



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:24 PM UTC

PDB ID : 9RUB / pdb_00009rub
Title : CRYSTAL STRUCTURE OF ACTIVATED RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE COMPLEXED WITH ITS SUBSTRATE, RIBULOSE-1,5-BISPHOSPHATE
Authors : Lundqvist, T.; Schneider, G.
Deposited on : 1990-11-28
Resolution : 2.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

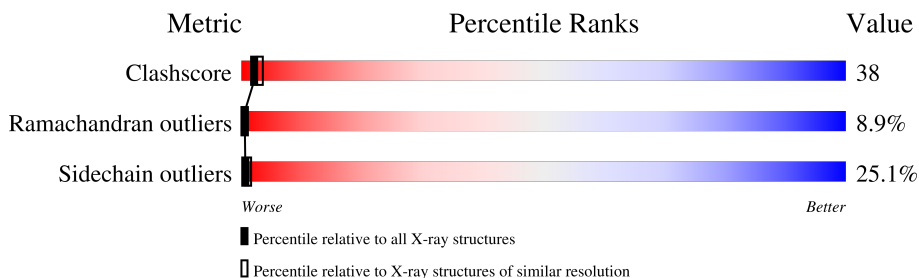
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	466	
1	B	466	

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
4	FMT	A	601	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7044 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.

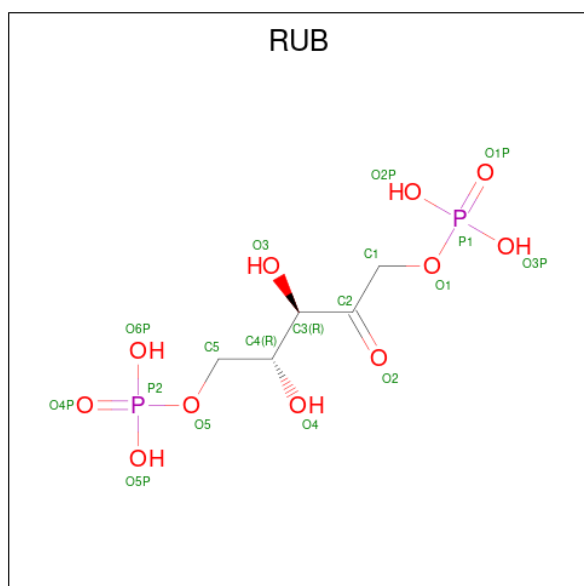
- Molecule 1 is a protein called RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	8	0	0
			3502	2213	613	658	18			
1	B	458	Total	C	N	O	S	1	0	0
			3498	2211	612	657	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	ASP	HIS	conflict	UNP P04718
B	91	ASP	HIS	conflict	UNP P04718

- Molecule 2 is RIBULOSE-1,5-DIPHOSPHATE (CCD ID: RUB) (formula: $C_5H_{12}O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	5	11	2		

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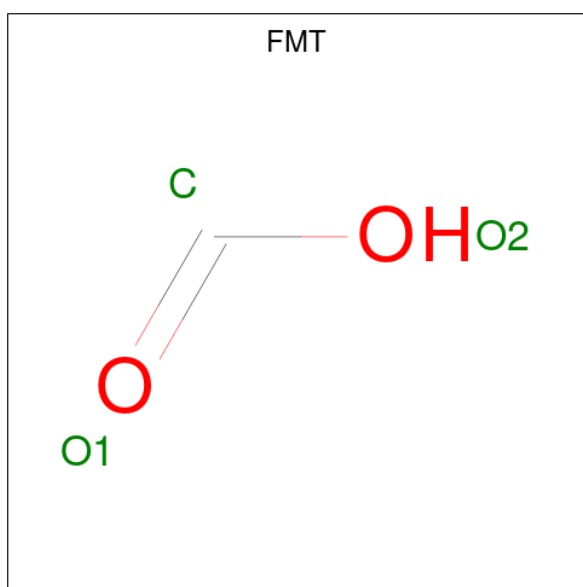
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			18	5	11	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



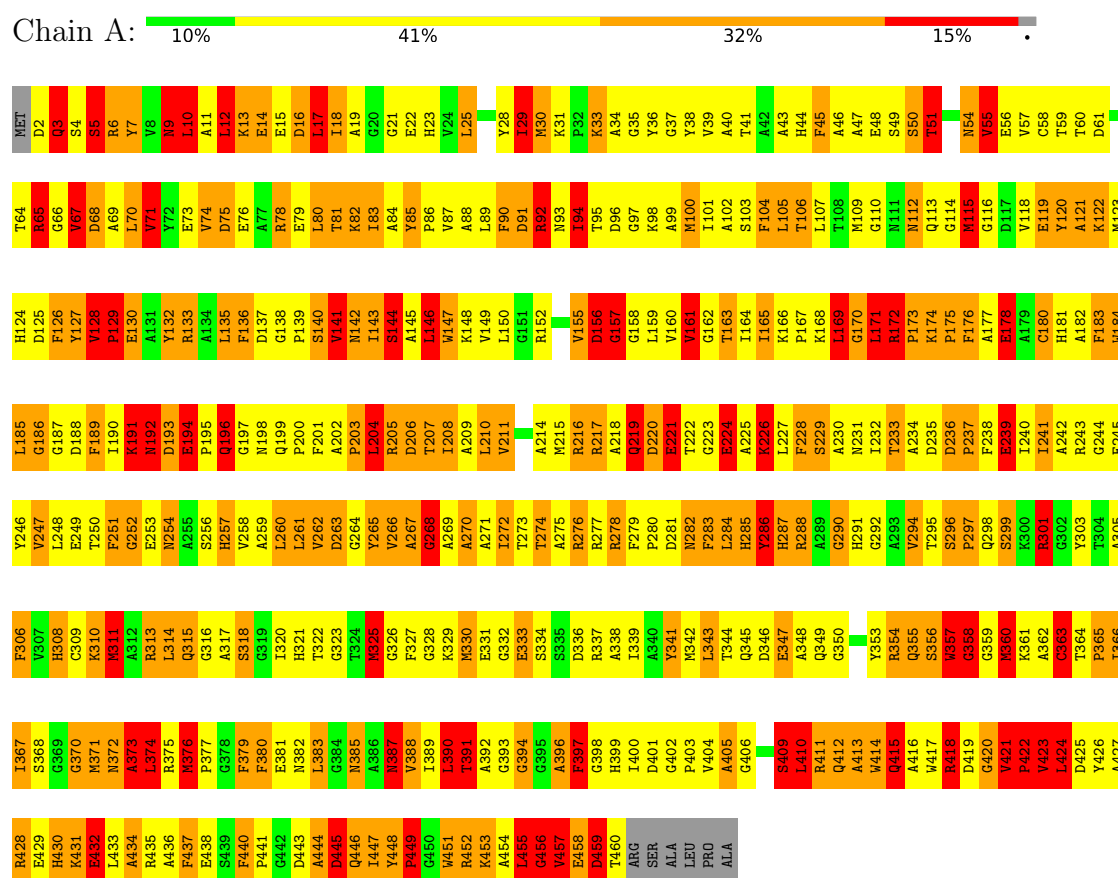
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	1	2		
4	B	1	Total	C	O	0	0
			3	1	2		

3 Residue-property plots

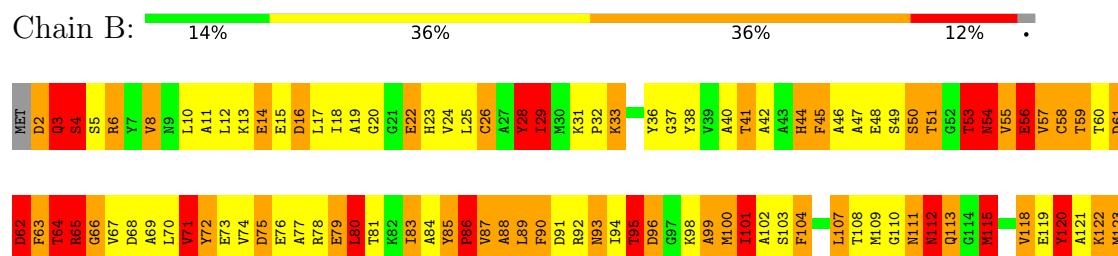
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE



• Molecule 1: RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.50Å 70.60Å 104.10Å 90.00° 92.10° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7044	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: FMT, MG, RUB

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	1.39	8/3586 (0.2%)	3.72	707/4859 (14.6%)
1	B	1.32	5/3582 (0.1%)	3.55	618/4854 (12.7%)
All	All	1.36	13/7168 (0.2%)	3.64	1325/9713 (13.6%)

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	B	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	ASP	CG-OD2	16.37	1.56	1.25
1	B	457	VAL	C-O	-14.33	1.05	1.23
1	A	458	GLU	CG-CD	12.90	1.84	1.52
1	A	460	THR	N-CA	-10.71	1.25	1.46
1	B	364	THR	CA-CB	8.26	1.64	1.53
1	A	192	ASN	N-CA	7.15	1.55	1.45
1	A	361	LYS	CA-CB	-6.45	1.46	1.54
1	A	460	THR	CA-C	6.16	1.65	1.52
1	A	193	ASP	N-CA	6.02	1.53	1.45
1	B	305	ALA	N-CA	5.63	1.53	1.46
1	A	361	LYS	C-O	5.23	1.27	1.24
1	B	135	LEU	N-CA	5.23	1.52	1.45
1	B	228	PHE	C-O	5.22	1.30	1.24

All (1325) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ARG	CD-NE-CZ	38.05	177.67	124.40
1	B	445	ASP	CA-CB-CG	28.79	141.39	112.60
1	A	459	ASP	CA-C-N	28.35	172.74	121.70
1	A	459	ASP	C-N-CA	28.35	172.74	121.70
1	B	65	ARG	CD-NE-CZ	26.39	161.35	124.40
1	A	56	GLU	CA-C-N	25.03	157.73	122.94
1	A	56	GLU	C-N-CA	25.03	157.73	122.94
1	A	333	GLU	CB-CG-CD	23.27	152.17	112.60
1	A	78	ARG	CD-NE-CZ	22.57	156.00	124.40
1	A	382	ASN	CA-CB-CG	22.55	135.15	112.60
1	B	62	ASP	CA-CB-CG	22.33	134.93	112.60
1	A	54	ASN	CA-CB-CG	21.43	134.03	112.60
1	B	206	ASP	CA-CB-CG	20.96	133.56	112.60
1	B	282	ASN	CA-CB-CG	-19.62	92.98	112.60
1	A	145	ALA	CA-C-N	19.06	146.55	120.63
1	A	145	ALA	C-N-CA	19.06	146.55	120.63
1	A	422	PRO	CB-CA-C	17.91	141.10	111.56
1	B	437	PHE	CA-CB-CG	17.75	131.55	113.80
1	B	334	SER	CA-C-N	17.58	155.12	121.54
1	B	334	SER	C-N-CA	17.58	155.12	121.54
1	A	127	TYR	CA-C-O	-17.15	101.74	120.43
1	A	156	ASP	CA-CB-CG	17.13	129.73	112.60
1	A	71	VAL	N-CA-CB	16.35	132.06	111.46
1	B	172	ARG	CD-NE-CZ	16.25	147.15	124.40
1	A	380	PHE	CA-CB-CG	15.49	129.29	113.80
1	A	105	LEU	CA-C-O	-15.13	104.51	120.55
1	B	92	ARG	CD-NE-CZ	15.05	145.47	124.40
1	B	212	ALA	O-C-N	14.86	137.38	122.07
1	B	315	GLN	OE1-CD-NE2	14.69	137.29	122.60
1	B	94	ILE	CA-C-O	14.50	134.57	119.20
1	B	16	ASP	CA-CB-CG	14.32	126.92	112.60
1	A	106	THR	N-CA-CB	14.28	131.47	110.20
1	A	188	ASP	CA-CB-CG	14.12	126.72	112.60
1	A	112	ASN	CA-CB-CG	14.11	126.71	112.60
1	A	189	PHE	N-CA-C	13.90	131.07	108.41
1	A	58	CYS	CA-C-N	13.88	141.63	123.03
1	A	58	CYS	C-N-CA	13.88	141.63	123.03
1	B	111	ASN	OD1-CG-ND2	13.86	136.46	122.60
1	B	408	ARG	CB-CG-CD	13.71	142.83	111.30
1	A	183	PHE	N-CA-C	-13.59	95.10	112.90
1	A	243	ARG	CD-NE-CZ	13.57	143.40	124.40
1	A	385	ASN	CA-CB-CG	13.44	126.04	112.60
1	A	410	LEU	CB-CA-C	13.42	135.45	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	90	PHE	CA-C-O	-13.39	103.99	119.79
1	A	183	PHE	N-CA-CB	13.29	130.27	110.33
1	A	225	ALA	CA-C-O	13.23	135.49	120.54
1	B	6	ARG	CD-NE-CZ	13.14	142.80	124.40
1	A	156	ASP	CA-C-N	13.07	147.04	121.41
1	A	156	ASP	C-N-CA	13.07	147.04	121.41
1	B	253	GLU	CB-CG-CD	13.05	134.78	112.60
1	B	126	PHE	CA-CB-CG	13.04	126.84	113.80
1	A	431	LYS	N-CA-C	13.04	125.02	111.07
1	A	310	LYS	CB-CG-CD	13.00	141.19	111.30
1	A	64	THR	CA-C-N	12.99	143.83	122.14
1	A	64	THR	C-N-CA	12.99	143.83	122.14
1	B	278	ARG	CD-NE-CZ	12.93	142.50	124.40
1	A	135	LEU	CA-C-O	-12.66	106.91	120.46
1	B	262	VAL	CA-C-O	12.62	133.74	120.36
1	A	146	LEU	CA-C-N	12.62	137.30	120.65
