10
1	C	185	GLU	CB-CG-CD	6.21	123.16	112.60
1	C	193	THR	CA-C-O	-6.21	113.61	120.38
1	C	24	ARG	NE-CZ-NH1	-6.21	115.29	121.50
1	C	67	SER	CA-CB-OG	-6.21	98.69	111.10
2	B	59	ASN	OD1-CG-ND2	-6.21	116.39	122.60
2	D	136	GLY	N-CA-C	-6.20	105.06	113.37
1	A	61	ARG	N-CA-C	-6.20	105.20	112.89
1	A	136	LEU	O-C-N	-6.20	114.81	122.68
2	B	194	SER	O-C-N	-6.20	114.34	122.59
1	A	198	HIS	CA-CB-CG	-6.20	107.60	113.80
2	B	143	SER	CA-CB-OG	-6.19	98.71	111.10
2	B	136	GLY	O-C-N	-6.19	114.65	122.70
1	C	172	THR	CA-CB-OG1	-6.19	100.32	109.60
1	A	138	ASN	CA-CB-CG	-6.18	106.42	112.60
2	D	18	ARG	O-C-N	6.18	129.47	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	174	THR	O-C-N	-6.18	115.70	123.05
2	B	154	TYR	O-C-N	6.17	130.21	122.43
2	B	154	TYR	N-CA-C	-6.17	100.85	110.17
1	A	194	CYS	O-C-N	-6.16	115.98	123.19
2	B	171	GLY	O-C-N	-6.16	119.47	123.35
1	C	166	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	C	155	ARG	NE-CZ-NH2	6.16	124.74	119.20
1	C	163	TRP	CG-CD2-CE3	6.15	140.05	133.90
1	A	153	SER	N-CA-CB	6.14	122.24	111.55
2	B	28	THR	N-CA-CB	-6.14	100.11	110.49
1	A	109	ALA	N-CA-C	-6.13	100.57	110.32
1	A	194	CYS	N-CA-C	-6.13	99.70	109.76
2	D	27	PHE	CA-C-N	-6.13	114.26	122.42
2	D	27	PHE	C-N-CA	-6.13	114.26	122.42
1	C	120	PRO	CA-C-O	-6.13	114.57	121.43
2	B	118	LEU	CA-C-N	-6.13	114.47	122.37
2	B	118	LEU	C-N-CA	-6.13	114.47	122.37
2	B	31	ASN	OD1-CG-ND2	-6.12	116.47	122.60
1	A	115	VAL	N-CA-C	6.12	119.28	110.09
2	D	171	GLY	CA-C-O	-6.12	115.35	120.92
1	C	171	SER	CA-C-O	-6.12	114.44	121.54
2	D	180	GLN	CA-C-O	6.12	128.47	120.21
1	A	106	ILE	CA-C-N	6.12	129.98	120.75
1	A	106	ILE	C-N-CA	6.12	129.98	120.75
2	D	190	VAL	CA-C-O	6.12	127.44	120.90
2	D	90	ASP	CA-CB-CG	6.11	118.71	112.60
2	B	7	SER	CA-CB-OG	6.11	123.32	111.10
1	A	201	SER	N-CA-C	6.11	116.66	108.23
1	C	48	ILE	CA-C-O	-6.11	114.20	121.28
1	C	191	SER	CA-C-N	-6.11	114.15	123.07
1	C	191	SER	C-N-CA	-6.11	114.15	123.07
2	D	204	CYS	CA-C-O	6.11	127.04	120.38
1	A	72	SER	N-CA-C	6.09	119.17	108.75
2	B	162	LYS	N-CA-C	-6.09	99.78	109.59
2	D	134	VAL	CB-CA-C	6.08	115.29	109.33
2	D	180	GLN	CA-C-N	-6.08	113.99	122.74
2	D	180	GLN	C-N-CA	-6.08	113.99	122.74
2	B	78	THR	CA-CB-OG1	-6.08	100.49	109.60
1	C	189	HIS	CA-CB-CG	-6.08	107.72	113.80
2	D	128	PRO	CA-N-CD	-6.08	103.49	112.00
2	B	165	TYR	N-CA-CB	6.07	120.30	110.41
1	C	37	GLN	CA-C-O	-6.07	113.65	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	192	VAL	O-C-N	6.07	127.24	121.11
2	B	150	LEU	N-CA-C	-6.06	99.36	109.24
2	B	114	GLN	CG-CD-NE2	6.06	125.49	116.40
1	A	90	GLN	CA-C-O	6.05	126.94	120.46
2	B	179	LEU	O-C-N	-6.05	116.28	123.06
2	B	157	GLY	CA-C-N	6.05	126.06	119.89
2	B	157	GLY	C-N-CA	6.05	126.06	119.89
1	A	3	GLN	N-CA-C	-6.04	100.71	110.32
1	C	153	SER	CA-C-O	-6.04	114.49	121.26
2	B	173	ARG	CB-CA-C	-6.04	100.13	110.16
1	A	147	LYS	CA-C-O	-6.03	114.56	121.68
1	A	153	SER	CB-CA-C	-6.03	97.44	109.79
2	B	213	THR	CA-CB-OG1	-6.03	100.56	109.60
2	B	152	LYS	N-CA-CB	-6.02	101.25	110.65
1	A	118	PHE	CA-C-O	-6.02	111.91	120.16
2	B	127	ALA	CA-C-N	6.02	126.52	120.14
2	B	127	ALA	C-N-CA	6.02	126.52	120.14
2	B	188	SER	N-CA-C	-6.01	99.20	109.24
1	C	189	HIS	CB-CG-CD2	-6.01	123.39	131.20
2	B	165	TYR	O-C-N	6.01	129.79	123.06
2	B	63	THR	O-C-N	-6.00	115.14	122.34
2	B	202	VAL	CB-CA-C	-6.00	101.45	111.29
1	A	1	ASP	N-CA-C	-6.00	94.21	111.00
2	D	60	TYR	O-C-N	-6.00	115.36	123.10
2	B	195	SER	CA-C-O	6.00	127.11	120.82
2	D	206	VAL	O-C-N	-6.00	116.08	123.10
2	D	170	SER	CA-C-O	5.99	129.08	120.51
1	A	168	SER	CA-CB-OG	-5.99	99.12	111.10
2	B	99	GLY	O-C-N	-5.99	114.92	122.70
2	B	104	ARG	CB-CG-CD	-5.99	97.53	111.30
2	B	114	GLN	N-CA-C	5.99	119.85	112.54
2	D	98	ARG	CB-CG-CD	-5.99	97.53	111.30
2	B	119	ILE	CA-C-N	-5.98	115.25	122.90
2	B	119	ILE	C-N-CA	-5.98	115.25	122.90
2	B	59	ASN	CA-C-O	5.97	127.68	120.27
2	D	125	THR	CB-CA-C	-5.97	98.47	109.46
2	D	22	CYS	O-C-N	-5.97	115.39	123.14
2	B	125	THR	N-CA-C	5.96	123.50	110.80
1	C	127	SER	CA-C-N	-5.96	114.15	122.86
1	C	127	SER	C-N-CA	-5.96	114.15	122.86
1	A	176	SER	CA-C-O	-5.96	112.93	120.20
1	A	87	PHE	CA-CB-CG	5.96	119.75	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	ASN	N-CA-C	5.95	123.48	110.80
1	C	35	TRP	CA-C-O	-5.95	113.93	120.36
1	A	175	MET	O-C-N	-5.95	117.26	123.56
2	D	162	LYS	N-CA-C	-5.94	100.39	109.41
1	C	199	LYS	N-CA-C	5.93	123.44	110.80
1	A	114	THR	CA-CB-CG2	5.93	120.58	110.50
2	D	115	GLY	CA-C-N	-5.93	112.51	122.29
2	D	115	GLY	C-N-CA	-5.93	112.51	122.29
2	D	2	VAL	CA-CB-CG1	-5.93	100.33	110.40
1	A	119	PRO	CA-C-N	5.92	127.24	119.84
1	A	119	PRO	C-N-CA	5.92	127.24	119.84
2	B	2	VAL	N-CA-CB	-5.92	101.45	111.23
2	D	158	PRO	O-C-N	5.92	132.35	121.10
2	D	156	PRO	N-CD-CG	-5.92	96.70	103.80
2	D	186	LEU	N-CA-C	5.92	117.53	108.42
1	A	37	GLN	O-C-N	-5.91	116.42	123.27
2	D	32	PHE	CA-CB-CG	5.90	119.70	113.80
1	C	159	VAL	N-CA-C	5.90	116.66	107.28
2	B	35	HIS	CB-CG-ND1	5.90	131.54	122.70
2	B	173	ARG	N-CA-CB	5.89	119.84	110.65
2	B	107	TYR	CA-CB-CG	-5.88	103.32	113.90
2	B	203	ILE	CA-C-N	-5.88	113.89	122.65
2	B	203	ILE	C-N-CA	-5.88	113.89	122.65
1	C	139	PHE	CA-CB-CG	-5.88	107.92	113.80
2	D	114	GLN	CA-CB-CG	-5.88	102.35	114.10
2	B	45	LEU	O-C-N	-5.87	116.38	123.13
2	B	55	GLY	O-C-N	-5.86	115.08	122.70
1	A	20	ILE	CA-C-O	-5.86	114.04	121.48
2	B	13	GLN	CA-CB-CG	5.86	125.82	114.10
2	B	85	SER	O-C-N	-5.86	115.94	122.91
1	C	177	SER	CA-CB-OG	5.86	122.81	111.10
2	D	183	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	150	ILE	CA-C-O	5.85	126.92	120.48
2	D	35	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	A	50	TYR	N-CA-C	-5.84	104.07	110.91
1	A	7	ILE	CA-C-O	-5.84	113.82	120.65
1	C	127	SER	N-CA-C	-5.84	104.75	112.34
2	B	195	SER	CA-CB-OG	-5.83	99.45	111.10
1	C	138	ASN	CB-CA-C	-5.83	103.71	111.63
1	A	26	SER	CA-C-N	-5.83	111.02	120.87
1	A	26	SER	C-N-CA	-5.83	111.02	120.87
2	B	35	HIS	CA-C-O	-5.83	115.20	121.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	150	LEU	CA-CB-CG	5.83	136.69	116.30
1	C	130	ALA	N-CA-C	5.83	117.93	108.26
1	A	147	LYS	N-CA-C	5.82	118.71	109.81
1	C	118	PHE	O-C-N	-5.81	114.91	121.36
1	A	198	HIS	O-C-N	-5.81	114.87	122.59
1	C	90	GLN	N-CA-C	-5.80	101.03	110.20
2	B	57	SER	O-C-N	-5.79	115.83	123.13
1	A	59	PRO	N-CA-C	-5.79	100.28	111.69
2	B	54	GLY	N-CA-C	5.79	126.91	113.18
1	C	8	THR	CA-CB-OG1	5.79	118.29	109.60
2	B	152	LYS	CG-CD-CE	-5.78	98.00	111.30
2	D	84	THR	N-CA-CB	-5.78	102.77	111.56
2	D	5	VAL	O-C-N	-5.77	116.95	123.18
1	C	124	GLN	OE1-CD-NE2	-5.77	116.83	122.60
1	A	18	ARG	CA-CB-CG	5.76	125.62	114.10
2	D	213	THR	N-CA-C	-5.76	97.95	108.02
1	A	156	GLN	CG-CD-NE2	5.75	125.03	116.40
1	A	176	SER	N-CA-CB	5.75	120.14	110.77
1	A	92	LYS	O-C-N	-5.75	116.01	122.10
1	A	32	PHE	CA-C-N	-5.74	112.88	122.64
1	A	32	PHE	C-N-CA	-5.74	112.88	122.64
1	C	172	THR	CB-CA-C	5.74	120.80	109.66
1	A	29	ILE	CA-CB-CG1	-5.74	100.65	110.40
2	B	169	SER	O-C-N	5.73	130.21	122.59
2	D	149	CYS	CA-C-O	-5.73	114.41	121.11
2	B	183	PHE	CA-CB-CG	-5.72	108.08	113.80
1	C	105	GLU	CB-CA-C	-5.72	99.83	109.50
1	C	8	THR	CA-CB-CG2	-5.72	100.77	110.50
2	D	194	SER	CA-C-N	-5.72	112.54	120.38
2	D	194	SER	C-N-CA	-5.72	112.54	120.38
2	D	63	THR	N-CA-C	5.72	122.98	110.80
1	C	14	SER	N-CA-C	-5.72	101.50	110.36
1	A	201	SER	N-CA-CB	5.71	118.61	110.51
1	A	21	ILE	CB-CG1-CD1	-5.70	101.83	113.80
1	A	180	THR	N-CA-C	-5.70	99.44	108.73
1	C	187	GLU	N-CA-CB	-5.70	100.86	110.49
2	D	102	GLY	O-C-N	5.70	130.11	122.70
1	A	118	PHE	CA-CB-CG	5.70	119.50	113.80
2	B	211	SER	CA-CB-OG	5.69	122.48	111.10
1	A	175	MET	N-CA-CB	-5.69	102.19	111.24
2	D	135	PRO	O-C-N	5.69	129.92	122.86
1	A	78	LEU	CA-C-O	-5.68	115.54	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	ALA	N-CA-CB	-5.68	101.94	109.78
1	C	2	ILE	CA-C-N	-5.68	114.77	122.77
1	C	2	ILE	C-N-CA	-5.68	114.77	122.77
1	A	15	LEU	O-C-N	-5.66	114.92	122.74
2	B	214	ASP	CA-C-N	-5.66	111.97	121.94
2	B	214	ASP	C-N-CA	-5.66	111.97	121.94
1	A	15	LEU	N-CA-C	-5.66	101.14	109.18
1	A	153	SER	CA-C-O	5.66	128.06	121.44
1	C	159	VAL	CA-C-O	-5.66	114.26	120.48
1	A	71	TYR	O-C-N	5.64	129.68	123.25
1	C	137	ASN	CA-CB-CG	5.64	118.24	112.60
2	D	72	ARG	CA-C-N	-5.63	114.86	122.86
2	D	72	ARG	C-N-CA	-5.63	114.86	122.86
2	B	109	PHE	CA-C-N	5.63	128.87	120.31
2	B	109	PHE	C-N-CA	5.63	128.87	120.31
2	D	120	VAL	CB-CA-C	5.63	117.77	111.80
2	B	139	ASP	N-CA-C	5.63	122.79	110.80
1	A	155	ARG	CB-CG-CD	-5.63	98.36	111.30
2	D	128	PRO	CA-C-N	5.62	130.47	122.72
2	D	128	PRO	C-N-CA	5.62	130.47	122.72
2	D	173	ARG	NE-CZ-NH1	-5.62	115.88	121.50
2	B	151	VAL	O-C-N	-5.61	116.99	122.99
2	D	192	VAL	N-CA-C	-5.61	100.94	107.61
1	C	145	ASN	CB-CG-OD1	-5.60	109.60	120.80
1	A	198	HIS	CB-CG-CD2	-5.60	123.92	131.20
2	D	129	SER	N-CA-CB	5.60	119.56	110.43
1	C	105	GLU	CB-CG-CD	-5.60	103.09	112.60
1	A	44	LEU	N-CA-C	5.59	118.46	110.24
1	C	59	PRO	CA-C-O	-5.59	115.04	121.86
1	A	43	SER	CA-CB-OG	-5.59	99.93	111.10
1	A	8	THR	CB-CA-C	-5.58	99.31	110.42
2	B	150	LEU	CA-C-O	-5.57	114.36	120.43
1	C	170	ASP	CA-C-N	-5.57	114.11	122.07
1	C	170	ASP	C-N-CA	-5.57	114.11	122.07
2	B	106	LEU	CA-CB-CG	-5.56	96.85	116.30
1	C	40	PRO	CA-CB-CG	-5.56	93.94	104.50
2	B	66	GLY	O-C-N	-5.55	115.48	122.70
2	B	77	ASN	CA-CB-CG	5.55	118.15	112.60
2	D	115	GLY	CA-C-O	-5.55	117.83	122.33
1	A	104	LEU	CB-CA-C	5.55	120.33	109.35
2	B	103	THR	CA-C-O	5.55	126.58	120.31
1	C	49	TYR	CA-C-O	-5.55	115.06	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	120	VAL	O-C-N	-5.55	116.52	122.45
2	D	38	ARG	CD-NE-CZ	-5.54	116.65	124.40
2	D	206	VAL	CA-C-O	-5.53	114.61	120.53
2	D	151	VAL	N-CA-C	-5.53	99.18	107.37
2	D	55	GLY	N-CA-C	5.52	122.95	115.00
2	B	65	LYS	O-C-N	-5.52	116.58	123.04
2	B	178	VAL	O-C-N	-5.52	116.69	123.09
2	B	163	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	C	132	VAL	O-C-N	-5.51	115.70	122.97
1	A	69	THR	N-CA-CB	5.50	118.24	110.98
2	B	170	SER	O-C-N	-5.49	115.28	122.59
1	C	75	ILE	CB-CA-C	-5.49	102.11	110.95
1	C	115	VAL	N-CA-CB	-5.49	103.56	110.31
1	A	17	ASP	CA-CB-CG	-5.49	107.11	112.60
1	C	198	HIS	O-C-N	-5.49	116.66	123.36
2	D	135	PRO	CA-N-CD	-5.49	104.32	112.00
1	A	167	ASP	CA-C-O	5.49	126.94	120.69
2	D	206	VAL	CA-C-N	-5.49	115.04	122.77
2	D	206	VAL	C-N-CA	-5.49	115.04	122.77
2	B	43	LYS	CA-C-N	-5.48	112.99	123.29
2	B	43	LYS	C-N-CA	-5.48	112.99	123.29
2	B	3	GLN	CA-C-N	5.47	130.05	122.77
2	B	3	GLN	C-N-CA	5.47	130.05	122.77
2	B	78	THR	OG1-CB-CG2	5.47	120.25	109.30
2	D	64	VAL	O-C-N	-5.47	115.73	122.57
2	D	79	LEU	CA-C-O	-5.47	115.38	121.51
2	D	62	ASP	CA-C-O	5.47	126.56	120.82
1	A	130	ALA	CA-C-N	-5.46	115.01	122.93
1	A	130	ALA	C-N-CA	-5.46	115.01	122.93
1	A	188	ARG	CA-C-N	-5.46	111.93	122.09
1	A	188	ARG	C-N-CA	-5.46	111.93	122.09
1	A	182	THR	O-C-N	-5.46	116.36	122.75
1	C	92	LYS	CB-CG-CD	-5.46	98.75	111.30
1	A	8	THR	CA-CB-OG1	5.45	117.78	109.60
1	A	98	PHE	CA-C-O	5.45	126.24	120.36
1	C	67	SER	N-CA-C	5.45	116.81	108.42
2	B	138	SER	CA-CB-OG	5.45	121.99	111.10
2	D	217	LYS	N-CA-C	-5.45	95.75	111.00
2	B	35	HIS	ND1-CG-CD2	5.44	111.54	106.10
2	B	33	GLY	N-CA-C	-5.44	100.29	113.18
1	C	157	ASN	O-C-N	-5.43	116.86	123.27
2	D	140	THR	N-CA-CB	5.43	119.67	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	141	SER	N-CA-C	-5.43	105.39	112.23
1	C	85	THR	OG1-CB-CG2	-5.42	98.45	109.30
2	D	77	ASN	N-CA-CB	-5.42	101.33	110.49
2	D	145	VAL	CA-C-N	-5.42	115.42	123.11
2	D	145	VAL	C-N-CA	-5.42	115.42	123.11
2	B	74	ASN	CA-CB-CG	-5.42	107.18	112.60
2	D	104	ARG	N-CA-C	5.41	119.18	112.47
2	D	153	GLY	O-C-N	-5.41	115.67	122.70
2	D	196	THR	CA-CB-OG1	-5.41	101.48	109.60
1	C	57	GLY	O-C-N	-5.41	115.67	122.70
2	B	197	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	C	104	LEU	N-CA-CB	-5.41	102.62	110.84
1	A	102	THR	O-C-N	-5.41	116.04	122.63
2	B	83	MET	CA-CB-CG	5.41	124.91	114.10
1	C	128	GLY	O-C-N	-5.40	116.55	122.65
2	D	130	VAL	CB-CA-C	-5.40	104.42	111.81
1	A	93	THR	O-C-N	-5.39	117.27	123.42
1	C	97	THR	CA-C-O	5.39	126.19	120.36
2	D	147	LEU	O-C-N	-5.39	116.70	122.85
2	B	91	THR	N-CA-CB	-5.39	101.12	109.48
1	C	142	LYS	O-C-N	5.39	127.83	122.12
1	C	111	ALA	CA-C-O	5.39	126.79	120.43
2	B	170	SER	CA-C-O	5.38	128.20	120.51
1	C	63	SER	CA-CB-OG	5.37	121.84	111.10
1	C	78	LEU	CA-C-N	-5.37	110.04	121.32
1	C	78	LEU	C-N-CA	-5.37	110.04	121.32
1	C	163	TRP	CE2-CD2-CG	-5.37	100.76	107.20
2	B	27	PHE	CA-CB-CG	5.36	119.16	113.80
2	D	128	PRO	O-C-N	5.36	129.88	122.64
2	D	190	VAL	N-CA-C	5.36	115.43	108.35
1	C	79	GLU	CA-C-N	5.36	131.77	121.54
1	C	79	GLU	C-N-CA	5.36	131.77	121.54
2	D	212	LYS	N-CA-C	5.36	118.05	110.50
1	A	1	ASP	CA-C-O	-5.35	111.70	120.80
1	A	17	ASP	CA-C-O	-5.35	115.20	121.46
1	C	155	ARG	N-CA-C	-5.35	100.57	109.46
1	C	52	SER	CA-C-N	-5.34	113.98	121.72
1	C	52	SER	C-N-CA	-5.34	113.98	121.72
2	D	104	ARG	CG-CD-NE	5.34	123.74	112.00
2	D	161	VAL	CA-C-O	-5.34	114.82	120.48
2	D	161	VAL	CB-CA-C	-5.34	102.88	110.83
1	A	19	VAL	CA-C-N	-5.34	114.05	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	VAL	C-N-CA	-5.34	114.05	122.64
2	D	16	GLY	N-CA-C	5.34	125.83	113.18
2	D	193	PRO	N-CA-CB	-5.33	97.65	103.25
1	A	185	GLU	N-CA-C	-5.33	106.45	113.17
2	B	172	VAL	N-CA-CB	-5.33	103.20	110.56
1	C	29	ILE	CB-CG1-CD1	-5.33	102.61	113.80
1	A	102	THR	N-CA-C	5.33	117.90	107.57
2	B	63	THR	CA-C-N	-5.33	112.39	121.97
2	B	63	THR	C-N-CA	-5.33	112.39	121.97
2	B	134	VAL	O-C-N	5.33	127.17	121.10
2	D	130	VAL	CA-C-O	-5.32	114.64	120.97
1	A	197	THR	CA-CB-OG1	-5.32	101.62	109.60
1	A	8	THR	CA-CB-CG2	-5.31	101.47	110.50
1	C	43	SER	N-CA-C	5.31	122.12	110.80
1	A	34	ASN	N-CA-C	-5.31	100.65	108.99
2	B	97	THR	CA-C-N	-5.31	110.18	121.32
2	B	97	THR	C-N-CA	-5.31	110.18	121.32
1	C	56	SER	CA-C-N	-5.30	111.01	121.41
1	C	56	SER	C-N-CA	-5.30	111.01	121.41
1	A	108	ARG	CD-NE-CZ	-5.30	116.98	124.40
2	B	48	VAL	N-CA-C	5.30	119.20	113.43
2	D	153	GLY	CA-C-N	-5.30	113.47	123.27
2	D	153	GLY	C-N-CA	-5.30	113.47	123.27
2	B	18	ARG	CA-C-N	-5.30	115.34	123.07
2	B	18	ARG	C-N-CA	-5.30	115.34	123.07
1	A	175	MET	CB-CG-SD	-5.29	96.81	112.70
2	B	59	ASN	O-C-N	-5.29	117.42	123.40
1	C	161	ASN	CA-CB-CG	-5.29	107.31	112.60
2	B	138	SER	CA-C-O	5.29	128.07	120.51
2	B	81	LEU	O-C-N	-5.29	116.37	123.14
2	D	193	PRO	CB-CA-C	5.29	120.28	111.56
1	C	148	TRP	CG-CD1-NE1	-5.29	103.33	110.20
1	A	52	SER	CB-CA-C	-5.28	100.61	109.27
2	D	101	THR	N-CA-CB	-5.28	104.16	112.13
1	A	56	SER	N-CA-C	5.28	117.88	109.96
2	D	60	TYR	N-CA-C	5.27	118.31	110.14
2	B	30	SER	O-C-N	-5.27	115.58	122.59
2	D	156	PRO	CA-CB-CG	-5.27	93.98	104.00
2	D	28	THR	CA-CB-OG1	-5.27	101.69	109.60
1	C	31	ASN	CA-C-N	-5.27	112.78	122.31
1	C	31	ASN	C-N-CA	-5.27	112.78	122.31
2	D	70	ILE	O-C-N	-5.27	116.11	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	112	TRP	CE2-CD2-CG	-5.26	100.89	107.20
2	B	70	ILE	O-C-N	-5.26	116.52	122.36
2	D	185	SER	N-CA-C	-5.26	101.30	109.24
1	C	82	ASP	N-CA-C	-5.25	105.95	114.09
2	D	34	MET	O-C-N	-5.25	115.81	122.43
2	D	105	SER	O-C-N	-5.25	115.35	121.97
2	D	187	SER	CA-CB-OG	5.25	121.60	111.10
2	B	70	ILE	CG1-CB-CG2	-5.25	94.96	110.70
1	A	44	LEU	CA-CB-CG	-5.24	97.95	116.30
1	A	24	ARG	CA-C-N	5.24	128.31	120.87
1	A	24	ARG	C-N-CA	5.24	128.31	120.87
1	A	31	ASN	CA-CB-CG	-5.24	107.36	112.60
2	D	175	VAL	CA-CB-CG2	-5.24	101.49	110.40
2	B	51	ILE	N-CA-CB	5.24	120.89	111.21
1	C	123	GLU	N-CA-C	5.24	117.07	111.36
2	D	68	PHE	CA-C-O	-5.24	115.22	121.56
2	D	78	THR	N-CA-CB	-5.23	103.20	111.05
2	D	178	VAL	CA-CB-CG2	-5.23	101.50	110.40
1	A	87	PHE	CA-C-N	-5.23	113.66	122.29
1	A	87	PHE	C-N-CA	-5.23	113.66	122.29
1	A	161	ASN	OD1-CG-ND2	-5.23	117.37	122.60
1	A	198	HIS	CB-CG-ND1	5.22	130.53	122.70
2	B	172	VAL	CB-CA-C	5.22	118.36	111.21
2	D	178	VAL	CA-CB-CG1	5.22	119.28	110.40
2	D	10	GLY	N-CA-C	5.22	117.66	110.56
2	D	197	TRP	CB-CG-CD1	-5.22	119.07	126.90
2	B	93	ILE	CA-CB-CG1	5.22	119.27	110.40
2	D	31	ASN	CA-C-N	-5.22	113.40	122.37
2	D	31	ASN	C-N-CA	-5.22	113.40	122.37
1	C	126	THR	O-C-N	-5.21	116.70	122.07
1	C	14	SER	CA-C-O	-5.21	115.51	121.82
2	B	197	TRP	CB-CA-C	-5.21	99.91	110.17
1	C	82	ASP	CA-CB-CG	5.21	117.81	112.60
2	B	40	ALA	N-CA-C	-5.21	103.62	110.39
2	B	119	ILE	N-CA-C	5.21	116.08	108.58
1	C	197	THR	CA-C-O	-5.20	115.19	120.71
2	D	120	VAL	CA-CB-CG2	-5.20	101.55	110.40
1	A	100	GLY	CA-C-O	-5.20	111.52	120.57
2	B	187	SER	N-CA-C	5.20	117.90	109.06
1	C	77	ASN	N-CA-C	-5.20	96.60	107.37
2	D	65	LYS	CA-CB-CG	5.20	124.50	114.10
2	B	57	SER	CA-CB-OG	5.19	121.48	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ALA	CA-C-O	5.19	126.56	120.80
2	B	145	VAL	CA-C-O	5.18	125.86	120.36
1	C	171	SER	CB-CA-C	-5.17	104.24	111.80
1	A	85	THR	O-C-N	-5.17	116.43	123.10
2	B	208	HIS	CA-C-N	5.17	126.30	119.84
2	B	208	HIS	C-N-CA	5.17	126.30	119.84
2	B	173	ARG	N-CA-C	-5.17	99.99	108.41
1	C	78	LEU	N-CA-C	5.17	121.81	110.80
2	D	59	ASN	N-CA-C	-5.17	99.69	108.26
1	A	46	LEU	O-C-N	-5.16	116.96	122.85
1	A	98	PHE	N-CA-CB	-5.16	102.00	110.68
2	D	173	ARG	CD-NE-CZ	-5.16	117.17	124.40
1	A	24	ARG	CA-C-O	5.16	127.17	120.21
2	B	67	ARG	N-CA-C	-5.16	106.67	113.12
2	B	118	LEU	N-CA-C	5.16	115.84	107.23
1	C	70	ASP	CB-CA-C	5.16	118.68	109.65
1	A	183	LYS	CA-C-N	-5.16	113.31	120.38
1	A	183	LYS	C-N-CA	-5.16	113.31	120.38
1	C	159	VAL	O-C-N	-5.15	117.48	122.99
1	A	205	ILE	CA-C-O	-5.15	114.65	120.67
2	B	155	PHE	CA-C-O	-5.15	114.77	119.76
1	C	149	LYS	CA-CB-CG	5.15	124.39	114.10
1	C	183	LYS	O-C-N	5.15	128.07	122.20
2	D	163	TRP	CE2-CD2-CG	-5.14	101.03	107.20
2	D	101	THR	CA-CB-CG2	5.14	119.24	110.50
1	C	30	GLY	CA-C-O	5.14	129.51	120.57
1	A	202	THR	CB-CA-C	5.14	116.11	109.28
2	D	109	PHE	CA-C-O	5.14	125.86	120.36
1	A	111	ALA	N-CA-C	5.13	116.00	107.73
2	D	162	LYS	CB-CG-CD	-5.13	99.49	111.30
2	D	197	TRP	CG-CD1-NE1	-5.13	103.53	110.20
1	A	104	LEU	N-CA-CB	-5.13	101.71	111.00
1	A	104	LEU	N-CA-C	-5.13	100.67	109.24
1	A	2	ILE	CA-CB-CG2	5.13	119.22	110.50
1	C	130	ALA	CA-C-O	5.13	126.46	120.20
2	D	72	ARG	CG-CD-NE	-5.12	100.72	112.00
1	A	195	GLU	CB-CG-CD	-5.11	103.91	112.60
2	B	77	ASN	N-CA-C	5.11	118.64	111.74
2	B	190	VAL	N-CA-C	-5.11	100.52	108.44
1	C	113	PRO	O-C-N	-5.11	115.75	122.64
2	D	17	SER	N-CA-C	5.11	115.08	107.88
2	D	164	ASN	O-C-N	5.11	129.86	123.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	CA-C-O	-5.10	114.02	120.55
1	C	56	SER	N-CA-CB	-5.10	102.96	110.26
1	A	147	LYS	CB-CG-CD	-5.10	99.57	111.30
2	B	134	VAL	CA-CB-CG2	-5.10	101.73	110.40
1	C	93	THR	OG1-CB-CG2	5.10	119.49	109.30
2	D	138	SER	N-CA-CB	-5.10	101.88	110.49
2	D	96	CYS	O-C-N	-5.09	116.71	123.13
1	A	192	TYR	CA-CB-CG	-5.09	104.73	113.90
2	B	13	GLN	N-CA-CB	-5.09	102.96	110.14
2	B	129	SER	CA-C-O	-5.09	115.35	120.84
2	D	38	ARG	NE-CZ-NH2	-5.09	114.62	119.20
2	D	197	TRP	CE2-CD2-CG	-5.08	101.10	107.20
1	C	18	ARG	NE-CZ-NH1	-5.08	116.42	121.50
1	C	93	THR	O-C-N	-5.08	116.03	122.78
1	C	113	PRO	N-CA-CB	-5.08	97.92	103.25
2	B	96	CYS	O-C-N	-5.08	116.70	122.89
1	C	64	GLY	CA-C-O	-5.08	116.53	121.76
1	C	131	SER	N-CA-CB	-5.07	102.16	110.68
2	D	172	VAL	CB-CA-C	5.07	119.11	110.95
1	C	107	LYS	CG-CD-CE	-5.07	99.65	111.30
1	A	130	ALA	CB-CA-C	-5.06	104.79	111.42
2	B	31	ASN	CB-CG-ND2	5.06	123.99	116.40
1	C	109	ALA	CA-C-O	-5.06	114.99	120.81
2	D	9	GLY	CA-C-O	-5.06	116.56	121.93
1	C	14	SER	CA-CB-OG	5.06	121.22	111.10
1	A	46	LEU	CA-CB-CG	5.06	134.00	116.30
2	D	49	ALA	N-CA-C	5.06	116.74	108.55
2	D	106	LEU	CA-C-O	-5.06	116.05	121.56
2	B	170	SER	CA-CB-OG	5.05	121.21	111.10
2	D	11	LEU	CA-C-N	-5.05	114.65	122.69
2	D	11	LEU	C-N-CA	-5.05	114.65	122.69
1	A	51	THR	CA-CB-CG2	5.05	119.09	110.50
1	C	81	GLU	CB-CG-CD	-5.05	104.01	112.60
1	C	3	GLN	N-CA-CB	-5.05	102.84	110.77
2	D	129	SER	CA-C-N	5.05	129.21	122.95
2	D	129	SER	C-N-CA	5.05	129.21	122.95
1	A	199	LYS	N-CA-CB	-5.05	101.96	110.49
1	A	186	TYR	N-CA-CB	5.04	117.59	110.13
1	A	37	GLN	CA-CB-CG	-5.04	104.02	114.10
1	C	192	TYR	CB-CG-CD1	-5.04	113.24	120.80
2	D	87	ARG	CA-CB-CG	-5.04	104.02	114.10
2	B	132	PRO	O-C-N	-5.04	117.06	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	18	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	199	LYS	O-C-N	-5.03	115.90	122.59
2	B	57	SER	N-CA-C	5.03	116.89	107.99
1	C	163	TRP	CB-CG-CD1	-5.02	119.36	126.90
2	B	82	GLN	CA-C-N	-5.02	114.93	122.81
2	B	82	GLN	C-N-CA	-5.02	114.93	122.81
1	C	46	LEU	CA-C-N	-5.02	113.17	122.60
1	C	46	LEU	C-N-CA	-5.02	113.17	122.60
1	C	137	ASN	N-CA-C	5.02	117.14	109.07
1	C	87	PHE	O-C-N	5.01	129.81	122.94
2	B	134	VAL	CA-C-N	5.01	126.11	119.84
2	B	134	VAL	C-N-CA	5.01	126.11	119.84
2	B	176	SER	N-CA-CB	-5.01	103.10	110.26
2	D	160	THR	N-CA-C	-5.00	100.89	109.24

