



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:56 PM UTC

PDB ID : 4CPA / pdb_00004cpa
Title : REFINED CRYSTAL STRUCTURE OF THE POTATO INHIBITOR COM-
PLEX OF CARBOXYPEPTIDASE A AT 2.5 ANGSTROMS RESOLUTION
Authors : Lipscomb, W.N.; Rees, D.C.
Deposited on : 1982-03-24
Resolution : 2.50 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

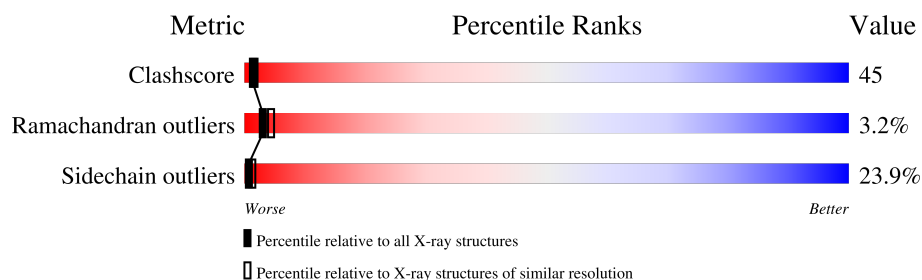
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	307	22% 34% 31% 13%
1	B	307	21% 35% 31% 12%
2	I	38	5% 39% 26% 26% .
2	J	38	5% 39% 26% 26% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLY	A	308	-	X	-	-
3	GLY	B	308	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5456 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 CARBOXYPEPTIDASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			
1	B	307	Total	C	N	O	S	0	0	0
			2437	1561	406	465	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	GLN	GLU	conflict	UNP P00730
A	31	GLU	GLN	conflict	UNP P00730
A	89	ASN	ASP	conflict	UNP P00730
A	93	ASN	ASP	conflict	UNP P00730
A	114	ASN	ASP	conflict	UNP P00730
A	122	GLU	GLN	conflict	UNP P00730
A	185	ASN	ASP	conflict	UNP P00730
A	228	ALA	GLU	conflict	UNP P00730
A	305	VAL	LEU	conflict	UNP P00730
B	28	GLN	GLU	conflict	UNP P00730
B	31	GLU	GLN	conflict	UNP P00730
B	89	ASN	ASP	conflict	UNP P00730
B	93	ASN	ASP	conflict	UNP P00730
B	114	ASN	ASP	conflict	UNP P00730
B	122	GLU	GLN	conflict	UNP P00730
B	185	ASN	ASP	conflict	UNP P00730
B	228	ALA	GLU	conflict	UNP P00730
B	305	VAL	LEU	conflict	UNP P00730

- Molecule 2 is a protein called METALLOCARBOXYPEPTIDASE INHIBITOR.

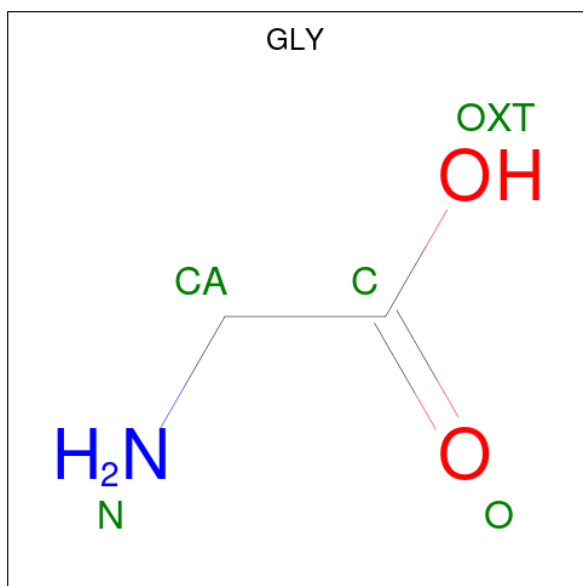
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	37	Total	C	N	O	S	0	0	0
			285	174	51	52	6			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	J	37	Total	C	N	O	S	X	0	0	0
			285	174	51	52	6	2			

- Molecule 3 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	2	1	2		
3	B	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

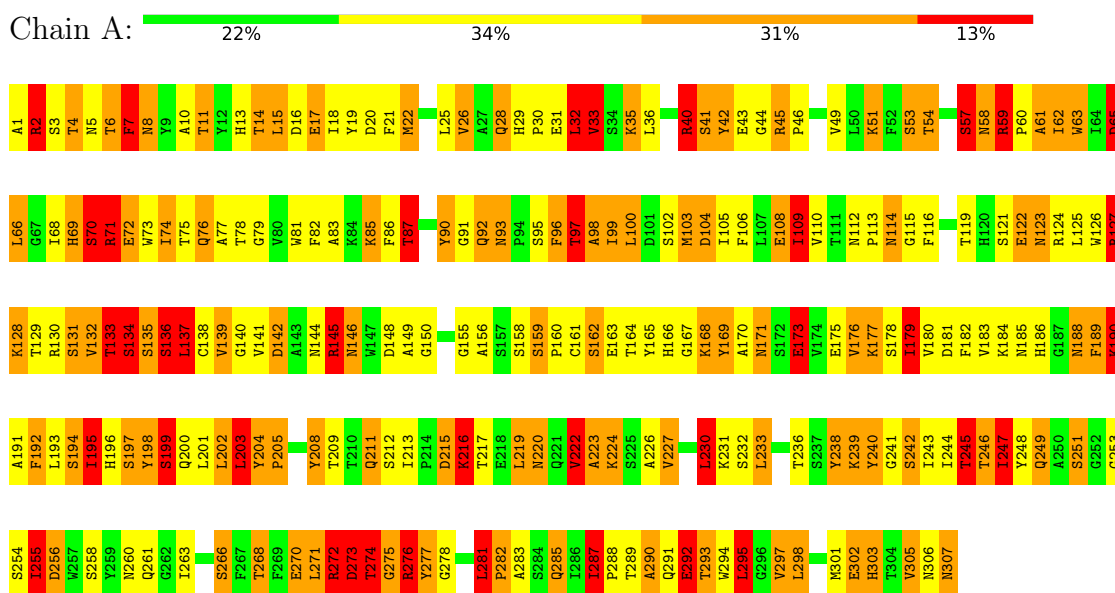
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	1	Total	Zn	0	0
			1	1		
4	J	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

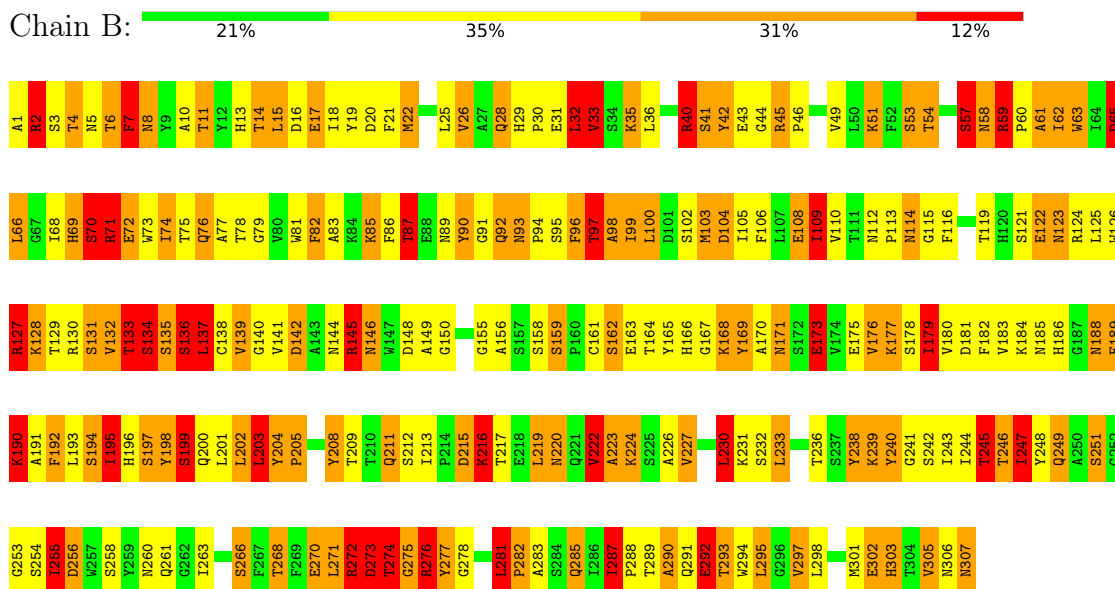
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

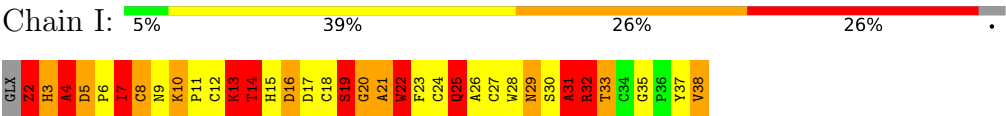
• Molecule 1: CARBOXYPEPTIDASE A



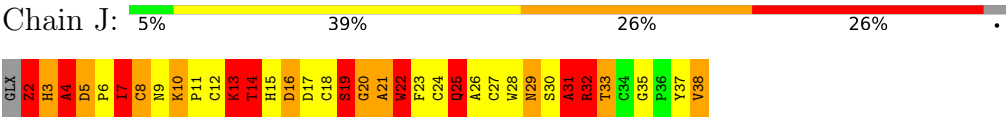
• Molecule 1: CARBOXYPEPTIDASE A



● Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR



● Molecule 2: METALLOCARBOXYPEPTIDASE INHIBITOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	53.45Å 53.45Å 218.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5456	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.63	21/2503 (0.8%)	3.28	351/3402 (10.3%)
1	B	1.63	20/2503 (0.8%)	3.28	352/3402 (10.3%)
2	I	1.85	4/287 (1.4%)	3.42	51/392 (13.0%)
2	J	1.85	4/287 (1.4%)	3.42	51/392 (13.0%)
All	All	1.66	49/5580 (0.9%)	3.29	805/7588 (10.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	B	0	12
2	I	0	3
2	J	0	3
All	All	0	30

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GLX	C-N	-10.96	1.32	1.43
2	J	2	GLX	C-N	-10.93	1.32	1.43
1	A	167	GLY	N-CA	7.63	1.53	1.45
1	B	167	GLY	N-CA	7.58	1.53	1.45
1	A	135	SER	N-CA	7.10	1.55	1.46
1	B	135	SER	N-CA	7.03	1.55	1.46
2	J	22	TRP	C-O	6.96	1.32	1.24
2	I	22	TRP	C-O	6.90	1.32	1.24
1	A	305	VAL	N-CA	6.80	1.54	1.46
1	B	305	VAL	N-CA	6.78	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2	ARG	CA-CB	-6.63	1.43	1.53
1	A	2	ARG	CA-CB	-6.59	1.43	1.53
1	A	2	ARG	CA-C	6.47	1.61	1.52
1	B	2	ARG	CA-C	6.45	1.61	1.52
1	A	253	GLY	N-CA	6.08	1.52	1.45
1	B	253	GLY	N-CA	6.03	1.52	1.45
1	A	293	THR	C-O	5.90	1.31	1.24
1	B	293	THR	C-O	5.81	1.31	1.24
1	B	73	TRP	N-CA	5.76	1.53	1.46
1	A	54	THR	N-CA	5.72	1.52	1.46
1	A	73	TRP	N-CA	5.70	1.53	1.46
1	B	54	THR	N-CA	5.65	1.52	1.46
1	A	109	ILE	CA-CB	5.58	1.62	1.54
1	B	109	ILE	CA-CB	5.54	1.61	1.54
1	B	176	VAL	C-N	-5.42	1.26	1.33
1	B	137	LEU	N-CA	-5.41	1.38	1.45
1	A	272	ARG	C-N	-5.39	1.25	1.33
1	A	176	VAL	C-N	-5.37	1.26	1.33
1	B	302	GLU	CD-OE2	5.37	1.35	1.25
1	B	136	SER	C-N	-5.36	1.25	1.33
1	B	272	ARG	C-N	-5.36	1.25	1.33
1	A	121	SER	C-N	-5.35	1.26	1.33
1	A	137	LEU	N-CA	-5.35	1.38	1.45
1	A	302	GLU	CD-OE2	5.35	1.35	1.25
1	A	136	SER	C-N	-5.34	1.25	1.33
1	B	196	HIS	CE1-NE2	-5.34	1.27	1.32
1	B	121	SER	C-N	-5.32	1.26	1.33
1	A	134	SER	C-O	5.30	1.30	1.24
2	J	33	THR	C-O	5.28	1.29	1.23
1	A	196	HIS	CE1-NE2	-5.27	1.27	1.32
1	B	134	SER	C-O	5.24	1.30	1.24
2	I	15	HIS	N-CA	5.23	1.52	1.46
2	J	15	HIS	N-CA	5.19	1.52	1.46
2	I	33	THR	C-O	5.14	1.29	1.23
1	A	276	ARG	C-O	-5.13	1.18	1.24
1	A	276	ARG	CA-CB	-5.09	1.45	1.53
1	B	276	ARG	C-O	-5.09	1.18	1.24
1	B	276	ARG	CA-CB	-5.04	1.45	1.53
1	A	66	LEU	N-CA	5.02	1.52	1.45