1	A	146	LEU	C-N-CA	12.62	137.30	120.65
1	A	460	THR	N-CA-C	12.60	146.28	111.00
1	B	61	ASP	CA-CB-CG	12.56	125.16	112.60
1	B	183	PHE	CA-CB-CG	12.39	126.19	113.80
1	A	249	GLU	CA-CB-CG	12.34	138.79	114.10
1	A	285	HIS	CA-CB-CG	12.32	126.12	113.80
1	B	171	LEU	O-C-N	12.30	137.17	123.27
1	B	140	SER	CA-C-N	12.28	142.09	122.68
1	B	140	SER	C-N-CA	12.28	142.09	122.68
1	A	394	GLY	CA-C-N	12.22	145.37	121.41
1	A	394	GLY	C-N-CA	12.22	145.37	121.41
1	A	56	GLU	CA-C-O	12.11	138.25	122.63
1	B	268	GLY	N-CA-C	12.11	128.40	112.65
1	A	173	PRO	N-CA-C	12.08	130.32	113.53
1	B	420	GLY	CA-C-N	12.00	134.08	123.04
1	B	420	GLY	C-N-CA	12.00	134.08	123.04
1	B	166	LYS	CB-CA-C	11.98	124.05	109.31
1	B	356	SER	N-CA-CB	11.95	130.25	110.77
1	B	135	LEU	N-CA-C	-11.88	98.77	113.97
1	A	66	GLY	CA-C-N	11.88	143.35	121.97
1	A	66	GLY	C-N-CA	11.88	143.35	121.97
1	A	390	LEU	CA-C-O	11.87	133.18	120.36
1	A	203	PRO	N-CA-C	11.84	129.62	110.21
1	B	412	GLN	CA-C-O	-11.81	108.42	120.82
1	A	198	ASN	CA-C-O	-11.80	107.41	122.63
1	A	284	LEU	N-CA-CB	11.77	127.90	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ALA	CA-C-N	11.74	139.58	122.21
1	B	386	ALA	C-N-CA	11.74	139.58	122.21
1	A	45	PHE	CA-CB-CG	11.73	125.53	113.80
1	B	334	SER	O-C-N	-11.70	110.47	122.99
1	B	56	GLU	N-CA-C	11.63	135.56	110.80
1	B	409	SER	CA-C-O	-11.52	108.33	120.55
1	B	390	LEU	CA-C-N	11.50	139.19	122.86
1	B	390	LEU	C-N-CA	11.50	139.19	122.86
1	A	206	ASP	CA-CB-CG	11.49	124.09	112.60
1	B	277	ARG	NE-CZ-NH2	11.37	129.43	119.20
1	B	327	PHE	CA-CB-CG	11.36	125.16	113.80
1	B	159	LEU	N-CA-C	11.30	126.54	109.25
1	B	144	SER	CA-C-O	-11.21	106.38	119.61
1	B	223	GLY	CA-C-N	11.21	137.45	121.42
1	B	223	GLY	C-N-CA	11.21	137.45	121.42
1	B	88	ALA	CA-C-O	-11.20	105.94	119.49
1	A	130	GLU	CB-CG-CD	11.19	131.62	112.60
1	B	75	ASP	CA-CB-CG	11.10	123.70	112.60
1	A	3	GLN	CA-C-N	11.09	142.73	121.54
1	A	3	GLN	C-N-CA	11.09	142.73	121.54
1	B	145	ALA	CA-C-N	11.02	141.80	121.52
1	B	145	ALA	C-N-CA	11.02	141.80	121.52
1	A	236	ASP	CA-CB-CG	10.94	123.54	112.60
1	B	211	VAL	CA-C-N	10.91	134.62	120.44
1	B	211	VAL	C-N-CA	10.91	134.62	120.44
1	B	413	ALA	CA-C-O	-10.90	107.78	120.10
1	B	315	GLN	O-C-N	10.90	133.30	122.07
1	B	2	ASP	CA-C-N	10.89	142.34	121.54
1	B	2	ASP	C-N-CA	10.89	142.34	121.54
1	A	201	PHE	CA-C-N	10.88	131.85	122.28
1	A	201	PHE	C-N-CA	10.88	131.85	122.28
1	A	414	TRP	CA-C-O	-10.87	106.72	120.31
1	A	257	HIS	CA-CB-CG	10.87	124.67	113.80
1	B	181	HIS	CA-C-O	10.86	132.41	121.00
1	A	262	VAL	CA-C-O	-10.83	109.34	120.27
1	B	274	THR	CA-C-N	10.80	134.91	120.65
1	B	274	THR	C-N-CA	10.80	134.91	120.65
1	A	194	GLU	CA-CB-CG	10.77	135.64	114.10
1	A	448	TYR	CA-C-N	10.77	133.30	119.84
1	A	448	TYR	C-N-CA	10.77	133.30	119.84
1	A	147	TRP	N-CA-CB	10.76	125.61	109.91
1	B	139	PRO	CB-CA-C	10.73	125.04	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	PRO	CB-CA-C	-10.68	101.68	111.40
1	A	158	GLY	N-CA-C	10.67	138.46	113.18
1	B	192	ASN	CA-CB-CG	10.60	123.20	112.60
1	A	336	ASP	CA-CB-CG	-10.60	102.00	112.60
1	B	57	VAL	CA-C-N	10.59	141.76	121.54
1	B	57	VAL	C-N-CA	10.59	141.76	121.54
1	A	165	ILE	CA-C-O	-10.58	107.55	120.78
1	A	263	ASP	CA-C-N	10.58	142.14	121.41
1	A	263	ASP	C-N-CA	10.58	142.14	121.41
1	A	278	ARG	CB-CG-CD	10.55	135.57	111.30
1	B	221	GLU	CB-CG-CD	10.52	130.48	112.60
1	A	236	ASP	CA-C-O	10.48	127.07	119.32
1	A	126	PHE	CA-CB-CG	10.46	124.26	113.80
1	A	10	LEU	N-CA-C	-10.41	92.53	108.67
1	A	337	ARG	CD-NE-CZ	10.39	138.95	124.40
1	B	14	GLU	CB-CG-CD	10.38	130.25	112.60
1	A	441	PRO	CA-C-N	10.37	133.11	120.14
1	A	441	PRO	C-N-CA	10.37	133.11	120.14
1	B	115	MET	CA-CB-CG	10.36	134.81	114.10
1	A	56	GLU	O-C-N	-10.30	109.83	122.71
1	B	278	ARG	CG-CD-NE	10.29	134.64	112.00
1	B	90	PHE	N-CA-C	10.16	125.03	112.23
1	B	350	GLY	N-CA-C	-10.16	99.94	112.23
1	B	128	VAL	N-CA-CB	-10.14	100.76	111.61
1	B	388	VAL	N-CA-CB	-10.13	91.23	112.00
1	A	198	ASN	CA-CB-CG	10.13	122.73	112.60
1	A	449	PRO	N-CA-C	10.11	133.30	112.47
1	B	253	GLU	CA-CB-CG	10.10	134.29	114.10
1	A	333	GLU	CA-C-N	10.07	140.78	121.54
1	A	333	GLU	C-N-CA	10.07	140.78	121.54
1	A	355	GLN	OE1-CD-NE2	10.02	132.62	122.60
1	A	361	LYS	N-CA-C	-10.01	94.42	108.23
1	B	268	GLY	CA-C-O	10.01	131.69	122.39
1	A	422	PRO	CA-N-CD	-9.99	98.02	112.00
1	A	438	GLU	CB-CG-CD	9.99	129.58	112.60
1	B	356	SER	CB-CA-C	-9.96	94.80	110.14
1	B	200	PRO	CA-C-N	9.96	139.18	122.65
1	B	200	PRO	C-N-CA	9.96	139.18	122.65
1	A	263	ASP	N-CA-C	9.93	127.07	113.37
1	B	235	ASP	N-CA-C	-9.93	97.96	111.96
1	A	34	ALA	CA-C-O	9.91	132.20	120.81
1	B	262	VAL	CB-CA-C	9.90	124.78	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	HIS	CA-C-N	9.89	134.53	120.28
1	A	181	HIS	C-N-CA	9.89	134.53	120.28
1	A	410	LEU	O-C-N	-9.82	110.73	122.22
1	A	245	GLU	CA-CB-CG	9.78	133.66	114.10
1	A	159	LEU	N-CA-C	9.75	124.63	110.10
1	A	290	GLY	CA-C-N	9.73	134.59	120.38
1	A	290	GLY	C-N-CA	9.73	134.59	120.38
1	A	268	GLY	CA-C-O	9.69	137.42	120.57
1	B	147	TRP	N-CA-C	-9.69	99.58	111.40
1	B	111	ASN	CA-C-N	9.68	139.41	122.09
1	B	111	ASN	C-N-CA	9.68	139.41	122.09
1	B	304	THR	CA-CB-OG1	-9.66	95.11	109.60
1	A	239	GLU	CA-CB-CG	-9.66	94.79	114.10
1	A	59	THR	CA-C-N	9.65	139.98	121.54