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	TYR	Sidechain
1	A	94	LEU	Peptide
2	B	107	TYR	Sidechain
2	B	154	TYR	Sidechain
2	B	157	GLY	Peptide
2	B	195	SER	Mainchain
2	B	208	HIS	Peptide
1	C	140	TYR	Peptide
1	C	167	ASP	Mainchain
1	C	203	SER	Peptide
1	C	96	TYR	Sidechain
2	D	102	GLY	Mainchain
2	D	107	TYR	Sidechain
2	D	123	ALA	Mainchain
2	D	169	SER	Mainchain
2	D	184	TYR	Sidechain
2	D	208	HIS	Peptide
2	D	40	ALA	Peptide
2	D	94	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1605	0	1540	384	0
1	C	1605	0	1538	382	2
2	B	1624	0	1583	372	2
2	D	1624	0	1586	366	0
All	All	6458	0	6247	1437	2

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 113.

All (1437) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:PRO:CB	1:A:125:LEU:HD21	1.39	1.51
1:C:78:LEU:HD12	1:C:78:LEU:C	1.30	1.42
2:B:133:LEU:CD1	2:B:189:LEU:HD11	1.48	1.41
2:D:163:TRP:CD1	2:D:172:VAL:HG21	1.63	1.34
1:C:78:LEU:C	1:C:78:LEU:CD1	1.99	1.32
2:D:11:LEU:CD2	2:D:119:ILE:CG2	2.09	1.31
2:B:158:PRO:O	2:B:209:PRO:HG2	1.22	1.29
2:D:38:ARG:NE	2:D:46:GLU:OE2	1.65	1.29
2:D:11:LEU:HD23	2:D:119:ILE:CG2	1.63	1.27
2:D:75:PRO:HG2	2:D:77:ASN:OD1	1.09	1.26
1:A:205:ILE:C	1:A:205:ILE:HD13	1.44	1.25
1:A:79:GLU:HB3	1:A:81:GLU:OE2	1.31	1.25
2:B:133:LEU:HB2	2:B:148:GLY:CA	1.66	1.24
2:B:204:CYS:N	2:B:216:ILE:O	1.67	1.24
1:A:205:ILE:HD13	1:A:206:VAL:N	1.51	1.24
2:B:106:LEU:HD23	2:B:108:TYR:CD1	1.72	1.23
2:D:147:LEU:HD12	2:D:217:LYS:NZ	1.51	1.22
2:B:133:LEU:HD12	2:B:189:LEU:CD1	1.69	1.21
2:B:166:GLY:O	2:B:168:LEU:CD1	1.88	1.21
1:A:12:SER:OG	1:A:107:LYS:HG3	1.33	1.20
2:D:163:TRP:CD1	2:D:172:VAL:CG2	2.23	1.20
2:B:13:GLN:HA	2:B:121:SER:O	1.39	1.19
2:B:195:SER:O	2:B:199:SER:OG	1.58	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:GLN:HG2	1:C:129:GLY:O	1.39	1.18
1:C:15:LEU:HD21	1:C:80:GLU:OE1	1.44	1.18
1:C:92:LYS:HG3	1:C:93:THR:OG1	1.42	1.18
1:C:78:LEU:HD12	1:C:78:LEU:O	1.40	1.17
1:A:18:ARG:HA	1:A:75:ILE:O	1.43	1.17
2:B:152:LYS:HG2	2:B:185:SER:OG	1.43	1.17
2:B:167:ALA:HA	2:B:170:SER:OG	1.40	1.16
1:A:56:SER:HB2	2:D:212:LYS:HD2	1.18	1.16
1:A:150:ILE:HG21	1:A:189:HIS:CD2	1.79	1.16
1:A:147:LYS:NZ	1:A:154:GLU:OE2	1.78	1.16
2:B:133:LEU:CD1	2:B:189:LEU:CD1	2.23	1.16
1:A:120:PRO:HB3	1:A:125:LEU:CD2	1.77	1.15
2:D:60:TYR:OH	2:D:69:THR:HA	1.47	1.14
2:D:34:MET:CE	2:D:34:MET:HA	1.77	1.14
2:B:41:PRO:O	2:B:43:LYS:N	1.79	1.13
1:C:108:ARG:HH21	1:C:108:ARG:HG3	1.06	1.13
1:A:17:ASP:O	1:A:78:LEU:N	1.81	1.12
2:B:88:SER:O	2:B:91:THR:HG22	1.45	1.12
1:C:7:ILE:HD13	1:C:7:ILE:O	1.45	1.12
2:D:216:ILE:HG12	2:D:217:LYS:N	1.57	1.12
2:D:75:PRO:CG	2:D:77:ASN:OD1	1.96	1.12
1:A:205:ILE:C	1:A:205:ILE:CD1	2.23	1.12
2:B:168:LEU:HD13	2:B:168:LEU:N	1.65	1.12
2:D:137:CYS:O	2:D:139:ASP:OD2	1.65	1.11
2:D:168:LEU:O	2:D:193:PRO:HG2	1.49	1.11
1:A:106:ILE:HD13	1:A:106:ILE:N	1.63	1.11
2:D:34:MET:HE1	2:D:98:ARG:HA	1.33	1.11
2:B:133:LEU:HD12	2:B:148:GLY:HA3	1.25	1.11
1:C:106:ILE:HG21	1:C:171:SER:OG	1.51	1.10
2:D:34:MET:HA	2:D:34:MET:HE2	1.20	1.10
1:C:20:ILE:HG13	1:C:74:THR:OG1	1.46	1.10
2:D:19:LYS:CD	2:D:82:GLN:OE1	1.99	1.10
2:B:133:LEU:HD13	2:B:189:LEU:HD11	1.21	1.10
2:D:11:LEU:CD2	2:D:119:ILE:HG22	1.72	1.09
1:C:144:ILE:HG23	1:C:144:ILE:O	1.49	1.09
2:B:103:THR:HG22	2:B:104:ARG:HG3	1.11	1.09
2:B:166:GLY:O	2:B:168:LEU:HD11	1.49	1.09
1:C:166:GLN:HG2	1:C:171:SER:HA	1.24	1.09
1:C:38:GLN:HB3	1:C:85:THR:HG22	1.11	1.08
1:C:49:TYR:CD2	1:C:53:ARG:HB2	1.87	1.08
1:C:86:PHE:HE2	1:C:104:LEU:HD13	1.16	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:74:ASN:O	2:D:77:ASN:HB2	1.54	1.08
2:D:179:LEU:C	2:D:179:LEU:HD23	1.79	1.08
2:B:60:TYR:OH	2:B:69:THR:HA	1.54	1.07
1:A:83:ILE:HD12	1:A:106:ILE:HD11	1.36	1.07
2:B:60:TYR:CD2	2:B:65:LYS:HD3	1.89	1.07
2:B:131:TYR:HD2	2:B:150:LEU:HD12	1.11	1.07
2:B:106:LEU:HD23	2:B:108:TYR:HD1	0.94	1.07
1:A:130:ALA:N	1:A:181:LEU:O	1.87	1.06
2:B:217:LYS:HE2	2:B:217:LYS:HA	1.37	1.05
1:A:130:ALA:O	1:A:181:LEU:N	1.89	1.05
2:D:38:ARG:CZ	2:D:46:GLU:OE2	2.02	1.05
2:D:147:LEU:HD12	2:D:217:LYS:HZ2	0.92	1.05
1:C:4:MET:CE	1:C:90:GLN:HG3	1.86	1.05
1:C:124:GLN:O	1:C:127:SER:HB2	1.55	1.05
2:B:203:ILE:HA	2:B:217:LYS:HB2	1.35	1.05
1:C:144:ILE:O	1:C:144:ILE:CG2	1.99	1.05
2:B:68:PHE:CE2	2:B:83:MET:HG2	1.91	1.04
1:C:12:SER:OG	1:C:105:GLU:HB3	1.54	1.04
2:D:19:LYS:HD3	2:D:82:GLN:OE1	1.57	1.04
2:D:88:SER:HA	2:D:120:VAL:CG1	1.87	1.04
2:D:11:LEU:HD23	2:D:119:ILE:CB	1.86	1.04
2:D:99:GLY:O	2:D:110:ASP:HB2	1.56	1.04
2:B:17:SER:CB	2:B:83:MET:O	2.05	1.04
2:D:169:SER:HB3	2:D:193:PRO:HD3	1.39	1.04
2:D:131:TYR:N	2:D:150:LEU:O	1.90	1.03
1:A:155:ARG:HG2	1:A:179:LEU:HD21	1.41	1.03
1:A:120:PRO:CB	1:A:125:LEU:CD2	2.34	1.03
1:A:15:LEU:HD21	1:A:80:GLU:HB3	1.40	1.02
2:B:140:THR:HG22	2:B:141:SER:N	1.67	1.02
1:C:15:LEU:CD2	1:C:80:GLU:OE1	2.07	1.02
1:C:108:ARG:HG2	1:C:140:TYR:CD1	1.94	1.02
2:D:11:LEU:HD23	2:D:119:ILE:HB	1.42	1.02
1:C:4:MET:HE1	1:C:90:GLN:CG	1.88	1.02
2:D:10:GLY:HA3	2:D:18:ARG:HH12	1.24	1.02
2:D:163:TRP:NE1	2:D:188:SER:OG	1.91	1.02
1:A:105:GLU:O	1:A:105:GLU:HG3	1.60	1.02
1:A:120:PRO:HB3	1:A:125:LEU:HD21	1.02	1.02
1:A:108:ARG:CD	1:A:171:SER:HB2	1.90	1.01
2:B:140:THR:OG1	2:B:145:VAL:HA	1.61	1.01
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.42	1.01
1:A:80:GLU:HG2	1:A:81:GLU:OE1	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:SER:HA	2:B:193:PRO:HA	1.03	1.01
1:A:12:SER:HA	1:A:105:GLU:O	1.59	1.00
1:C:166:GLN:HE21	1:C:171:SER:HB3	1.25	1.00
1:C:160:LEU:HD22	2:D:178:VAL:HG21	1.42	1.00
2:D:11:LEU:HD21	2:D:119:ILE:HG21	1.40	1.00
1:A:24:ARG:HG3	1:A:70:ASP:OD2	1.59	1.00
1:C:133:VAL:HG21	2:D:133:LEU:HD21	1.38	0.99
1:A:108:ARG:HD2	1:A:171:SER:HB2	1.00	0.99
2:B:131:TYR:CD2	2:B:150:LEU:HD12	1.98	0.99
2:D:2:VAL:HG12	2:D:2:VAL:O	1.60	0.99
1:A:148:TRP:O	1:A:155:ARG:N	1.94	0.99
1:A:8:THR:HG21	1:A:11:LEU:HD13	1.42	0.98
2:B:131:TYR:HD2	2:B:150:LEU:CD1	1.76	0.98
1:C:21:ILE:HB	1:C:73:LEU:HB3	1.44	0.98
1:A:33:LEU:HD13	1:A:71:TYR:CG	1.97	0.98
1:A:19:VAL:CG2	1:A:78:LEU:HD12	1.92	0.98
2:B:144:SER:CA	2:B:193:PRO:HA	1.93	0.98
1:A:12:SER:OG	1:A:107:LYS:CG	2.12	0.98
1:A:122:SER:O	1:A:123:GLU:C	2.03	0.98
2:B:133:LEU:HB2	2:B:148:GLY:HA3	1.46	0.98
2:B:171:GLY:O	2:B:190:VAL:HA	1.62	0.98
2:B:133:LEU:HD12	2:B:189:LEU:HD13	1.43	0.97
1:C:2:ILE:O	1:C:3:GLN:HG3	1.64	0.97
2:B:158:PRO:O	2:B:209:PRO:CG	2.11	0.97
1:A:18:ARG:HH21	1:A:74:THR:HG21	1.27	0.97
1:C:49:TYR:N	1:C:53:ARG:O	1.97	0.97
2:D:73:ASP:O	2:D:77:ASN:HB3	1.63	0.97
2:D:125:THR:HG22	2:D:126:THR:N	1.75	0.97
1:A:136:LEU:HD13	1:A:144:ILE:HD12	1.47	0.97
2:D:216:ILE:CG1	2:D:217:LYS:H	1.77	0.97
2:D:11:LEU:CD2	2:D:119:ILE:HG21	1.86	0.96
2:D:104:ARG:O	2:D:105:SER:CB	2.10	0.96
1:A:4:MET:HE2	1:A:4:MET:HA	1.44	0.96
2:B:168:LEU:CD1	2:B:168:LEU:N	2.29	0.96
2:B:154:TYR:OH	2:B:186:LEU:HD23	1.65	0.96
1:A:6:GLN:OE1	1:A:101:GLY:N	1.96	0.96
1:A:13:VAL:CG2	1:A:78:LEU:HD13	1.96	0.96
1:A:108:ARG:HD2	1:A:171:SER:CB	1.95	0.96
2:D:216:ILE:HG12	2:D:217:LYS:H	1.19	0.96
2:D:10:GLY:HA3	2:D:18:ARG:NH1	1.80	0.96
1:A:135:PHE:CE2	1:A:174:SER:HB3	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:LEU:CD1	2:D:217:LYS:NZ	2.28	0.95
2:B:121:SER:OG	2:B:122:SER:N	1.97	0.95
1:C:196:ALA:HB3	1:C:205:ILE:CG2	1.96	0.95
2:B:130:VAL:HG22	2:B:206:VAL:HG21	1.47	0.95
2:D:163:TRP:HD1	2:D:172:VAL:HG21	1.04	0.95
1:C:50:TYR:O	1:C:52:SER:N	1.99	0.95
2:D:11:LEU:HD21	2:D:119:ILE:CG2	1.88	0.95
1:A:198:HIS:O	1:A:200:THR:N	2.00	0.94
1:C:108:ARG:NH2	1:C:109:ALA:O	2.00	0.94
1:A:41:ASP:OD1	1:A:41:ASP:N	1.96	0.94
2:B:6:GLU:CB	2:B:116:ALA:HB2	1.98	0.94
1:A:149:LYS:HA	1:A:153:SER:O	1.66	0.94
1:C:108:ARG:HG3	1:C:109:ALA:N	1.81	0.94
1:A:27:GLN:O	1:A:29:ILE:HD13	1.65	0.94
1:C:23:CYS:HB2	1:C:35:TRP:HH2	1.32	0.94
1:C:86:PHE:CE2	1:C:104:LEU:HD13	2.02	0.94
1:C:4:MET:HE1	1:C:90:GLN:HG3	1.43	0.94
2:D:27:PHE:CD2	2:D:32:PHE:HE1	1.84	0.94
2:D:216:ILE:O	2:D:217:LYS:HB2	1.68	0.94
1:A:12:SER:HB3	1:A:107:LYS:NZ	1.82	0.94
2:B:156:PRO:O	2:B:208:HIS:HE1	1.48	0.94
1:A:135:PHE:HE2	1:A:174:SER:HB3	1.32	0.93
2:D:133:LEU:HD12	2:D:148:GLY:HA3	1.50	0.93
1:A:51:THR:OG1	1:A:71:TYR:HE2	1.51	0.93
2:B:19:LYS:HA	2:B:82:GLN:HA	1.51	0.93
1:A:29:ILE:HG23	1:A:32:PHE:HB2	1.50	0.93
1:C:91:GLY:O	2:D:107:TYR:N	2.00	0.93
1:C:150:ILE:O	1:C:152:GLY:N	2.01	0.93
2:B:125:THR:HG22	2:B:125:THR:O	1.68	0.92
2:D:216:ILE:CG1	2:D:217:LYS:N	2.25	0.92
1:A:12:SER:CB	1:A:107:LYS:HG3	1.97	0.92
1:A:135:PHE:CE1	2:B:189:LEU:HD23	2.04	0.92
2:B:133:LEU:CD1	2:B:148:GLY:HA3	1.98	0.92
2:D:19:LYS:HD2	2:D:82:GLN:OE1	1.66	0.92
1:C:108:ARG:HG3	1:C:108:ARG:NH2	1.79	0.91
2:D:67:ARG:HD2	2:D:85:SER:O	1.70	0.91
2:D:71:SER:O	2:D:79:LEU:HD12	1.70	0.91
2:B:144:SER:HA	2:B:193:PRO:CA	1.98	0.90
2:D:67:ARG:O	2:D:84:THR:HG22	1.70	0.90
2:B:103:THR:HG22	2:B:104:ARG:CG	2.00	0.90
2:B:133:LEU:HB2	2:B:148:GLY:N	1.86	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HD13	1:C:90:GLN:NE2	1.86	0.90
1:C:61:ARG:NH2	1:C:82:ASP:OD1	2.05	0.90
1:A:12:SER:OG	1:A:140:TYR:OH	1.90	0.90
2:B:87:ARG:NH1	2:B:89:GLU:HB2	1.86	0.90
2:B:100:GLY:O	2:B:101:THR:HB	1.70	0.90
1:C:127:SER:OG	2:D:131:TYR:OH	1.60	0.90
2:B:98:ARG:N	2:B:111:TYR:O	2.05	0.89
2:B:140:THR:CG2	2:B:141:SER:N	2.27	0.89
2:D:1:ASP:O	2:D:2:VAL:HB	1.72	0.89
1:A:31:ASN:HA	1:A:71:TYR:OH	1.72	0.89
2:B:6:GLU:HB3	2:B:116:ALA:HB2	1.52	0.89
1:C:108:ARG:NH2	1:C:109:ALA:HB3	1.86	0.89
2:B:101:THR:CG2	2:B:101:THR:O	2.21	0.89
1:C:108:ARG:CG	1:C:109:ALA:N	2.27	0.89
2:B:104:ARG:O	2:B:106:LEU:N	2.05	0.89
2:B:204:CYS:SG	2:B:216:ILE:HG22	2.12	0.89
2:D:163:TRP:HE1	2:D:188:SER:HG	1.17	0.89
2:D:104:ARG:O	2:D:105:SER:HB2	1.72	0.89
2:B:110:ASP:OD2	2:B:111:TYR:CE2	2.26	0.88
1:C:56:SER:O	1:C:58:VAL:N	2.06	0.88
2:D:6:GLU:OE2	2:D:6:GLU:N	2.04	0.88
1:C:80:GLU:O	1:C:83:ILE:HG22	1.73	0.88
1:C:12:SER:OG	1:C:105:GLU:CB	2.21	0.88
2:D:217:LYS:HE2	2:D:217:LYS:O	1.74	0.88
1:C:190:ASN:N	1:C:190:ASN:HD22	1.69	0.87
2:B:133:LEU:HB2	2:B:148:GLY:C	1.99	0.87
1:A:19:VAL:CG2	1:A:78:LEU:CD1	2.53	0.87
1:A:31:ASN:HD21	1:A:67:SER:HA	1.40	0.87
2:B:106:LEU:CD2	2:B:108:TYR:HD1	1.85	0.87
1:C:78:LEU:HD12	1:C:79:GLU:N	1.88	0.87
2:B:97:THR:HG21	2:B:109:PHE:HB3	1.57	0.87
1:C:55:GLN:HG3	1:C:56:SER:N	1.90	0.87
2:B:67:ARG:HG2	2:B:67:ARG:HH21	1.38	0.86
2:B:8:GLY:O	2:B:18:ARG:NH1	2.08	0.86
1:C:4:MET:HE3	1:C:90:GLN:H	1.38	0.86
1:C:23:CYS:HB2	1:C:35:TRP:CH2	2.09	0.86
1:A:120:PRO:HB2	1:A:125:LEU:HD21	1.54	0.86
1:A:162:SER:HB2	2:B:175:VAL:CG1	2.05	0.86
2:B:87:ARG:HB3	2:B:89:GLU:OE1	1.76	0.86
1:C:49:TYR:O	1:C:53:ARG:N	2.09	0.86
1:C:169:LYS:O	1:C:169:LYS:HG2	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:PRO:HD2	2:D:128:PRO:O	1.75	0.86
2:D:196:THR:OG1	2:D:197:TRP:N	2.06	0.86
2:B:87:ARG:NH1	2:B:89:GLU:CB	2.39	0.85
2:B:167:ALA:CA	2:B:170:SER:OG	2.23	0.85
1:A:131:SER:OG	1:A:180:THR:HG23	1.76	0.85
1:A:189:HIS:HB2	1:A:192:TYR:OH	1.74	0.85
2:D:19:LYS:HA	2:D:82:GLN:HA	1.58	0.85
1:A:65:TRP:CD1	1:A:65:TRP:N	2.43	0.85
1:A:185:GLU:HA	1:A:188:ARG:HG3	1.57	0.85
2:D:34:MET:CE	2:D:98:ARG:HA	2.05	0.85
1:A:8:THR:HG21	1:A:11:LEU:CD1	2.06	0.85
2:D:97:THR:HG22	2:D:112:TRP:HA	1.57	0.85
1:A:7:ILE:HD13	1:A:7:ILE:N	1.91	0.84
1:A:135:PHE:CD1	2:B:189:LEU:HD23	2.12	0.84
1:A:79:GLU:CB	1:A:81:GLU:OE2	2.23	0.84
2:B:106:LEU:CD2	2:B:108:TYR:CD1	2.58	0.84
1:C:20:ILE:HA	1:C:74:THR:HA	1.60	0.84
2:D:75:PRO:HG2	2:D:77:ASN:CG	2.02	0.84
1:A:120:PRO:CG	1:A:125:LEU:HD21	2.05	0.84
1:A:41:ASP:OD2	1:A:43:SER:OG	1.96	0.84
1:A:60:SER:O	1:C:126:THR:HG23	1.78	0.84
2:B:139:ASP:C	2:B:145:VAL:HG13	2.03	0.84
1:C:133:VAL:HG21	2:D:133:LEU:CD2	2.06	0.84
2:B:51:ILE:HG13	2:B:58:ILE:HG12	1.59	0.84
2:B:140:THR:CG2	2:B:141:SER:H	1.78	0.84
1:C:38:GLN:HB3	1:C:85:THR:CG2	2.04	0.84
1:C:89:GLN:HG2	1:C:98:PHE:CE2	2.12	0.84
1:A:49:TYR:CZ	1:A:53:ARG:HB3	2.13	0.84
1:A:83:ILE:HD12	1:A:106:ILE:CD1	2.08	0.84
1:C:39:LYS:HB2	1:C:43:SER:HB2	1.60	0.83
1:C:83:ILE:HA	1:C:104:LEU:HD22	1.58	0.83
1:C:183:LYS:HE2	1:C:187:GLU:OE2	1.78	0.83
2:D:125:THR:CG2	2:D:126:THR:N	2.41	0.83
2:D:88:SER:HA	2:D:120:VAL:HG12	1.58	0.83
2:D:11:LEU:HD11	2:D:155:PHE:HE2	1.43	0.83
2:B:102:GLY:HA3	2:B:108:TYR:OH	1.79	0.83
1:C:36:TYR:CE2	1:C:46:LEU:HD23	2.14	0.83
1:C:83:ILE:HA	1:C:104:LEU:CD2	2.08	0.83
1:C:166:GLN:HG2	1:C:171:SER:CA	2.07	0.83
2:B:134:VAL:HG23	2:B:135:PRO:HD2	1.61	0.83
2:B:91:THR:HB	2:B:120:VAL:H	1.43	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ALA:C	2:D:70:ILE:HD11	2.04	0.83