All (805) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	SER	CA-C-N	30.24	169.72	122.24
1	A	136	SER	C-N-CA	30.24	169.72	122.24
1	B	136	SER	CA-C-N	30.21	169.67	122.24
1	B	136	SER	C-N-CA	30.21	169.67	122.24
1	A	2	ARG	CA-CB-CG	25.73	165.56	114.10
1	B	2	ARG	CA-CB-CG	25.71	165.53	114.10
1	B	260	ASN	CA-CB-CG	16.56	129.16	112.60
1	A	260	ASN	CA-CB-CG	16.55	129.15	112.60
1	B	211	GLN	OE1-CD-NE2	16.36	138.96	122.60
1	A	211	GLN	OE1-CD-NE2	16.23	138.83	122.60
1	A	272	ARG	CA-C-N	15.93	150.38	121.70
1	A	272	ARG	C-N-CA	15.93	150.38	121.70
1	B	272	ARG	CA-C-N	15.91	150.34	121.70
1	B	272	ARG	C-N-CA	15.91	150.34	121.70
1	B	127	ARG	NE-CZ-NH2	15.24	132.91	119.20
1	A	127	ARG	NE-CZ-NH2	15.14	132.83	119.20
2	J	5	ASP	CA-CB-CG	-14.85	97.75	112.60
2	I	5	ASP	CA-CB-CG	-14.81	97.79	112.60
2	I	28	TRP	CA-C-O	-14.05	105.93	120.54
2	J	28	TRP	CA-C-O	-13.98	106.00	120.54
1	B	137	LEU	CA-C-N	13.80	142.46	123.00
1	B	137	LEU	C-N-CA	13.80	142.46	123.00
1	A	137	LEU	CA-C-N	13.79	142.45	123.00
1	A	137	LEU	C-N-CA	13.79	142.45	123.00
1	B	65	ASP	CA-CB-CG	13.77	126.37	112.60
1	A	65	ASP	CA-CB-CG	13.73	126.33	112.60
1	A	137	LEU	CA-C-O	13.39	133.63	118.77
1	B	137	LEU	CA-C-O	13.34	133.58	118.77
1	A	302	GLU	CB-CG-CD	13.09	134.86	112.60
1	B	302	GLU	CB-CG-CD	13.07	134.82	112.60
1	A	93	ASN	CA-CB-CG	12.95	125.55	112.60
1	B	93	ASN	CA-CB-CG	12.94	125.54	112.60
1	B	127	ARG	NH1-CZ-NH2	-12.75	102.73	119.30
1	A	127	ARG	NH1-CZ-NH2	-12.74	102.74	119.30
1	B	5	ASN	OD1-CG-ND2	12.38	134.98	122.60
1	A	5	ASN	OD1-CG-ND2	12.29	134.89	122.60
1	A	96	PHE	CA-C-O	-11.88	108.35	120.82
1	B	96	PHE	CA-C-O	-11.86	108.37	120.82
1	B	179	ILE	O-C-N	11.76	134.06	121.94
1	A	179	ILE	O-C-N	11.74	134.03	121.94
2	J	8	CYS	CA-C-O	-11.69	108.29	121.15
2	I	8	CYS	CA-C-O	-11.66	108.32	121.15
1	B	136	SER	CA-C-O	11.54	134.45	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	SER	CA-C-O	11.51	134.41	120.60
1	B	98	ALA	CA-C-N	11.51	135.06	120.56
1	B	98	ALA	C-N-CA	11.51	135.06	120.56
1	A	98	ALA	CA-C-N	11.49	135.03	120.56
1	A	98	ALA	C-N-CA	11.49	135.03	120.56
2	J	15	HIS	CA-C-O	11.03	133.22	119.11
2	I	15	HIS	CA-C-O	11.02	133.21	119.11
2	J	32	ARG	CA-CB-CG	10.98	136.05	114.10
2	I	32	ARG	CA-CB-CG	10.96	136.03	114.10
1	A	179	ILE	N-CA-CB	10.96	122.57	110.62
1	B	179	ILE	N-CA-CB	10.96	122.57	110.62
1	A	256	ASP	CA-CB-CG	-10.86	101.74	112.60
1	B	256	ASP	CA-CB-CG	-10.83	101.77	112.60
2	I	20	GLY	O-C-N	10.74	136.66	122.70
2	J	20	GLY	O-C-N	10.71	136.63	122.70
1	B	305	VAL	CB-CA-C	10.59	126.43	112.24
1	A	305	VAL	CB-CA-C	10.59	126.42	112.24
1	A	181	ASP	CA-C-N	10.56	135.00	120.63
1	A	181	ASP	C-N-CA	10.56	135.00	120.63
1	B	181	ASP	CA-C-N	10.56	134.99	120.63
1	B	181	ASP	C-N-CA	10.56	134.99	120.63
1	B	270	GLU	CA-C-O	-10.55	109.18	120.46
1	B	247	ILE	N-CA-CB	10.53	128.61	111.23
1	A	270	GLU	CA-C-O	-10.53	109.19	120.46
1	A	247	ILE	N-CA-CB	10.51	128.56	111.23
1	A	73	TRP	CA-C-O	-10.50	109.29	120.63
1	B	73	TRP	CA-C-O	-10.50	109.29	120.63
1	A	253	GLY	CA-C-N	10.44	134.26	120.28
1	A	253	GLY	C-N-CA	10.44	134.26	120.28
1	B	253	GLY	CA-C-N	10.44	134.26	120.28
1	B	253	GLY	C-N-CA	10.44	134.26	120.28
1	A	113	PRO	CA-C-N	10.21	134.98	120.79
1	A	113	PRO	C-N-CA	10.21	134.98	120.79
1	B	113	PRO	CA-C-N	10.20	134.97	120.79
1	B	113	PRO	C-N-CA	10.20	134.97	120.79
1	B	62	ILE	CA-C-O	-10.14	109.54	120.59
1	A	62	ILE	CA-C-O	-10.12	109.56	120.59
2	J	29	ASN	CA-CB-CG	-10.05	102.55	112.60
1	A	282	PRO	O-C-N	-10.05	110.55	123.01
2	I	29	ASN	CA-CB-CG	-10.02	102.58	112.60
1	B	40	ARG	NE-CZ-NH1	9.98	131.49	121.50
1	A	40	ARG	NE-CZ-NH1	9.94	131.44	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	282	PRO	O-C-N	-9.93	110.70	123.01
2	J	13	LYS	CA-C-N	9.86	138.13	122.36
2	J	13	LYS	C-N-CA	9.86	138.13	122.36
2	I	13	LYS	CA-C-N	9.83	138.09	122.36
2	I	13	LYS	C-N-CA	9.83	138.09	122.36
1	B	71	ARG	NE-CZ-NH2	9.82	128.04	119.20
1	A	136	SER	O-C-N	-9.81	111.46	123.33
1	B	136	SER	O-C-N	-9.80	111.48	123.33
1	A	71	ARG	NE-CZ-NH2	9.76	127.99	119.20
1	A	137	LEU	N-CA-CB	-9.76	97.92	110.90
1	B	137	LEU	N-CA-CB	-9.76	97.93	110.90
1	A	282	PRO	CA-C-N	9.75	134.33	120.28
1	A	282	PRO	C-N-CA	9.75	134.33	120.28
1	B	282	PRO	CA-C-N	9.75	134.32	120.28
1	B	282	PRO	C-N-CA	9.75	134.32	120.28
1	B	165	TYR	CA-C-O	-9.63	109.94	120.92
2	I	21	ALA	N-CA-CB	-9.63	96.50	110.56
1	B	254	SER	CA-C-N	9.62	135.95	120.55
1	B	254	SER	C-N-CA	9.62	135.95	120.55
1	A	165	TYR	CA-C-O	-9.62	109.95	120.92
2	J	21	ALA	N-CA-CB	-9.60	96.54	110.56
1	A	254	SER	CA-C-N	9.58	135.88	120.55
1	A	254	SER	C-N-CA	9.58	135.88	120.55
1	A	127	ARG	CB-CG-CD	9.58	133.33	111.30
1	B	127	ARG	CB-CG-CD	9.56	133.30	111.30
2	I	35	GLY	O-C-N	9.44	131.21	121.77
2	J	35	GLY	O-C-N	9.41	131.18	121.77
1	A	133	THR	CB-CA-C	-9.31	91.90	110.42
1	B	133	THR	CB-CA-C	-9.31	91.90	110.42
1	B	287	ILE	O-C-N	9.30	126.37	120.42
1	A	281	LEU	CA-C-O	-9.26	111.53	119.59
1	B	177	LYS	CA-CB-CG	9.26	132.63	114.10
1	A	287	ILE	O-C-N	9.26	126.35	120.42
1	A	177	LYS	CA-CB-CG	9.26	132.62	114.10
1	B	281	LEU	CA-C-O	-9.26	111.53	119.59
1	B	247	ILE	CA-CB-CG1	9.21	126.05	110.40
1	A	185	ASN	O-C-N	9.19	133.29	122.17
1	A	247	ILE	CA-CB-CG1	9.18	126.00	110.40
1	B	185	ASN	O-C-N	9.17	133.26	122.17
1	A	276	ARG	CA-CB-CG	9.04	132.19	114.10
1	B	276	ARG	CA-CB-CG	9.03	132.16	114.10
1	B	58	ASN	N-CA-C	-9.02	99.61	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	PHE	N-CA-CB	9.01	123.07	110.01
1	B	96	PHE	N-CA-CB	9.01	123.07	110.01
1	B	273	ASP	CA-C-N	9.00	136.36	122.23
1	B	273	ASP	C-N-CA	9.00	136.36	122.23
1	A	273	ASP	CA-C-N	8.99	136.35	122.23
1	A	273	ASP	C-N-CA	8.99	136.35	122.23
1	A	58	ASN	N-CA-C	-8.99	99.66	110.44
1	A	62	ILE	CA-C-N	-8.98	109.91	122.93
1	A	62	ILE	C-N-CA	-8.98	109.91	122.93
1	B	108	GLU	CA-C-N	8.97	134.90	120.55
1	B	108	GLU	C-N-CA	8.97	134.90	120.55
2	I	25	GLN	OE1-CD-NE2	-8.97	113.63	122.60
1	B	62	ILE	CA-C-N	-8.96	109.94	122.93
1	B	62	ILE	C-N-CA	-8.96	109.94	122.93
1	A	108	GLU	CA-C-N	8.93	134.83	120.55
1	A	108	GLU	C-N-CA	8.93	134.83	120.55
2	J	25	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	A	8	ASN	CA-CB-CG	8.90	121.50	112.60
1	B	8	ASN	CA-CB-CG	8.88	121.47	112.60
1	A	223	ALA	CA-C-O	8.87	129.96	120.55
1	B	44	GLY	N-CA-C	8.87	127.10	115.40
1	B	2	ARG	N-CA-CB	8.86	123.99	110.61
1	A	44	GLY	N-CA-C	8.86	127.09	115.40
1	B	230	LEU	CA-C-O	8.86	130.29	119.31
1	A	2	ARG	N-CA-CB	8.82	123.93	110.61
1	B	175	GLU	O-C-N	8.82	133.12	122.27
1	B	71	ARG	NE-CZ-NH1	-8.81	112.69	121.50
1	B	223	ALA	CA-C-O	8.81	129.89	120.55
1	B	180	VAL	CA-C-N	8.81	132.08	120.28
1	B	180	VAL	C-N-CA	8.81	132.08	120.28
1	A	230	LEU	CA-C-O	8.81	130.23	119.31
1	B	215	ASP	CA-C-N	8.78	132.39	120.54
1	B	215	ASP	C-N-CA	8.78	132.39	120.54
1	A	71	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	A	215	ASP	CA-C-N	8.77	132.37	120.54
1	A	215	ASP	C-N-CA	8.77	132.37	120.54
1	A	180	VAL	CA-C-N	8.76	132.02	120.28
1	A	180	VAL	C-N-CA	8.76	132.02	120.28
1	A	20	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	175	GLU	O-C-N	8.74	133.02	122.27
1	B	11	THR	CA-CB-OG1	8.74	122.71	109.60
1	A	11	THR	CA-CB-OG1	8.74	122.70	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	ASP	CA-CB-CG	8.73	121.33	112.60
1	B	114	ASN	CA-C-N	8.71	129.60	119.94
1	B	114	ASN	C-N-CA	8.71	129.60	119.94
1	A	114	ASN	CA-C-N	8.66	129.55	119.94
1	A	114	ASN	C-N-CA	8.66	129.55	119.94
1	A	287	ILE	N-CA-CB	8.65	117.19	110.45
1	B	287	ILE	N-CA-CB	8.64	117.19	110.45
1	B	33	VAL	CA-C-N	8.56	135.97	122.62
1	B	33	VAL	C-N-CA	8.56	135.97	122.62
1	A	33	VAL	CA-C-N	8.55	135.96	122.62
1	A	33	VAL	C-N-CA	8.55	135.96	122.62
1	B	276	ARG	CB-CA-C	-8.49	97.55	110.88
1	A	276	ARG	CB-CA-C	-8.48	97.57	110.88
1	B	179	ILE	CB-CA-C	-8.46	101.24	111.81
1	B	164	THR	CA-C-N	8.45	132.73	120.82
1	B	164	THR	C-N-CA	8.45	132.73	120.82
1	A	164	THR	CA-C-N	8.41	132.68	120.82
1	A	164	THR	C-N-CA	8.41	132.68	120.82
1	A	179	ILE	CB-CA-C	-8.41	101.30	111.81
1	B	273	ASP	CB-CG-OD1	8.40	137.72	118.40
1	A	273	ASP	CB-CG-OD1	8.38	137.68	118.40
1	B	171	ASN	CA-CB-CG	-8.37	104.23	112.60
1	A	171	ASN	CA-CB-CG	-8.34	104.26	112.60
1	B	161	CYS	O-C-N	8.32	134.58	122.43
1	A	43	GLU	CB-CA-C	-8.31	101.00	111.22
1	B	43	GLU	CB-CA-C	-8.31	101.00	111.22
1	A	161	CYS	O-C-N	8.28	134.52	122.43
1	B	204	TYR	O-C-N	8.22	127.96	121.55
1	B	178	SER	CA-C-N	8.21	130.97	120.70
1	B	178	SER	C-N-CA	8.21	130.97	120.70
1	B	145	ARG	CD-NE-CZ	8.20	135.88	124.40
1	A	178	SER	CA-C-N	8.18	130.93	120.70
1	A	178	SER	C-N-CA	8.18	130.93	120.70
2	J	17	ASP	CA-CB-CG	-8.16	104.44	112.60
1	A	145	ARG	CD-NE-CZ	8.16	135.82	124.40
2	I	17	ASP	CA-CB-CG	-8.16	104.44	112.60
1	B	192	PHE	CA-CB-CG	8.15	121.95	113.80
1	A	192	PHE	CA-CB-CG	8.13	121.93	113.80
1	A	204	TYR	O-C-N	8.13	127.89	121.55
1	A	112	ASN	CA-C-N	8.05	127.62	118.85
1	A	112	ASN	C-N-CA	8.05	127.62	118.85
1	B	211	GLN	CG-CD-OE1	-8.05	104.71	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	LYS	CA-C-N	8.04	134.30	123.05
1	B	51	LYS	C-N-CA	8.04	134.30	123.05
1	B	99	ILE	CA-C-O	-8.04	112.65	121.17
1	B	112	ASN	CA-C-N	8.02	127.60	118.85
1	B	112	ASN	C-N-CA	8.02	127.60	118.85
1	B	133	THR	N-CA-CB	8.02	124.04	110.49
1	A	133	THR	N-CA-CB	8.00	124.01	110.49
1	A	211	GLN	CG-CD-OE1	-8.00	104.80	120.80
1	A	99	ILE	CA-C-O	-7.99	112.70	121.17
1	A	51	LYS	CA-C-N	7.98	134.23	123.05
1	A	51	LYS	C-N-CA	7.98	134.23	123.05
1	B	96	PHE	O-C-N	7.96	130.26	122.07
1	A	96	PHE	O-C-N	7.95	130.26	122.07
1	A	10	ALA	CA-C-N	7.92	135.04	122.21
1	A	10	ALA	C-N-CA	7.92	135.04	122.21
1	B	45	ARG	CA-C-O	7.90	128.78	120.25
1	B	10	ALA	CA-C-N	7.90	135.00	122.21
1	B	10	ALA	C-N-CA	7.90	135.00	122.21
1	B	130	ARG	NH1-CZ-NH2	-7.90	109.03	119.30
1	A	130	ARG	NH1-CZ-NH2	-7.88	109.06	119.30
1	A	45	ARG	CA-C-O	7.87	128.75	120.25
1	A	305	VAL	CA-CB-CG1	7.87	123.77	110.40
1	B	124	ARG	CD-NE-CZ	7.86	135.41	124.40
1	A	79	GLY	CA-C-N	7.83	131.57	120.53
1	A	79	GLY	C-N-CA	7.83	131.57	120.53
1	B	79	GLY	CA-C-N	7.82	131.56	120.53
1	B	79	GLY	C-N-CA	7.82	131.56	120.53
1	A	124	ARG	CD-NE-CZ	7.82	135.34	124.40
1	B	305	VAL	CA-CB-CG1	7.82	123.69	110.40
1	A	28	GLN	O-C-N	-7.77	112.71	122.27
1	B	28	GLN	O-C-N	-7.75	112.73	122.27
1	A	179	ILE	CA-C-O	-7.70	113.06	121.29
1	B	179	ILE	CA-C-O	-7.68	113.07	121.29
1	A	16	ASP	CA-CB-CG	-7.67	104.93	112.60
1	A	45	ARG	NE-CZ-NH1	-7.63	113.87	121.50
1	B	45	ARG	NE-CZ-NH1	-7.61	113.89	121.50
1	B	16	ASP	CA-CB-CG	-7.60	105.00	112.60
1	B	167	GLY	CA-C-O	-7.58	115.59	122.57
1	A	167	GLY	CA-C-O	-7.57	115.60	122.57
1	B	2	ARG	N-CA-C	-7.57	103.16	113.30
1	B	77	ALA	CA-C-N	7.56	131.02	120.29
1	B	77	ALA	C-N-CA	7.56	131.02	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77	ALA	CA-C-N	7.55	131.01	120.29
1	A	77	ALA	C-N-CA	7.55	131.01	120.29
1	A	2	ARG	N-CA-C	-7.54	103.19	113.30
2	I	32	ARG	NH1-CZ-NH2	-7.44	109.62	119.30
1	A	132	VAL	O-C-N	-7.44	113.27	122.57
1	B	132	VAL	O-C-N	-7.42	113.29	122.57
1	A	135	SER	N-CA-C	-7.42	97.60	109.39
1	A	133	THR	O-C-N	7.41	132.45	122.59
1	B	135	SER	N-CA-C	-7.40	97.63	109.39
1	B	133	THR	O-C-N	7.40	132.43	122.59
2	J	32	ARG	NH1-CZ-NH2	-7.40	109.68	119.30
1	A	268	THR	N-CA-CB	7.39	123.10	110.68
1	B	181	ASP	CA-C-O	7.38	128.37	120.55
1	B	268	THR	N-CA-CB	7.36	123.05	110.68