1	A	59	THR	C-N-CA	9.65	139.98	121.54
1	B	287	HIS	CA-CB-CG	-9.65	104.15	113.80
1	A	85	TYR	CB-CA-C	-9.61	101.79	110.44
1	B	422	PRO	N-CA-C	9.61	132.27	112.47
1	A	61	ASP	CA-C-N	9.60	139.87	121.54
1	A	61	ASP	C-N-CA	9.60	139.87	121.54
1	A	259	ALA	N-CA-C	-9.59	96.32	110.52
1	B	261	LEU	CA-C-O	9.53	130.82	120.43
1	B	418	ARG	NE-CZ-NH1	-9.53	111.97	121.50
1	B	100	MET	CG-SD-CE	9.51	121.81	100.90
1	A	226	LYS	CA-C-N	9.50	137.19	122.94
1	A	226	LYS	C-N-CA	9.50	137.19	122.94
1	B	57	VAL	N-CA-C	9.50	122.45	108.96
1	A	313	ARG	NE-CZ-NH2	9.49	127.74	119.20
1	A	139	PRO	CA-C-O	-9.49	110.09	121.67
1	A	146	LEU	CB-CA-C	9.48	125.64	110.95
1	A	420	GLY	N-CA-C	9.41	132.98	114.16
1	A	64	THR	CA-C-O	9.41	137.63	122.20
1	A	183	PHE	CA-C-O	-9.41	108.59	119.60
1	A	25	LEU	CA-C-O	-9.40	110.75	120.71
1	B	212	ALA	CA-C-O	-9.37	110.98	120.82
1	A	420	GLY	CA-C-N	9.36	139.45	122.13
1	A	420	GLY	C-N-CA	9.36	139.45	122.13
1	A	169	LEU	CA-C-O	-9.34	109.75	120.31
1	A	234	ALA	CA-C-O	-9.33	110.53	120.99
1	B	148	LYS	CA-C-O	-9.32	109.56	120.10
1	B	112	ASN	N-CA-CB	-9.30	96.89	110.47
1	A	277	ARG	NE-CZ-NH2	9.29	127.56	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	LEU	CB-CA-C	9.27	124.65	109.07
1	A	379	PHE	N-CA-C	-9.25	97.41	111.56
1	A	104	PHE	CA-CB-CG	-9.22	104.58	113.80
1	A	189	PHE	CA-C-O	-9.22	110.44	120.30
1	B	413	ALA	N-CA-CB	9.21	124.40	110.22
1	A	56	GLU	N-CA-C	9.19	123.40	109.62
1	A	202	ALA	N-CA-CB	-9.18	99.58	111.23
1	A	414	TRP	N-CA-CB	9.16	124.39	110.19
1	B	399	HIS	CA-CB-CG	9.14	122.94	113.80
1	B	418	ARG	CG-CD-NE	9.10	132.01	112.00
1	B	57	VAL	CA-C-O	9.09	131.31	121.67
1	A	198	ASN	OD1-CG-ND2	-9.09	113.51	122.60
1	B	157	GLY	CA-C-O	-9.09	108.19	119.09
1	A	457	VAL	CA-CB-CG1	9.08	125.84	110.40
1	B	363	CYS	N-CA-C	-9.08	94.08	109.24
1	A	37	GLY	CA-C-N	9.07	138.87	121.54
1	A	37	GLY	C-N-CA	9.07	138.87	121.54
1	A	411	ARG	NE-CZ-NH2	9.07	127.37	119.20
1	A	128	VAL	CA-C-N	9.05	131.16	119.84
1	A	128	VAL	C-N-CA	9.05	131.16	119.84
1	B	346	ASP	CA-CB-CG	9.05	121.65	112.60
1	B	96	ASP	CA-C-O	-9.03	109.31	119.78
1	B	112	ASN	CA-CB-CG	9.02	121.62	112.60
1	A	363	CYS	CB-CA-C	9.02	125.14	110.16
1	B	23	HIS	N-CA-C	9.01	124.09	109.40
1	A	373	ALA	N-CA-CB	-9.00	95.27	110.49
1	B	280	PRO	CA-C-N	9.00	132.68	120.44
1	B	280	PRO	C-N-CA	9.00	132.68	120.44
1	B	355	GLN	CA-C-N	8.98	135.68	122.39
1	B	355	GLN	C-N-CA	8.98	135.68	122.39
1	A	223	GLY	CA-C-N	8.97	138.71	122.92
1	A	223	GLY	C-N-CA	8.97	138.71	122.92
1	A	393	GLY	CA-C-O	-8.96	113.10	120.81
1	A	98	LYS	O-C-N	8.96	133.43	122.86
1	A	243	ARG	CA-C-O	8.95	130.40	121.00
1	B	143	ILE	CB-CA-C	8.95	125.12	112.05
1	B	184	TRP	CA-C-N	8.95	138.90	121.18
1	B	184	TRP	C-N-CA	8.95	138.90	121.18
1	B	19	ALA	CA-C-N	8.94	129.83	120.00
1	B	19	ALA	C-N-CA	8.94	129.83	120.00
1	A	365	PRO	CB-CA-C	8.92	122.97	111.46
1	A	176	PHE	N-CA-C	-8.91	101.52	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	380	PHE	CA-CB-CG	8.90	122.70	113.80
1	A	176	PHE	CA-C-O	-8.88	111.55	120.70
1	B	362	ALA	N-CA-C	-8.88	98.81	110.53
1	A	232	ILE	CA-C-N	8.86	134.26	122.30
1	A	232	ILE	C-N-CA	8.86	134.26	122.30
1	A	115	MET	CB-CA-C	8.82	123.54	109.61
1	A	313	ARG	NE-CZ-NH1	-8.82	112.68	121.50
1	A	458	GLU	CB-CG-CD	-8.77	97.69	112.60
1	B	276	ARG	NE-CZ-NH1	-8.77	112.73	121.50
1	A	235	ASP	CB-CA-C	-8.76	97.12	110.88
1	B	180	CYS	CA-C-N	8.76	132.21	120.65
1	B	180	CYS	C-N-CA	8.76	132.21	120.65
1	B	389	ILE	CA-C-O	-8.76	109.34	121.51
1	A	59	THR	N-CA-C	-8.73	94.08	108.49
1	B	80	LEU	N-CA-C	8.71	124.77	107.62
1	B	167	PRO	CA-C-N	8.70	135.03	121.19
1	B	167	PRO	C-N-CA	8.70	135.03	121.19
1	A	147	TRP	CB-CA-C	-8.70	97.56	110.96
1	A	125	ASP	CA-C-O	-8.70	112.14	121.45
1	B	411	ARG	N-CA-C	-8.69	101.89	111.36
1	B	240	ILE	N-CA-C	-8.69	102.08	110.42
1	A	382	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	A	199	GLN	N-CA-C	-8.68	97.57	110.24
1	B	133	ARG	O-C-N	-8.67	113.14	122.07
1	A	397	PHE	CA-CB-CG	8.67	122.47	113.80
1	A	71	VAL	N-CA-C	-8.67	95.23	107.80
1	B	199	GLN	OE1-CD-NE2	-8.66	113.94	122.60
1	A	203	PRO	O-C-N	-8.66	114.53	122.93
1	B	334	SER	N-CA-C	8.65	120.06	108.38
1	B	217	ARG	CA-C-O	-8.65	111.74	120.82
1	A	149	VAL	N-CA-CB	8.64	124.28	112.35
1	B	252	GLY	CA-C-N	8.63	134.41	120.60
1	B	252	GLY	C-N-CA	8.63	134.41	120.60
1	B	334	SER	CA-C-O	8.63	130.54	121.31
1	B	409	SER	O-C-N	8.63	131.27	122.12
1	A	449	PRO	CA-N-CD	-8.61	99.95	112.00
1	B	83	ILE	CA-C-N	8.61	134.81	122.85
1	B	83	ILE	C-N-CA	8.61	134.81	122.85
1	B	443	ASP	CA-CB-CG	8.61	121.21	112.60
1	B	245	GLU	N-CA-CB	8.60	123.46	110.22
1	B	152	ARG	CA-CB-CG	8.58	131.27	114.10
1	B	164	ILE	N-CA-CB	8.57	122.78	111.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	GLU	CA-CB-CG	8.56	131.22	114.10
1	B	215	MET	N-CA-C	-8.56	101.29	112.68
1	A	234	ALA	CA-C-N	8.56	131.56	120.44
1	A	234	ALA	C-N-CA	8.56	131.56	120.44
1	A	275	ALA	O-C-N	8.55	130.88	122.07
1	B	262	VAL	O-C-N	-8.54	113.97	123.20
1	A	207	THR	CA-CB-CG2	8.53	125.01	110.50
1	A	411	ARG	CD-NE-CZ	-8.52	112.47	124.40
1	A	374	LEU	N-CA-C	8.51	121.69	111.82
1	B	4	SER	CA-C-N	8.51	133.64	119.35
1	B	4	SER	C-N-CA	8.51	133.64	119.35
1	B	277	ARG	O-C-N	-8.51	111.28	122.59
1	B	283	PHE	CA-C-O	-8.49	110.64	120.49