1:A:19:VAL:HG23	1:A:78:LEU:HD12	1.58	0.82
1:A:142:LYS:HG3	1:A:173:TYR:CE1	2.14	0.82
1:C:49:TYR:CD2	1:C:53:ARG:CB	2.62	0.82
1:C:196:ALA:HB3	1:C:205:ILE:HG22	1.59	0.82
1:A:39:LYS:HB2	1:A:40:PRO:HD2	1.61	0.82
2:D:179:LEU:C	2:D:179:LEU:CD2	2.50	0.82
1:A:2:ILE:CD1	1:A:29:ILE:HD11	2.09	0.82
2:D:19:LYS:HD2	2:D:82:GLN:HB2	1.60	0.81
2:D:88:SER:HA	2:D:120:VAL:HG11	1.62	0.81
2:B:144:SER:OG	2:B:193:PRO:HB3	1.78	0.81
2:B:217:LYS:HA	2:B:217:LYS:CE	2.09	0.81
1:C:108:ARG:HH21	1:C:108:ARG:CG	1.88	0.81
1:C:108:ARG:HH22	1:C:109:ALA:HB3	1.42	0.81
1:C:9:SER:HA	1:C:102:THR:HA	1.61	0.81
1:A:36:TYR:HE1	1:A:89:GLN:HG2	1.42	0.81
2:B:107:TYR:HD1	2:B:107:TYR:N	1.73	0.81
1:A:85:THR:HB	1:A:103:LYS:HA	1.61	0.81
2:D:38:ARG:NH1	2:D:46:GLU:OE2	2.12	0.81
2:D:204:CYS:O	2:D:216:ILE:N	2.12	0.81
2:D:140:THR:OG1	2:D:144:SER:HB3	1.81	0.81
2:D:78:THR:HG22	2:D:79:LEU:N	1.93	0.80
2:D:159:VAL:CG2	2:D:208:HIS:HB2	2.11	0.80
2:B:103:THR:CG2	2:B:104:ARG:HG3	2.03	0.80
1:C:2:ILE:HG12	1:C:29:ILE:CD1	2.12	0.80
1:A:66:GLY:HA3	1:A:71:TYR:CD2	2.16	0.80
1:A:13:VAL:HG21	1:A:78:LEU:HD13	1.62	0.80
2:D:179:LEU:HB2	2:D:184:TYR:CD1	2.17	0.80
1:C:20:ILE:HD11	1:C:65:TRP:HE1	1.47	0.80
1:C:2:ILE:HD13	1:C:90:GLN:CD	2.07	0.80
1:A:170:ASP:O	1:A:172:THR:N	2.15	0.80
2:D:100:GLY:O	2:D:101:THR:HB	1.80	0.80
1:C:78:LEU:HD11	1:C:79:GLU:O	1.80	0.79
1:A:79:GLU:O	1:A:81:GLU:N	2.15	0.79
2:B:64:VAL:HB	2:B:68:PHE:CD1	2.17	0.79
2:D:78:THR:CG2	2:D:79:LEU:N	2.45	0.79
2:D:27:PHE:CD2	2:D:32:PHE:CE1	2.71	0.79
2:D:89:GLU:OE2	2:D:89:GLU:N	2.16	0.79
2:D:128:PRO:O	2:D:128:PRO:CD	2.28	0.79
2:B:139:ASP:O	2:B:145:VAL:HG13	1.82	0.79
1:C:143:ASP:OD1	1:C:143:ASP:N	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TYR:CG	1:C:53:ARG:HB2	2.17	0.79
1:A:13:VAL:HG22	1:A:78:LEU:HD13	1.62	0.79
1:A:136:LEU:HD22	1:A:144:ILE:HD11	1.63	0.79
1:C:71:TYR:CD1	1:C:71:TYR:N	2.51	0.79
1:C:135:PHE:CD2	2:D:189:LEU:HG	2.17	0.79
1:A:15:LEU:HD21	1:A:80:GLU:CB	2.12	0.78
2:B:147:LEU:O	2:B:189:LEU:HD12	1.83	0.78
2:D:128:PRO:HB3	2:D:154:TYR:HB3	1.65	0.78
1:A:106:ILE:HD13	1:A:106:ILE:H	1.47	0.78
2:B:138:SER:O	2:B:145:VAL:HG22	1.83	0.78
2:B:139:ASP:O	2:B:145:VAL:CG1	2.31	0.78
2:B:203:ILE:CA	2:B:217:LYS:HB2	2.12	0.78
1:C:70:ASP:C	1:C:71:TYR:CD1	2.61	0.78
2:D:34:MET:CE	2:D:34:MET:CA	2.62	0.78
2:D:204:CYS:SG	2:D:216:ILE:HG23	2.24	0.78
1:A:4:MET:HE2	1:A:4:MET:CA	2.14	0.78
1:C:94:LEU:HD11	1:C:96:TYR:OH	1.83	0.78
2:D:87:ARG:O	2:D:89:GLU:N	2.16	0.78
1:A:135:PHE:CD1	2:B:189:LEU:CD2	2.67	0.78
2:D:179:LEU:HD23	2:D:180:GLN:N	1.97	0.78
1:C:203:SER:HB2	1:C:204:PRO:HD3	1.64	0.78
2:D:156:PRO:O	2:D:208:HIS:HE1	1.66	0.77
2:B:98:ARG:HG2	2:B:99:GLY:N	1.99	0.77
2:B:151:VAL:O	2:B:151:VAL:HG22	1.84	0.77
2:D:145:VAL:O	2:D:191:THR:HA	1.84	0.77
2:D:146:THR:OG1	2:D:191:THR:HG23	1.84	0.77
1:A:48:ILE:HA	1:A:53:ARG:O	1.84	0.77
2:B:22:CYS:O	2:B:79:LEU:N	2.15	0.77
2:B:34:MET:O	2:B:50:TYR:CD2	2.37	0.77
2:B:146:THR:HA	2:B:191:THR:HG22	1.67	0.77
1:C:29:ILE:HG12	1:C:90:GLN:CB	2.14	0.77
1:A:106:ILE:N	1:A:106:ILE:CD1	2.41	0.77
2:D:30:SER:O	2:D:53:SER:HB2	1.84	0.77
2:D:204:CYS:N	2:D:216:ILE:O	2.16	0.77
1:A:108:ARG:CZ	1:A:172:THR:HG23	2.14	0.77
2:B:13:GLN:CA	2:B:121:SER:O	2.29	0.77
2:B:97:THR:CG2	2:B:109:PHE:HB3	2.14	0.77
2:B:156:PRO:O	2:B:208:HIS:CE1	2.36	0.77
1:C:117:ILE:HG23	1:C:117:ILE:O	1.85	0.77
1:C:124:GLN:HG2	1:C:129:GLY:C	2.09	0.77
2:D:151:VAL:CG1	2:D:186:LEU:HD12	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ASN:OD1	1:A:51:THR:HG21	1.84	0.77
1:C:7:ILE:O	1:C:7:ILE:CD1	2.29	0.77
1:C:36:TYR:HE1	1:C:89:GLN:CG	1.98	0.77
2:B:83:MET:SD	2:B:86:LEU:HD21	2.25	0.77
2:B:33:GLY:HA2	2:B:72:ARG:HH22	1.50	0.76
1:C:29:ILE:HG12	1:C:90:GLN:HB3	1.66	0.76
1:A:121:SER:O	1:A:125:LEU:HG	1.84	0.76
2:B:101:THR:O	2:B:101:THR:HG22	1.83	0.76
2:B:200:GLN:N	2:B:200:GLN:OE1	2.18	0.76
1:C:108:ARG:HG3	1:C:109:ALA:O	1.85	0.76
2:D:163:TRP:CD1	2:D:172:VAL:HG23	2.20	0.76
1:A:18:ARG:HH21	1:A:74:THR:CG2	1.97	0.76
1:A:149:LYS:CA	1:A:153:SER:O	2.33	0.76
1:A:140:TYR:CD2	1:A:141:PRO:HA	2.21	0.76
2:B:87:ARG:HH11	2:B:89:GLU:HG2	1.50	0.76
2:B:159:VAL:HG12	2:B:159:VAL:O	1.86	0.76
2:D:11:LEU:HD11	2:D:155:PHE:CE2	2.20	0.76
2:B:34:MET:O	2:B:50:TYR:HD2	1.68	0.76
1:A:32:PHE:HD2	2:B:106:LEU:HD12	1.50	0.75
2:D:179:LEU:HD23	2:D:179:LEU:O	1.86	0.75
1:A:18:ARG:NH2	1:A:74:THR:HG21	2.00	0.75
1:A:23:CYS:O	1:A:71:TYR:N	2.17	0.75
1:A:50:TYR:OH	2:B:104:ARG:HD2	1.86	0.75
1:C:190:ASN:O	1:C:192:TYR:CD2	2.39	0.75
2:D:18:ARG:HG3	2:D:118:LEU:HD11	1.67	0.75
1:A:51:THR:HG1	1:A:71:TYR:HE2	0.79	0.75
1:A:102:THR:O	1:A:102:THR:HG22	1.85	0.75
2:B:167:ALA:C	2:B:168:LEU:CD1	2.58	0.75
2:B:17:SER:HB3	2:B:83:MET:O	1.85	0.75
1:C:106:ILE:CG2	1:C:171:SER:OG	2.34	0.75
2:D:39:GLN:HA	2:D:44:GLY:O	1.86	0.75
1:C:78:LEU:C	1:C:78:LEU:HD13	2.12	0.75
2:D:193:PRO:O	2:D:196:THR:HG22	1.86	0.74
1:A:33:LEU:HD13	1:A:71:TYR:CB	2.17	0.74
1:A:164:THR:OG1	1:A:174:SER:N	2.20	0.74
2:D:73:ASP:O	2:D:77:ASN:CB	2.36	0.74
2:B:60:TYR:CG	2:B:65:LYS:HD3	2.23	0.74
1:C:6:GLN:OE1	1:C:101:GLY:N	2.21	0.74
2:B:87:ARG:HB3	2:B:89:GLU:CD	2.12	0.74
1:C:78:LEU:CD1	1:C:79:GLU:O	2.35	0.74
1:A:39:LYS:O	1:A:41:ASP:N	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ARG:NH1	2:B:110:ASP:OD1	2.19	0.74
2:D:179:LEU:HG	2:D:183:PHE:O	1.87	0.74
1:A:155:ARG:HG2	1:A:179:LEU:CD2	2.16	0.74
1:C:203:SER:CB	1:C:204:PRO:HD3	2.17	0.74
2:D:150:LEU:HD13	2:D:152:LYS:HB2	1.69	0.74
1:A:56:SER:CB	2:D:212:LYS:HD2	2.10	0.74
2:B:168:LEU:HD13	2:B:168:LEU:H	1.47	0.73
2:D:107:TYR:N	2:D:107:TYR:CD1	2.54	0.73
1:A:13:VAL:HG21	1:A:78:LEU:CD1	2.18	0.73
1:A:12:SER:CA	1:A:105:GLU:O	2.35	0.73
1:A:136:LEU:HD11	1:A:146:VAL:HG21	1.71	0.73
2:B:133:LEU:CB	2:B:148:GLY:HA3	2.17	0.73
1:A:29:ILE:CD1	1:A:29:ILE:N	2.51	0.73
2:B:89:GLU:CD	2:B:89:GLU:H	1.96	0.73
2:B:143:SER:C	2:B:194:SER:OG	2.31	0.73
1:A:136:LEU:HD22	1:A:144:ILE:CD1	2.17	0.73
1:C:81:GLU:N	1:C:81:GLU:OE2	2.21	0.73
1:A:135:PHE:CD1	2:B:189:LEU:HG	2.23	0.73
2:B:151:VAL:O	2:B:151:VAL:CG2	2.36	0.73
2:D:33:GLY:O	2:D:34:MET:HE3	1.88	0.73
2:B:107:TYR:N	2:B:107:TYR:CD1	2.50	0.73
2:B:168:LEU:O	2:B:169:SER:HB3	1.86	0.73
1:C:4:MET:CE	1:C:90:GLN:CG	2.58	0.73
1:C:79:GLU:O	1:C:82:ASP:HB2	1.88	0.73
1:A:123:GLU:O	1:A:124:GLN:C	2.29	0.73
1:C:166:GLN:NE2	1:C:171:SER:HB3	2.00	0.73
2:B:146:THR:CA	2:B:191:THR:HG22	2.19	0.73
1:C:166:GLN:CG	1:C:171:SER:HA	2.14	0.73
1:A:56:SER:HB2	2:D:212:LYS:CD	2.10	0.72
1:A:196:ALA:O	1:A:205:ILE:HG22	1.89	0.72
2:B:61:ALA:O	2:B:63:THR:N	2.20	0.72
1:C:12:SER:HB3	1:C:107:LYS:HB2	1.71	0.72
1:A:150:ILE:N	1:A:153:SER:O	2.22	0.72
1:A:21:ILE:O	1:A:72:SER:HA	1.88	0.72
2:B:87:ARG:HH11	2:B:89:GLU:CG	2.02	0.72
2:B:172:VAL:HA	2:B:189:LEU:O	1.88	0.72
1:A:88:CYS:O	1:A:99:GLY:N	2.16	0.72
2:B:106:LEU:C	2:B:107:TYR:HD1	1.98	0.72
2:D:93:ILE:HA	2:D:117:THR:HA	1.69	0.72
2:D:147:LEU:CD1	2:D:217:LYS:HZ3	2.02	0.72
2:B:68:PHE:CZ	2:B:83:MET:HG2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PHE:HD1	2:B:189:LEU:CD2	2.02	0.72
2:D:112:TRP:N	2:D:112:TRP:CD1	2.57	0.72
2:D:159:VAL:HG23	2:D:208:HIS:HB2	1.71	0.72
2:D:216:ILE:O	2:D:217:LYS:CB	2.38	0.72
1:A:37:GLN:HB2	1:A:47:LEU:CD1	2.19	0.72
2:D:17:SER:HB3	2:D:84:THR:HA	1.70	0.72
1:A:12:SER:HB3	1:A:107:LYS:HZ2	1.54	0.72
1:A:7:ILE:HD13	1:A:7:ILE:H	1.52	0.72
2:B:17:SER:HB3	2:B:84:THR:HA	1.72	0.71
1:C:75:ILE:HG22	1:C:76:SER:N	2.03	0.71
1:C:93:THR:C	1:C:94:LEU:HD12	2.14	0.71
1:C:155:ARG:HH12	1:C:185:GLU:CD	1.98	0.71
1:A:162:SER:HB2	2:B:175:VAL:HG12	1.71	0.71
2:B:148:GLY:HA3	2:B:189:LEU:CD1	2.21	0.71
1:A:12:SER:HB3	1:A:107:LYS:HZ1	1.54	0.71
1:C:124:GLN:OE1	1:C:131:SER:N	2.20	0.71
2:D:130:VAL:HG11	2:D:216:ILE:HG22	1.72	0.71
2:B:134:VAL:CG2	2:B:135:PRO:HD2	2.20	0.71
2:B:166:GLY:O	2:B:168:LEU:HD13	1.88	0.71
2:B:167:ALA:C	2:B:168:LEU:HD12	2.16	0.71
2:D:68:PHE:CD2	2:D:81:LEU:HD21	2.26	0.71
1:C:92:LYS:HG3	1:C:93:THR:HG1	1.53	0.71
2:B:68:PHE:CE2	2:B:83:MET:CG	2.71	0.71
2:D:89:GLU:CD	2:D:89:GLU:H	1.99	0.71
2:D:212:LYS:HE3	2:D:214:ASP:OD1	1.91	0.70
2:D:30:SER:HA	2:D:74:ASN:ND2	2.06	0.70
2:B:88:SER:O	2:B:91:THR:CG2	2.34	0.70
1:C:158:GLY:O	1:C:179:LEU:HA	1.91	0.70
2:B:91:THR:O	2:B:92:ALA:HB2	1.89	0.70
2:B:17:SER:CA	2:B:83:MET:O	2.40	0.70
1:A:184:ASP:O	1:A:188:ARG:HG3	1.91	0.70
1:A:21:ILE:N	1:A:73:LEU:O	2.21	0.70
1:A:124:GLN:O	1:A:127:SER:N	2.24	0.70
2:B:133:LEU:CB	2:B:148:GLY:CA	2.58	0.70
1:C:2:ILE:CD1	1:C:90:GLN:NE2	2.55	0.70
1:C:33:LEU:HD23	1:C:34:ASN:N	2.07	0.70
1:C:80:GLU:O	1:C:82:ASP:N	2.25	0.70
1:A:8:THR:CG2	1:A:11:LEU:HD13	2.21	0.70
1:A:144:ILE:O	1:A:144:ILE:HG22	1.92	0.69
2:B:73:ASP:O	2:B:74:ASN:C	2.31	0.69
2:D:67:ARG:CD	2:D:85:SER:O	2.39	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:ALA:HB1	2:B:70:ILE:HG13	1.72	0.69
2:D:204:CYS:SG	2:D:216:ILE:CG2	2.80	0.69
2:B:148:GLY:HA3	2:B:189:LEU:HD13	1.74	0.69
1:C:55:GLN:HG3	1:C:56:SER:H	1.56	0.69
2:D:137:CYS:HA	2:D:197:TRP:CH2	2.27	0.69
1:A:32:PHE:HD2	2:B:106:LEU:CD1	2.04	0.69
1:A:150:ILE:CG2	1:A:189:HIS:CD2	2.70	0.69
2:B:167:ALA:HA	2:B:170:SER:HG	1.57	0.69
2:D:34:MET:O	2:D:50:TYR:HD2	1.75	0.69
1:C:125:LEU:C	1:C:128:GLY:H	1.99	0.69
2:B:152:LYS:HG2	2:B:185:SER:HG	1.56	0.69
1:C:36:TYR:HE1	1:C:89:GLN:HG2	1.58	0.69
1:C:124:GLN:O	1:C:127:SER:CB	2.38	0.69
1:A:203:SER:C	1:A:204:PRO:O	2.30	0.69
1:C:64:GLY:HA2	1:C:72:SER:O	1.92	0.69
2:D:49:ALA:HB1	2:D:70:ILE:HD11	1.75	0.69
1:C:146:VAL:O	1:C:147:LYS:HB2	1.93	0.69
1:C:183:LYS:CE	1:C:187:GLU:OE2	2.41	0.69
1:A:143:ASP:O	1:A:198:HIS:CD2	2.46	0.68
1:A:164:THR:HG1	1:A:174:SER:H	1.37	0.68
2:D:168:LEU:O	2:D:169:SER:HB2	1.91	0.68
2:B:2:VAL:HG12	2:B:2:VAL:O	1.93	0.68
2:B:6:GLU:HB3	2:B:116:ALA:CB	2.23	0.68
1:C:4:MET:HE3	1:C:90:GLN:N	2.07	0.68
1:C:38:GLN:CB	1:C:85:THR:HG22	2.06	0.68
2:D:130:VAL:HG21	2:D:214:ASP:HB3	1.76	0.68
2:B:4:LEU:O	2:B:114:GLN:NE2	2.26	0.68
1:C:10:SER:HA	1:C:103:LYS:O	1.93	0.68
1:C:108:ARG:HG3	1:C:109:ALA:H	1.54	0.68
1:A:49:TYR:CZ	1:A:53:ARG:CB	2.76	0.68
2:B:197:TRP:CD1	2:B:198:PRO:HA	2.28	0.68
2:D:168:LEU:O	2:D:193:PRO:CG	2.37	0.68
1:A:51:THR:OG1	1:A:71:TYR:CE2	2.33	0.68
2:D:67:ARG:O	2:D:84:THR:CG2	2.42	0.68
1:A:33:LEU:HD13	1:A:71:TYR:HB2	1.76	0.68
1:A:201:SER:OG	1:A:203:SER:N	2.27	0.68
1:A:83:ILE:CD1	1:A:106:ILE:HD11	2.20	0.68
1:A:108:ARG:HG2	1:A:108:ARG:HH21	1.60	0.67
1:A:39:LYS:H	1:A:43:SER:HB2	1.59	0.67
2:B:87:ARG:HH11	2:B:89:GLU:CB	2.07	0.67
1:C:155:ARG:HG2	1:C:179:LEU:HD21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:146:THR:HA	2:D:190:VAL:O	1.94	0.67
1:A:2:ILE:HD13	1:A:29:ILE:HD11	1.75	0.67
1:C:108:ARG:CG	1:C:109:ALA:O	2.42	0.67
1:A:48:ILE:HG12	1:A:54:LEU:HD12	1.74	0.67
1:C:4:MET:HE1	1:C:90:GLN:HG2	1.76	0.67
1:C:91:GLY:O	2:D:106:LEU:HD12	1.94	0.67
2:D:169:SER:HB2	2:D:193:PRO:CG	2.24	0.67
1:C:115:VAL:HG22	1:C:136:LEU:HG	1.75	0.67
2:B:17:SER:HB2	2:B:83:MET:O	1.94	0.67
2:B:22:CYS:O	2:B:78:THR:HA	1.95	0.67
2:B:164:ASN:ND2	2:B:164:ASN:O	2.28	0.67
1:C:108:ARG:HD3	1:C:140:TYR:CG	2.30	0.67
1:C:183:LYS:HZ3	1:C:187:GLU:CD	2.03	0.67
2:D:134:VAL:HG22	2:D:135:PRO:O	1.94	0.67
1:A:80:GLU:HG2	1:A:81:GLU:CD	2.19	0.67
1:A:108:ARG:HG2	1:A:108:ARG:NH2	2.08	0.67
1:A:167:ASP:O	1:A:171:SER:N	2.25	0.67
1:C:67:SER:O	1:C:69:THR:N	2.27	0.67
1:C:115:VAL:HG21	1:C:205:ILE:CG2	2.25	0.67
2:B:67:ARG:HG2	2:B:67:ARG:NH2	2.10	0.67
2:B:217:LYS:HE2	2:B:217:LYS:CA	2.21	0.67
2:D:139:ASP:HA	2:D:142:GLY:O	1.95	0.67
2:B:42:GLU:OE2	2:B:43:LYS:HG3	1.95	0.67
2:D:180:GLN:O	2:D:181:SER:HB2	1.93	0.67
2:B:203:ILE:HA	2:B:217:LYS:CB	2.20	0.66
1:A:24:ARG:NE	1:A:70:ASP:OD2	2.28	0.66
1:A:136:LEU:HD13	1:A:144:ILE:CD1	2.24	0.66
1:A:183:LYS:HE2	1:A:187:GLU:OE2	1.96	0.66
1:C:108:ARG:O	1:C:140:TYR:CE1	2.48	0.66
2:D:151:VAL:CG1	2:D:186:LEU:CD1	2.73	0.66
2:D:159:VAL:HG22	2:D:208:HIS:HB2	1.77	0.66
1:A:27:GLN:O	1:A:29:ILE:CD1	2.42	0.66
1:A:31:ASN:OD1	1:A:66:GLY:O	2.14	0.66
1:A:86:PHE:O	1:A:101:GLY:HA2	1.95	0.66
1:A:29:ILE:CG2	1:A:32:PHE:HB2	2.22	0.66
1:C:108:ARG:CG	1:C:109:ALA:H	2.09	0.66
2:B:133:LEU:CB	2:B:148:GLY:C	2.68	0.66
2:D:140:THR:N	2:D:142:GLY:O	2.28	0.66
1:A:198:HIS:O	1:A:199:LYS:C	2.36	0.66
1:C:108:ARG:O	1:C:140:TYR:HE1	1.77	0.66
2:B:166:GLY:C	2:B:168:LEU:CD1	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:VAL:O	1:C:74:THR:HA	1.97	0.65
1:C:20:ILE:CG1	1:C:74:THR:OG1	2.36	0.65
1:C:65:TRP:HZ2	1:C:74:THR:HG1	1.44	0.65
2:D:196:THR:HG1	2:D:197:TRP:H	1.43	0.65
1:A:21:ILE:O	1:A:73:LEU:N	2.27	0.65