1	B	205	PRO	O-C-N	-7.35	112.72	122.64
1	B	6	THR	CA-CB-OG1	-7.33	98.61	109.60
1	A	6	THR	CA-CB-OG1	-7.32	98.61	109.60
1	B	226	ALA	CA-C-O	-7.31	112.67	120.42
1	A	205	PRO	O-C-N	-7.31	112.78	122.64
1	B	42	TYR	CA-CB-CG	-7.30	100.75	113.90
1	A	181	ASP	CA-C-O	7.29	128.28	120.55
1	A	226	ALA	CA-C-O	-7.29	112.69	120.42
1	A	42	TYR	CA-CB-CG	-7.29	100.78	113.90
1	A	177	LYS	CG-CD-CE	7.28	128.03	111.30
1	A	273	ASP	CB-CG-OD2	-7.28	101.67	118.40
1	B	276	ARG	CD-NE-CZ	-7.27	114.22	124.40
1	B	273	ASP	CB-CG-OD2	-7.27	101.67	118.40
1	B	61	ALA	CA-C-N	7.27	132.21	122.90
1	B	61	ALA	C-N-CA	7.27	132.21	122.90
1	B	177	LYS	CG-CD-CE	7.27	128.02	111.30
1	A	61	ALA	CA-C-N	7.26	132.20	122.90
1	A	61	ALA	C-N-CA	7.26	132.20	122.90
1	A	123	ASN	OD1-CG-ND2	7.25	129.85	122.60
1	A	276	ARG	CD-NE-CZ	-7.23	114.28	124.40
1	A	249	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	B	249	GLN	OE1-CD-NE2	-7.23	115.37	122.60
1	B	123	ASN	OD1-CG-ND2	7.21	129.81	122.60
1	B	182	PHE	CA-CB-CG	-7.16	106.64	113.80
1	A	182	PHE	CA-CB-CG	-7.16	106.64	113.80
1	B	188	ASN	OD1-CG-ND2	7.14	129.74	122.60
1	A	188	ASN	OD1-CG-ND2	7.11	129.71	122.60
1	A	274	THR	N-CA-CB	7.11	120.69	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	LEU	O-C-N	-7.11	114.52	122.34
1	B	274	THR	N-CA-CB	7.10	120.68	110.88
1	A	185	ASN	CB-CA-C	-7.09	98.88	110.79
1	B	185	ASN	CB-CA-C	-7.09	98.88	110.79
1	A	93	ASN	OD1-CG-ND2	-7.07	115.53	122.60
1	A	130	ARG	NE-CZ-NH2	7.07	125.56	119.20
1	B	137	LEU	O-C-N	-7.05	114.58	122.34
1	B	130	ARG	NE-CZ-NH2	7.05	125.54	119.20
2	I	20	GLY	CA-C-N	-7.04	111.38	122.65
2	I	20	GLY	C-N-CA	-7.04	111.38	122.65
1	B	227	VAL	CA-CB-CG1	7.04	122.36	110.40
2	J	20	GLY	CA-C-N	-7.04	111.39	122.65
2	J	20	GLY	C-N-CA	-7.04	111.39	122.65
1	B	93	ASN	OD1-CG-ND2	-7.03	115.57	122.60
1	A	227	VAL	CA-CB-CG1	7.02	122.33	110.40
1	A	302	GLU	CA-CB-CG	7.01	128.12	114.10
2	I	31	ALA	CA-C-O	-7.01	110.49	120.51
2	J	33	THR	CA-C-O	-7.01	111.66	120.28
1	B	108	GLU	CA-C-O	6.99	130.23	120.52
1	B	195	ILE	CA-C-O	6.98	128.03	120.57
2	J	31	ALA	CA-C-O	-6.97	110.55	120.51
1	A	276	ARG	CA-C-O	6.96	128.13	120.82
2	I	33	THR	CA-C-O	-6.96	111.72	120.28
1	B	276	ARG	CA-C-O	6.96	128.13	120.82
1	B	302	GLU	CA-CB-CG	6.96	128.02	114.10
1	B	268	THR	CA-C-N	6.96	132.32	122.72
1	B	268	THR	C-N-CA	6.96	132.32	122.72
1	A	108	GLU	CA-C-O	6.95	130.18	120.52
1	A	268	THR	CA-C-N	6.94	132.30	122.72
1	A	268	THR	C-N-CA	6.94	132.30	122.72
1	A	195	ILE	CA-C-O	6.94	127.99	120.57
1	A	17	GLU	CG-CD-OE1	6.92	134.33	118.40
1	A	190	LYS	N-CA-CB	6.91	121.05	110.61
1	B	17	GLU	CG-CD-OE1	6.91	134.28	118.40
1	B	190	LYS	N-CA-CB	6.90	121.02	110.61
1	A	70	SER	N-CA-C	6.89	118.79	111.28
1	A	209	THR	O-C-N	-6.88	115.41	123.25
1	B	209	THR	O-C-N	-6.88	115.41	123.25
1	B	33	VAL	CA-C-O	6.86	130.12	121.40
1	A	33	VAL	CA-C-O	6.86	130.11	121.40
1	B	70	SER	N-CA-C	6.86	118.75	111.28
1	A	87	THR	O-C-N	-6.83	114.42	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	SER	CA-CB-OG	-6.81	97.49	111.10
1	B	87	THR	O-C-N	-6.81	114.44	122.20
1	B	159	SER	CA-CB-OG	-6.80	97.49	111.10
1	A	140	GLY	N-CA-C	6.80	120.71	112.48
1	A	220	ASN	O-C-N	6.78	129.08	122.03
1	A	17	GLU	CG-CD-OE2	-6.78	102.81	118.40
1	B	275	GLY	CA-C-O	-6.78	108.78	120.57
1	B	140	GLY	N-CA-C	6.77	120.67	112.48
2	I	35	GLY	N-CA-C	-6.76	98.55	112.34
1	A	275	GLY	CA-C-O	-6.76	108.81	120.57
1	B	125	LEU	O-C-N	6.75	130.57	122.26
1	B	17	GLU	CG-CD-OE2	-6.75	102.88	118.40
1	A	197	SER	CA-C-N	6.74	133.84	121.70
1	A	197	SER	C-N-CA	6.74	133.84	121.70
2	J	35	GLY	N-CA-C	-6.74	98.58	112.34
1	B	220	ASN	O-C-N	6.74	129.04	122.03
1	B	197	SER	CA-C-N	6.74	133.83	121.70
1	B	197	SER	C-N-CA	6.74	133.83	121.70
1	B	261	GLN	OE1-CD-NE2	-6.74	115.86	122.60
1	A	125	LEU	O-C-N	6.72	130.53	122.26
1	A	32	LEU	CA-C-O	-6.72	110.99	120.07
1	A	76	GLN	CA-C-N	6.71	132.10	120.68
1	A	76	GLN	C-N-CA	6.71	132.10	120.68
1	B	32	LEU	CA-C-O	-6.71	111.02	120.07
1	B	41	SER	CA-C-O	6.68	130.06	120.51
1	B	76	GLN	CA-C-N	6.67	132.02	120.68
1	B	76	GLN	C-N-CA	6.67	132.02	120.68
1	A	261	GLN	OE1-CD-NE2	-6.67	115.93	122.60
1	B	93	ASN	CB-CA-C	6.67	117.45	109.85
1	A	93	ASN	CB-CA-C	6.66	117.45	109.85
1	A	41	SER	CA-C-O	6.65	130.02	120.51
1	B	236	THR	CA-CB-OG1	-6.64	99.64	109.60
1	B	104	ASP	CA-CB-CG	6.63	119.23	112.60
2	I	4	ALA	O-C-N	6.62	131.40	122.59
1	B	199	SER	N-CA-CB	6.62	121.68	110.49
1	A	236	THR	CA-CB-OG1	-6.62	99.67	109.60
1	A	54	THR	N-CA-C	-6.62	104.51	112.59
1	B	277	TYR	CA-C-O	-6.62	112.06	119.67
1	A	185	ASN	N-CA-CB	6.61	119.92	110.13
1	B	54	THR	N-CA-C	-6.61	104.53	112.59
1	B	185	ASN	N-CA-CB	6.61	119.91	110.13
1	A	199	SER	N-CA-CB	6.60	121.64	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	LYS	CA-C-N	6.60	133.27	121.66
1	A	231	LYS	C-N-CA	6.60	133.27	121.66
1	B	231	LYS	CA-C-N	6.60	133.27	121.66
1	B	231	LYS	C-N-CA	6.60	133.27	121.66
1	A	76	GLN	OE1-CD-NE2	6.59	129.19	122.60
2	J	4	ALA	O-C-N	6.59	131.36	122.59
1	A	104	ASP	CA-CB-CG	6.59	119.19	112.60
1	A	276	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	B	276	ARG	NE-CZ-NH1	-6.58	114.92	121.50
1	A	277	TYR	CA-C-O	-6.57	112.12	119.67
2	J	16	ASP	N-CA-CB	-6.55	100.21	110.30
1	A	40	ARG	NE-CZ-NH2	-6.55	113.30	119.20
2	J	32	ARG	CA-C-N	6.55	133.33	122.33
2	J	32	ARG	C-N-CA	6.55	133.33	122.33
1	A	105	ILE	O-C-N	6.54	130.24	123.18
2	I	16	ASP	N-CA-CB	-6.54	100.23	110.30
1	B	173	GLU	CB-CG-CD	6.53	123.70	112.60
1	B	40	ARG	NE-CZ-NH2	-6.52	113.33	119.20
2	I	32	ARG	CA-C-N	6.52	133.28	122.33
2	I	32	ARG	C-N-CA	6.52	133.28	122.33
1	B	76	GLN	OE1-CD-NE2	6.52	129.12	122.60
1	A	140	GLY	CA-C-N	6.51	131.50	123.10
1	A	140	GLY	C-N-CA	6.51	131.50	123.10
2	I	27	CYS	O-C-N	6.51	130.71	123.16
2	J	27	CYS	O-C-N	6.50	130.71	123.16
1	B	57	SER	CA-C-N	6.50	135.04	123.34
1	B	57	SER	C-N-CA	6.50	135.04	123.34
1	B	105	ILE	O-C-N	6.50	130.20	123.18
1	B	140	GLY	CA-C-N	6.50	131.48	123.10
1	B	140	GLY	C-N-CA	6.50	131.48	123.10
1	A	173	GLU	CB-CG-CD	6.49	123.64	112.60
1	A	248	TYR	CA-CB-CG	6.49	125.58	113.90
1	A	20	ASP	CA-C-O	-6.47	113.62	120.55
1	B	20	ASP	CA-C-O	-6.47	113.63	120.55
1	B	245	THR	CA-CB-CG2	6.47	121.50	110.50
1	A	57	SER	CA-C-N	6.46	134.98	123.34
1	A	57	SER	C-N-CA	6.46	134.98	123.34
1	B	248	TYR	CA-CB-CG	6.46	125.54	113.90
1	A	245	THR	CA-CB-CG2	6.44	121.45	110.50
1	B	17	GLU	CA-C-N	6.44	131.77	121.34
1	B	17	GLU	C-N-CA	6.44	131.77	121.34
1	B	145	ARG	NE-CZ-NH2	6.44	124.99	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	CA-C-N	6.39	131.70	121.34
1	A	17	GLU	C-N-CA	6.39	131.70	121.34
1	A	43	GLU	CA-C-N	6.39	132.89	122.09
1	A	43	GLU	C-N-CA	6.39	132.89	122.09
1	A	145	ARG	NE-CZ-NH2	6.38	124.95	119.20
1	B	189	PHE	CA-CB-CG	-6.38	107.42	113.80
2	J	5	ASP	CB-CG-OD1	6.38	133.07	118.40
2	I	5	ASP	CB-CG-OD1	6.37	133.06	118.40
1	A	189	PHE	CA-CB-CG	-6.36	107.44	113.80
1	B	43	GLU	CA-C-N	6.36	132.84	122.09
1	B	43	GLU	C-N-CA	6.36	132.84	122.09
1	A	142	ASP	CA-CB-CG	-6.35	106.25	112.60
1	B	211	GLN	N-CA-C	-6.35	101.98	110.24
2	J	6	PRO	CB-CA-C	6.35	123.09	112.62
1	A	211	GLN	N-CA-C	-6.34	101.99	110.24
1	B	131	SER	CA-C-N	6.34	133.39	121.97
1	B	131	SER	C-N-CA	6.34	133.39	121.97
1	A	131	SER	CA-C-N	6.34	133.38	121.97
1	A	131	SER	C-N-CA	6.34	133.38	121.97
1	B	142	ASP	CA-CB-CG	-6.34	106.26	112.60
1	B	227	VAL	CA-C-N	6.33	128.67	120.44
1	B	227	VAL	C-N-CA	6.33	128.67	120.44
2	I	6	PRO	CB-CA-C	6.32	123.05	112.62
1	B	302	GLU	N-CA-C	-6.32	103.52	111.11
2	J	31	ALA	CA-C-N	6.32	133.61	121.54
2	J	31	ALA	C-N-CA	6.32	133.61	121.54
1	A	7	PHE	CB-CA-C	6.32	120.13	109.84
2	I	31	ALA	CA-C-N	6.31	133.60	121.54
2	I	31	ALA	C-N-CA	6.31	133.60	121.54
1	A	227	VAL	CA-C-N	6.30	128.62	120.44
1	A	227	VAL	C-N-CA	6.30	128.62	120.44
1	B	7	PHE	CB-CA-C	6.29	120.10	109.84
2	I	14	THR	CA-CB-CG2	6.29	121.20	110.50
1	A	148	ASP	O-C-N	6.29	129.65	122.55
1	B	222	VAL	CB-CA-C	6.28	120.62	112.14
1	B	266	SER	O-C-N	6.28	131.04	123.13
2	J	14	THR	CA-CB-CG2	6.27	121.16	110.50
2	I	16	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	281	LEU	O-C-N	6.26	126.36	121.47
2	I	11	PRO	N-CA-CB	6.26	108.31	103.30
1	A	222	VAL	CB-CA-C	6.26	120.59	112.14
1	A	302	GLU	N-CA-C	-6.26	103.60	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	SER	O-C-N	6.26	131.01	123.13
2	J	11	PRO	N-CA-CB	6.26	108.31	103.30
1	A	19	TYR	CA-C-N	6.25	131.15	120.71
1	A	19	TYR	C-N-CA	6.25	131.15	120.71
1	B	281	LEU	O-C-N	6.24	126.34	121.47
2	J	16	ASP	CA-CB-CG	6.24	118.84	112.60
2	I	33	THR	CA-CB-CG2	6.22	121.07	110.50
1	B	148	ASP	O-C-N	6.22	129.57	122.55
1	A	161	CYS	CA-CB-SG	-6.21	100.11	114.40
1	A	167	GLY	N-CA-C	-6.21	103.62	112.81
1	B	255	ILE	CA-C-O	6.21	127.35	120.71
1	A	72	GLU	CA-C-N	6.20	128.88	120.38
1	A	72	GLU	C-N-CA	6.20	128.88	120.38
1	A	97	THR	CA-C-O	-6.20	113.97	120.55
1	B	19	TYR	CA-C-N	6.20	131.07	120.71
1	B	19	TYR	C-N-CA	6.20	131.07	120.71
1	B	97	THR	CA-C-O	-6.20	113.98	120.55
1	B	167	GLY	N-CA-C	-6.20	103.64	112.81
2	I	12	CYS	N-CA-CB	-6.19	101.47	110.70
1	B	72	GLU	CA-C-N	6.19	128.86	120.38
1	B	72	GLU	C-N-CA	6.19	128.86	120.38
1	B	161	CYS	CA-CB-SG	-6.19	100.17	114.40
1	B	22	MET	N-CA-C	-6.18	104.54	111.28
2	J	19	SER	CA-CB-OG	6.18	123.45	111.10
2	J	33	THR	CA-CB-CG2	6.18	121.00	110.50
2	J	12	CYS	N-CA-CB	-6.17	101.51	110.70
2	I	19	SER	CA-CB-OG	6.16	123.42	111.10
1	A	22	MET	N-CA-C	-6.16	104.57	111.28
2	I	5	ASP	O-C-N	6.16	126.55	121.44
1	A	18	ILE	N-CA-C	6.15	118.10	111.58
1	A	255	ILE	CA-C-O	6.13	127.27	120.71
1	A	285	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	B	285	GLN	OE1-CD-NE2	-6.12	116.48	122.60
1	A	220	ASN	CA-CB-CG	-6.12	106.48	112.60
1	A	287	ILE	CA-C-O	-6.11	114.60	118.69
1	B	124	ARG	CA-C-O	6.11	126.89	119.38
1	B	171	ASN	OD1-CG-ND2	6.11	128.71	122.60
1	A	233	LEU	N-CA-CB	-6.11	100.07	110.33
1	B	161	CYS	CA-C-O	-6.10	111.30	119.11
1	B	287	ILE	CA-C-O	-6.10	114.60	118.69
1	B	131	SER	CA-C-O	6.10	127.82	120.81
2	I	7	ILE	CB-CG1-CD1	6.09	126.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	CA-C-O	6.09	126.87	119.38
1	B	233	LEU	N-CA-CB	-6.08	100.11	110.33
1	A	190	LYS	CA-C-N	6.08	132.33	122.29
1	A	190	LYS	C-N-CA	6.08	132.33	122.29
1	B	18	ILE	N-CA-C	6.08	118.03	111.58
1	A	131	SER	CA-C-O	6.07	127.80	120.81
1	B	215	ASP	CA-CB-CG	-6.07	106.53	112.60
1	A	215	ASP	CA-CB-CG	-6.07	106.53	112.60
1	A	171	ASN	OD1-CG-ND2	6.07	128.67	122.60
2	J	7	ILE	CB-CG1-CD1	6.07	126.55	113.80
1	A	285	GLN	CA-C-N	6.07	129.41	120.74
1	A	285	GLN	C-N-CA	6.07	129.41	120.74
1	B	285	GLN	CA-C-N	6.07	129.41	120.74
1	B	285	GLN	C-N-CA	6.07	129.41	120.74
1	A	161	CYS	CA-C-O	-6.05	111.37	119.11
1	B	220	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	190	LYS	CA-C-N	6.05	132.27	122.29
1	B	190	LYS	C-N-CA	6.05	132.27	122.29
1	B	209	THR	CA-C-N	6.04	132.90	122.09
1	B	209	THR	C-N-CA	6.04	132.90	122.09
2	J	5	ASP	O-C-N	6.04	126.45	121.44
1	A	266	SER	CA-C-O	-6.03	114.00	120.46
1	A	209	THR	CA-C-N	6.03	132.88	122.09
1	A	209	THR	C-N-CA	6.03	132.88	122.09
1	B	247	ILE	CB-CA-C	-6.02	101.41	111.29
1	B	42	TYR	O-C-N	6.02	128.52	122.08
1	A	247	ILE	CB-CA-C	-6.01	101.43	111.29
1	B	266	SER	CA-C-O	-6.01	114.03	120.46
1	A	42	TYR	O-C-N	6.00	128.50	122.08
1	B	194	SER	N-CA-CB	6.00	120.02	110.65
1	A	236	THR	O-C-N	5.99	130.30	122.93
1	A	110	VAL	CA-C-N	5.99	128.80	120.29