1	B	239	GLU	CA-C-O	8.47	128.98	119.41
1	A	314	LEU	CA-C-N	8.44	131.42	120.44
1	A	314	LEU	C-N-CA	8.44	131.42	120.44
1	A	332	GLY	CA-C-N	8.44	137.66	121.54
1	A	332	GLY	C-N-CA	8.44	137.66	121.54
1	B	57	VAL	N-CA-CB	-8.44	101.71	112.60
1	A	308	HIS	CA-CB-CG	8.43	122.23	113.80
1	A	230	ALA	CA-C-N	8.43	136.40	122.07
1	A	230	ALA	C-N-CA	8.43	136.40	122.07
1	A	445	ASP	CA-CB-CG	8.43	121.03	112.60
1	B	207	THR	CA-CB-OG1	-8.42	96.97	109.60
1	A	353	TYR	CA-C-O	8.39	131.72	121.56
1	B	372	ASN	OD1-CG-ND2	-8.39	114.20	122.60
1	B	51	THR	N-CA-C	8.38	124.19	113.88
1	B	335	SER	N-CA-C	8.36	128.60	110.80
1	A	23	HIS	CA-C-N	8.35	133.14	122.37
1	A	23	HIS	C-N-CA	8.35	133.14	122.37
1	B	363	CYS	CA-C-O	-8.34	111.07	120.66
1	B	24	VAL	CA-C-O	-8.34	110.90	120.74
1	B	409	SER	CA-C-N	8.34	131.78	120.44
1	B	409	SER	C-N-CA	8.34	131.78	120.44
1	A	301	ARG	NE-CZ-NH2	8.32	126.69	119.20
1	A	361	LYS	CA-C-O	-8.30	112.51	120.56
1	B	362	ALA	CA-C-N	8.30	136.18	122.73
1	B	362	ALA	C-N-CA	8.30	136.18	122.73
1	A	428	ARG	N-CA-C	-8.30	102.19	111.07
1	B	57	VAL	O-C-N	-8.30	114.26	122.97
1	B	287	HIS	CA-C-N	8.27	137.34	121.54
1	B	287	HIS	C-N-CA	8.27	137.34	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	ALA	N-CA-C	8.25	123.16	109.46
1	B	418	ARG	CA-CB-CG	8.25	130.59	114.10
1	A	76	GLU	CB-CG-CD	8.24	126.61	112.60
1	A	75	ASP	N-CA-CB	8.24	123.55	110.86
1	A	207	THR	CA-CB-OG1	-8.21	97.28	109.60
1	B	122	LYS	CA-CB-CG	8.21	130.52	114.10
1	A	359	GLY	O-C-N	8.21	131.58	122.47
1	A	389	ILE	O-C-N	8.20	132.16	123.05
1	B	222	THR	CA-C-O	8.20	127.75	118.97
1	B	339	ILE	CA-C-N	8.19	131.47	120.65
1	B	339	ILE	C-N-CA	8.19	131.47	120.65
1	B	201	PHE	CA-CB-CG	8.18	121.98	113.80
1	B	286	TYR	CA-CB-CG	8.18	128.62	113.90
1	B	271	ALA	N-CA-C	-8.17	101.96	111.03
1	A	155	VAL	CA-C-O	-8.15	112.80	121.93
1	B	112	ASN	CA-C-O	8.13	128.60	119.41
1	A	143	ILE	CA-C-O	-8.13	110.62	120.78
1	B	259	ALA	CB-CA-C	8.12	124.88	109.37
1	A	233	THR	CA-CB-CG2	8.12	124.30	110.50
1	A	271	ALA	CA-C-N	8.11	130.78	120.56
1	A	271	ALA	C-N-CA	8.11	130.78	120.56
1	A	375	ARG	NE-CZ-NH2	8.11	126.50	119.20
1	B	133	ARG	CA-CB-CG	8.11	130.31	114.10
1	A	96	ASP	CB-CG-OD1	8.10	137.03	118.40
1	B	219	GLN	CB-CG-CD	8.10	126.36	112.60
1	B	418	ARG	NE-CZ-NH2	8.09	126.48	119.20
1	A	178	GLU	CA-C-O	-8.09	112.25	120.90
1	B	192	ASN	N-CA-CB	8.08	124.14	110.49
1	A	278	ARG	CD-NE-CZ	8.07	135.70	124.40
1	A	393	GLY	O-C-N	8.07	128.43	123.35
1	A	243	ARG	N-CA-C	-8.07	102.18	110.97
1	B	267	ALA	CA-C-O	8.06	127.66	118.47
1	B	179	ALA	N-CA-C	-8.03	103.48	113.28
1	B	366	ILE	CA-C-O	-8.03	111.64	121.04
1	B	371	MET	N-CA-C	-8.03	96.19	108.96
1	A	141	VAL	N-CA-CB	-8.03	99.24	109.84
1	B	53	THR	N-CA-C	-8.02	101.53	110.91
1	A	418	ARG	CA-C-N	8.02	131.36	120.38
1	A	418	ARG	C-N-CA	8.02	131.36	120.38
1	B	428	ARG	NE-CZ-NH1	8.01	129.51	121.50
1	A	58	CYS	O-C-N	8.00	131.29	123.29
1	A	25	LEU	O-C-N	7.99	133.36	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	GLN	CA-C-N	7.99	130.83	120.44
1	B	219	GLN	C-N-CA	7.99	130.83	120.44
1	A	354	ARG	N-CA-C	-7.99	96.38	109.40
1	A	262	VAL	N-CA-CB	-7.99	100.96	111.82
1	B	347	GLU	CA-C-O	-7.99	110.64	119.98
1	B	452	ARG	CA-C-N	7.99	131.32	120.54
1	B	452	ARG	C-N-CA	7.99	131.32	120.54
1	A	112	ASN	N-CA-C	-7.98	103.33	113.23
1	A	135	LEU	N-CA-C	-7.98	93.86	107.99
1	A	413	ALA	CA-C-O	-7.97	111.27	120.20
1	A	138	GLY	O-C-N	7.96	129.73	121.77
1	A	189	PHE	N-CA-CB	-7.94	98.26	110.65
1	A	456	GLY	N-CA-C	7.94	132.00	113.18
1	B	163	THR	CA-C-N	7.93	133.65	123.10
1	B	163	THR	C-N-CA	7.93	133.65	123.10
1	A	423	VAL	CA-C-N	7.92	131.22	120.38
1	A	423	VAL	C-N-CA	7.92	131.22	120.38
1	A	344	THR	CA-C-O	7.91	128.76	119.67
1	B	136	PHE	CA-CB-CG	-7.89	105.91	113.80
1	B	401	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	331	GLU	CB-CG-CD	7.87	125.98	112.60
1	A	91	ASP	CA-CB-CG	7.85	120.45	112.60
1	A	192	ASN	CA-CB-CG	7.84	120.44	112.60
1	A	310	LYS	CA-CB-CG	7.84	129.78	114.10
1	B	177	ALA	CA-C-O	-7.84	112.16	120.63
1	A	192	ASN	CA-C-O	-7.82	112.94	121.94
1	B	36	TYR	N-CA-C	7.82	121.52	110.50
1	A	250	THR	CA-CB-CG2	7.81	123.78	110.50
1	B	364	THR	N-CA-C	7.81	121.09	110.31
1	B	134	ALA	N-CA-C	7.80	122.18	113.21
1	A	145	ALA	N-CA-C	-7.80	104.28	113.88
1	A	308	HIS	CB-CG-CD2	-7.80	121.06	131.20
1	A	457	VAL	CA-C-N	7.80	134.24	122.93
1	A	457	VAL	C-N-CA	7.80	134.24	122.93
1	A	298	GLN	N-CA-C	-7.79	103.77	113.28
1	A	92	ARG	O-C-N	-7.79	113.64	122.20
1	A	280	PRO	CA-C-N	7.78	139.72	121.52
1	A	280	PRO	C-N-CA	7.78	139.72	121.52
1	B	243	ARG	CD-NE-CZ	7.77	135.28	124.40
1	B	375	ARG	CD-NE-CZ	7.76	135.27	124.40
1	A	373	ALA	CA-C-N	7.75	132.08	120.31
1	A	373	ALA	C-N-CA	7.75	132.08	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASP	CA-CB-CG	7.74	120.34	112.60
1	B	171	LEU	CA-C-O	-7.74	111.99	120.43
1	A	296	SER	O-C-N	7.74	127.51	121.47
1	A	220	ASP	N-CA-C	-7.71	94.37	110.80
1	B	8	VAL	N-CA-CB	7.70	123.98	111.36
1	A	60	THR	CA-C-N	7.69	131.61	120.38
1	A	60	THR	C-N-CA	7.69	131.61	120.38
1	B	31	LYS	CA-C-O	-7.69	112.17	119.55
1	B	147	TRP	CA-C-O	7.69	128.78	120.55
1	A	344	THR	CA-C-N	7.68	132.49	121.50
1	A	344	THR	C-N-CA	7.68	132.49	121.50
1	B	401	ASP	CA-C-N	7.67	133.91	121.87
1	B	401	ASP	C-N-CA	7.67	133.91	121.87