1:A:29:ILE:HD13	1:A:29:ILE:N	2.12	0.65
1:A:89:GLN:HB3	1:A:98:PHE:CE2	2.31	0.65
1:C:78:LEU:HD12	1:C:79:GLU:CA	2.25	0.65
1:C:160:LEU:HD13	2:D:178:VAL:HG13	1.77	0.65
1:C:190:ASN:N	1:C:190:ASN:ND2	2.40	0.65
2:B:98:ARG:HH11	2:B:110:ASP:CG	2.05	0.65
1:C:66:GLY:HA3	1:C:71:TYR:CD2	2.32	0.65
1:C:89:GLN:HB3	1:C:98:PHE:CD2	2.31	0.65
2:B:64:VAL:HB	2:B:68:PHE:CG	2.32	0.64
2:D:1:ASP:O	2:D:2:VAL:CB	2.40	0.64
2:D:169:SER:HB3	2:D:193:PRO:CD	2.22	0.64
2:D:169:SER:CB	2:D:193:PRO:HD3	2.23	0.64
2:B:140:THR:HG22	2:B:141:SER:H	1.42	0.64
2:D:158:PRO:O	2:D:208:HIS:ND1	2.23	0.64
1:A:18:ARG:CG	1:A:74:THR:HG23	2.26	0.64
1:A:2:ILE:HG23	1:A:27:GLN:N	2.13	0.64
1:C:2:ILE:HG12	1:C:29:ILE:HD13	1.79	0.64
1:C:78:LEU:CD1	1:C:79:GLU:N	2.53	0.64
1:C:49:TYR:HE1	1:C:55:GLN:HA	1.61	0.63
1:C:55:GLN:O	1:C:58:VAL:HB	1.98	0.63
1:A:89:GLN:HB3	1:A:98:PHE:CD2	2.33	0.63
1:C:115:VAL:HG21	1:C:205:ILE:HG23	1.79	0.63
1:C:196:ALA:CB	1:C:205:ILE:HG22	2.26	0.63
2:B:124:THR:HG23	2:B:124:THR:O	1.97	0.63
2:B:202:VAL:O	2:B:203:ILE:HG13	1.98	0.63
1:C:46:LEU:HD11	1:C:49:TYR:HB3	1.81	0.63
1:C:80:GLU:H	1:C:80:GLU:CD	2.06	0.63
1:C:153:SER:OG	1:C:154:GLU:N	2.28	0.63
2:D:34:MET:HA	2:D:34:MET:HE3	1.75	0.63
1:A:134:CYS:HB2	1:A:148:TRP:CZ2	2.33	0.63
2:B:53:SER:O	2:B:54:GLY:C	2.42	0.63
2:B:202:VAL:O	2:B:217:LYS:HB3	1.99	0.63
1:C:15:LEU:HD23	1:C:80:GLU:OE1	1.99	0.63
1:C:160:LEU:HD13	2:D:178:VAL:CG1	2.29	0.63
1:C:155:ARG:NH1	1:C:185:GLU:OE2	2.31	0.63
1:A:24:ARG:CG	1:A:70:ASP:OD2	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD11	1:A:62:PHE:O	1.99	0.63
2:B:131:TYR:CD2	2:B:150:LEU:CD1	2.69	0.63
2:B:131:TYR:O	2:B:149:CYS:HA	1.98	0.63
1:C:144:ILE:O	1:C:144:ILE:HG22	1.95	0.63
2:B:130:VAL:HG23	2:B:214:ASP:CB	2.28	0.62
2:D:50:TYR:N	2:D:70:ILE:HD11	2.13	0.62
2:D:139:ASP:O	2:D:145:VAL:HA	1.99	0.62
1:A:47:LEU:O	1:A:48:ILE:HG13	1.98	0.62
1:A:134:CYS:HB2	1:A:148:TRP:CH2	2.34	0.62
1:C:81:GLU:N	1:C:81:GLU:CD	2.56	0.62
2:D:169:SER:HB3	2:D:191:THR:O	1.98	0.62
1:C:2:ILE:HD13	1:C:90:GLN:HE21	1.65	0.62
1:C:2:ILE:HG12	1:C:29:ILE:HD11	1.82	0.62
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.79	0.62
1:C:108:ARG:HG2	1:C:140:TYR:CE1	2.33	0.62
1:A:205:ILE:CD1	1:A:206:VAL:N	2.46	0.62
1:C:3:GLN:N	1:C:26:SER:OG	2.31	0.62
1:C:85:THR:HG23	1:C:87:PHE:CE1	2.35	0.62
1:C:139:PHE:CE1	1:C:141:PRO:O	2.53	0.62
1:A:7:ILE:H	1:A:7:ILE:CD1	2.10	0.62
2:B:29:PHE:O	2:B:31:ASN:N	2.33	0.62
1:C:123:GLU:O	1:C:126:THR:HG22	2.00	0.62
1:A:18:ARG:HG3	1:A:74:THR:HG23	1.82	0.61
1:A:135:PHE:HE1	2:B:189:LEU:HD23	1.61	0.61
2:D:72:ARG:HG2	2:D:74:ASN:OD1	2.01	0.61
2:D:92:ALA:O	2:D:117:THR:OG1	2.18	0.61
2:D:93:ILE:HG13	2:D:117:THR:HB	1.82	0.61
1:C:2:ILE:HD13	1:C:90:GLN:CG	2.30	0.61
1:A:17:ASP:OD2	1:A:78:LEU:HB3	2.00	0.61
1:A:30:GLY:O	1:A:32:PHE:CD1	2.53	0.61
1:C:135:PHE:CE2	2:D:189:LEU:HG	2.36	0.61
2:D:72:ARG:HE	2:D:74:ASN:HD21	1.49	0.61
2:D:130:VAL:HG11	2:D:216:ILE:CG2	2.31	0.61
2:B:20:LEU:HD21	2:B:94:TYR:CB	2.31	0.61
2:B:69:THR:O	2:B:81:LEU:HA	2.00	0.61
2:D:74:ASN:C	2:D:77:ASN:HB2	2.25	0.61
1:A:120:PRO:HB2	1:A:125:LEU:HD11	1.82	0.61
2:B:148:GLY:CA	2:B:189:LEU:HD13	2.30	0.61
2:D:84:THR:O	2:D:85:SER:C	2.39	0.61
2:D:156:PRO:O	2:D:156:PRO:HG2	2.01	0.61
2:B:4:LEU:N	2:B:4:LEU:HD23	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:49:ALA:HB1	2:D:70:ILE:CD1	2.31	0.61
1:A:153:SER:OG	1:A:154:GLU:N	2.34	0.61
2:D:179:LEU:HD23	2:D:180:GLN:CA	2.30	0.61
1:C:17:ASP:N	1:C:17:ASP:OD1	2.33	0.61
1:A:135:PHE:CD1	2:B:189:LEU:CG	2.84	0.60
2:B:128:PRO:HD3	2:B:208:HIS:CD2	2.36	0.60
1:C:94:LEU:HD12	1:C:94:LEU:N	2.16	0.60
2:D:144:SER:HA	2:D:192:VAL:O	2.02	0.60
2:D:212:LYS:HE3	2:D:214:ASP:HB2	1.82	0.60
1:A:12:SER:HA	1:A:105:GLU:HG3	1.82	0.60
1:A:173:TYR:N	1:A:173:TYR:HD2	1.99	0.60
2:B:18:ARG:N	2:B:83:MET:O	2.30	0.60
1:C:35:TRP:CE3	1:C:73:LEU:HD22	2.37	0.60
1:C:61:ARG:NH2	1:C:82:ASP:CG	2.58	0.60
1:A:122:SER:O	1:A:123:GLU:O	2.19	0.60
2:B:49:ALA:HB1	2:B:70:ILE:CG1	2.31	0.60
1:A:132:VAL:O	1:A:178:THR:HA	2.02	0.60
2:D:132:PRO:O	2:D:132:PRO:HG2	2.00	0.60
2:D:151:VAL:HG11	2:D:186:LEU:CD1	2.31	0.60
1:A:19:VAL:HG22	1:A:78:LEU:CD1	2.31	0.60
2:B:162:LYS:O	2:B:205:ASN:N	2.23	0.60
2:D:13:GLN:HG2	2:D:14:PRO:CD	2.30	0.60
1:A:29:ILE:HG22	1:A:32:PHE:H	1.66	0.60
2:D:58:ILE:HG22	2:D:60:TYR:CE2	2.37	0.60
2:B:128:PRO:HG2	2:B:212:LYS:HD3	1.83	0.60
1:C:117:ILE:O	1:C:117:ILE:CG2	2.49	0.60
1:A:31:ASN:ND2	1:A:67:SER:HA	2.12	0.60
1:A:92:LYS:HG3	1:A:93:THR:OG1	2.02	0.60
2:D:91:THR:HA	2:D:118:LEU:O	2.00	0.60
1:A:146:VAL:HG22	1:A:196:ALA:HB2	1.84	0.60
2:D:212:LYS:CE	2:D:214:ASP:HB2	2.31	0.60
1:A:12:SER:HB3	1:A:107:LYS:HG3	1.84	0.59
1:A:17:ASP:OD2	1:A:17:ASP:N	2.28	0.59
1:A:37:GLN:HE21	1:A:84:ALA:HB3	1.66	0.59
1:A:143:ASP:O	1:A:198:HIS:HD2	1.84	0.59
1:C:24:ARG:NH1	1:C:69:THR:HB	2.17	0.59
2:D:151:VAL:HG11	2:D:186:LEU:HD11	1.84	0.59
1:A:70:ASP:C	1:A:71:TYR:CD1	2.80	0.59
2:B:174:THR:HG23	2:B:188:SER:HB2	1.84	0.59
1:C:54:LEU:HD21	1:C:58:VAL:O	2.02	0.59
1:C:170:ASP:O	1:C:171:SER:C	2.44	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HD2	2:D:82:GLN:CD	2.27	0.59
1:A:138:ASN:OD1	1:A:138:ASN:N	2.24	0.59
1:A:85:THR:HG22	1:A:103:LYS:HG2	1.84	0.59
2:B:64:VAL:HA	2:B:67:ARG:HH11	1.67	0.59
2:B:164:ASN:ND2	2:B:164:ASN:C	2.61	0.59
1:A:18:ARG:HD3	1:A:74:THR:HG23	1.84	0.59
1:A:26:SER:OG	1:A:27:GLN:N	2.35	0.59
1:C:125:LEU:O	1:C:128:GLY:N	2.34	0.59
2:D:11:LEU:HA	2:D:119:ILE:HB	1.83	0.59
2:D:50:TYR:CD2	2:D:51:ILE:N	2.71	0.59
2:D:103:THR:HG22	2:D:104:ARG:HG3	1.85	0.59
2:B:101:THR:O	2:B:101:THR:HG23	2.03	0.59
2:D:58:ILE:CG2	2:D:60:TYR:CE2	2.86	0.59
1:A:49:TYR:CE1	1:A:53:ARG:CB	2.85	0.59
2:B:102:GLY:C	2:B:103:THR:OG1	2.42	0.59
2:B:167:ALA:C	2:B:168:LEU:HD13	2.21	0.59
1:C:24:ARG:NH1	1:C:69:THR:CB	2.66	0.59
2:D:119:ILE:HD13	2:D:156:PRO:HB2	1.85	0.59
1:A:21:ILE:O	1:A:72:SER:CA	2.51	0.59
1:C:89:GLN:HA	1:C:97:THR:O	2.03	0.59
1:A:17:ASP:OD2	1:A:78:LEU:CB	2.50	0.58
1:C:2:ILE:C	1:C:3:GLN:HG3	2.28	0.58
2:B:98:ARG:HG2	2:B:99:GLY:H	1.66	0.58
2:B:98:ARG:O	2:B:109:PHE:HA	2.03	0.58
1:C:57:GLY:O	1:C:58:VAL:C	2.44	0.58
2:D:133:LEU:HD12	2:D:148:GLY:CA	2.30	0.58
2:D:167:ALA:C	2:D:170:SER:OG	2.47	0.58
1:A:163:TRP:N	1:A:163:TRP:CE3	2.71	0.58
2:B:19:LYS:HD3	2:B:80:PHE:CD1	2.38	0.58
1:C:39:LYS:C	1:C:41:ASP:H	2.11	0.58
1:C:152:GLY:O	1:C:153:SER:CB	2.46	0.58
1:C:196:ALA:HB3	1:C:205:ILE:HG21	1.81	0.58
2:D:13:GLN:CD	2:D:14:PRO:HD2	2.29	0.58
1:A:136:LEU:HD12	1:A:175:MET:SD	2.44	0.58
2:D:154:TYR:CE2	2:D:184:TYR:HB2	2.38	0.58
1:A:110:ASP:O	1:A:111:ALA:HB2	2.03	0.58
1:C:41:ASP:CG	1:C:41:ASP:O	2.47	0.58
1:A:49:TYR:CD1	1:A:49:TYR:N	2.72	0.58
1:A:156:GLN:OE1	1:A:156:GLN:HA	2.03	0.58
1:A:173:TYR:N	1:A:173:TYR:CD2	2.72	0.58
2:B:128:PRO:CG	2:B:212:LYS:HD3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:140:THR:HG1	2:B:145:VAL:HA	1.66	0.58
2:B:174:THR:HA	2:B:188:SER:HA	1.86	0.58
2:D:146:THR:CG2	2:D:189:LEU:HB3	2.34	0.58
1:A:163:TRP:N	1:A:163:TRP:HE3	2.02	0.58
2:B:139:ASP:OD1	2:B:145:VAL:HG11	2.03	0.58
2:B:168:LEU:O	2:B:169:SER:CB	2.52	0.58
1:A:12:SER:CB	1:A:107:LYS:HZ1	2.17	0.58
1:A:105:GLU:C	1:A:106:ILE:HD13	2.29	0.58
1:C:65:TRP:HZ2	1:C:74:THR:OG1	1.86	0.58
1:C:67:SER:O	1:C:68:GLY:C	2.45	0.58
1:A:22:SER:HA	1:A:72:SER:HA	1.86	0.57
2:B:65:LYS:HD2	2:B:66:GLY:H	1.69	0.57
2:B:130:VAL:HG22	2:B:206:VAL:CG2	2.27	0.57
2:D:179:LEU:HA	2:D:184:TYR:HA	1.86	0.57
1:A:49:TYR:CD1	1:A:53:ARG:HB2	2.39	0.57
1:C:35:TRP:CD2	1:C:73:LEU:HD22	2.40	0.57
1:C:163:TRP:CH2	1:C:175:MET:HE2	2.39	0.57
1:C:182:THR:C	1:C:184:ASP:N	2.59	0.57
1:A:34:ASN:HD21	2:B:106:LEU:HD21	1.69	0.57
2:D:29:PHE:O	2:D:72:ARG:NH1	2.35	0.57
2:B:61:ALA:O	2:B:62:ASP:C	2.46	0.57
1:C:170:ASP:O	1:C:172:THR:HG23	2.05	0.57
1:C:189:HIS:C	1:C:190:ASN:HD22	2.12	0.57
2:D:49:ALA:HB1	2:D:70:ILE:CG1	2.35	0.57
1:A:18:ARG:CD	1:A:74:THR:HG23	2.35	0.57
2:B:41:PRO:C	2:B:43:LYS:N	2.62	0.57
2:B:87:ARG:NE	2:B:89:GLU:OE1	2.33	0.57
2:B:133:LEU:CG	2:B:148:GLY:HA3	2.35	0.57
1:A:77:ASN:O	1:A:78:LEU:C	2.45	0.57
1:A:148:TRP:HA	1:A:193:THR:O	2.05	0.57
2:B:9:GLY:C	2:B:18:ARG:HH12	2.13	0.57
2:B:146:THR:HG23	2:B:191:THR:HG23	1.86	0.57
1:C:124:GLN:NE2	1:C:131:SER:N	2.53	0.57
2:D:145:VAL:HG23	2:D:192:VAL:O	2.05	0.57
1:C:167:ASP:O	1:C:171:SER:N	2.38	0.57
1:C:183:LYS:NZ	1:C:187:GLU:OE2	2.37	0.57
1:C:203:SER:HB2	1:C:204:PRO:CD	2.31	0.57
1:A:185:GLU:HA	1:A:188:ARG:CG	2.31	0.56
2:B:68:PHE:HD2	2:B:81:LEU:HD11	1.69	0.56
1:C:35:TRP:CE3	1:C:73:LEU:CD2	2.88	0.56
1:C:49:TYR:O	1:C:53:ARG:HG2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:O	1:A:41:ASP:OD1	2.21	0.56
1:C:137:ASN:O	1:C:138:ASN:HB2	2.05	0.56
1:A:107:LYS:HA	1:A:140:TYR:OH	2.05	0.56
1:A:144:ILE:O	1:A:144:ILE:CG2	2.49	0.56
1:C:78:LEU:CD1	1:C:79:GLU:C	2.77	0.56
1:C:150:ILE:C	1:C:152:GLY:H	2.10	0.56
2:D:87:ARG:O	2:D:88:SER:C	2.42	0.56
1:C:164:THR:HG22	2:D:175:VAL:HA	1.86	0.56
2:D:74:ASN:O	2:D:77:ASN:CB	2.43	0.56
1:A:108:ARG:NE	1:A:170:ASP:O	2.36	0.56
2:B:180:GLN:O	2:B:181:SER:CB	2.52	0.56
1:A:85:THR:CG2	1:A:103:LYS:HG2	2.36	0.56
2:D:68:PHE:CE2	2:D:81:LEU:HD21	2.39	0.56
2:D:93:ILE:HG22	2:D:115:GLY:HA3	1.87	0.56
2:B:28:THR:O	2:B:29:PHE:C	2.49	0.56
2:B:203:ILE:HG21	2:B:215:LEU:HD11	1.87	0.56
1:C:183:LYS:O	1:C:183:LYS:HG2	2.06	0.56
2:D:74:ASN:N	2:D:75:PRO:HD2	2.21	0.56
1:A:17:ASP:O	1:A:78:LEU:HB2	2.06	0.56
1:C:2:ILE:HD13	1:C:90:GLN:HG2	1.88	0.56
2:D:34:MET:HB3	2:D:79:LEU:HD22	1.87	0.56
1:C:12:SER:HA	1:C:105:GLU:O	2.06	0.55
1:A:33:LEU:CD1	1:A:71:TYR:HB2	2.36	0.55
1:A:90:GLN:HG3	1:A:97:THR:H	1.71	0.55
1:A:136:LEU:CD1	1:A:175:MET:SD	2.94	0.55
1:A:147:LYS:CE	1:A:154:GLU:OE2	2.55	0.55
2:B:128:PRO:HD2	2:B:212:LYS:HD3	1.87	0.55
2:D:49:ALA:CB	2:D:70:ILE:HD11	2.35	0.55
2:D:91:THR:O	2:D:92:ALA:HB2	2.05	0.55
1:A:197:THR:O	1:A:198:HIS:HB2	2.06	0.55
1:C:139:PHE:N	1:C:173:TYR:O	2.38	0.55
2:D:10:GLY:CA	2:D:18:ARG:NH1	2.64	0.55
2:D:215:LEU:O	2:D:216:ILE:HB	2.07	0.55
2:D:89:GLU:N	2:D:89:GLU:CD	2.63	0.55
1:A:39:LYS:CB	1:A:40:PRO:HD2	2.30	0.55
1:A:115:VAL:HG21	1:A:205:ILE:HD12	1.88	0.55
1:A:120:PRO:HB3	1:A:125:LEU:CG	2.37	0.55
1:C:107:LYS:HA	1:C:140:TYR:OH	2.06	0.55
1:A:197:THR:HG22	1:A:198:HIS:N	2.22	0.55
2:B:179:LEU:HG	2:B:184:TYR:CZ	2.42	0.55
1:C:182:THR:O	1:C:184:ASP:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:ASP:OD2	2:B:111:TYR:HE2	1.87	0.55
1:C:49:TYR:CE2	1:C:53:ARG:CB	2.89	0.55
1:C:148:TRP:HA	1:C:193:THR:O	2.06	0.55
1:C:196:ALA:CB	1:C:205:ILE:CG2	2.79	0.55
2:D:4:LEU:HD12	2:D:96:CYS:O	2.07	0.55
1:A:135:PHE:CE1	2:B:189:LEU:HB2	2.41	0.55
1:A:135:PHE:HE1	2:B:189:LEU:HB2	1.72	0.55
1:C:81:GLU:CD	1:C:81:GLU:H	2.14	0.55
2:B:67:ARG:HD3	2:B:67:ARG:N	2.22	0.55
2:B:99:GLY:O	2:B:110:ASP:HB3	2.07	0.55
2:B:180:GLN:O	2:B:181:SER:HB2	2.07	0.55
2:B:201:THR:HG22	2:B:202:VAL:O	2.07	0.55
2:D:38:ARG:O	2:D:45:LEU:HA	2.07	0.55
1:A:48:ILE:CG1	1:A:54:LEU:HD12	2.37	0.54
2:D:13:GLN:CG	2:D:14:PRO:HD2	2.36	0.54
1:A:2:ILE:HD12	1:A:29:ILE:HD11	1.88	0.54
1:A:7:ILE:N	1:A:7:ILE:CD1	2.60	0.54
1:A:49:TYR:CE1	1:A:53:ARG:HB2	2.42	0.54
2:B:143:SER:CA	2:B:194:SER:OG	2.55	0.54
1:C:78:LEU:HD12	1:C:79:GLU:C	2.32	0.54
2:D:169:SER:HB2	2:D:193:PRO:HG3	1.89	0.54
1:A:39:LYS:HG3	1:A:43:SER:CB	2.37	0.54
1:A:135:PHE:CE1	2:B:189:LEU:CD2	2.83	0.54
2:B:164:ASN:HD22	2:B:165:TYR:C	2.14	0.54
1:C:85:THR:CG2	1:C:87:PHE:CE1	2.91	0.54
2:D:91:THR:O	2:D:91:THR:HG22	2.06	0.54
1:A:15:LEU:CD2	1:A:80:GLU:HB3	2.25	0.54
1:A:48:ILE:HD11	1:A:54:LEU:CD1	2.38	0.54
2:B:30:SER:HB3	2:B:74:ASN:HD22	1.71	0.54
2:B:159:VAL:O	2:B:159:VAL:CG1	2.36	0.54
1:C:166:GLN:O	1:C:167:ASP:C	2.44	0.54
2:D:179:LEU:CD2	2:D:179:LEU:O	2.53	0.54
1:A:57:GLY:O	1:A:58:VAL:C	2.44	0.54
2:B:130:VAL:CG2	2:B:206:VAL:HG21	2.31	0.54
1:C:147:LYS:HE2	1:C:154:GLU:OE2	2.08	0.54
1:A:18:ARG:NH2	1:A:74:THR:CG2	2.66	0.54
1:A:137:ASN:O	1:A:139:PHE:HD2	1.90	0.54
2:B:100:GLY:O	2:B:101:THR:CB	2.40	0.54
1:C:29:ILE:HG12	1:C:90:GLN:HB2	1.89	0.54
2:D:93:ILE:CG2	2:D:115:GLY:HA3	2.38	0.54
2:B:51:ILE:HG21	2:B:72:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:LEU:HD12	2:D:184:TYR:CE2	2.43	0.54
2:B:133:LEU:HD13	2:B:189:LEU:CD1	2.10	0.54
1:C:83:ILE:HG13	1:C:104:LEU:O	2.08	0.54
2:D:168:LEU:N	2:D:170:SER:OG	2.40	0.54
1:A:46:LEU:HD22	1:A:47:LEU:H	1.73	0.53
2:B:87:ARG:O	2:B:120:VAL:HG11	2.08	0.53
1:C:37:GLN:HG3	1:C:86:PHE:CE1	2.42	0.53
1:C:136:LEU:HD23	1:C:144:ILE:HD11	1.90	0.53
1:C:182:THR:O	1:C:183:LYS:C	2.46	0.53