1	A	110	VAL	C-N-CA	5.99	128.80	120.29
1	A	194	SER	N-CA-CB	5.99	119.99	110.65
1	B	71	ARG	CA-C-O	5.97	126.84	119.97
1	A	140	GLY	CA-C-O	-5.97	117.05	122.24
1	A	71	ARG	CA-C-O	5.96	126.83	119.97
1	B	223	ALA	N-CA-C	-5.96	104.79	111.28
1	B	110	VAL	CA-C-N	5.95	128.74	120.29
1	B	110	VAL	C-N-CA	5.95	128.74	120.29
1	B	236	THR	O-C-N	5.94	130.23	122.93
1	A	223	ALA	N-CA-C	-5.93	104.81	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	38	VAL	N-CA-CB	-5.93	101.42	111.50
2	I	38	VAL	N-CA-CB	-5.92	101.44	111.50
1	B	140	GLY	CA-C-O	-5.92	117.09	122.24
1	B	202	LEU	CA-C-N	5.90	131.49	122.93
1	B	202	LEU	C-N-CA	5.90	131.49	122.93
1	B	185	ASN	CB-CG-ND2	-5.90	107.55	116.40
1	A	93	ASN	CB-CG-OD1	5.90	132.59	120.80
1	B	93	ASN	CB-CG-OD1	5.90	132.59	120.80
1	A	185	ASN	CB-CG-ND2	-5.88	107.58	116.40
1	A	208	TYR	CB-CG-CD1	5.87	129.60	120.80
1	A	109	ILE	CB-CA-C	-5.87	104.38	112.24
1	B	208	TYR	CB-CG-CD1	5.86	129.59	120.80
1	A	202	LEU	CA-C-N	5.86	131.42	122.93
1	A	202	LEU	C-N-CA	5.86	131.42	122.93
1	B	109	ILE	CB-CA-C	-5.85	104.40	112.24
1	B	129	THR	CA-CB-OG1	-5.85	100.82	109.60
1	A	70	SER	CA-C-N	5.84	129.18	120.31
1	A	70	SER	C-N-CA	5.84	129.18	120.31
1	B	175	GLU	CA-C-O	-5.84	113.26	119.97
1	A	129	THR	CA-CB-OG1	-5.83	100.85	109.60
2	J	18	CYS	CA-C-O	-5.83	112.17	120.51
1	A	135	SER	CA-CB-OG	5.83	122.75	111.10
1	B	135	SER	CA-CB-OG	5.82	122.74	111.10
1	A	20	ASP	O-C-N	5.82	129.21	122.17
2	J	26	ALA	CA-C-O	-5.82	114.55	120.71
1	B	20	ASP	O-C-N	5.81	129.20	122.17
2	I	18	CYS	CA-C-O	-5.80	112.21	120.51
1	B	70	SER	CA-C-N	5.80	129.13	120.31
1	B	70	SER	C-N-CA	5.80	129.13	120.31
1	A	189	PHE	CA-C-O	-5.79	113.94	120.43
1	B	189	PHE	CA-C-O	-5.78	113.95	120.43
1	B	180	VAL	O-C-N	-5.77	116.17	121.94
1	A	175	GLU	CA-C-O	-5.77	113.34	119.97
1	B	70	SER	CA-CB-OG	5.77	122.63	111.10
1	A	180	VAL	O-C-N	-5.74	116.20	121.94
2	I	26	ALA	CA-C-O	-5.73	114.64	120.71
2	I	35	GLY	CA-C-O	-5.73	113.33	121.52
1	A	70	SER	CA-CB-OG	5.72	122.55	111.10
2	J	35	GLY	CA-C-O	-5.72	113.34	121.52
1	A	59	ARG	NH1-CZ-NH2	5.71	126.73	119.30
1	A	169	TYR	CB-CA-C	5.71	121.24	110.62
1	A	28	GLN	CB-CA-C	5.71	121.63	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	59	ARG	NH1-CZ-NH2	5.70	126.71	119.30
1	B	169	TYR	CB-CA-C	5.70	121.23	110.62
2	I	32	ARG	CB-CG-CD	5.69	124.39	111.30
1	B	28	GLN	CB-CA-C	5.69	121.59	110.67
1	B	142	ASP	CA-C-O	-5.68	114.48	121.02
1	B	93	ASN	CA-C-O	5.68	125.68	119.32
1	B	203	LEU	CA-C-O	-5.68	114.69	120.71
1	A	203	LEU	CA-C-O	-5.68	114.69	120.71
1	A	85	LYS	CA-C-O	-5.67	114.54	120.55
1	B	85	LYS	CA-C-O	-5.67	114.54	120.55
2	J	32	ARG	CB-CG-CD	5.67	124.34	111.30
1	A	93	ASN	CA-C-O	5.67	125.67	119.32
1	A	69	HIS	CB-CA-C	-5.65	101.64	110.74
1	B	69	HIS	CB-CA-C	-5.64	101.66	110.74
1	A	109	ILE	CA-C-N	5.64	128.32	122.96
1	A	109	ILE	C-N-CA	5.64	128.32	122.96
1	A	19	TYR	N-CA-C	-5.63	105.67	112.54
1	B	109	ILE	CA-C-N	5.63	128.31	122.96
1	B	109	ILE	C-N-CA	5.63	128.31	122.96
1	A	142	ASP	CA-C-O	-5.63	114.55	121.02
1	B	19	TYR	N-CA-C	-5.62	105.68	112.54
2	I	3	HIS	N-CA-CB	5.62	120.06	110.50
1	A	133	THR	OG1-CB-CG2	5.62	120.54	109.30
1	A	217	THR	CA-C-O	5.61	126.71	120.82
2	I	32	ARG	NE-CZ-NH1	5.61	127.11	121.50
2	J	32	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	B	159	SER	CA-C-N	5.60	125.44	119.28
1	B	159	SER	C-N-CA	5.60	125.44	119.28
1	B	276	ARG	CG-CD-NE	-5.60	99.67	112.00
1	B	133	THR	OG1-CB-CG2	5.60	120.50	109.30
1	A	159	SER	CA-C-N	5.60	125.44	119.28
1	A	159	SER	C-N-CA	5.60	125.44	119.28
1	A	276	ARG	CG-CD-NE	-5.59	99.70	112.00
1	A	114	ASN	CA-CB-CG	-5.58	107.02	112.60
1	A	166	HIS	CA-C-N	-5.58	113.97	122.06
1	A	166	HIS	C-N-CA	-5.58	113.97	122.06
1	A	183	VAL	O-C-N	5.58	127.28	121.87
1	B	220	ASN	OD1-CG-ND2	-5.58	117.02	122.60
2	J	3	HIS	N-CA-CB	5.57	119.97	110.50
1	A	220	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	166	HIS	CA-C-N	-5.57	113.98	122.06
1	B	166	HIS	C-N-CA	-5.57	113.98	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	183	VAL	O-C-N	5.56	127.26	121.87
1	A	136	SER	N-CA-C	5.56	118.51	109.06
1	B	114	ASN	CA-CB-CG	-5.55	107.05	112.60
2	I	28	TRP	O-C-N	5.53	129.63	123.05
2	J	28	TRP	O-C-N	5.53	129.63	123.05
1	A	19	TYR	CA-C-O	5.52	126.17	119.38
1	A	209	THR	CA-C-O	5.51	127.28	121.33
1	B	136	SER	N-CA-C	5.51	118.43	109.06
1	B	19	TYR	CA-C-O	5.51	126.16	119.38
1	B	217	THR	CA-C-O	5.51	126.61	120.82
2	I	19	SER	O-C-N	-5.51	115.26	122.59
1	B	224	LYS	CA-C-N	5.50	127.97	120.54
1	B	224	LYS	C-N-CA	5.50	127.97	120.54
1	A	219	LEU	CA-C-O	-5.49	114.60	120.42
1	B	219	LEU	CA-C-O	-5.49	114.60	120.42
1	A	224	LYS	CA-C-N	5.49	127.94	120.54
1	A	224	LYS	C-N-CA	5.49	127.94	120.54
2	J	19	SER	O-C-N	-5.49	115.29	122.59
1	B	146	ASN	CA-C-N	5.48	130.94	120.97
1	B	146	ASN	C-N-CA	5.48	130.94	120.97
1	A	290	ALA	CA-C-O	-5.48	115.07	120.82
1	B	93	ASN	CA-C-N	5.48	125.13	119.05
1	B	93	ASN	C-N-CA	5.48	125.13	119.05
1	A	291	GLN	CB-CA-C	-5.47	101.70	110.79
1	B	256	ASP	O-C-N	5.47	127.93	122.08
1	B	291	GLN	CB-CA-C	-5.47	101.71	110.79
1	A	146	ASN	CA-C-N	5.47	130.92	120.97
1	A	146	ASN	C-N-CA	5.47	130.92	120.97
1	A	46	PRO	CB-CA-C	5.46	118.47	111.21
1	B	290	ALA	CA-C-O	-5.46	115.09	120.82
1	A	93	ASN	CA-C-N	5.45	125.10	119.05
1	A	93	ASN	C-N-CA	5.45	125.10	119.05
1	B	46	PRO	CB-CA-C	5.45	118.46	111.21
1	A	256	ASP	O-C-N	5.44	127.90	122.08
1	B	209	THR	CA-C-O	5.44	127.21	121.33
2	J	27	CYS	N-CA-CB	5.44	119.04	110.23
1	A	53	SER	N-CA-C	5.43	117.52	108.99
1	B	11	THR	N-CA-CB	-5.43	102.24	111.69
1	B	90	TYR	CA-C-O	5.43	127.11	120.92
1	A	297	VAL	CA-C-N	5.42	127.99	120.29
1	A	297	VAL	C-N-CA	5.42	127.99	120.29
1	A	217	THR	CA-CB-CG2	5.42	119.72	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	SER	N-CA-C	5.42	117.50	108.99
2	I	27	CYS	N-CA-CB	5.41	119.00	110.23
1	B	297	VAL	CA-C-N	5.41	127.98	120.29
1	B	297	VAL	C-N-CA	5.41	127.98	120.29
1	A	90	TYR	CA-C-O	5.41	127.09	120.92
1	A	11	THR	N-CA-CB	-5.41	102.28	111.69
1	B	33	VAL	CA-CB-CG2	5.40	119.58	110.40
1	B	175	GLU	N-CA-C	-5.40	105.55	111.82
1	B	217	THR	CA-CB-CG2	5.40	119.68	110.50
1	A	199	SER	CA-CB-OG	5.40	121.90	111.10
1	B	199	SER	CA-CB-OG	5.40	121.89	111.10
1	B	41	SER	CA-C-N	5.39	128.29	120.79
1	B	41	SER	C-N-CA	5.39	128.29	120.79
1	A	33	VAL	CA-CB-CG2	5.39	119.56	110.40
1	A	175	GLU	N-CA-C	-5.39	105.57	111.82
1	A	59	ARG	NE-CZ-NH1	-5.38	116.12	121.50
1	A	71	ARG	CD-NE-CZ	-5.38	116.87	124.40
1	A	41	SER	CA-C-N	5.37	128.26	120.79
1	A	41	SER	C-N-CA	5.37	128.26	120.79
1	A	306	ASN	CB-CG-ND2	5.37	124.45	116.40
1	A	63	TRP	CB-CA-C	5.35	119.02	109.38
1	A	251	SER	CA-CB-OG	-5.35	100.40	111.10
1	A	28	GLN	CB-CG-CD	5.35	121.70	112.60
1	B	59	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	71	ARG	CD-NE-CZ	-5.35	116.91	124.40
1	A	76	GLN	N-CA-C	-5.34	105.54	111.36
2	J	21	ALA	O-C-N	-5.34	115.93	122.34
1	B	251	SER	CA-CB-OG	-5.34	100.43	111.10
1	B	69	HIS	N-CA-CB	5.33	119.08	110.65
1	B	63	TRP	CB-CA-C	5.33	118.97	109.38
2	I	16	ASP	CB-CA-C	5.33	121.24	110.38
1	A	297	VAL	O-C-N	5.32	127.82	121.80
1	B	28	GLN	CB-CG-CD	5.32	121.64	112.60
1	B	292	GLU	CA-CB-CG	5.32	124.74	114.10
1	B	297	VAL	O-C-N	5.32	127.81	121.80
1	B	306	ASN	CB-CG-ND2	5.31	124.36	116.40
1	B	76	GLN	N-CA-C	-5.30	105.58	111.36
1	A	216	LYS	CB-CA-C	-5.30	102.34	110.81
1	A	219	LEU	CB-CA-C	5.29	119.85	110.85
1	B	216	LYS	CB-CA-C	-5.29	102.35	110.81
2	J	16	ASP	CB-CA-C	5.29	121.17	110.38
1	A	292	GLU	CA-CB-CG	5.28	124.66	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	GLN	O-C-N	-5.28	116.01	122.34
1	B	219	LEU	CB-CA-C	5.27	119.81	110.85
1	A	69	HIS	N-CA-CB	5.27	118.98	110.65
1	B	246	THR	O-C-N	-5.27	116.10	122.48
1	B	5	ASN	CA-C-O	5.26	125.85	119.38
1	A	59	ARG	CA-C-N	5.25	125.55	119.93
1	A	59	ARG	C-N-CA	5.25	125.55	119.93
1	A	246	THR	O-C-N	-5.25	116.13	122.48
2	J	11	PRO	CA-C-N	5.25	132.45	123.05
2	J	11	PRO	C-N-CA	5.25	132.45	123.05
2	J	5	ASP	CB-CG-OD2	-5.25	106.33	118.40
2	I	5	ASP	CB-CG-OD2	-5.25	106.34	118.40
1	A	5	ASN	CA-C-O	5.24	125.83	119.38
1	B	59	ARG	CA-C-N	5.24	125.54	119.93
1	B	59	ARG	C-N-CA	5.24	125.54	119.93
2	I	21	ALA	O-C-N	-5.23	116.06	122.34
1	A	128	LYS	CA-C-O	-5.23	115.08	121.78
1	A	285	GLN	O-C-N	-5.23	116.07	122.34
1	A	96	PHE	N-CA-C	-5.23	105.48	111.07
2	I	11	PRO	CA-C-N	5.22	132.40	123.05
2	I	11	PRO	C-N-CA	5.22	132.40	123.05
1	B	128	LYS	CA-C-O	-5.22	115.09	121.78
1	A	104	ASP	CA-C-N	-5.22	115.85	123.06
1	A	104	ASP	C-N-CA	-5.22	115.85	123.06
1	B	134	SER	CA-C-N	-5.22	114.19	122.23
1	B	134	SER	C-N-CA	-5.22	114.19	122.23
1	B	96	PHE	N-CA-C	-5.22	105.49	111.07
1	A	134	SER	CA-C-N	-5.21	114.20	122.23
1	A	134	SER	C-N-CA	-5.21	114.20	122.23
1	B	104	ASP	CA-C-N	-5.21	115.87	123.06
1	B	104	ASP	C-N-CA	-5.21	115.87	123.06
1	B	270	GLU	CB-CA-C	-5.18	102.35	110.79
1	A	270	GLU	CB-CA-C	-5.18	102.35	110.79
1	B	124	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	B	148	ASP	CA-C-N	5.17	131.41	121.54
1	B	148	ASP	C-N-CA	5.17	131.41	121.54
1	B	7	PHE	CA-C-O	5.17	126.58	120.69
1	A	124	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	A	198	TYR	CA-C-O	-5.16	112.02	120.80
1	A	97	THR	N-CA-CB	5.16	117.70	110.12
1	B	97	THR	N-CA-CB	5.16	117.70	110.12
1	B	66	LEU	CB-CA-C	5.16	120.36	109.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	7	PHE	CA-C-O	5.15	126.56	120.69
1	A	230	LEU	N-CA-CB	-5.14	102.01	110.40
1	B	198	TYR	CA-C-O	-5.14	112.05	120.80
1	A	66	LEU	CB-CA-C	5.14	120.32	109.79
1	A	148	ASP	CA-C-N	5.13	131.35	121.54
1	A	148	ASP	C-N-CA	5.13	131.35	121.54
1	B	305	VAL	CA-C-N	5.13	128.88	120.63
1	B	305	VAL	C-N-CA	5.13	128.88	120.63
1	A	156	ALA	O-C-N	5.12	129.61	123.36
1	A	45	ARG	NE-CZ-NH2	5.12	123.80	119.20
1	B	230	LEU	N-CA-CB	-5.11	102.07	110.40
1	A	40	ARG	CA-C-O	-5.11	114.65	120.32
1	B	40	ARG	CA-C-O	-5.11	114.65	120.32
1	A	240	TYR	CA-C-N	5.10	128.81	121.56
1	A	240	TYR	C-N-CA	5.10	128.81	121.56
1	B	58	ASN	O-C-N	5.09	128.60	121.83
1	A	21	PHE	CA-C-O	5.09	125.95	120.55
1	A	4	THR	CA-CB-OG1	-5.09	101.97	109.60
1	A	305	VAL	CA-C-N	5.08	128.82	120.63
1	A	305	VAL	C-N-CA	5.08	128.82	120.63
1	B	197	SER	O-C-N	-5.08	117.19	123.33
1	A	197	SER	O-C-N	-5.07	117.19	123.33
1	B	240	TYR	CA-C-N	5.07	128.76	121.56
1	B	240	TYR	C-N-CA	5.07	128.76	121.56
1	B	156	ALA	O-C-N	5.07	129.55	123.36
1	B	45	ARG	NE-CZ-NH2	5.07	123.76	119.20
1	A	58	ASN	O-C-N	5.07	128.57	121.83
1	B	181	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	35	LYS	CA-CB-CG	5.06	124.21	114.10
1	B	21	PHE	CA-C-O	5.05	125.91	120.55
1	B	254	SER	CA-C-O	5.05	125.91	120.55
1	A	35	LYS	CA-CB-CG	5.04	124.18	114.10
1	B	4	THR	CA-CB-OG1	-5.04	102.04	109.60
1	A	92	GLN	O-C-N	5.04	128.14	122.19
1	A	254	SER	CA-C-O	5.03	125.88	120.55
1	B	89	ASN	CA-CB-CG	5.03	117.63	112.60
1	B	92	GLN	O-C-N	5.03	128.12	122.19
1	A	242	SER	N-CA-C	-5.02	103.85	110.43
1	A	303	HIS	N-CA-CB	5.02	117.29	110.01
1	B	219	LEU	N-CA-C	-5.01	105.89	111.36
1	B	243	ILE	CB-CG1-CD1	5.01	124.32	113.80
1	B	303	HIS	N-CA-CB	5.01	117.28	110.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	LEU	CA-C-N	5.01	131.22	121.41
1	A	295	LEU	C-N-CA	5.01	131.22	121.41
1	A	298	LEU	O-C-N	5.01	127.86	122.15
1	B	82	PHE	CA-C-O	-5.01	115.56	121.07
1	B	2	ARG	NE-CZ-NH2	5.00	123.70	119.20
1	A	243	ILE	CB-CG1-CD1	5.00	124.30	113.80