1	B	435	ARG	NE-CZ-NH1	7.67	129.17	121.50
1	A	277	ARG	NE-CZ-NH1	-7.67	113.83	121.50
1	B	326	GLY	CA-C-N	7.66	136.17	121.54
1	B	326	GLY	C-N-CA	7.66	136.17	121.54
1	B	91	ASP	CA-C-O	7.65	131.45	120.51
1	A	68	ASP	CA-CB-CG	7.65	120.25	112.60
1	A	243	ARG	CA-C-N	7.63	129.74	120.13
1	A	243	ARG	C-N-CA	7.63	129.74	120.13
1	B	98	LYS	N-CA-C	7.61	121.74	110.48
1	B	79	GLU	CB-CG-CD	7.61	125.53	112.60
1	B	154	GLU	CG-CD-OE1	-7.59	100.93	118.40
1	A	444	ALA	CA-C-O	7.58	131.35	120.51
1	A	152	ARG	O-C-N	7.58	130.04	121.32
1	A	421	VAL	N-CA-CB	-7.58	100.60	111.21
1	A	367	ILE	CB-CA-C	7.54	122.04	111.63
1	B	183	PHE	N-CA-C	-7.54	103.64	114.12
1	A	338	ALA	CA-C-N	7.54	130.12	120.70
1	A	338	ALA	C-N-CA	7.54	130.12	120.70
1	B	282	ASN	OD1-CG-ND2	7.53	130.13	122.60
1	A	272	ILE	CB-CA-C	-7.52	102.34	111.97
1	A	233	THR	CA-CB-OG1	-7.52	98.32	109.60
1	B	438	GLU	CA-C-N	7.51	130.85	120.63
1	B	438	GLU	C-N-CA	7.51	130.85	120.63
1	A	171	LEU	N-CA-CB	-7.51	97.81	110.49
1	B	384	GLY	CA-C-O	-7.50	113.03	119.56
1	A	22	GLU	CA-CB-CG	7.50	129.11	114.10
1	A	393	GLY	N-CA-C	-7.50	96.57	111.34
1	B	352	PHE	CA-CB-CG	-7.50	106.30	113.80
1	B	3	GLN	CA-C-O	-7.50	109.79	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	ASP	CB-CA-C	7.48	125.31	110.42
1	A	387	ASN	CA-CB-CG	7.48	120.08	112.60
1	A	308	HIS	CB-CG-ND1	7.47	133.91	122.70
1	A	146	LEU	N-CA-C	-7.47	102.74	111.03
1	A	457	VAL	CA-C-O	7.47	130.11	120.78
1	B	254	ASN	CA-C-N	7.46	130.61	120.38
1	B	254	ASN	C-N-CA	7.46	130.61	120.38
1	B	297	PRO	CA-C-N	7.46	130.59	120.44
1	B	297	PRO	C-N-CA	7.46	130.59	120.44
1	B	162	GLY	CA-C-O	7.46	129.56	121.57
1	B	389	ILE	O-C-N	7.46	131.94	122.61
1	A	401	ASP	CA-CB-CG	7.45	120.05	112.60
1	B	22	GLU	N-CA-CB	7.44	121.47	110.53
1	A	286	TYR	CB-CG-CD1	7.44	131.96	120.80
1	A	92	ARG	CA-C-N	7.43	133.46	122.99
1	A	92	ARG	C-N-CA	7.43	133.46	122.99
1	A	249	GLU	CA-C-O	-7.43	110.94	120.00
1	B	311	MET	O-C-N	7.43	131.41	122.27
1	B	87	VAL	CA-C-O	-7.41	112.24	120.25
1	B	72	TYR	O-C-N	7.39	131.45	122.35
1	B	95	THR	CA-CB-OG1	-7.38	98.52	109.60
1	A	92	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	A	341	TYR	CA-C-O	-7.38	112.60	120.42
1	B	220	ASP	CA-CB-CG	-7.37	105.23	112.60
1	B	235	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	75	ASP	N-CA-C	-7.36	94.69	107.20
1	A	75	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	315	GLN	CG-CD-NE2	-7.35	105.38	116.40
1	B	207	THR	N-CA-C	-7.35	101.76	111.24
1	A	376	MET	CA-C-N	7.33	127.01	119.82
1	A	376	MET	C-N-CA	7.33	127.01	119.82
1	A	362	ALA	O-C-N	7.32	131.52	123.10
1	A	172	ARG	CD-NE-CZ	7.31	134.64	124.40
1	A	175	PRO	CA-C-N	7.31	130.39	120.44
1	A	175	PRO	C-N-CA	7.31	130.39	120.44
1	A	67	VAL	CA-C-N	7.31	132.50	122.19
1	A	67	VAL	C-N-CA	7.31	132.50	122.19
1	B	81	THR	CA-CB-OG1	-7.31	98.63	109.60
1	B	187	GLY	CA-C-O	-7.31	113.55	121.88
1	B	88	ALA	N-CA-CB	7.30	122.72	110.32
1	B	345	GLN	CA-CB-CG	7.30	128.69	114.10
1	A	283	PHE	CB-CA-C	7.29	121.20	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	MET	CA-C-O	-7.29	110.17	120.16
1	B	44	HIS	N-CA-C	-7.29	102.94	111.03
1	B	65	ARG	NH1-CZ-NH2	-7.28	109.83	119.30
1	B	176	PHE	CA-CB-CG	-7.28	106.52	113.80
1	A	191	LYS	CA-C-O	-7.28	111.86	120.60
1	B	133	ARG	NE-CZ-NH2	7.27	125.74	119.20
1	B	333	GLU	CB-CG-CD	7.26	124.94	112.60
1	B	159	LEU	CA-CB-CG	7.25	141.68	116.30
1	B	196	GLN	OE1-CD-NE2	-7.25	115.35	122.60
1	A	94	ILE	CA-C-N	7.25	135.06	122.09
1	A	94	ILE	C-N-CA	7.25	135.06	122.09
1	A	414	TRP	O-C-N	7.25	132.08	122.30
1	B	447	ILE	N-CA-C	-7.25	103.90	111.58
1	B	277	ARG	NE-CZ-NH1	-7.24	114.26	121.50
1	A	140	SER	CA-C-N	7.23	129.20	121.97
1	A	140	SER	C-N-CA	7.23	129.20	121.97
1	A	355	GLN	N-CA-CB	-7.23	98.67	110.81
1	A	56	GLU	CB-CG-CD	7.22	124.88	112.60
1	B	431	LYS	CA-C-N	7.22	130.83	120.79
1	B	431	LYS	C-N-CA	7.22	130.83	120.79
1	A	125	ASP	N-CA-CB	-7.22	100.15	111.56
1	A	170	GLY	N-CA-C	-7.21	96.09	113.18
1	A	287	HIS	CA-C-N	7.21	135.30	121.54
1	A	287	HIS	C-N-CA	7.21	135.30	121.54
1	A	313	ARG	CG-CD-NE	7.20	127.85	112.00
1	A	17	LEU	N-CA-C	-7.20	103.36	111.14
1	B	64	THR	CA-C-O	7.20	128.18	120.55
1	B	282	ASN	N-CA-CB	-7.20	99.97	110.26
1	A	337	ARG	CA-CB-CG	7.20	128.49	114.10
1	A	391	THR	N-CA-C	-7.20	96.68	108.41
1	A	136	PHE	CA-CB-CG	7.19	120.99	113.80
1	A	120	TYR	N-CA-CB	7.17	122.61	110.49
1	B	23	HIS	N-CA-CB	-7.17	98.35	110.83
1	A	173	PRO	CA-C-N	7.16	128.66	119.78
1	A	173	PRO	C-N-CA	7.16	128.66	119.78
1	B	215	MET	O-C-N	7.16	131.56	122.19
1	A	306	PHE	CA-C-N	7.15	129.56	120.56
1	A	306	PHE	C-N-CA	7.15	129.56	120.56
1	A	79	GLU	CB-CG-CD	7.13	124.73	112.60
1	A	235	ASP	CA-CB-CG	7.13	119.73	112.60
1	B	354	ARG	CB-CG-CD	7.13	127.70	111.30
1	B	394	GLY	N-CA-C	7.12	121.51	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ALA	CA-C-N	7.12	135.98	122.60
1	B	214	ALA	C-N-CA	7.12	135.98	122.60
1	A	227	LEU	CA-C-O	7.11	128.38	120.70
1	B	423	VAL	CA-C-N	7.11	129.81	120.28
1	B	423	VAL	C-N-CA	7.11	129.81	120.28
1	B	44	HIS	O-C-N	7.10	129.70	122.03
1	B	307	VAL	CA-C-O	-7.09	113.90	121.27
1	A	421	VAL	CA-CB-CG2	7.08	122.44	110.40
1	A	286	TYR	CA-CB-CG	7.08	126.64	113.90
1	B	337	ARG	CD-NE-CZ	7.08	134.31	124.40
1	A	325	MET	N-CA-C	-7.08	103.57	111.28
1	A	416	ALA	CA-C-N	7.07	129.98	120.65