2:D:41:PRO:HA	2:D:43:LYS:O	2.07	0.53
1:A:156:GLN:O	1:A:157:ASN:C	2.47	0.53
2:B:134:VAL:CG2	2:B:135:PRO:CD	2.86	0.53
2:D:79:LEU:HD12	2:D:80:PHE:H	1.73	0.53
2:B:63:THR:O	2:B:64:VAL:CG1	2.56	0.53
2:B:216:ILE:HG23	2:B:217:LYS:N	2.22	0.53
2:B:104:ARG:C	2:B:106:LEU:H	2.16	0.53
1:C:93:THR:HG22	1:C:94:LEU:N	2.24	0.53
1:C:146:VAL:O	1:C:147:LYS:CB	2.50	0.53
2:B:51:ILE:HB	2:B:70:ILE:HG22	1.91	0.53
1:C:34:ASN:OD1	2:D:106:LEU:HD21	2.08	0.53
1:A:79:GLU:O	1:A:80:GLU:C	2.52	0.53
1:C:124:GLN:CD	1:C:130:ALA:HA	2.34	0.53
1:A:2:ILE:HG23	1:A:27:GLN:H	1.73	0.53
1:C:85:THR:CG2	1:C:87:PHE:CZ	2.91	0.53
1:C:152:GLY:O	1:C:153:SER:HB2	2.08	0.53
1:C:89:GLN:HB3	1:C:98:PHE:HA	1.91	0.53
1:C:108:ARG:HD3	1:C:140:TYR:CB	2.39	0.53
1:A:34:ASN:ND2	2:B:108:TYR:HB3	2.23	0.53
1:A:62:PHE:CE2	1:A:75:ILE:HD13	2.44	0.53
2:B:88:SER:N	2:B:89:GLU:OE2	2.42	0.53
2:B:90:ASP:O	2:B:91:THR:C	2.47	0.53
1:C:83:ILE:CG1	1:C:104:LEU:O	2.57	0.53
2:D:9:GLY:O	2:D:18:ARG:CZ	2.58	0.53
1:A:19:VAL:O	1:A:75:ILE:N	2.42	0.52
1:A:49:TYR:CE1	1:A:53:ARG:HB3	2.43	0.52
1:A:125:LEU:O	1:A:126:THR:C	2.51	0.52
1:A:139:PHE:O	1:A:173:TYR:N	2.42	0.52
2:B:87:ARG:CB	2:B:89:GLU:OE1	2.53	0.52
1:A:66:GLY:HA3	1:A:71:TYR:CG	2.43	0.52
1:C:20:ILE:CD1	1:C:72:SER:HB2	2.40	0.52
1:C:31:ASN:HD21	1:C:67:SER:HA	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:LEU:CD1	1:C:78:LEU:O	2.30	0.52
2:D:13:GLN:CG	2:D:14:PRO:CD	2.87	0.52
2:D:126:THR:C	2:D:127:ALA:O	2.46	0.52
1:A:4:MET:CA	1:A:4:MET:CE	2.86	0.52
2:B:63:THR:O	2:B:64:VAL:HG12	2.10	0.52
1:C:89:GLN:HG2	1:C:98:PHE:CD2	2.45	0.52
1:C:136:LEU:HD23	1:C:144:ILE:CD1	2.40	0.52
2:B:32:PHE:O	2:B:72:ARG:NH1	2.42	0.52
2:B:143:SER:HB3	2:B:194:SER:OG	2.10	0.52
1:C:71:TYR:N	1:C:71:TYR:HD1	2.03	0.52
2:D:73:ASP:O	2:D:77:ASN:CG	2.52	0.52
2:D:199:SER:HB2	2:D:200:GLN:OE1	2.10	0.52
1:C:56:SER:C	1:C:58:VAL:N	2.67	0.52
2:D:40:ALA:HB2	2:D:92:ALA:HB2	1.91	0.52
2:B:98:ARG:HD2	2:B:111:TYR:HD2	1.75	0.52
2:B:144:SER:OG	2:B:193:PRO:CB	2.55	0.52
2:B:150:LEU:HD13	2:B:152:LYS:HB2	1.91	0.52
1:C:32:PHE:HB3	2:D:106:LEU:CD1	2.40	0.52
2:B:130:VAL:CG2	2:B:214:ASP:CB	2.88	0.52
2:B:147:LEU:O	2:B:189:LEU:CD1	2.53	0.52
1:A:43:SER:O	1:A:44:LEU:C	2.47	0.52
2:B:65:LYS:HD2	2:B:66:GLY:N	2.24	0.52
2:B:152:LYS:HD3	2:B:152:LYS:C	2.34	0.52
2:D:13:GLN:HG2	2:D:14:PRO:HD3	1.90	0.52
2:D:179:LEU:HD21	2:D:182:GLY:H	1.75	0.52
2:B:20:LEU:N	2:B:81:LEU:O	2.42	0.52
1:C:75:ILE:CG2	1:C:76:SER:N	2.71	0.52
2:D:100:GLY:O	2:D:101:THR:C	2.42	0.52
2:D:192:VAL:O	2:D:192:VAL:HG23	2.07	0.52
1:A:39:LYS:CB	1:A:40:PRO:CD	2.88	0.51
1:C:125:LEU:CD2	1:C:130:ALA:HB2	2.41	0.51
1:A:54:LEU:HD23	1:A:58:VAL:O	2.10	0.51
1:A:81:GLU:N	1:A:81:GLU:CD	2.67	0.51
1:A:108:ARG:CZ	1:A:172:THR:CG2	2.86	0.51
1:A:141:PRO:HD2	1:A:198:HIS:CE1	2.45	0.51
1:C:36:TYR:CE1	1:C:89:GLN:HG2	2.42	0.51
1:C:71:TYR:C	1:C:72:SER:OG	2.34	0.51
2:B:33:GLY:HA2	2:B:72:ARG:NH2	2.23	0.51
2:B:60:TYR:CD2	2:B:65:LYS:CD	2.79	0.51
1:A:62:PHE:CE2	1:A:75:ILE:CD1	2.94	0.51
1:A:163:TRP:CE2	1:A:175:MET:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ILE:HG21	1:C:171:SER:HG	1.70	0.51
1:C:160:LEU:HD22	2:D:178:VAL:CG2	2.27	0.51
1:C:164:THR:CG2	2:D:175:VAL:HG23	2.40	0.51
1:C:32:PHE:HB3	2:D:106:LEU:HD13	1.91	0.51
1:C:33:LEU:HD23	1:C:33:LEU:C	2.36	0.51
1:C:83:ILE:O	1:C:84:ALA:HB2	2.09	0.51
1:A:39:LYS:HG3	1:A:43:SER:HB3	1.93	0.51
2:D:34:MET:CB	2:D:79:LEU:HD22	2.40	0.51
2:D:125:THR:CG2	2:D:126:THR:H	2.20	0.51
1:A:34:ASN:OD1	1:A:49:TYR:HA	2.11	0.51
1:A:107:LYS:HA	1:A:140:TYR:HH	1.76	0.51
2:B:2:VAL:HG11	2:B:111:TYR:CE1	2.46	0.51
2:B:29:PHE:O	2:B:30:SER:C	2.52	0.51
1:C:38:GLN:O	1:C:84:ALA:HB1	2.10	0.51
2:D:30:SER:HA	2:D:74:ASN:HD22	1.74	0.51
2:D:177:SER:HA	2:D:185:SER:O	2.11	0.51
1:A:111:ALA:N	1:A:200:THR:HG21	2.25	0.51
1:A:136:LEU:HD21	1:A:146:VAL:CG2	2.41	0.51
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.93	0.51
1:C:118:PHE:CE1	2:D:135:PRO:HD3	2.46	0.51
1:C:126:THR:C	1:C:128:GLY:N	2.69	0.51
2:D:130:VAL:CG1	2:D:216:ILE:CG2	2.88	0.51
2:D:130:VAL:HG12	2:D:216:ILE:HG21	1.93	0.51
1:A:136:LEU:HD21	1:A:146:VAL:HG21	1.93	0.51
1:A:150:ILE:HG21	1:A:189:HIS:CG	2.38	0.51
1:C:4:MET:HE3	1:C:90:GLN:HG3	1.83	0.51
1:C:124:GLN:CD	1:C:131:SER:N	2.68	0.51
2:D:146:THR:OG1	2:D:191:THR:CG2	2.56	0.51
2:D:169:SER:CB	2:D:193:PRO:CD	2.87	0.51
1:A:25:ALA:HB1	1:A:27:GLN:O	2.11	0.50
1:A:31:ASN:CA	1:A:71:TYR:OH	2.53	0.50
1:A:80:GLU:O	1:A:83:ILE:CG2	2.58	0.50
2:B:22:CYS:HB3	2:B:79:LEU:HB3	1.92	0.50
2:B:58:ILE:HG23	2:B:70:ILE:HB	1.93	0.50
1:A:18:ARG:CA	1:A:75:ILE:O	2.37	0.50
1:A:28:ASP:C	1:A:29:ILE:CD1	2.84	0.50
1:C:139:PHE:N	1:C:139:PHE:CD2	2.78	0.50
1:C:159:VAL:HA	1:C:178:THR:O	2.10	0.50
2:D:100:GLY:O	2:D:101:THR:CB	2.41	0.50
2:B:17:SER:HA	2:B:83:MET:O	2.11	0.50
1:C:85:THR:HG21	1:C:87:PHE:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ARG:C	1:C:140:TYR:CE1	2.90	0.50
1:C:166:GLN:CG	1:C:171:SER:CA	2.83	0.50
2:D:75:PRO:CD	2:D:77:ASN:OD1	2.58	0.50
2:D:112:TRP:CD1	2:D:112:TRP:H	2.30	0.50
1:A:79:GLU:C	1:A:81:GLU:H	2.20	0.50
1:A:186:TYR:O	1:A:187:GLU:C	2.52	0.50
2:D:41:PRO:O	2:D:42:GLU:HB3	2.11	0.50
2:D:52:SER:O	2:D:53:SER:C	2.50	0.50
2:D:73:ASP:OD1	2:D:77:ASN:OD1	2.29	0.50
1:A:108:ARG:NE	1:A:172:THR:HG23	2.26	0.50
1:A:130:ALA:CA	1:A:181:LEU:O	2.59	0.50
2:B:91:THR:HA	2:B:118:LEU:O	2.11	0.50
1:C:49:TYR:CE2	1:C:53:ARG:HB3	2.46	0.50
1:C:90:GLN:OE1	1:C:92:LYS:HB3	2.11	0.50
1:C:120:PRO:HG3	1:C:132:VAL:HG22	1.94	0.50
1:C:126:THR:O	1:C:127:SER:C	2.51	0.50
1:C:150:ILE:C	1:C:152:GLY:N	2.66	0.50
2:D:13:GLN:HG2	2:D:14:PRO:HD2	1.93	0.50
1:A:19:VAL:O	1:A:74:THR:HA	2.12	0.50
2:B:52:SER:O	2:B:72:ARG:NH2	2.45	0.50
1:C:139:PHE:HE1	1:C:141:PRO:O	1.93	0.50
2:D:33:GLY:C	2:D:34:MET:HE3	2.37	0.50
2:D:42:GLU:O	2:D:42:GLU:HG2	2.12	0.50
2:D:174:THR:HG22	2:D:175:VAL:O	2.12	0.50
2:B:63:THR:C	2:B:64:VAL:HG13	2.37	0.50
2:B:159:VAL:HG13	2:B:160:THR:N	2.12	0.50
2:B:212:LYS:HE3	2:B:213:THR:C	2.37	0.50
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.94	0.50
2:D:169:SER:CB	2:D:193:PRO:CG	2.90	0.50
1:A:49:TYR:CG	1:A:53:ARG:HB2	2.47	0.49
1:A:133:VAL:HG12	1:A:134:CYS:N	2.26	0.49
2:B:2:VAL:CG1	2:B:111:TYR:CD1	2.95	0.49
1:C:5:THR:HB	1:C:24:ARG:HG2	1.93	0.49
1:A:13:VAL:HG21	1:A:19:VAL:HG22	1.94	0.49
1:A:19:VAL:HG21	1:A:78:LEU:CD1	2.41	0.49
1:C:50:TYR:C	1:C:52:SER:N	2.70	0.49
1:A:46:LEU:HD22	1:A:47:LEU:N	2.28	0.49
1:A:135:PHE:HZ	2:B:173:ARG:HB2	1.76	0.49
1:C:8:THR:HG21	1:C:11:LEU:HD22	1.94	0.49
2:D:20:LEU:HD13	2:D:83:MET:HE1	1.94	0.49
1:C:166:GLN:NE2	1:C:171:SER:CB	2.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:VAL:HG13	2:D:186:LEU:HD12	1.92	0.49
2:B:128:PRO:CD	2:B:212:LYS:HD3	2.42	0.49
1:C:56:SER:O	1:C:57:GLY:C	2.49	0.49
1:C:136:LEU:HD21	1:C:196:ALA:HB2	1.94	0.49
1:A:90:GLN:NE2	1:A:93:THR:O	2.44	0.49
2:B:103:THR:O	2:B:106:LEU:CB	2.61	0.49
2:B:130:VAL:HG23	2:B:214:ASP:HB2	1.94	0.49
2:B:130:VAL:CG2	2:B:214:ASP:HB3	2.42	0.49
1:C:32:PHE:HD1	1:C:92:LYS:HD3	1.78	0.49
1:A:135:PHE:HD1	2:B:189:LEU:HG	1.71	0.49
2:B:87:ARG:CZ	2:B:89:GLU:HB2	2.42	0.49
2:B:104:ARG:C	2:B:106:LEU:N	2.71	0.49
1:C:13:VAL:HG21	1:C:19:VAL:HG22	1.95	0.49
1:C:66:GLY:HA3	1:C:71:TYR:CB	2.42	0.49
2:D:137:CYS:HA	2:D:197:TRP:HH2	1.77	0.49
2:D:146:THR:HG22	2:D:189:LEU:HB3	1.95	0.49
1:A:48:ILE:CD1	1:A:54:LEU:HD12	2.43	0.49
2:B:61:ALA:C	2:B:63:THR:N	2.70	0.49
1:C:37:GLN:HG3	1:C:86:PHE:HE1	1.78	0.49
2:B:29:PHE:HB2	2:B:77:ASN:ND2	2.27	0.49
2:D:11:LEU:HD22	2:D:119:ILE:HG22	1.81	0.49
2:D:104:ARG:O	2:D:105:SER:HB3	2.07	0.49
2:D:197:TRP:C	2:D:199:SER:H	2.21	0.49
2:B:27:PHE:HD2	2:B:28:THR:H	1.59	0.48
2:B:52:SER:CB	2:B:57:SER:H	2.25	0.48
2:B:108:TYR:C	2:B:109:PHE:CD1	2.90	0.48
1:C:20:ILE:HD11	1:C:72:SER:HB2	1.94	0.48
2:D:11:LEU:HD21	2:D:119:ILE:HG22	1.68	0.48
2:D:165:TYR:C	2:D:165:TYR:HD1	2.21	0.48
1:C:9:SER:OG	1:C:10:SER:N	2.43	0.48
2:D:132:PRO:O	2:D:132:PRO:CG	2.61	0.48
2:D:162:LYS:N	2:D:205:ASN:O	2.38	0.48
2:D:166:GLY:O	2:D:170:SER:OG	2.31	0.48
1:A:2:ILE:HA	1:A:26:SER:OG	2.12	0.48
1:A:28:ASP:C	1:A:29:ILE:HD12	2.38	0.48
2:B:134:VAL:HG22	2:B:135:PRO:N	2.26	0.48
1:C:133:VAL:CG2	2:D:133:LEU:CD2	2.86	0.48
2:D:112:TRP:H	2:D:112:TRP:HD1	1.62	0.48
2:D:168:LEU:O	2:D:169:SER:CB	2.60	0.48
1:A:89:GLN:HA	1:A:97:THR:O	2.13	0.48
1:A:170:ASP:OD2	1:A:172:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:CG1	1:C:90:GLN:HB2	2.43	0.48
1:C:32:PHE:CD1	1:C:92:LYS:HD3	2.48	0.48
1:C:167:ASP:O	1:C:168:SER:C	2.56	0.48
2:D:6:GLU:CD	2:D:115:GLY:H	2.21	0.48
2:B:14:PRO:HD3	2:B:121:SER:O	2.13	0.48
1:A:61:ARG:NH2	1:A:82:ASP:OD1	2.46	0.48
2:B:104:ARG:O	2:B:105:SER:C	2.52	0.48
2:B:135:PRO:HD3	2:B:147:LEU:HD12	1.96	0.48
1:C:66:GLY:HA3	1:C:71:TYR:CG	2.49	0.48
1:C:183:LYS:O	1:C:187:GLU:HG3	2.13	0.48
2:D:147:LEU:N	2:D:190:VAL:O	2.43	0.48
2:D:168:LEU:C	2:D:193:PRO:HG2	2.34	0.48
1:A:34:ASN:HD21	2:B:108:TYR:HB3	1.79	0.48
1:C:32:PHE:HE1	1:C:92:LYS:HZ3	1.61	0.48
1:C:39:LYS:C	1:C:41:ASP:N	2.71	0.48
1:C:81:GLU:HG2	1:C:81:GLU:O	2.13	0.48
1:A:79:GLU:C	1:A:81:GLU:N	2.71	0.48
1:A:110:ASP:HB3	1:A:200:THR:CG2	2.44	0.48
2:D:17:SER:HA	2:D:86:LEU:CD1	2.44	0.48
1:A:24:ARG:HA	1:A:69:THR:O	2.13	0.48
1:A:135:PHE:HZ	2:B:173:ARG:HG3	1.79	0.48
2:B:73:ASP:OD1	2:B:76:LYS:HB2	2.14	0.48
1:C:7:ILE:HD13	1:C:7:ILE:C	2.33	0.48
1:C:59:PRO:O	1:C:62:PHE:HD1	1.97	0.48
1:C:150:ILE:HG23	1:C:192:TYR:CE1	2.48	0.48
1:A:36:TYR:CE1	1:A:89:GLN:HG2	2.34	0.48
2:B:63:THR:C	2:B:64:VAL:CG1	2.86	0.47
1:C:106:ILE:HB	1:C:166:GLN:CD	2.38	0.47
2:D:130:VAL:CG1	2:D:216:ILE:HG21	2.43	0.47
1:C:125:LEU:HD23	1:C:129:GLY:O	2.13	0.47
2:D:194:SER:C	2:D:196:THR:N	2.71	0.47
1:C:32:PHE:CD2	2:D:106:LEU:HD13	2.49	0.47
1:C:90:GLN:OE1	1:C:90:GLN:C	2.58	0.47
1:C:184:ASP:O	1:C:185:GLU:C	2.54	0.47
2:D:34:MET:N	2:D:51:ILE:O	2.45	0.47
1:C:93:THR:O	1:C:96:TYR:CE2	2.67	0.47
1:C:94:LEU:N	1:C:94:LEU:CD1	2.77	0.47
1:A:50:TYR:CZ	2:B:104:ARG:HD2	2.49	0.47
1:A:115:VAL:HG21	1:A:205:ILE:CD1	2.43	0.47
1:C:54:LEU:HD11	1:C:58:VAL:HG12	1.96	0.47
2:D:19:LYS:CD	2:D:82:GLN:HB2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:LYS:CE	2:B:217:LYS:CA	2.87	0.47
1:C:83:ILE:HA	1:C:104:LEU:HD23	1.95	0.47
2:D:11:LEU:HD23	2:D:119:ILE:HG22	1.52	0.47
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.95	0.47
2:B:2:VAL:HG11	2:B:111:TYR:CZ	2.49	0.47
2:B:148:GLY:CA	2:B:189:LEU:CD1	2.90	0.47
1:C:47:LEU:O	1:C:58:VAL:HG21	2.15	0.47
1:C:116:SER:N	1:C:135:PHE:O	2.44	0.47
1:C:167:ASP:OD2	1:C:168:SER:N	2.48	0.47
2:D:147:LEU:HA	2:D:147:LEU:HD13	1.45	0.47
2:D:165:TYR:C	2:D:165:TYR:CD1	2.93	0.47
2:D:194:SER:O	2:D:195:SER:C	2.53	0.47
2:B:3:GLN:C	2:B:4:LEU:HD23	2.40	0.47
2:B:166:GLY:C	2:B:168:LEU:HD12	2.40	0.47
1:C:9:SER:O	1:C:103:LYS:O	2.33	0.47
2:D:179:LEU:HD11	2:D:182:GLY:O	2.15	0.47
1:A:29:ILE:HD12	1:A:29:ILE:HA	1.32	0.47
1:A:136:LEU:CD1	1:A:146:VAL:HG21	2.42	0.47
1:C:118:PHE:CD1	2:D:135:PRO:HD3	2.49	0.47
1:C:139:PHE:CD1	1:C:141:PRO:O	2.68	0.47
2:D:49:ALA:HB1	2:D:70:ILE:HG12	1.97	0.47
2:D:123:ALA:HB3	2:D:155:PHE:CE2	2.50	0.47
1:A:65:TRP:HD1	1:A:72:SER:O	1.97	0.46
2:D:9:GLY:O	2:D:18:ARG:NH1	2.48	0.46
1:A:57:GLY:HA2	2:D:214:ASP:OD1	2.15	0.46
1:A:116:SER:HB3	1:A:118:PHE:CE2	2.50	0.46
2:B:67:ARG:NH2	2:B:67:ARG:CG	2.72	0.46
1:C:36:TYR:HE2	1:C:46:LEU:HD23	1.72	0.46
1:C:144:ILE:HG13	1:C:198:HIS:HD2	1.80	0.46
1:A:26:SER:O	1:A:27:GLN:C	2.56	0.46
1:A:162:SER:C	1:A:163:TRP:CE3	2.93	0.46
2:B:17:SER:HA	2:B:86:LEU:HD12	1.97	0.46
2:B:130:VAL:HG12	2:B:131:TYR:N	2.30	0.46
2:B:174:THR:O	2:B:175:VAL:C	2.56	0.46
1:C:39:LYS:O	1:C:41:ASP:N	2.49	0.46
2:D:8:GLY:O	2:D:18:ARG:HD2	2.15	0.46
2:D:53:SER:HA	2:D:72:ARG:CZ	2.45	0.46
1:A:73:LEU:CD2	1:A:86:PHE:CD1	2.98	0.46
1:A:115:VAL:CG1	1:A:116:SER:N	2.79	0.46
2:B:3:GLN:N	2:B:25:SER:O	2.43	0.46
2:B:164:ASN:C	2:B:164:ASN:HD22	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ARG:NH1	1:C:69:THR:OG1	2.47	0.46
2:D:155:PHE:CD2	2:D:156:PRO:N	2.83	0.46
2:D:168:LEU:HD12	2:D:168:LEU:HA	1.60	0.46
1:A:25:ALA:HB3	1:A:69:THR:HB	1.98	0.46
2:B:6:GLU:HB2	2:B:116:ALA:HB2	1.91	0.46
2:B:133:LEU:HD12	2:B:148:GLY:CA	2.18	0.46
2:D:92:ALA:O	2:D:117:THR:HA	2.15	0.46
1:A:33:LEU:O	1:A:51:THR:N	2.49	0.46
1:A:48:ILE:HD11	1:A:54:LEU:HD11	1.98	0.46
1:A:149:LYS:C	1:A:153:SER:O	2.59	0.46
2:B:64:VAL:O	2:B:67:ARG:N	2.46	0.46
2:B:91:THR:O	2:B:92:ALA:CB	2.58	0.46
1:C:119:PRO:HA	1:C:120:PRO:HD3	1.87	0.46
2:D:6:GLU:OE2	2:D:114:GLN:OE1	2.33	0.46