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	135	SER	Mainchain
1	A	145	ARG	Sidechain
1	A	2	ARG	Sidechain
1	A	238	TYR	Mainchain
1	A	247	ILE	Mainchain
1	A	272	ARG	Sidechain,Peptide
1	A	276	ARG	Sidechain
1	A	40	ARG	Sidechain
1	A	59	ARG	Sidechain
1	A	71	ARG	Sidechain
1	B	127	ARG	Sidechain
1	B	135	SER	Mainchain
1	B	145	ARG	Sidechain
1	B	2	ARG	Sidechain
1	B	238	TYR	Mainchain
1	B	247	ILE	Mainchain
1	B	272	ARG	Sidechain,Peptide
1	B	276	ARG	Sidechain
1	B	40	ARG	Sidechain
1	B	59	ARG	Sidechain
1	B	71	ARG	Sidechain
2	I	2	GLX	Mainchain
2	I	31	ALA	Mainchain
2	I	32	ARG	Sidechain
2	J	2	GLX	Mainchain
2	J	31	ALA	Mainchain
2	J	32	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2437	0	2350	207	0
1	B	2437	0	2350	201	0
2	I	285	0	243	44	0
2	J	285	0	243	45	0
3	A	5	0	2	1	0
3	B	5	0	2	1	0
4	I	1	0	0	0	0
4	J	1	0	0	0	0
All	All	5456	0	5190	480	0