1	A	416	ALA	C-N-CA	7.07	129.98	120.65
1	A	241	ILE	N-CA-C	7.06	117.82	110.62
1	B	120	TYR	CA-C-O	7.06	130.61	120.51
1	A	85	TYR	CA-C-O	-7.06	113.99	119.71
1	A	133	ARG	NE-CZ-NH1	-7.05	114.44	121.50
1	B	104	PHE	CA-C-N	7.05	129.60	120.44
1	B	104	PHE	C-N-CA	7.05	129.60	120.44
1	A	106	THR	CB-CA-C	-7.05	97.80	110.70
1	A	119	GLU	CB-CG-CD	7.04	124.57	112.60
1	B	406	GLY	CA-C-N	7.04	129.71	120.28
1	B	406	GLY	C-N-CA	7.04	129.71	120.28
1	A	139	PRO	CB-CA-C	7.03	120.19	110.98
1	B	203	PRO	CA-C-N	7.03	129.93	120.65
1	B	203	PRO	C-N-CA	7.03	129.93	120.65
1	A	70	LEU	N-CA-C	7.02	120.92	110.52
1	B	11	ALA	CA-C-O	7.01	126.76	119.05
1	B	20	GLY	CA-C-O	7.01	128.09	120.66
1	B	189	PHE	CA-CB-CG	7.00	120.80	113.80
1	A	265	TYR	CB-CA-C	6.99	123.26	110.88
1	B	361	LYS	N-CA-C	6.99	120.13	110.35
1	A	411	ARG	CA-C-O	6.98	127.95	120.55
1	B	6	ARG	CA-CB-CG	6.98	128.06	114.10
1	B	414	TRP	CB-CA-C	6.98	121.76	110.95
1	A	430	HIS	CB-CA-C	6.96	121.72	110.16
1	A	246	TYR	CA-C-N	6.96	129.40	120.70
1	A	246	TYR	C-N-CA	6.96	129.40	120.70
1	A	146	LEU	N-CA-CB	-6.96	99.89	109.98
1	A	389	ILE	CA-C-O	-6.94	113.13	120.76
1	B	269	ALA	CA-C-N	6.93	133.92	121.92
1	B	269	ALA	C-N-CA	6.93	133.92	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	LYS	CA-CB-CG	6.93	127.95	114.10
1	B	212	ALA	N-CA-C	-6.92	103.66	111.07
1	B	12	LEU	CB-CA-C	6.92	120.95	109.89
1	A	284	LEU	CB-CA-C	-6.91	100.07	111.68
1	B	265	TYR	N-CA-CB	6.91	120.89	110.19
1	A	276	ARG	CA-C-O	-6.90	113.51	120.90
1	B	59	THR	CB-CA-C	6.90	124.16	110.42
1	A	458	GLU	N-CA-CB	-6.90	99.58	110.69
1	A	455	LEU	N-CA-C	6.90	119.89	109.41
1	B	188	ASP	CB-CA-C	-6.90	97.48	109.07
1	A	182	ALA	N-CA-CB	6.89	120.83	110.22
1	B	155	VAL	CA-C-O	-6.89	113.31	120.27
1	B	285	HIS	CA-CB-CG	6.89	120.69	113.80
1	B	451	TRP	CA-C-N	6.88	134.68	121.54
1	B	451	TRP	C-N-CA	6.88	134.68	121.54
1	A	34	ALA	CA-C-N	6.87	130.58	123.30
1	A	34	ALA	C-N-CA	6.87	130.58	123.30
1	B	164	ILE	N-CA-C	-6.84	97.77	107.75
1	B	128	VAL	CB-CA-C	6.83	117.68	110.37
1	B	316	GLY	O-C-N	6.83	131.58	122.70
1	A	249	GLU	CA-C-N	6.83	129.73	120.44
1	A	249	GLU	C-N-CA	6.83	129.73	120.44
1	A	410	LEU	N-CA-CB	-6.83	99.71	110.22
1	B	4	SER	CA-C-O	6.82	130.27	120.51
1	A	197	GLY	O-C-N	6.82	131.56	122.70
1	B	169	LEU	CB-CA-C	6.80	123.18	109.38
1	B	209	ALA	N-CA-C	-6.80	103.11	111.40
1	A	406	GLY	CA-C-N	6.78	132.04	120.72
1	A	406	GLY	C-N-CA	6.78	132.04	120.72
1	B	377	PRO	CA-C-N	6.77	128.81	120.22
1	B	377	PRO	C-N-CA	6.77	128.81	120.22
1	B	102	ALA	CA-C-O	-6.76	113.11	121.02
1	A	209	ALA	O-C-N	6.76	129.86	122.15
1	A	33	LYS	CB-CG-CD	6.76	126.84	111.30
1	A	74	VAL	CA-C-N	6.75	130.78	121.33
1	A	74	VAL	C-N-CA	6.75	130.78	121.33
1	B	401	ASP	CA-C-O	6.75	127.56	119.59
1	B	239	GLU	N-CA-C	-6.75	105.18	113.41
1	B	64	THR	CA-C-N	6.75	134.43	121.54
1	B	64	THR	C-N-CA	6.75	134.43	121.54
1	A	299	SER	CA-C-O	-6.74	113.08	120.43
1	B	272	ILE	N-CA-C	6.74	118.30	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	VAL	CB-CA-C	6.74	120.50	111.88
1	B	200	PRO	CA-C-O	6.73	129.50	119.74
1	A	270	ALA	CB-CA-C	6.73	124.11	110.38
1	B	227	LEU	N-CA-C	6.73	119.38	108.41
1	B	436	ALA	N-CA-C	-6.73	104.02	111.36
1	B	251	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	17	LEU	CA-C-O	-6.73	113.77	120.70
1	A	341	TYR	CB-CA-C	6.73	122.28	110.85
1	A	186	GLY	O-C-N	6.72	131.44	122.70
1	B	272	ILE	CB-CA-C	-6.72	103.23	112.04
1	A	372	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	422	PRO	CA-C-O	6.72	132.83	120.60
1	A	238	PHE	CA-C-O	-6.72	112.25	119.97
1	A	409	SER	CA-CB-OG	6.71	124.53	111.10
1	B	286	TYR	CB-CG-CD1	6.71	130.87	120.80
1	A	35	GLY	N-CA-C	-6.71	106.41	113.58
1	A	458	GLU	N-CA-C	6.70	120.38	109.59
1	B	41	THR	O-C-N	6.70	130.51	122.27
1	A	288	ARG	N-CA-C	6.69	125.05	110.80
1	A	189	PHE	O-C-N	6.67	131.01	123.27
1	A	79	GLU	CA-C-N	-6.67	114.17	122.84
1	A	79	GLU	C-N-CA	-6.67	114.17	122.84
1	B	14	GLU	CA-C-N	6.67	133.79	121.52
1	B	14	GLU	C-N-CA	6.67	133.79	121.52
1	A	371	MET	N-CA-C	-6.67	94.29	107.69
1	A	98	LYS	CA-C-O	-6.66	114.30	121.56
1	B	256	SER	CB-CA-C	-6.66	96.38	110.31
1	B	184	TRP	CA-C-O	6.66	127.71	119.05
1	A	149	VAL	N-CA-C	-6.65	105.64	113.42
1	B	111	ASN	CB-CG-OD1	-6.65	107.50	120.80
1	B	413	ALA	O-C-N	6.64	129.99	122.22
1	A	418	ARG	CD-NE-CZ	-6.64	115.10	124.40
1	B	28	TYR	CA-CB-CG	6.64	125.86	113.90
1	B	388	VAL	CA-CB-CG2	6.64	121.69	110.40
1	A	425	ASP	CA-C-O	6.64	127.54	119.31
1	A	235	ASP	CA-C-N	6.62	130.82	121.61
1	A	235	ASP	C-N-CA	6.62	130.82	121.61
1	A	145	ALA	CA-C-O	6.62	126.72	119.24
1	A	185	LEU	N-CA-CB	-6.62	101.64	111.43
1	B	138	GLY	O-C-N	6.61	128.38	121.77
1	A	245	GLU	N-CA-CB	-6.60	100.70	110.53
1	A	19	ALA	N-CA-C	6.60	119.31	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	TRP	CA-C-N	6.60	134.34	121.41
1	A	357	TRP	C-N-CA	6.60	134.34	121.41
1	A	161	VAL	O-C-N	6.59	129.87	123.14
1	B	354	ARG	N-CA-C	-6.59	98.52	109.46
1	A	203	PRO	CA-C-N	6.59	134.12	121.54
1	A	203	PRO	C-N-CA	6.59	134.12	121.54
1	A	355	GLN	CA-C-N	6.59	134.35	122.62
1	A	355	GLN	C-N-CA	6.59	134.35	122.62
1	A	176	PHE	N-CA-CB	6.56	119.58	110.07
1	A	201	PHE	CA-CB-CG	6.56	120.36	113.80
1	B	443	ASP	N-CA-C	-6.56	103.97	112.23
1	A	238	PHE	O-C-N	6.55	130.33	122.27