1:A:174:SER:OG	2:B:173:ARG:HD2	2.15	0.46
2:B:146:THR:HA	2:B:191:THR:CG2	2.40	0.46
1:C:61:ARG:HD3	1:C:77:ASN:O	2.16	0.46
1:C:149:LYS:O	1:C:193:THR:N	2.39	0.46
1:A:17:ASP:OD2	1:A:78:LEU:HB2	2.15	0.46
1:A:29:ILE:O	1:A:32:PHE:HD1	1.98	0.46
1:A:123:GLU:O	1:A:126:THR:HB	2.14	0.46
1:A:135:PHE:CE1	2:B:189:LEU:CG	2.99	0.46
1:A:205:ILE:HD12	1:A:205:ILE:HG23	1.71	0.46
2:B:68:PHE:CD1	2:B:68:PHE:N	2.84	0.46
2:B:74:ASN:HB2	2:B:75:PRO:CD	2.46	0.46
1:C:58:VAL:HA	1:C:59:PRO:HD3	1.63	0.46
2:D:38:ARG:HD3	2:D:48:VAL:HG21	1.98	0.46
2:B:61:ALA:O	2:B:64:VAL:N	2.39	0.46
2:B:64:VAL:HG23	2:B:68:PHE:HB2	1.98	0.46
1:C:16:GLY:O	1:C:77:ASN:HA	2.15	0.46
1:C:92:LYS:C	1:C:93:THR:OG1	2.58	0.46
2:D:19:LYS:HD2	2:D:82:GLN:CB	2.38	0.46
2:D:180:GLN:C	2:D:180:GLN:CD	2.84	0.46
1:A:38:GLN:HB2	1:A:44:LEU:HG	1.98	0.45
1:A:147:LYS:HB3	1:A:147:LYS:HE2	1.28	0.45
1:A:175:MET:SD	1:A:175:MET:C	2.99	0.45
2:D:216:ILE:HG12	2:D:217:LYS:CA	2.41	0.45
1:C:54:LEU:HG	1:C:58:VAL:HB	1.98	0.45
1:C:91:GLY:C	2:D:106:LEU:HD12	2.40	0.45
1:A:48:ILE:HG12	1:A:54:LEU:HA	1.99	0.45
1:A:108:ARG:HH21	1:A:108:ARG:CG	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ASN:HB3	1:A:138:ASN:OD1	2.15	0.45
1:A:195:GLU:HG3	1:A:204:PRO:HB3	1.98	0.45
1:C:98:PHE:CZ	2:D:109:PHE:HE2	2.34	0.45
2:B:17:SER:CB	2:B:84:THR:HA	2.44	0.45
2:D:18:ARG:HG3	2:D:118:LEU:CD1	2.42	0.45
1:C:12:SER:HB3	1:C:107:LYS:CB	2.43	0.45
1:C:13:VAL:HG23	1:C:17:ASP:OD2	2.16	0.45
1:C:21:ILE:HG22	1:C:22:SER:N	2.21	0.45
1:C:41:ASP:O	1:C:42:GLY:C	2.60	0.45
2:B:146:THR:OG1	2:B:191:THR:HG22	2.17	0.45
1:C:21:ILE:CG2	1:C:22:SER:N	2.72	0.45
2:D:98:ARG:HD3	2:D:110:ASP:HB3	1.99	0.45
1:A:155:ARG:HD2	1:A:155:ARG:HA	1.54	0.45
2:B:117:THR:OG1	2:B:118:LEU:N	2.49	0.45
2:B:146:THR:OG1	2:B:191:THR:CG2	2.65	0.45
1:C:92:LYS:CG	1:C:93:THR:OG1	2.36	0.45
1:C:130:ALA:O	1:C:180:THR:HG23	2.17	0.45
1:A:33:LEU:HD13	1:A:71:TYR:CD2	2.47	0.45
1:A:60:SER:O	1:C:126:THR:CG2	2.56	0.45
1:A:131:SER:HG	1:A:180:THR:HG23	1.80	0.45
2:B:52:SER:HB2	2:B:57:SER:H	1.82	0.45
1:C:94:LEU:HD21	2:D:59:ASN:HB3	1.98	0.45
1:C:108:ARG:N	1:C:140:TYR:OH	2.45	0.45
2:D:33:GLY:O	2:D:34:MET:CE	2.62	0.45
2:D:39:GLN:O	2:D:39:GLN:CG	2.64	0.45
2:D:97:THR:CG2	2:D:112:TRP:HA	2.38	0.45
2:B:74:ASN:O	2:B:77:ASN:N	2.45	0.45
2:B:212:LYS:O	2:B:212:LYS:HG3	2.11	0.45
1:C:50:TYR:CE2	2:D:104:ARG:NH1	2.84	0.45
1:C:108:ARG:HG2	1:C:140:TYR:CG	2.46	0.45
2:D:17:SER:HB2	2:D:83:MET:O	2.17	0.45
1:A:135:PHE:HZ	2:B:173:ARG:CB	2.30	0.45
2:D:24:ALA:HB3	2:D:77:ASN:O	2.17	0.45
2:D:204:CYS:SG	2:D:216:ILE:HG22	2.55	0.45
2:D:209:PRO:O	2:D:211:SER:N	2.40	0.45
1:A:111:ALA:O	1:A:200:THR:HG21	2.17	0.44
1:C:12:SER:OG	1:C:105:GLU:HB2	2.09	0.44
1:C:59:PRO:O	1:C:62:PHE:HB2	2.18	0.44
1:C:85:THR:HA	1:C:102:THR:O	2.16	0.44
1:A:32:PHE:CD2	2:B:106:LEU:HD12	2.40	0.44
1:A:144:ILE:HG23	1:A:144:ILE:HD13	1.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:VAL:HG21	1:C:78:LEU:HD22	1.99	0.44
2:D:137:CYS:HA	2:D:197:TRP:CZ3	2.52	0.44
2:D:147:LEU:HD11	2:D:217:LYS:HZ3	1.82	0.44
1:A:7:ILE:O	1:A:8:THR:CB	2.65	0.44
2:B:2:VAL:HG12	2:B:111:TYR:CD1	2.52	0.44
2:B:102:GLY:HA3	2:B:108:TYR:HH	1.77	0.44
2:B:106:LEU:HD12	2:B:106:LEU:HA	1.75	0.44
2:B:130:VAL:CG2	2:B:214:ASP:HB2	2.47	0.44
2:B:146:THR:CB	2:B:191:THR:HG22	2.47	0.44
2:B:162:LYS:HA	2:B:162:LYS:HD2	1.26	0.44
1:C:9:SER:CA	1:C:102:THR:HA	2.42	0.44
2:D:97:THR:HG22	2:D:111:TYR:O	2.17	0.44
2:B:11:LEU:C	2:B:11:LEU:HD23	2.43	0.44
2:B:143:SER:CB	2:B:194:SER:OG	2.65	0.44
2:B:212:LYS:HZ2	2:B:213:THR:C	2.25	0.44
1:C:32:PHE:CB	2:D:106:LEU:HD13	2.47	0.44
1:C:98:PHE:HZ	2:D:109:PHE:HE2	1.64	0.44
2:D:58:ILE:HG21	2:D:60:TYR:CE2	2.52	0.44
1:A:30:GLY:C	1:A:32:PHE:HD1	2.25	0.44
1:A:57:GLY:CA	2:D:214:ASP:OD1	2.65	0.44
1:A:64:GLY:C	1:A:65:TRP:CD1	2.95	0.44
2:B:106:LEU:C	2:B:107:TYR:CD1	2.88	0.44
2:D:50:TYR:N	2:D:70:ILE:CD1	2.81	0.44
1:A:47:LEU:HD23	1:A:58:VAL:HG21	2.00	0.44
2:B:2:VAL:O	2:B:2:VAL:CG1	2.63	0.44
2:B:138:SER:O	2:B:145:VAL:CG2	2.61	0.44
2:D:145:VAL:HG11	2:D:197:TRP:CZ3	2.52	0.44
2:B:48:VAL:CG2	2:B:64:VAL:HG11	2.48	0.44
2:B:139:ASP:O	2:B:145:VAL:HG12	2.17	0.44
1:A:144:ILE:HD12	1:A:144:ILE:HG21	1.60	0.44
2:D:33:GLY:HA3	2:D:50:TYR:HE2	1.83	0.44
2:D:126:THR:HG21	2:D:183:PHE:CE2	2.53	0.44
2:D:144:SER:C	2:D:145:VAL:HG22	2.43	0.44
1:A:112:ALA:HB1	1:A:113:PRO:HD2	1.99	0.44
2:B:198:PRO:O	2:B:199:SER:C	2.61	0.43
1:C:190:ASN:O	1:C:192:TYR:HD2	1.94	0.43
2:D:70:ILE:HG21	2:D:70:ILE:HD13	1.37	0.43
2:B:17:SER:HB3	2:B:84:THR:CA	2.45	0.43
2:B:51:ILE:HB	2:B:70:ILE:CG2	2.48	0.43
2:B:217:LYS:O	2:B:217:LYS:HD3	2.18	0.43
1:C:85:THR:HG23	1:C:87:PHE:CZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:CD	2:D:82:GLN:CD	2.87	0.43
2:D:20:LEU:HD13	2:D:83:MET:CE	2.48	0.43
1:A:111:ALA:C	1:A:200:THR:HG21	2.43	0.43
1:A:148:TRP:CZ2	1:A:194:CYS:HB2	2.53	0.43
2:B:11:LEU:HD23	2:B:12:VAL:N	2.33	0.43
2:B:110:ASP:OD2	2:B:111:TYR:CD2	2.68	0.43
1:C:169:LYS:NZ	1:C:170:ASP:HB3	2.33	0.43
2:D:20:LEU:N	2:D:81:LEU:O	2.35	0.43
2:D:94:TYR:O	2:D:115:GLY:HA2	2.19	0.43
2:D:146:THR:HA	2:D:191:THR:HA	1.99	0.43
1:A:7:ILE:O	1:A:8:THR:HB	2.19	0.43
1:A:182:THR:HG22	1:A:184:ASP:N	2.33	0.43
2:B:2:VAL:HG11	2:B:111:TYR:CD1	2.54	0.43
2:B:68:PHE:CD2	2:B:83:MET:HG2	2.48	0.43
1:C:41:ASP:O	1:C:41:ASP:OD1	2.35	0.43
1:C:61:ARG:HB3	1:C:75:ILE:HG23	1.99	0.43
1:C:65:TRP:HZ2	1:C:74:THR:CB	2.30	0.43
1:C:163:TRP:CZ2	1:C:175:MET:HE2	2.54	0.43
2:D:74:ASN:O	2:D:75:PRO:C	2.62	0.43
1:A:135:PHE:HD1	2:B:189:LEU:CG	2.25	0.43
1:A:151:ASP:OD2	1:A:191:SER:N	2.43	0.43
2:B:130:VAL:HG23	2:B:214:ASP:HB3	1.98	0.43
1:C:182:THR:HG22	1:C:184:ASP:H	1.83	0.43
1:A:22:SER:HA	1:A:72:SER:CA	2.48	0.43
1:A:47:LEU:C	1:A:48:ILE:HG13	2.42	0.43
2:D:45:LEU:HA	2:D:45:LEU:HD23	1.56	0.43
2:D:100:GLY:HA3	2:D:108:TYR:CZ	2.54	0.43
2:B:209:PRO:O	2:B:211:SER:N	2.42	0.43
1:C:153:SER:O	1:C:154:GLU:C	2.49	0.43
2:D:100:GLY:C	2:D:102:GLY:N	2.65	0.43
2:D:129:SER:O	2:D:152:LYS:N	2.48	0.43
1:A:150:ILE:CG2	1:A:189:HIS:CG	2.99	0.43
1:A:137:ASN:O	1:A:138:ASN:C	2.61	0.43
1:C:49:TYR:O	1:C:50:TYR:C	2.62	0.43
1:A:135:PHE:CZ	2:B:173:ARG:HG3	2.54	0.42
1:C:199:LYS:O	1:C:199:LYS:HG2	2.16	0.42
2:D:13:GLN:HA	2:D:14:PRO:HD3	1.66	0.42
2:D:150:LEU:CD1	2:D:152:LYS:HB2	2.44	0.42
1:A:59:PRO:HD2	1:A:59:PRO:O	2.18	0.42
1:A:125:LEU:HA	1:A:129:GLY:O	2.19	0.42
2:B:2:VAL:CG1	2:B:111:TYR:CE1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLY:CA	2:D:107:TYR:HB2	2.49	0.42
1:C:181:LEU:HD12	1:C:186:TYR:HD2	1.84	0.42
1:A:47:LEU:HD23	1:A:58:VAL:CG2	2.49	0.42
1:A:124:GLN:O	1:A:125:LEU:C	2.62	0.42
2:B:22:CYS:O	2:B:78:THR:CA	2.66	0.42
2:B:164:ASN:O	2:B:164:ASN:CG	2.62	0.42
2:D:202:VAL:O	2:D:203:ILE:HG13	2.19	0.42
2:D:212:LYS:HE3	2:D:214:ASP:CB	2.49	0.42
2:B:29:PHE:C	2:B:31:ASN:N	2.78	0.42
2:B:45:LEU:HD23	2:B:45:LEU:HA	1.75	0.42
2:B:70:ILE:HG23	2:B:70:ILE:HD13	1.19	0.42
2:B:203:ILE:CG2	2:B:215:LEU:HD11	2.47	0.42
1:C:110:ASP:OD2	1:C:199:LYS:CE	2.67	0.42
2:D:1:ASP:O	2:D:1:ASP:OD1	2.37	0.42
2:D:74:ASN:C	2:D:77:ASN:CB	2.92	0.42
1:A:107:LYS:HA	1:A:140:TYR:CZ	2.55	0.42
2:B:38:ARG:O	2:B:46:GLU:N	2.44	0.42
1:C:14:SER:C	1:C:15:LEU:O	2.52	0.42
1:A:156:GLN:HB3	1:A:157:ASN:H	1.67	0.42
1:C:169:LYS:HZ2	1:C:170:ASP:HB3	1.85	0.42
2:D:34:MET:CA	2:D:34:MET:HE3	2.44	0.42
1:A:30:GLY:C	1:A:32:PHE:CD1	2.98	0.42
2:B:91:THR:CB	2:B:120:VAL:H	2.22	0.42
2:D:17:SER:HA	2:D:86:LEU:HD11	2.02	0.42
2:D:17:SER:CB	2:D:83:MET:O	2.68	0.42
1:A:34:ASN:HD22	1:A:89:GLN:HE21	1.67	0.42
1:A:148:TRP:CH2	1:A:194:CYS:HB2	2.54	0.42
1:A:173:TYR:HD2	1:A:173:TYR:H	1.67	0.42
2:B:163:TRP:CE3	2:B:203:ILE:O	2.72	0.42
1:C:29:ILE:CG1	1:C:90:GLN:CB	2.93	0.42
1:C:136:LEU:O	1:C:175:MET:N	2.40	0.42
2:D:101:THR:O	2:D:101:THR:HG22	2.20	0.42
2:D:171:GLY:O	2:D:190:VAL:HG23	2.20	0.42
1:A:49:TYR:CE2	1:A:53:ARG:CB	3.03	0.42
2:B:60:TYR:OH	2:B:70:ILE:N	2.44	0.42
2:D:51:ILE:O	2:D:51:ILE:HG23	2.19	0.42
2:D:92:ALA:O	2:D:117:THR:CA	2.68	0.42
2:D:125:THR:HG23	2:D:155:PHE:O	2.19	0.42
2:D:196:THR:HA	2:D:200:GLN:OE1	2.20	0.42
1:A:155:ARG:NE	1:A:157:ASN:O	2.53	0.42
2:B:20:LEU:HD21	2:B:94:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG11	2:B:112:TRP:HH2	1.84	0.42
2:B:88:SER:C	2:B:90:ASP:H	2.28	0.42
1:C:46:LEU:CD1	1:C:49:TYR:HD1	2.33	0.42
2:D:27:PHE:CE2	2:D:32:PHE:CE1	3.08	0.42
2:D:88:SER:C	2:D:90:ASP:H	2.26	0.42
1:A:6:GLN:NE2	1:A:86:PHE:O	2.48	0.41
1:A:197:THR:O	1:A:198:HIS:CB	2.65	0.41
2:B:17:SER:CA	2:B:86:LEU:HD12	2.50	0.41
1:C:6:GLN:CD	1:C:101:GLY:H	2.25	0.41
1:C:39:LYS:HB2	1:C:41:ASP:O	2.20	0.41
1:C:135:PHE:C	1:C:136:LEU:HD12	2.45	0.41
1:A:121:SER:O	1:A:125:LEU:CG	2.63	0.41
2:B:50:TYR:HD1	2:B:59:ASN:HB3	1.85	0.41
1:C:53:ARG:HD3	1:C:53:ARG:HA	1.81	0.41
1:C:93:THR:O	1:C:96:TYR:CD2	2.73	0.41
1:A:3:GLN:H	1:A:26:SER:HB3	1.85	0.41
1:A:60:SER:C	1:C:126:THR:CG2	2.93	0.41
1:A:60:SER:C	1:C:126:THR:HG23	2.45	0.41
2:B:70:ILE:HG21	2:B:70:ILE:HD12	1.41	0.41
2:D:72:ARG:CD	2:D:74:ASN:OD1	2.68	0.41
1:A:88:CYS:SG	1:A:99:GLY:HA3	2.60	0.41
1:C:7:ILE:O	1:C:8:THR:CB	2.68	0.41
1:A:65:TRP:CD1	1:A:72:SER:O	2.74	0.41
1:C:66:GLY:HA3	1:C:71:TYR:HB3	2.03	0.41
1:C:93:THR:O	1:C:94:LEU:HD12	2.19	0.41
2:D:148:GLY:HA3	2:D:189:LEU:HD13	2.03	0.41
2:D:192:VAL:HA	2:D:193:PRO:HD3	1.59	0.41
2:D:203:ILE:HG23	2:D:215:LEU:HG	2.03	0.41
1:A:31:ASN:HA	1:A:71:TYR:CZ	2.54	0.41
2:B:51:ILE:HG12	2:B:52:SER:N	2.36	0.41
2:B:202:VAL:C	2:B:203:ILE:HG13	2.44	0.41
1:C:29:ILE:HD12	1:C:29:ILE:HA	1.38	0.41
1:C:89:GLN:HB3	1:C:98:PHE:CG	2.56	0.41
1:C:115:VAL:CG2	1:C:205:ILE:CG2	2.98	0.41
1:C:196:ALA:H	1:C:205:ILE:HG22	1.86	0.41
2:D:67:ARG:NH2	2:D:90:ASP:OD1	2.49	0.41
1:A:102:THR:O	1:A:103:LYS:C	2.58	0.41
1:C:147:LYS:O	1:C:195:GLU:N	2.51	0.41
2:D:10:GLY:CA	2:D:18:ARG:HH12	2.12	0.41
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.54	0.41
1:A:64:GLY:C	1:A:65:TRP:CG	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:SER:OG	1:A:180:THR:HA	2.21	0.41
2:B:39:GLN:O	2:B:93:ILE:HD12	2.20	0.41
2:B:128:PRO:HD2	2:B:212:LYS:HG2	2.02	0.41
1:C:183:LYS:O	1:C:183:LYS:CG	2.68	0.41
2:D:39:GLN:HB2	2:D:45:LEU:CD2	2.51	0.41
2:D:93:ILE:CG1	2:D:117:THR:HB	2.47	0.41
2:D:111:TYR:CE1	2:D:112:TRP:O	2.73	0.41
2:D:123:ALA:HB3	2:D:155:PHE:CZ	2.56	0.41
2:D:143:SER:C	2:D:144:SER:O	2.59	0.41
1:A:48:ILE:HD11	1:A:54:LEU:HD12	2.03	0.41
1:A:112:ALA:CB	1:A:113:PRO:HD2	2.49	0.41
2:B:19:LYS:HA	2:B:81:LEU:O	2.21	0.41
2:B:20:LEU:O	2:B:80:PHE:HA	2.20	0.41
2:B:21:SER:HA	2:B:80:PHE:HA	2.02	0.41
2:B:61:ALA:C	2:B:63:THR:H	2.29	0.41
2:B:154:TYR:CD1	2:B:154:TYR:N	2.88	0.41
1:C:61:ARG:CB	1:C:75:ILE:HG23	2.51	0.41
1:C:80:GLU:C	1:C:82:ASP:N	2.79	0.41
1:C:106:ILE:HB	1:C:166:GLN:NE2	2.36	0.41
1:C:106:ILE:HG22	1:C:166:GLN:NE2	2.34	0.41
2:D:179:LEU:HD23	2:D:180:GLN:HA	2.03	0.41
1:C:35:TRP:CE3	1:C:73:LEU:HD23	2.56	0.41
1:C:106:ILE:HB	1:C:166:GLN:OE1	2.21	0.41
1:C:166:GLN:O	1:C:168:SER:N	2.54	0.41
2:D:126:THR:HG22	2:D:127:ALA:O	2.21	0.41
2:B:65:LYS:HD2	2:B:65:LYS:HA	1.61	0.40
2:B:71:SER:HB2	2:B:80:PHE:HB2	2.02	0.40
2:B:98:ARG:NH1	2:B:111:TYR:CE2	2.90	0.40
1:C:80:GLU:C	1:C:82:ASP:H	2.26	0.40
1:C:99:GLY:O	1:C:100:GLY:C	2.64	0.40
2:D:17:SER:HB3	2:D:84:THR:CA	2.47	0.40
1:A:42:GLY:O	1:A:43:SER:C	2.58	0.40
2:B:34:MET:HB3	2:B:79:LEU:HD22	2.04	0.40
1:C:10:SER:CA	1:C:103:LYS:O	2.67	0.40
2:D:73:ASP:OD1	2:D:73:ASP:C	2.64	0.40
2:D:86:LEU:HD22	2:D:118:LEU:CD2	2.50	0.40
2:D:129:SER:O	2:D:151:VAL:HA	2.21	0.40
2:D:209:PRO:C	2:D:211:SER:H	2.28	0.40
1:A:134:CYS:CB	1:A:148:TRP:CZ2	3.01	0.40
1:A:137:ASN:OD1	2:B:173:ARG:HG3	2.22	0.40
2:B:64:VAL:O	2:B:68:PHE:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:PRO:HB2	2:B:139:ASP:CG	2.46	0.40
1:C:11:LEU:O	1:C:104:LEU:HA	2.21	0.40
2:D:136:GLY:O	2:D:137:CYS:SG	2.80	0.40
1:A:70:ASP:C	1:A:71:TYR:HD1	2.26	0.40
1:A:111:ALA:CA	1:A:200:THR:HG21	2.52	0.40
1:A:181:LEU:HD23	1:A:181:LEU:HA	1.66	0.40
2:B:36:TRP:HB3	2:B:48:VAL:HG12	2.03	0.40
2:B:130:VAL:CG2	2:B:206:VAL:CG2	2.96	0.40
1:C:24:ARG:HH11	1:C:70:ASP:CG	2.28	0.40
1:C:55:GLN:HG3	1:C:56:SER:OG	2.20	0.40
1:C:96:TYR:CZ	2:D:107:TYR:CG	3.10	0.40
1:C:164:THR:HG22	2:D:175:VAL:HG23	2.04	0.40
2:D:34:MET:HE2	2:D:34:MET:CA	2.13	0.40
2:D:111:TYR:C	2:D:111:TYR:CD1	3.00	0.40
1:A:16:GLY:HA2	1:A:77:ASN:OD1	2.21	0.40
1:A:28:ASP:C	1:A:29:ILE:HD13	2.46	0.40
2:B:12:VAL:O	2:B:120:VAL:HA	2.22	0.40
1:C:50:TYR:HD2	1:C:53:ARG:NH2	2.19	0.40
1:C:54:LEU:HD11	1:C:58:VAL:CG1	2.51	0.40
2:D:60:TYR:OH	2:D:69:THR:CA	2.40	0.40