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 45.

All (480) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:SER:HB3	1:B:136:SER:HB2	1.25	1.18
1:A:134:SER:HB3	1:A:136:SER:HB2	1.25	1.17
1:B:136:SER:HA	1:B:137:LEU:HD22	1.32	1.10
1:B:60:PRO:HB3	1:B:190:LYS:HD2	1.33	1.09
1:A:136:SER:HA	1:A:137:LEU:HD22	1.32	1.08
1:B:208:TYR:HB3	1:B:251:SER:HA	1.31	1.08
1:A:60:PRO:HB3	1:A:190:LYS:HD2	1.33	1.04
1:A:208:TYR:HB3	1:A:251:SER:HA	1.31	1.04
2:I:5:ASP:CG	2:I:21:ALA:HB1	1.86	0.99
2:J:5:ASP:CG	2:J:21:ALA:HB1	1.86	0.99
1:B:74:ILE:HD13	1:B:281:LEU:HD12	1.45	0.98
2:J:21:ALA:O	2:J:23:PHE:N	1.97	0.97
1:A:74:ILE:HD13	1:A:281:LEU:HD12	1.44	0.96
2:I:21:ALA:O	2:I:23:PHE:N	1.97	0.96
1:B:74:ILE:HD13	1:B:281:LEU:CD1	1.96	0.95
1:A:74:ILE:HD13	1:A:281:LEU:CD1	1.96	0.94
1:B:134:SER:CB	1:B:136:SER:HB2	1.98	0.93
2:I:9:ASN:HA	2:I:33:THR:HG23	1.51	0.93
2:J:9:ASN:HA	2:J:33:THR:HG23	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:SER:CB	1:A:136:SER:HB2	1.98	0.92
1:A:186:HIS:HD2	1:A:188:ASN:H	1.11	0.92
1:B:186:HIS:HD2	1:B:188:ASN:H	1.11	0.92
1:A:289:THR:O	1:A:293:THR:HG22	1.70	0.92
1:B:289:THR:O	1:B:293:THR:HG22	1.70	0.91
1:A:283:ALA:HB3	1:B:122:GLU:HG3	1.52	0.89
1:A:122:GLU:HG3	1:B:283:ALA:HB3	1.53	0.89
1:B:132:VAL:O	1:B:133:THR:OG1	1.90	0.89
1:A:132:VAL:O	1:A:133:THR:OG1	1.90	0.88
2:J:5:ASP:OD2	2:J:21:ALA:O	1.92	0.88
2:J:5:ASP:OD1	2:J:21:ALA:HB1	1.73	0.87
2:I:5:ASP:OD2	2:I:21:ALA:O	1.92	0.86
1:B:171:ASN:O	1:B:177:LYS:HE2	1.75	0.86
1:A:92:GLN:HA	1:A:92:GLN:NE2	1.90	0.86
1:B:92:GLN:HA	1:B:92:GLN:NE2	1.90	0.86
1:A:136:SER:HA	1:A:137:LEU:CD2	2.05	0.86
1:B:136:SER:HA	1:B:137:LEU:CD2	2.05	0.86
2:I:5:ASP:OD1	2:I:21:ALA:HB1	1.74	0.85
1:A:283:ALA:HB2	1:B:122:GLU:HA	1.58	0.85
1:A:171:ASN:O	1:A:177:LYS:HE2	1.75	0.85
1:A:245:THR:HG22	1:A:246:THR:CG2	2.08	0.84
1:A:122:GLU:HA	1:B:283:ALA:HB2	1.60	0.84
1:A:245:THR:HG22	1:A:246:THR:HG23	1.59	0.83
1:B:245:THR:HG22	1:B:246:THR:CG2	2.08	0.83
1:B:245:THR:HG22	1:B:246:THR:HG23	1.59	0.82
2:J:31:ALA:HA	2:J:32:ARG:NH1	1.95	0.81
1:B:134:SER:HB3	1:B:136:SER:CB	2.09	0.81
2:J:5:ASP:OD2	2:J:21:ALA:HB1	1.80	0.81
2:I:31:ALA:HA	2:I:32:ARG:NH1	1.95	0.80
1:A:93:ASN:O	1:A:97:THR:HG23	1.82	0.80
1:A:134:SER:HB3	1:A:136:SER:CB	2.09	0.80
1:A:186:HIS:CD2	1:A:188:ASN:H	1.99	0.79
2:I:5:ASP:OD2	2:I:21:ALA:HB1	1.80	0.79
1:A:208:TYR:CB	1:A:251:SER:HA	2.13	0.78
1:B:93:ASN:O	1:B:97:THR:HG23	1.82	0.78
1:B:208:TYR:CB	1:B:251:SER:HA	2.13	0.78
1:A:91:GLY:H	1:A:97:THR:HG22	1.48	0.78
1:B:186:HIS:CD2	1:B:188:ASN:H	1.99	0.78
1:A:131:SER:O	1:A:139:VAL:HG23	1.83	0.77
1:B:131:SER:O	1:B:139:VAL:HG23	1.83	0.77
2:J:5:ASP:HB3	2:J:8:CYS:SG	2.24	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:ASP:HB3	2:I:8:CYS:SG	2.24	0.77
2:I:7:ILE:HD12	2:I:20:GLY:H	1.50	0.77
1:B:91:GLY:H	1:B:97:THR:HG22	1.48	0.77
2:J:7:ILE:HD12	2:J:20:GLY:H	1.50	0.76
1:B:297:VAL:HG12	1:B:301:MET:HE3	1.68	0.76
1:A:297:VAL:HG12	1:A:301:MET:HE3	1.68	0.76
1:B:26:VAL:HG13	1:B:33:VAL:HG23	1.68	0.75
1:A:26:VAL:HG13	1:A:33:VAL:HG23	1.68	0.75
1:A:91:GLY:H	1:A:97:THR:CG2	2.00	0.75
1:B:91:GLY:H	1:B:97:THR:CG2	2.00	0.74
1:A:159:SER:O	1:A:162:SER:HB2	1.88	0.74
2:I:31:ALA:CA	2:I:32:ARG:NH1	2.51	0.74
1:B:159:SER:O	1:B:162:SER:HB2	1.88	0.73
1:B:224:LYS:HD2	1:B:240:TYR:OH	1.88	0.73
1:A:224:LYS:HD2	1:A:240:TYR:OH	1.88	0.73
2:J:31:ALA:CA	2:J:32:ARG:NH1	2.51	0.73
1:B:26:VAL:HA	1:B:33:VAL:HG22	1.72	0.72
1:B:297:VAL:HG12	1:B:301:MET:CE	2.19	0.72
1:A:297:VAL:HG12	1:A:301:MET:CE	2.19	0.72
1:B:136:SER:CA	1:B:137:LEU:HD22	2.16	0.72
1:A:297:VAL:O	1:A:301:MET:HG3	1.90	0.72
1:B:303:HIS:O	1:B:307:ASN:ND2	2.23	0.72
1:B:297:VAL:O	1:B:301:MET:HG3	1.90	0.71
1:A:303:HIS:O	1:A:307:ASN:ND2	2.23	0.71
2:J:32:ARG:HH11	2:J:32:ARG:H	1.40	0.70
1:A:26:VAL:HA	1:A:33:VAL:HG22	1.72	0.70
2:I:31:ALA:CA	2:I:32:ARG:HH11	2.05	0.70
1:B:83:ALA:O	1:B:87:THR:HG23	1.92	0.70
1:A:136:SER:CA	1:A:137:LEU:HD22	2.16	0.69
2:J:5:ASP:OD1	2:J:21:ALA:CB	2.40	0.69
1:A:273:ASP:OD2	1:A:274:THR:N	2.22	0.69
2:I:32:ARG:HH11	2:I:32:ARG:H	1.40	0.69
1:A:83:ALA:O	1:A:87:THR:HG23	1.92	0.69
2:J:31:ALA:CA	2:J:32:ARG:HH11	2.05	0.69
1:B:273:ASP:OD2	1:B:274:THR:N	2.22	0.69
2:I:5:ASP:OD1	2:I:21:ALA:CB	2.40	0.68
2:I:32:ARG:HH11	2:I:32:ARG:N	1.92	0.68
1:A:119:THR:HA	1:A:123:ASN:O	1.94	0.68
1:B:213:ILE:O	1:B:216:LYS:HB2	1.94	0.68
1:B:91:GLY:N	1:B:97:THR:HG22	2.09	0.68
1:A:213:ILE:O	1:A:216:LYS:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:SER:HA	1:B:28:GLN:HE22	1.59	0.67
1:A:3:SER:HA	1:A:28:GLN:HE22	1.59	0.67
1:A:91:GLY:N	1:A:97:THR:HG22	2.09	0.67
1:B:119:THR:HA	1:B:123:ASN:O	1.94	0.67
1:A:273:ASP:OD2	1:A:275:GLY:N	2.27	0.67
2:J:32:ARG:HH11	2:J:32:ARG:N	1.92	0.67
2:I:9:ASN:HD21	2:J:3:HIS:H	1.42	0.67
2:J:7:ILE:O	2:J:10:LYS:HB3	1.94	0.67
2:J:31:ALA:HA	2:J:32:ARG:HH12	1.59	0.67
2:I:7:ILE:O	2:I:10:LYS:HB3	1.94	0.67
1:A:58:ASN:HD21	1:A:188:ASN:HB2	1.60	0.67
2:I:31:ALA:O	2:I:33:THR:HB	1.95	0.67
1:A:179:ILE:N	1:A:179:ILE:HD12	2.10	0.66
1:B:26:VAL:HG13	1:B:33:VAL:CG2	2.25	0.66
2:I:3:HIS:H	2:J:9:ASN:HD21	1.44	0.66
1:B:273:ASP:OD2	1:B:275:GLY:N	2.27	0.66
1:B:192:PHE:O	1:B:266:SER:HA	1.95	0.66
2:J:31:ALA:O	2:J:33:THR:HB	1.95	0.66
1:A:26:VAL:HG13	1:A:33:VAL:CG2	2.25	0.66
1:A:192:PHE:O	1:A:266:SER:HA	1.95	0.66
1:B:179:ILE:HD12	1:B:179:ILE:N	2.10	0.65
1:A:70:SER:HB3	1:A:116:PHE:N	2.11	0.65
1:A:186:HIS:HD2	1:A:188:ASN:N	1.92	0.65
1:B:58:ASN:HD21	1:B:188:ASN:HB2	1.60	0.65
2:I:31:ALA:HA	2:I:32:ARG:HH12	1.60	0.65
1:B:70:SER:HB3	1:B:116:PHE:N	2.11	0.65
1:A:201:LEU:HA	1:A:239:LYS:O	1.97	0.65
1:B:201:LEU:HA	1:B:239:LYS:O	1.97	0.65
1:B:81:TRP:CH2	1:B:85:LYS:HD3	2.32	0.64
1:A:81:TRP:CH2	1:A:85:LYS:HD3	2.32	0.64
1:A:42:TYR:C	1:A:42:TYR:CD2	2.75	0.64
1:A:149:ALA:HB1	1:A:256:ASP:HB3	1.80	0.64
1:B:42:TYR:C	1:B:42:TYR:CD2	2.75	0.64
1:A:283:ALA:CB	1:B:122:GLU:HA	2.28	0.63
1:B:149:ALA:HB1	1:B:256:ASP:HB3	1.80	0.63
1:A:179:ILE:H	1:A:179:ILE:CD1	2.12	0.63
2:I:21:ALA:O	2:I:22:TRP:CD1	2.52	0.63
1:B:91:GLY:HA2	1:B:97:THR:HG21	1.81	0.63
1:B:69:HIS:NE2	1:B:127:ARG:NH2	2.46	0.63
1:A:122:GLU:HA	1:B:283:ALA:CB	2.29	0.62
1:A:91:GLY:HA2	1:A:97:THR:HG21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:21:ALA:O	2:J:22:TRP:CD1	2.52	0.62
1:A:51:LYS:HG3	1:A:106:PHE:CZ	2.35	0.62
1:B:69:HIS:CE1	1:B:127:ARG:NH2	2.68	0.61
1:B:179:ILE:H	1:B:179:ILE:CD1	2.12	0.61
2:I:7:ILE:HB	2:I:21:ALA:HB2	1.82	0.61
1:A:69:HIS:CE1	1:A:127:ARG:NH2	2.68	0.61
1:B:186:HIS:HD2	1:B:188:ASN:N	1.92	0.61
1:A:103:MET:HE2	1:A:305:VAL:HB	1.83	0.61
1:B:103:MET:HE2	1:B:305:VAL:HB	1.83	0.61
1:B:51:LYS:HG3	1:B:106:PHE:CZ	2.35	0.61
1:A:213:ILE:CD1	1:A:219:LEU:HD22	2.31	0.61
1:A:146:ASN:O	1:A:170:ALA:HA	2.01	0.61
1:A:91:GLY:N	1:A:97:THR:CG2	2.64	0.60
1:B:213:ILE:CD1	1:B:219:LEU:HD22	2.31	0.60
2:J:3:HIS:O	2:J:4:ALA:HB2	2.01	0.60
2:J:7:ILE:HB	2:J:21:ALA:HB2	1.82	0.60
2:I:3:HIS:O	2:I:4:ALA:HB2	2.01	0.60
1:A:69:HIS:NE2	1:A:127:ARG:NH2	2.46	0.60
1:A:91:GLY:CA	1:A:97:THR:HG21	2.31	0.60
1:B:91:GLY:CA	1:B:97:THR:HG21	2.31	0.60
1:B:146:ASN:O	1:B:170:ALA:HA	2.01	0.60
1:B:171:ASN:O	1:B:177:LYS:CE	2.49	0.60
1:B:233:LEU:CD1	1:B:295:LEU:HD22	2.33	0.59
1:A:131:SER:C	1:A:139:VAL:HG23	2.28	0.59
1:A:233:LEU:CD1	1:A:295:LEU:HD22	2.33	0.59
1:A:63:TRP:HB2	1:A:189:PHE:CE2	2.38	0.59
1:B:63:TRP:HB2	1:B:189:PHE:CE2	2.38	0.59
1:B:242:SER:OG	1:B:245:THR:HB	2.03	0.59
1:B:289:THR:O	1:B:293:THR:CG2	2.49	0.59
1:A:70:SER:HB2	1:A:119:THR:HG21	1.85	0.59
1:B:58:ASN:ND2	1:B:188:ASN:HB2	2.18	0.59
1:B:150:GLY:O	1:B:251:SER:HB2	2.03	0.59
1:B:211:GLN:HG2	1:B:212:SER:N	2.17	0.59
1:A:127:ARG:NH2	1:A:142:ASP:OD2	2.36	0.58
2:I:31:ALA:C	2:I:32:ARG:HH11	2.11	0.58
1:B:66:LEU:N	1:B:108:GLU:O	2.36	0.58
1:B:70:SER:HB2	1:B:119:THR:HG21	1.85	0.58
1:B:198:TYR:HA	1:B:271:LEU:O	2.03	0.58
1:A:150:GLY:O	1:A:251:SER:HB2	2.03	0.58
1:A:242:SER:OG	1:A:245:THR:HB	2.03	0.58
1:A:7:PHE:CD1	1:A:7:PHE:C	2.82	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:NH2	1:B:142:ASP:OD2	2.36	0.58
1:B:131:SER:C	1:B:139:VAL:HG23	2.27	0.58
1:A:171:ASN:HD22	1:A:176:VAL:HG12	1.68	0.58
1:A:192:PHE:HB2	1:A:263:ILE:HG21	1.86	0.58
1:A:211:GLN:HG2	1:A:212:SER:N	2.18	0.58
1:A:198:TYR:HA	1:A:271:LEU:O	2.03	0.58
1:B:192:PHE:HB2	1:B:263:ILE:HG21	1.86	0.58
1:A:58:ASN:ND2	1:A:188:ASN:HB2	2.18	0.58
1:A:136:SER:CA	1:A:137:LEU:HD13	2.34	0.58
1:B:91:GLY:N	1:B:97:THR:CG2	2.64	0.58
1:A:171:ASN:O	1:A:177:LYS:CE	2.49	0.57
1:A:22:MET:HE2	1:A:109:ILE:HG13	1.86	0.57
2:J:31:ALA:C	2:J:32:ARG:HH11	2.11	0.57
1:B:22:MET:HE2	1:B:109:ILE:HG13	1.86	0.57
1:B:136:SER:CA	1:B:137:LEU:HD13	2.34	0.57
1:B:195:ILE:CG2	1:B:271:LEU:HD21	2.35	0.57
1:A:41:SER:N	1:A:45:ARG:O	2.30	0.57
1:B:233:LEU:HD12	1:B:295:LEU:HD22	1.87	0.57
1:B:245:THR:HG22	1:B:246:THR:HG22	1.85	0.57
1:A:86:PHE:HE1	1:A:294:TRP:HE1	1.53	0.57
1:B:171:ASN:HD22	1:B:176:VAL:HG12	1.68	0.57
3:B:308:GLY:HA2	2:J:38:VAL:OXT	2.04	0.57
1:A:179:ILE:HD12	1:A:179:ILE:H	1.68	0.57
1:A:233:LEU:HD12	1:A:295:LEU:HD22	1.87	0.57
1:A:74:ILE:CD1	1:A:281:LEU:HD12	2.29	0.57
1:B:61:ALA:HA	1:B:104:ASP:O	2.05	0.57
1:A:215:ASP:O	1:A:219:LEU:HD13	2.05	0.57
1:A:25:LEU:HD11	1:A:87:THR:HG21	1.87	0.56
3:A:308:GLY:HA2	2:I:38:VAL:OXT	2.05	0.56
1:A:66:LEU:N	1:A:108:GLU:O	2.36	0.56
1:B:7:PHE:CD1	1:B:7:PHE:C	2.81	0.56
1:A:195:ILE:CG2	1:A:271:LEU:HD21	2.35	0.56
1:A:245:THR:HG22	1:A:246:THR:HG22	1.85	0.56
1:B:72:GLU:HB3	1:B:197:SER:HB3	1.87	0.56
1:B:86:PHE:HE1	1:B:294:TRP:HE1	1.53	0.56
2:J:21:ALA:O	2:J:22:TRP:CG	2.59	0.56
1:A:289:THR:O	1:A:293:THR:CG2	2.49	0.56
1:B:25:LEU:HD11	1:B:87:THR:HG21	1.87	0.56
1:B:179:ILE:HD12	1:B:179:ILE:H	1.68	0.56
2:I:21:ALA:O	2:I:22:TRP:CG	2.59	0.56
1:A:61:ALA:HA	1:A:104:ASP:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:ARG:HG2	1:A:276:ARG:HH11	1.71	0.56
1:A:69:HIS:CE1	1:A:127:ARG:HH21	2.24	0.56
1:B:276:ARG:HG2	1:B:276:ARG:HH11	1.71	0.56
1:A:115:GLY:O	1:A:119:THR:HG23	2.06	0.56
1:A:212:SER:OG	1:A:216:LYS:HG3	2.06	0.55
1:A:281:LEU:HD21	1:A:285:GLN:NE2	2.22	0.55
1:B:215:ASP:O	1:B:219:LEU:HD13	2.05	0.55
1:B:258:SER:HB2	1:B:263:ILE:HD12	1.89	0.55
1:A:208:TYR:HD1	1:A:256:ASP:OD2	1.89	0.55
1:A:72:GLU:HB3	1:A:197:SER:HB3	1.87	0.55
1:A:74:ILE:HG13	1:A:74:ILE:O	2.05	0.55
1:B:95:SER:OG	1:B:302:GLU:OE2	2.25	0.55
1:A:66:LEU:HD22	1:A:75:THR:O	2.07	0.55
2:I:29:ASN:N	2:I:29:ASN:HD22	2.04	0.55
1:B:115:GLY:O	1:B:119:THR:HG23	2.06	0.55
1:B:74:ILE:HG13	1:B:74:ILE:O	2.05	0.54
1:B:127:ARG:HH11	2:J:37:TYR:CB	2.20	0.54
1:B:63:TRP:HE1	1:B:65:ASP:HB3	1.72	0.54
1:B:281:LEU:HD21	1:B:285:GLN:NE2	2.22	0.54