1	B	356	SER	O-C-N	6.55	131.66	123.28
1	B	327	PHE	N-CA-C	-6.55	96.86	110.80
1	B	122	LYS	CB-CG-CD	6.54	126.36	111.30
1	B	279	PHE	CA-C-N	6.54	126.25	119.64
1	B	279	PHE	C-N-CA	6.54	126.25	119.64
1	B	261	LEU	CA-C-N	6.52	132.05	122.99
1	B	261	LEU	C-N-CA	6.52	132.05	122.99
1	B	450	GLY	CA-C-N	6.51	130.21	120.31
1	B	450	GLY	C-N-CA	6.51	130.21	120.31
1	B	6	ARG	NE-CZ-NH1	6.51	128.01	121.50
1	A	83	ILE	N-CA-C	6.51	118.15	108.46
1	A	39	VAL	N-CA-CB	6.50	118.15	110.55
1	A	160	VAL	CA-C-O	-6.50	113.51	120.59
1	A	443	ASP	N-CA-C	-6.49	103.42	112.12
1	B	71	VAL	N-CA-C	-6.49	99.24	108.58
1	B	418	ARG	CA-C-O	6.49	127.43	120.55
1	B	344	THR	N-CA-C	6.49	121.86	113.88
1	B	54	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	A	216	ARG	CA-C-O	-6.48	111.65	119.49
1	A	198	ASN	N-CA-CB	-6.48	102.63	110.53
1	A	74	VAL	N-CA-CB	6.47	122.00	112.35
1	B	78	ARG	CA-C-N	6.47	133.90	121.54
1	B	78	ARG	C-N-CA	6.47	133.90	121.54
1	A	116	GLY	N-CA-C	6.46	123.79	115.32
1	B	19	ALA	N-CA-C	6.46	119.14	111.71
1	A	192	ASN	CB-CA-C	6.45	123.76	110.40
1	B	120	TYR	CA-CB-CG	6.44	125.50	113.90
1	B	441	PRO	N-CA-C	6.44	124.21	113.78
1	A	95	THR	CA-CB-CG2	6.43	121.44	110.50
1	A	421	VAL	N-CA-C	6.43	122.78	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	ASP	N-CA-C	6.43	120.84	113.19
1	A	455	LEU	N-CA-CB	-6.43	101.20	111.43
1	A	43	ALA	CA-C-O	6.43	127.32	120.70
1	A	163	THR	CA-C-O	6.43	128.95	121.49
1	A	246	TYR	N-CA-C	-6.43	103.56	111.40
1	A	254	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	18	ILE	O-C-N	6.42	128.56	121.94
1	A	194	GLU	CB-CG-CD	6.42	123.52	112.60
1	B	372	ASN	N-CA-CB	-6.42	100.55	110.56
1	B	87	VAL	CA-CB-CG1	6.41	121.30	110.40
1	A	325	MET	CA-CB-CG	6.41	126.92	114.10
1	B	172	ARG	NE-CZ-NH1	6.40	127.90	121.50
1	B	189	PHE	O-C-N	6.40	131.07	123.27
1	A	330	MET	CA-C-O	6.39	127.57	120.92
1	A	102	ALA	CA-C-N	6.39	129.32	120.63
1	A	102	ALA	C-N-CA	6.39	129.32	120.63
1	A	178	GLU	O-C-N	6.38	128.72	122.09
1	A	417	TRP	CA-C-N	6.37	133.71	121.54
1	A	417	TRP	C-N-CA	6.37	133.71	121.54
1	B	276	ARG	CA-C-O	-6.37	111.40	120.51
1	B	287	HIS	N-CA-C	-6.37	100.13	110.20
1	B	51	THR	N-CA-CB	-6.37	102.12	110.59
1	B	192	ASN	N-CA-C	-6.37	97.23	110.80
1	A	142	ASN	CB-CG-OD1	6.37	133.53	120.80
1	B	229	SER	CA-CB-OG	-6.37	98.37	111.10
1	B	243	ARG	O-C-N	-6.36	114.13	122.59
1	B	238	PHE	O-C-N	6.36	129.93	122.24
1	B	246	TYR	CA-C-N	6.35	133.41	121.97
1	B	246	TYR	C-N-CA	6.35	133.41	121.97
1	A	348	ALA	CA-C-O	-6.35	114.70	121.88
1	A	95	THR	CA-C-O	-6.35	112.24	119.41
1	A	357	TRP	O-C-N	-6.34	114.15	122.59
1	A	236	ASP	OD1-CG-OD2	-6.32	107.73	122.90
1	A	209	ALA	CB-CA-C	-6.32	100.11	110.85
1	A	157	GLY	N-CA-C	6.31	128.14	113.18
1	A	40	ALA	CA-C-N	6.31	129.37	120.28
1	A	40	ALA	C-N-CA	6.31	129.37	120.28
1	B	192	ASN	O-C-N	6.31	130.98	122.59
1	B	3	GLN	N-CA-C	6.31	124.24	110.80
1	A	39	VAL	CA-C-O	-6.31	114.48	121.17
1	B	45	PHE	CA-CB-CG	6.30	120.10	113.80
1	A	414	TRP	N-CA-C	-6.30	102.97	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	TYR	CA-C-O	-6.29	112.54	120.28
1	A	177	ALA	CA-C-N	6.29	129.02	120.54
1	A	177	ALA	C-N-CA	6.29	129.02	120.54
1	B	89	LEU	CB-CA-C	-6.29	98.08	110.27
1	B	85	TYR	N-CA-C	6.28	119.72	108.47
1	A	390	LEU	CB-CA-C	6.28	121.20	109.71
1	A	412	GLN	OE1-CD-NE2	6.27	128.87	122.60
1	A	166	LYS	CB-CA-C	6.27	119.18	109.15
1	B	303	TYR	CA-CB-CG	6.27	125.18	113.90
1	B	335	SER	CA-C-N	6.27	132.45	122.86
1	B	335	SER	C-N-CA	6.27	132.45	122.86
1	A	354	ARG	CB-CA-C	6.27	121.34	109.37
1	B	294	VAL	N-CA-CB	-6.27	103.70	112.35
1	B	61	ASP	N-CA-CB	-6.26	99.90	110.49
1	A	15	GLU	CB-CG-CD	6.26	123.25	112.60
1	A	75	ASP	O-C-N	6.25	130.00	123.62
1	B	31	LYS	O-C-N	6.25	128.78	121.10
1	B	70	LEU	N-CA-CB	-6.25	100.63	110.69
1	A	22	GLU	N-CA-C	-6.24	105.60	113.72
1	A	250	THR	CA-C-N	6.24	131.14	120.72
1	A	250	THR	C-N-CA	6.24	131.14	120.72
1	B	385	ASN	CA-C-O	-6.23	111.60	120.51
1	B	118	VAL	CA-C-O	6.23	127.23	120.57
1	B	80	LEU	CA-C-O	-6.22	113.61	120.70
1	B	333	GLU	CA-CB-CG	6.21	126.53	114.10
1	A	43	ALA	N-CA-C	-6.20	104.44	111.14
1	A	112	ASN	CA-C-N	6.20	130.68	122.06
1	A	112	ASN	C-N-CA	6.20	130.68	122.06
1	A	177	ALA	CA-C-O	6.20	127.33	120.82
1	A	34	ALA	N-CA-C	6.20	119.25	109.96
1	A	379	PHE	CA-CB-CG	-6.20	107.60	113.80
1	B	54	ASN	CB-CG-ND2	6.18	125.68	116.40
1	A	381	GLU	CB-CA-C	-6.18	98.43	110.11
1	B	143	ILE	O-C-N	-6.18	115.66	121.90
1	A	409	SER	N-CA-C	-6.18	104.24	110.97
1	A	160	VAL	CA-C-N	-6.17	115.14	123.10
1	A	160	VAL	C-N-CA	-6.17	115.14	123.10
1	B	316	GLY	CA-C-N	6.17	130.67	121.72
1	B	316	GLY	C-N-CA	6.17	130.67	121.72
1	A	22	GLU	CB-CG-CD	6.17	123.09	112.60
1	B	93	ASN	CA-C-N	6.17	130.65	121.77
1	B	93	ASN	C-N-CA	6.17	130.65	121.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	LEU	N-CA-C	6.17	120.06	112.54
1	B	3	GLN	N-CA-CB	6.17	120.91	110.49
1	A	315	GLN	CB-CA-C	-6.16	101.20	110.88
1	A	225	ALA	CA-C-N	6.16	131.86	122.93
1	A	225	ALA	C-N-CA	6.16	131.86	122.93
1	B	284	LEU	O-C-N	6.16	130.50	122.68
1	B	320	ILE	N-CA-CB	-6.16	101.27	111.36
1	A	306	PHE	CB-CA-C	6.15	120.54	110.88
1	A	328	GLY	CA-C-N	6.15	133.29	121.54
1	A	328	GLY	C-N-CA	6.15	133.29	121.54
1	A	415	GLN	CA-C-N	6.15	128.84	120.54
1	A	415	GLN	C-N-CA	6.15	128.84	120.54