All (2) 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:1:ASP:N	1:C:77:ASN:OD1[2_656]	2.01	0.19
2:B:124:THR:CG2	1:C:156:GLN:NE2[1_565]	2.04	0.16

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	204/206 (99%)	166 (81%)	26 (13%)	12 (6%)	1	8
1	C	204/206 (99%)	162 (79%)	24 (12%)	18 (9%)	0	3
2	B	215/217 (99%)	163 (76%)	26 (12%)	26 (12%)	0	1
2	D	215/217 (99%)	169 (79%)	25 (12%)	21 (10%)	0	3
All	All	838/846 (99%)	660 (79%)	101 (12%)	77 (9%)	0	3

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	51	THR
1	A	80	GLU
1	A	199	LYS
2	B	42	GLU
2	B	105	SER
2	B	170	SER
2	B	194	SER
2	B	209	PRO
2	B	211	SER
1	C	8	THR
1	C	31	ASN
1	C	51	THR
1	C	78	LEU
1	C	81	GLU
1	C	151	ASP
2	D	42	GLU
2	D	75	PRO
2	D	88	SER
2	D	123	ALA
2	D	128	PRO
2	D	137	CYS
2	D	138	SER
2	D	167	ALA
2	D	169	SER
2	D	170	SER
2	D	197	TRP
2	D	216	ILE
1	A	8	THR
1	A	26	SER
1	A	123	GLU
1	A	171	SER
1	A	188	ARG