1:B:66:LEU:HD22	1:B:75:THR:O	2.07	0.54
1:B:179:ILE:N	1:B:179:ILE:CD1	2.70	0.54
1:B:208:TYR:HD1	1:B:256:ASP:OD2	1.89	0.54
1:B:212:SER:OG	1:B:216:LYS:HG3	2.06	0.54
1:A:95:SER:OG	1:A:302:GLU:OE2	2.25	0.54
1:A:1:ALA:N	1:A:7:PHE:HB2	2.23	0.54
1:A:63:TRP:HE1	1:A:65:ASP:HB3	1.73	0.54
1:B:45:ARG:HH11	1:B:114:ASN:ND2	2.06	0.54
1:A:70:SER:HB2	1:A:119:THR:CG2	2.38	0.54
1:B:70:SER:HB2	1:B:119:THR:CG2	2.38	0.54
2:J:7:ILE:CD1	2:J:20:GLY:H	2.20	0.54
1:A:127:ARG:HH11	2:I:37:TYR:CB	2.21	0.53
1:A:136:SER:HA	1:A:137:LEU:HD13	1.90	0.53
1:B:136:SER:HA	1:B:137:LEU:HD13	1.91	0.53
1:A:258:SER:HB2	1:A:263:ILE:HD12	1.89	0.53
1:B:195:ILE:HG22	1:B:271:LEU:CD2	2.38	0.53
1:A:45:ARG:HH11	1:A:114:ASN:ND2	2.06	0.53
1:A:195:ILE:HG22	1:A:271:LEU:CD2	2.39	0.53
1:B:1:ALA:H2	1:B:7:PHE:HB2	1.74	0.53
1:B:93:ASN:O	1:B:97:THR:CG2	2.56	0.53
1:B:199:SER:N	1:B:271:LEU:O	2.42	0.53
1:B:1:ALA:N	1:B:7:PHE:HB2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:HB2	1:A:33:VAL:HG13	1.92	0.52
2:I:7:ILE:CD1	2:I:20:GLY:H	2.21	0.52
1:A:204:TYR:HB2	1:A:205:PRO:HD2	1.91	0.52
2:J:21:ALA:C	2:J:23:PHE:H	2.14	0.52
1:A:133:THR:O	1:A:134:SER:HB2	2.10	0.52
1:A:144:ASN:C	1:A:145:ARG:HD2	2.35	0.52
1:A:199:SER:N	1:A:271:LEU:O	2.42	0.52
1:B:204:TYR:HB2	1:B:205:PRO:HD2	1.91	0.52
1:A:60:PRO:HA	1:A:188:ASN:O	2.10	0.52
1:A:26:VAL:HG12	1:A:33:VAL:O	2.11	0.51
1:A:213:ILE:HD11	1:A:216:LYS:HA	1.91	0.51
1:B:204:TYR:O	1:B:242:SER:HA	2.10	0.51
1:B:213:ILE:HD11	1:B:216:LYS:HA	1.91	0.51
1:A:25:LEU:CD2	1:A:83:ALA:HB1	2.41	0.51
1:B:25:LEU:CD2	1:B:83:ALA:HB1	2.41	0.51
1:B:74:ILE:CD1	1:B:281:LEU:HD12	2.29	0.51
1:A:69:HIS:HE2	1:A:127:ARG:HH21	1.54	0.51
1:B:41:SER:N	1:B:45:ARG:O	2.30	0.51
1:B:144:ASN:C	1:B:145:ARG:HD2	2.35	0.51
1:B:95:SER:O	1:B:99:ILE:HD12	2.10	0.51
1:B:133:THR:O	1:B:134:SER:HB2	2.10	0.51
1:A:179:ILE:N	1:A:179:ILE:CD1	2.70	0.51
1:A:136:SER:HA	1:A:137:LEU:CD1	2.41	0.51
1:B:26:VAL:HG12	1:B:33:VAL:O	2.11	0.51
1:B:136:SER:HA	1:B:137:LEU:CD1	2.41	0.51
1:B:136:SER:C	1:B:137:LEU:HD13	2.36	0.51
1:B:213:ILE:O	1:B:213:ILE:HG13	2.10	0.51
1:B:60:PRO:HA	1:B:188:ASN:O	2.10	0.50
1:A:95:SER:O	1:A:99:ILE:HD12	2.10	0.50
1:A:213:ILE:O	1:A:213:ILE:HG13	2.10	0.50
1:A:136:SER:C	1:A:137:LEU:HD13	2.36	0.50
1:A:204:TYR:O	1:A:242:SER:HA	2.10	0.50
1:B:293:THR:O	1:B:297:VAL:HG23	2.12	0.50
1:A:1:ALA:H2	1:A:7:PHE:HB2	1.75	0.50
1:B:29:HIS:HB2	1:B:33:VAL:HG13	1.92	0.50
2:I:21:ALA:C	2:I:23:PHE:N	2.70	0.50
1:A:93:ASN:ND2	1:A:96:PHE:HB2	2.27	0.49
1:A:293:THR:O	1:A:297:VAL:HG23	2.12	0.49
1:B:69:HIS:CE1	1:B:127:ARG:HH21	2.24	0.49
1:B:54:THR:HG21	1:B:90:TYR:CZ	2.47	0.49
1:A:54:THR:HG21	1:A:90:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:ASN:N	2:J:29:ASN:HD22	2.04	0.49
1:A:93:ASN:O	1:A:97:THR:CG2	2.56	0.49
1:A:133:THR:O	1:A:134:SER:CB	2.61	0.49
1:A:195:ILE:HG22	1:A:271:LEU:HD22	1.95	0.49
2:I:2:GLX:O	2:I:2:GLX:HG2	2.12	0.49
1:A:93:ASN:HD22	1:A:96:PHE:CB	2.26	0.49
1:A:203:LEU:HD11	1:A:246:THR:OG1	2.13	0.49
1:B:93:ASN:ND2	1:B:96:PHE:HB2	2.27	0.49
1:A:134:SER:C	1:A:136:SER:N	2.71	0.49
1:B:144:ASN:O	1:B:145:ARG:HD2	2.12	0.49
1:A:93:ASN:HD22	1:A:96:PHE:HB2	1.78	0.48
1:B:134:SER:C	1:B:136:SER:N	2.71	0.48
1:A:144:ASN:O	1:A:145:ARG:HD2	2.13	0.48
1:B:93:ASN:HD22	1:B:96:PHE:CB	2.26	0.48
2:J:2:GLX:O	2:J:2:GLX:HG2	2.12	0.48
2:I:9:ASN:HA	2:I:33:THR:CG2	2.34	0.48
1:A:204:TYR:HB2	1:A:205:PRO:CD	2.44	0.48
1:B:93:ASN:HD22	1:B:96:PHE:HB2	1.78	0.48
1:B:195:ILE:HG21	1:B:271:LEU:HD21	1.96	0.48
1:B:133:THR:O	1:B:134:SER:CB	2.61	0.48
1:B:203:LEU:HD11	1:B:246:THR:OG1	2.13	0.48
1:A:195:ILE:HG21	1:A:271:LEU:HD21	1.96	0.48
2:I:31:ALA:O	2:I:33:THR:N	2.47	0.48
1:B:203:LEU:HD12	1:B:241:GLY:O	2.14	0.48
2:J:14:THR:HB	2:J:16:ASP:HB3	1.95	0.48
1:A:203:LEU:HD12	1:A:241:GLY:O	2.14	0.47
2:J:9:ASN:HA	2:J:33:THR:CG2	2.34	0.47
1:A:8:ASN:O	1:A:11:THR:CG2	2.62	0.47
2:I:14:THR:HB	2:I:16:ASP:HB3	1.95	0.47
1:B:272:ARG:HD3	1:B:285:GLN:HE21	1.79	0.47
2:J:21:ALA:C	2:J:23:PHE:N	2.69	0.47
1:A:127:ARG:HH11	2:I:37:TYR:HB2	1.79	0.47
1:A:272:ARG:HD3	1:A:285:GLN:HE21	1.79	0.47
1:B:186:HIS:CD2	1:B:188:ASN:N	2.76	0.47
1:B:136:SER:OG	1:B:138:CYS:HB2	2.15	0.47
1:B:8:ASN:O	1:B:11:THR:CG2	2.62	0.47
1:B:69:HIS:HE2	1:B:127:ARG:HH21	1.54	0.47
1:B:127:ARG:HH11	2:J:37:TYR:HB2	1.78	0.47
1:B:195:ILE:HG22	1:B:271:LEU:HD22	1.95	0.47
1:B:205:PRO:HB2	1:B:213:ILE:HG21	1.97	0.47
2:J:31:ALA:O	2:J:33:THR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:PHE:CE1	1:A:294:TRP:HB2	2.49	0.47
1:A:276:ARG:HG2	1:A:276:ARG:NH1	2.30	0.47
1:B:62:ILE:HD12	1:B:191:ALA:HB3	1.97	0.47
1:B:132:VAL:O	1:B:133:THR:CB	2.60	0.47
1:A:136:SER:OG	1:A:138:CYS:HB2	2.15	0.47
1:A:62:ILE:HD12	1:A:191:ALA:HB3	1.97	0.47
1:A:36:LEU:HB2	1:A:49:VAL:O	2.15	0.47
1:B:36:LEU:HB2	1:B:49:VAL:O	2.15	0.47
1:A:200:GLN:HB3	1:A:238:TYR:CD1	2.50	0.46
1:A:205:PRO:HB2	1:A:213:ILE:HG21	1.97	0.46
1:B:195:ILE:CG2	1:B:271:LEU:CD2	2.93	0.46
1:B:297:VAL:HG12	1:B:301:MET:HE2	1.96	0.46
1:B:204:TYR:HB2	1:B:205:PRO:CD	2.44	0.46
1:A:277:TYR:CG	1:A:282:PRO:HD3	2.51	0.46
2:I:3:HIS:O	2:I:4:ALA:CB	2.61	0.46
2:I:5:ASP:OD2	2:I:21:ALA:CB	2.59	0.46
1:B:82:PHE:CE1	1:B:294:TRP:HB2	2.49	0.46
1:B:200:GLN:HB3	1:B:238:TYR:CD1	2.50	0.46
1:A:54:THR:HG21	1:A:90:TYR:CE1	2.51	0.46
1:A:4:THR:HG23	1:A:28:GLN:OE1	2.15	0.46
1:A:132:VAL:O	1:A:133:THR:CB	2.60	0.46
1:B:93:ASN:HA	1:B:94:PRO:HD2	1.64	0.46
1:B:95:SER:O	1:B:98:ALA:HB3	2.15	0.46
1:B:4:THR:HG23	1:B:28:GLN:OE1	2.15	0.46
1:B:14:THR:O	1:B:15:LEU:C	2.59	0.46
1:B:54:THR:HG21	1:B:90:TYR:CE1	2.51	0.46
1:B:126:TRP:NE1	1:B:128:LYS:O	2.50	0.46
1:B:277:TYR:O	1:B:278:GLY:C	2.59	0.46
1:A:95:SER:O	1:A:98:ALA:HB3	2.15	0.45
2:I:31:ALA:O	2:I:33:THR:CB	2.63	0.45
2:J:21:ALA:O	2:J:22:TRP:C	2.47	0.45
1:A:287:ILE:HD13	1:A:287:ILE:N	2.32	0.45
1:B:15:LEU:HD23	1:B:15:LEU:HA	1.79	0.45
1:B:271:LEU:HB3	1:B:272:ARG:H	1.63	0.45
1:A:36:LEU:O	1:A:49:VAL:N	2.40	0.45
2:I:29:ASN:N	2:I:29:ASN:ND2	2.63	0.45
1:B:287:ILE:HD13	1:B:287:ILE:N	2.31	0.45
1:A:126:TRP:NE1	1:A:128:LYS:O	2.50	0.45
1:A:168:LYS:HG3	1:A:169:TYR:CD2	2.51	0.45
1:A:277:TYR:O	1:A:278:GLY:C	2.59	0.45
1:B:220:ASN:O	1:B:223:ALA:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ASN:HB3	1:B:177:LYS:HD3	1.99	0.45
1:B:203:LEU:HD12	1:B:203:LEU:HA	1.75	0.45
1:A:13:HIS:HA	1:A:17:GLU:OE1	2.17	0.45
1:B:13:HIS:HA	1:B:17:GLU:OE1	2.17	0.45
1:B:277:TYR:CG	1:B:282:PRO:HD3	2.51	0.45
1:A:198:TYR:O	1:A:199:SER:CB	2.65	0.45
1:A:220:ASN:O	1:A:223:ALA:HB3	2.16	0.45
1:A:14:THR:O	1:A:15:LEU:C	2.60	0.45
1:B:276:ARG:HG2	1:B:276:ARG:NH1	2.30	0.45
1:B:168:LYS:HG3	1:B:169:TYR:CD2	2.51	0.44
1:A:230:LEU:HD23	1:A:230:LEU:C	2.43	0.44
1:B:205:PRO:HG3	1:B:255:ILE:HG23	2.00	0.44
1:A:195:ILE:CG2	1:A:271:LEU:CD2	2.93	0.44
2:J:31:ALA:O	2:J:33:THR:CB	2.63	0.44
2:J:29:ASN:N	2:J:29:ASN:ND2	2.63	0.44
1:A:287:ILE:N	1:A:288:PRO:CD	2.81	0.44
1:B:290:ALA:HA	1:B:293:THR:CG2	2.48	0.44
1:A:76:GLN:HG3	1:A:109:ILE:O	2.18	0.44
1:A:290:ALA:HA	1:A:293:THR:CG2	2.48	0.44
1:B:186:HIS:NE2	1:B:188:ASN:HB3	2.33	0.44
2:J:5:ASP:OD2	2:J:21:ALA:CB	2.59	0.44
1:A:45:ARG:HH11	1:A:45:ARG:HD2	1.50	0.44
1:A:208:TYR:CD1	1:A:256:ASP:OD2	2.69	0.44
1:B:29:HIS:N	1:B:30:PRO:HD3	2.33	0.44
1:B:100:LEU:HD23	1:B:100:LEU:HA	1.86	0.44
1:A:127:ARG:NH1	2:I:37:TYR:HB3	2.33	0.44
2:J:3:HIS:O	2:J:4:ALA:CB	2.61	0.44
1:A:186:HIS:NE2	1:A:188:ASN:HB3	2.33	0.43
1:B:127:ARG:NH1	2:J:37:TYR:HB3	2.33	0.43
1:B:230:LEU:C	1:B:230:LEU:HD23	2.43	0.43
1:A:171:ASN:HB3	1:A:177:LYS:HD3	1.99	0.43
1:B:76:GLN:HG3	1:B:109:ILE:O	2.18	0.43
1:B:198:TYR:O	1:B:199:SER:CB	2.65	0.43
1:A:194:SER:O	1:A:268:THR:HG23	2.19	0.43
1:A:205:PRO:HG3	1:A:255:ILE:HG23	2.00	0.43
1:B:287:ILE:HB	1:B:288:PRO:HD3	2.01	0.43
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.86	0.43
2:J:7:ILE:HG13	2:J:21:ALA:HB2	2.01	0.43
1:A:29:HIS:N	1:A:30:PRO:HD3	2.33	0.43
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.75	0.42
1:A:233:LEU:HD12	1:A:292:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:SER:HB3	1:B:58:ASN:H	1.66	0.42
1:B:287:ILE:N	1:B:288:PRO:CD	2.81	0.42
1:B:220:ASN:O	1:B:224:LYS:N	2.52	0.42
1:B:247:ILE:HD13	1:B:247:ILE:HG21	1.85	0.42
1:A:142:ASP:HB2	1:A:163:GLU:O	2.20	0.42
1:A:159:SER:HA	1:A:160:PRO:HD3	1.75	0.42
1:B:142:ASP:HB2	1:B:163:GLU:O	2.19	0.42
1:A:287:ILE:HB	1:A:288:PRO:HD3	2.01	0.42
1:B:208:TYR:CD1	1:B:256:ASP:OD2	2.69	0.42
1:A:54:THR:H	1:A:59:ARG:HH22	1.68	0.42
1:A:136:SER:HB3	1:A:138:CYS:O	2.19	0.42
1:B:222:VAL:HG21	1:B:303:HIS:CG	2.55	0.42
2:I:7:ILE:HG13	2:I:21:ALA:HB2	2.01	0.42
1:B:233:LEU:HD12	1:B:292:GLU:HA	2.01	0.42
1:A:186:HIS:CD2	1:A:188:ASN:N	2.76	0.42
1:B:54:THR:H	1:B:59:ARG:HH22	1.68	0.42
1:A:276:ARG:O	2:J:22:TRP:CZ2	2.73	0.42
1:A:297:VAL:HG12	1:A:301:MET:HE2	1.96	0.42
1:B:91:GLY:CA	1:B:97:THR:CG2	2.98	0.42
1:B:194:SER:O	1:B:268:THR:HG23	2.19	0.42
1:A:127:ARG:NH1	2:I:37:TYR:CB	2.83	0.42
1:A:239:LYS:HZ3	1:A:239:LYS:HG2	1.81	0.42
1:A:247:ILE:HD13	1:A:247:ILE:HG21	1.85	0.42
1:B:69:HIS:HB2	1:B:72:GLU:CD	2.45	0.42
1:B:136:SER:HB3	1:B:138:CYS:O	2.19	0.42
1:A:71:ARG:HH11	1:A:71:ARG:HD2	1.48	0.42
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.79	0.41
2:I:22:TRP:CZ2	1:B:276:ARG:O	2.73	0.41
1:A:287:ILE:N	1:A:287:ILE:CD1	2.84	0.41
1:B:155:GLY:HA3	1:B:251:SER:H	1.86	0.41
1:B:168:LYS:H	1:B:168:LYS:HG2	1.48	0.41
2:J:8:CYS:HA	2:J:24:CYS:CB	2.50	0.41
1:B:59:ARG:HA	1:B:60:PRO:HD3	1.76	0.41
1:B:141:VAL:HG21	1:B:173:GLU:OE2	2.21	0.41
1:A:91:GLY:CA	1:A:97:THR:CG2	2.98	0.41
1:A:290:ALA:HA	1:A:293:THR:HG22	2.03	0.41
2:I:8:CYS:HA	2:I:24:CYS:CB	2.50	0.41
1:A:69:HIS:HB2	1:A:72:GLU:CD	2.45	0.41
1:A:222:VAL:HG21	1:A:303:HIS:CG	2.55	0.41
1:A:155:GLY:HA3	1:A:251:SER:H	1.86	0.41
1:A:58:ASN:ND2	1:A:188:ASN:CB	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:VAL:HG21	1:A:173:GLU:OE2	2.21	0.41
1:A:301:MET:O	1:A:302:GLU:C	2.64	0.41
1:A:220:ASN:O	1:A:224:LYS:N	2.52	0.40
1:A:70:SER:HB3	1:A:115:GLY:C	2.46	0.40
2:I:23:PHE:O	2:I:25:GLN:HG3	2.21	0.40
1:B:32:LEU:HD11	1:B:54:THR:HG22	2.02	0.40
1:B:287:ILE:N	1:B:287:ILE:CD1	2.83	0.40
1:A:198:TYR:CA	1:A:271:LEU:O	2.70	0.40
2:J:23:PHE:O	2:J:25:GLN:HG3	2.21	0.40
1:A:32:LEU:HD11	1:A:54:THR:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	9	18
1	B	305/307 (99%)	274 (90%)	27 (9%)	4 (1%)	9	18
2	I	35/38 (92%)	22 (63%)	6 (17%)	7 (20%)	0	0
2	J	35/38 (92%)	22 (63%)	6 (17%)	7 (20%)	0	0
All	All	680/690 (99%)	592 (87%)	66 (10%)	22 (3%)	3	4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	134	SER
1	A	199	SER
1	A	273	ASP
2	I	4	ALA