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Mol	Chain	Res	Type
1	A	198	HIS
2	B	2	VAL
2	B	54	GLY
2	B	62	ASP
2	B	73	ASP
2	B	89	GLU
2	B	100	GLY
2	B	125	THR
2	B	139	ASP
1	C	40	PRO
1	C	42	GLY
1	C	57	GLY
1	C	68	GLY
1	C	199	LYS
2	D	48	VAL
1	A	138	ASN
2	B	7	SER
2	B	30	SER
2	B	104	ARG
2	B	135	PRO
2	B	210	ALA
1	C	43	SER
1	C	80	GLU
1	C	113	PRO
2	B	169	SER
2	B	199	SER
1	C	84	ALA
2	D	211	SER
1	C	141	PRO
2	D	2	VAL
2	D	41	PRO
2	D	127	ALA
2	B	144	SER
2	D	100	GLY
2	D	144	SER
1	A	100	GLY
2	D	16	GLY
2	D	99	GLY
2	B	166	GLY
1	C	144	ILE
2	B	197	TRP
2	B	216	ILE

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Mol	Chain	Res	Type
1	C	30	GLY
2	B	74	ASN

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	184/184 (100%)	128 (70%)	56 (30%)	0	0
1	C	184/184 (100%)	134 (73%)	50 (27%)	0	1
2	B	181/181 (100%)	126 (70%)	55 (30%)	0	0
2	D	181/181 (100%)	122 (67%)	59 (33%)	0	0
All	All	730/730 (100%)	510 (70%)	220 (30%)	0	1

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	4	MET
1	A	5	THR
1	A	7	ILE
1	A	10	SER
1	A	11	LEU
1	A	13	VAL
1	A	15	LEU
1	A	17	ASP
1	A	27	GLN
1	A	29	ILE
1	A	39	LYS
1	A	40	PRO
1	A	41	ASP
1	A	43	SER
1	A	44	LEU
1	A	46	LEU
1	A	49	TYR
1	A	54	LEU

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Mol	Chain	Res	Type
1	A	55	GLN
1	A	58	VAL
1	A	65	TRP
1	A	71	TYR
1	A	72	SER
1	A	76	SER
1	A	77	ASN
1	A	78	LEU
1	A	80	GLU
1	A	81	GLU
1	A	83	ILE
1	A	85	THR
1	A	89	GLN
1	A	106	ILE
1	A	114	THR
1	A	119	PRO
1	A	120	PRO
1	A	122	SER
1	A	126	THR
1	A	135	PHE
1	A	136	LEU
1	A	142	LYS
1	A	144	ILE
1	A	147	LYS
1	A	160	LEU
1	A	162	SER
1	A	163	TRP
1	A	164	THR
1	A	168	SER
1	A	171	SER
1	A	173	TYR
1	A	179	LEU
1	A	183	LYS
1	A	184	ASP
1	A	194	CYS
1	A	204	PRO
1	A	205	ILE
2	B	7	SER
2	B	13	GLN
2	B	17	SER
2	B	20	LEU
2	B	28	THR

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Mol	Chain	Res	Type
2	B	31	ASN
2	B	37	VAL
2	B	48	VAL
2	B	51	ILE
2	B	56	SER
2	B	63	THR
2	B	67	ARG
2	B	70	ILE
2	B	77	ASN
2	B	84	THR
2	B	85	SER
2	B	89	GLU
2	B	93	ILE
2	B	97	THR
2	B	98	ARG
2	B	101	THR
2	B	103	THR
2	B	114	GLN
2	B	117	THR
2	B	126	THR
2	B	135	PRO
2	B	144	SER
2	B	145	VAL
2	B	147	LEU
2	B	150	LEU
2	B	151	VAL
2	B	152	LYS
2	B	154	TYR
2	B	158	PRO
2	B	168	LEU
2	B	170	SER
2	B	172	VAL
2	B	178	VAL
2	B	179	LEU
2	B	180	GLN
2	B	185	SER
2	B	186	LEU
2	B	191	THR
2	B	192	VAL
2	B	194	SER
2	B	195	SER
2	B	196	THR

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Mol	Chain	Res	Type
2	B	199	SER
2	B	202	VAL
2	B	204	CYS
2	B	205	ASN
2	B	212	LYS
2	B	213	THR
2	B	216	ILE
2	B	217	LYS
1	C	4	MET
1	C	7	ILE
1	C	10	SER
1	C	12	SER
1	C	13	VAL
1	C	15	LEU
1	C	17	ASP
1	C	20	ILE
1	C	22	SER
1	C	24	ARG
1	C	27	GLN
1	C	40	PRO
1	C	44	LEU
1	C	48	ILE
1	C	60	SER
1	C	65	TRP
1	C	67	SER
1	C	71	TYR
1	C	72	SER
1	C	78	LEU
1	C	79	GLU
1	C	80	GLU
1	C	81	GLU
1	C	83	ILE
1	C	89	GLN
1	C	95	PRO
1	C	103	LYS
1	C	105	GLU
1	C	107	LYS
1	C	108	ARG
1	C	114	THR
1	C	123	GLU
1	C	126	THR
1	C	131	SER

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Mol	Chain	Res	Type
1	C	141	PRO
1	C	142	LYS
1	C	143	ASP
1	C	169	LYS
1	C	172	THR
1	C	175	MET
1	C	178	THR
1	C	179	LEU
1	C	182	THR
1	C	190	ASN
1	C	193	THR
1	C	197	THR
1	C	200	THR
1	C	202	THR
1	C	205	ILE
1	C	206	VAL
2	D	3	GLN
2	D	4	LEU
2	D	11	LEU
2	D	13	GLN
2	D	17	SER
2	D	18	ARG
2	D	20	LEU
2	D	30	SER
2	D	34	MET
2	D	39	GLN
2	D	48	VAL
2	D	56	SER
2	D	59	ASN
2	D	64	VAL
2	D	65	LYS
2	D	69	THR
2	D	70	ILE
2	D	71	SER
2	D	77	ASN
2	D	87	ARG
2	D	91	THR
2	D	93	ILE
2	D	101	THR
2	D	103	THR
2	D	105	SER
2	D	114	GLN

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Mol	Chain	Res	Type
2	D	122	SER
2	D	128	PRO
2	D	132	PRO
2	D	135	PRO
2	D	139	ASP
2	D	144	SER
2	D	145	VAL
2	D	147	LEU
2	D	149	CYS
2	D	151	VAL
2	D	152	LYS
2	D	156	PRO
2	D	159	VAL
2	D	162	LYS
2	D	168	LEU
2	D	170	SER
2	D	173	ARG
2	D	175	VAL
2	D	178	VAL
2	D	179	LEU
2	D	180	GLN
2	D	184	TYR
2	D	189	LEU
2	D	191	THR
2	D	194	SER
2	D	195	SER
2	D	199	SER
2	D	200	GLN
2	D	201	THR
2	D	202	VAL
2	D	203	ILE
2	D	215	LEU
2	D	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	37	GLN
1	A	89	GLN
1	A	190	ASN
2	B	59	ASN

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Mol	Chain	Res	Type
2	B	164	ASN
2	B	180	GLN
2	B	208	HIS
1	C	27	GLN
1	C	31	ASN
1	C	34	ASN
1	C	77	ASN
1	C	166	GLN
1	C	190	ASN
2	D	3	GLN
2	D	59	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	206/206 (100%)	-0.47	1 (0%) 87 73	28, 28, 28, 28	0
1	C	206/206 (100%)	-0.56	0 100 100	28, 28, 28, 28	0
2	B	217/217 (100%)	-0.41	3 (1%) 73 53	28, 28, 28, 28	0
2	D	217/217 (100%)	-0.38	6 (2%) 55 34	28, 28, 28, 28	0
All	All	846/846 (100%)	-0.45	10 (1%) 76 58	28, 28, 28, 28	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	166	GLY	4.3
2	B	140	THR	3.1
2	D	1	ASP	3.0
2	D	142	GLY	2.9
2	D	169	SER	2.3
2	D	195	SER	2.3
1	A	12	SER	2.3
2	B	138	SER	2.2
2	D	164	ASN	2.2
2	B	141	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.