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Mol	Chain	Res	Type
2	I	32	ARG
1	B	57	SER
1	B	134	SER
1	B	199	SER
1	B	273	ASP
2	J	4	ALA
2	J	32	ARG
2	I	19	SER
2	I	22	TRP
2	I	31	ALA
2	J	19	SER
2	J	22	TRP
2	J	31	ALA
2	I	30	SER
2	J	30	SER
2	I	13	LYS
2	J	13	LYS

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	263/263 (100%)	200 (76%)	63 (24%)	1	1
1	B	263/263 (100%)	200 (76%)	63 (24%)	1	1
2	I	30/30 (100%)	23 (77%)	7 (23%)	1	1
2	J	30/30 (100%)	23 (77%)	7 (23%)	1	1
All	All	586/586 (100%)	446 (76%)	140 (24%)	1	1

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	THR
1	A	7	PHE
1	A	14	THR

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Mol	Chain	Res	Type
1	A	15	LEU
1	A	26	VAL
1	A	31	GLU
1	A	32	LEU
1	A	33	VAL
1	A	35	LYS
1	A	40	ARG
1	A	53	SER
1	A	57	SER
1	A	65	ASP
1	A	68	ILE
1	A	70	SER
1	A	71	ARG
1	A	74	ILE
1	A	78	THR
1	A	87	THR
1	A	97	THR
1	A	100	LEU
1	A	102	SER
1	A	103	MET
1	A	109	ILE
1	A	122	GLU
1	A	127	ARG
1	A	133	THR
1	A	136	SER
1	A	137	LEU
1	A	139	VAL
1	A	158	SER
1	A	162	SER
1	A	168	LYS
1	A	173	GLU
1	A	179	ILE
1	A	184	LYS
1	A	190	LYS
1	A	193	LEU
1	A	195	ILE
1	A	202	LEU
1	A	203	LEU
1	A	216	LYS
1	A	222	VAL
1	A	227	VAL
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	232	SER
1	A	239	LYS
1	A	244	ILE
1	A	245	THR
1	A	247	ILE
1	A	249	GLN
1	A	255	ILE
1	A	270	GLU
1	A	271	LEU
1	A	272	ARG
1	A	274	THR
1	A	281	LEU
1	A	287	ILE
1	A	292	GLU
1	A	295	LEU
1	A	298	LEU
1	A	307	ASN
2	I	7	ILE
2	I	10	LYS
2	I	13	LYS
2	I	14	THR
2	I	19	SER
2	I	25	GLN
2	I	32	ARG
1	B	2	ARG
1	B	6	THR
1	B	7	PHE
1	B	14	THR
1	B	15	LEU
1	B	26	VAL
1	B	31	GLU
1	B	32	LEU
1	B	33	VAL
1	B	35	LYS
1	B	40	ARG
1	B	53	SER
1	B	57	SER
1	B	65	ASP
1	B	68	ILE
1	B	70	SER
1	B	71	ARG
1	B	74	ILE

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Mol	Chain	Res	Type
1	B	78	THR
1	B	87	THR
1	B	97	THR
1	B	100	LEU
1	B	102	SER
1	B	103	MET
1	B	109	ILE
1	B	122	GLU
1	B	127	ARG
1	B	133	THR
1	B	136	SER
1	B	137	LEU
1	B	139	VAL
1	B	158	SER
1	B	162	SER
1	B	168	LYS
1	B	173	GLU
1	B	179	ILE
1	B	184	LYS
1	B	190	LYS
1	B	193	LEU
1	B	195	ILE
1	B	202	LEU
1	B	203	LEU
1	B	216	LYS
1	B	222	VAL
1	B	227	VAL
1	B	230	LEU
1	B	232	SER
1	B	239	LYS
1	B	244	ILE
1	B	245	THR
1	B	247	ILE
1	B	249	GLN
1	B	255	ILE
1	B	270	GLU
1	B	271	LEU
1	B	272	ARG
1	B	274	THR
1	B	281	LEU
1	B	287	ILE
1	B	292	GLU

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Mol	Chain	Res	Type
1	B	295	LEU
1	B	298	LEU
1	B	307	ASN
2	J	7	ILE
2	J	10	LYS
2	J	13	LYS
2	J	14	THR
2	J	19	SER
2	J	25	GLN
2	J	32	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	58	ASN
1	A	92	GLN
1	A	93	ASN
1	A	120	HIS
1	A	171	ASN
1	A	186	HIS
1	A	221	GLN
1	A	285	GLN
2	I	9	ASN
2	I	25	GLN
2	I	29	ASN
1	B	29	HIS
1	B	58	ASN
1	B	92	GLN
1	B	93	ASN
1	B	120	HIS
1	B	171	ASN
1	B	186	HIS
1	B	220	ASN
1	B	221	GLN
1	B	285	GLN
2	J	9	ASN
2	J	25	GLN
2	J	29	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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GLY	B	308	-	4,4,4	1.24	1 (25%)	3,4,4	1.88	1 (33%)
3	GLY	A	308	-	4,4,4	1.25	1 (25%)	3,4,4	1.88	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GLY	B	308	-	-	2/2/2/2	-
3	GLY	A	308	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	308	GLY	O-C	2.07	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	308	GLY	O-C	2.07	1.28	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	308	GLY	OXT-C-O	-3.21	115.06	123.33
3	A	308	GLY	OXT-C-O	-3.21	115.07	123.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	308	GLY	O-C-CA-N
3	B	308	GLY	O-C-CA-N
3	A	308	GLY	OXT-C-CA-N
3	B	308	GLY	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	308	GLY	1	0
3	A	308	GLY	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.