1	A	333	GLU	CA-C-O	6.15	129.30	120.51
1	A	282	ASN	CA-C-O	-6.14	114.26	121.44
1	B	234	ALA	CA-C-N	6.14	131.93	122.42
1	B	234	ALA	C-N-CA	6.14	131.93	122.42
1	A	95	THR	CA-CB-OG1	-6.13	100.40	109.60
1	A	125	ASP	CB-CG-OD1	6.13	132.50	118.40
1	A	136	PHE	O-C-N	6.13	130.74	122.59
1	B	384	GLY	N-CA-C	6.13	120.96	113.79
1	A	61	ASP	CA-C-O	6.12	127.06	120.20
1	B	412	GLN	N-CA-CB	6.12	118.89	110.01
1	A	221	GLU	CG-CD-OE1	6.12	132.48	118.40
1	B	424	LEU	CA-C-N	6.12	128.76	120.44
1	B	424	LEU	C-N-CA	6.12	128.76	120.44
1	A	424	LEU	N-CA-C	6.12	118.74	111.33
1	A	3	GLN	CA-CB-CG	6.11	126.33	114.10
1	B	71	VAL	N-CA-CB	6.11	117.38	110.72
1	B	286	TYR	O-C-N	6.11	130.39	122.87
1	A	337	ARG	NE-CZ-NH1	6.11	127.61	121.50
1	A	150	LEU	N-CA-C	-6.11	104.73	111.82
1	A	219	GLN	N-CA-CB	6.11	119.80	110.70
1	A	343	LEU	CA-CB-CG	6.11	137.68	116.30
1	A	173	PRO	O-C-N	-6.10	114.91	122.23
1	A	260	LEU	CB-CA-C	6.10	120.20	110.19
1	B	375	ARG	N-CA-C	-6.10	104.19	111.69
1	A	432	GLU	O-C-N	6.10	130.60	122.43
1	B	457	VAL	CA-C-N	6.10	133.19	121.54
1	B	457	VAL	C-N-CA	6.10	133.19	121.54
1	B	318	SER	O-C-N	6.09	129.77	122.27
1	B	148	LYS	N-CA-CB	6.09	119.60	110.22
1	B	279	PHE	CA-C-O	-6.09	112.29	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	VAL	CA-CB-CG1	6.09	120.75	110.40
1	B	44	HIS	N-CA-CB	6.09	118.81	109.98
1	B	188	ASP	O-C-N	6.09	129.84	122.48
1	B	259	ALA	N-CA-C	-6.08	99.48	109.40
1	A	36	TYR	CA-C-O	-6.08	114.50	121.19
1	B	66	GLY	CA-C-N	6.08	132.91	121.97
1	B	66	GLY	C-N-CA	6.08	132.91	121.97
1	A	286	TYR	CB-CG-CD2	-6.08	111.69	120.80
1	B	305	ALA	CB-CA-C	6.07	120.87	110.79
1	A	31	LYS	CB-CA-C	-6.07	103.17	110.15
1	A	298	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	B	259	ALA	CA-C-N	6.07	130.49	122.30
1	B	259	ALA	C-N-CA	6.07	130.49	122.30
1	A	10	LEU	O-C-N	6.07	130.71	122.82
1	B	458	GLU	CG-CD-OE1	6.07	132.35	118.40
1	A	104	PHE	CA-C-O	6.06	128.11	121.02
1	B	182	ALA	CA-C-O	-6.06	112.46	119.61
1	B	65	ARG	NE-CZ-NH2	6.06	124.65	119.20
1	B	269	ALA	CA-C-O	-6.05	111.86	120.51
1	B	337	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	134	ALA	CB-CA-C	-6.05	100.02	110.72
1	A	61	ASP	CA-CB-CG	6.04	118.64	112.60
1	B	373	ALA	CA-C-O	-6.04	111.87	120.51
1	B	102	ALA	O-C-N	6.04	129.50	122.20
1	B	148	LYS	N-CA-C	-6.03	104.77	111.71
1	A	358	GLY	N-CA-C	6.03	127.47	113.18
1	B	354	ARG	CD-NE-CZ	6.03	132.84	124.40
1	B	236	ASP	CA-C-O	6.02	125.45	119.49
1	B	339	ILE	CA-C-O	6.02	127.23	120.85
1	A	54	ASN	N-CA-CB	6.02	119.69	110.60
1	A	55	VAL	CA-CB-CG2	6.02	120.63	110.40
1	B	150	LEU	CA-C-N	6.02	133.20	121.41
1	B	150	LEU	C-N-CA	6.02	133.20	121.41
1	A	228	PHE	CA-CB-CG	-6.01	107.78	113.80
1	A	446	GLN	CA-C-O	-6.01	114.45	121.07
1	A	224	GLU	CA-C-O	6.01	128.83	121.56
1	A	282	ASN	CB-CG-OD1	6.01	132.82	120.80
1	B	144	SER	CB-CA-C	-6.01	96.72	110.18
1	A	189	PHE	CA-CB-CG	6.01	119.81	113.80
1	A	438	GLU	N-CA-CB	5.99	119.05	110.06
1	A	398	GLY	N-CA-C	-5.99	98.98	113.18
1	B	188	ASP	N-CA-C	5.99	121.63	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	LYS	N-CA-CB	5.97	117.46	110.42
1	B	255	ALA	CA-C-O	-5.96	114.19	120.63
1	A	18	ILE	O-C-N	-5.96	115.69	121.83
1	B	95	THR	N-CA-CB	-5.96	101.64	110.10
1	A	269	ALA	N-CA-CB	-5.95	100.73	110.14
1	B	313	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	A	421	VAL	CA-C-N	5.95	127.28	119.84
1	A	421	VAL	C-N-CA	5.95	127.28	119.84
1	A	64	THR	CA-CB-OG1	-5.95	100.68	109.60
1	A	242	ALA	CA-C-N	5.95	128.50	120.65
1	A	242	ALA	C-N-CA	5.95	128.50	120.65
1	B	13	LYS	CA-C-O	5.95	127.47	120.69
1	A	419	ASP	CA-C-N	5.94	133.18	121.06
1	A	419	ASP	C-N-CA	5.94	133.18	121.06
1	B	354	ARG	CG-CD-NE	5.94	125.06	112.00
1	B	270	ALA	CB-CA-C	5.94	120.09	109.29
1	A	382	ASN	N-CA-C	-5.93	105.54	112.89
1	A	277	ARG	CG-CD-NE	5.92	125.03	112.00
1	A	23	HIS	N-CA-C	5.92	119.05	109.40
1	B	274	THR	CA-CB-OG1	-5.92	100.72	109.60
1	B	99	ALA	O-C-N	-5.92	114.72	122.59
1	B	132	TYR	CB-CA-C	5.91	118.61	109.03
1	B	243	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	158	GLY	CA-C-N	5.91	129.16	120.82
1	A	158	GLY	C-N-CA	5.91	129.16	120.82
1	A	46	ALA	CA-C-O	-5.91	113.17	119.97
1	B	76	GLU	CA-C-N	5.91	130.59	120.72
1	B	76	GLU	C-N-CA	5.91	130.59	120.72
1	A	257	HIS	CB-CA-C	-5.91	100.19	110.17
1	A	451	TRP	N-CA-C	5.90	123.37	110.80
1	A	192	ASN	OD1-CG-ND2	-5.90	116.70	122.60
1	A	180	CYS	CA-C-N	5.89	128.97	120.79
1	A	180	CYS	C-N-CA	5.89	128.97	120.79
1	A	383	LEU	CA-C-O	-5.89	112.09	120.51
1	A	455	LEU	CA-C-O	5.88	128.40	121.58
1	A	95	THR	CB-CA-C	-5.88	98.95	109.24
1	B	205	ARG	CA-C-N	5.88	132.01	121.66
1	B	205	ARG	C-N-CA	5.88	132.01	121.66
1	B	70	LEU	CA-C-O	-5.88	114.48	120.71
1	A	305	ALA	CA-C-O	-5.87	113.22	119.97
1	A	391	THR	N-CA-CB	-5.87	101.49	110.65
1	B	423	VAL	N-CA-C	5.87	121.54	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	ASP	CA-CB-CG	5.86	118.46	112.60
1	A	33	LYS	CA-C-O	-5.86	115.18	121.56
1	B	426	TYR	N-CA-C	-5.85	104.98	111.71
1	A	449	PRO	N-CA-CB	-5.85	97.11	103.25
1	A	217	ARG	CG-CD-NE	5.84	124.85	112.00
1	B	78	ARG	N-CA-C	-5.84	106.01	114.12
1	A	285	HIS	N-CA-CB	-5.83	100.60	109.94
1	A	244	GLY	CA-C-O	-5.83	114.51	120.45
1	B	444	ALA	CA-C-N	5.83	132.67	121.54
1	B	444	ALA	C-N-CA	5.83	132.67	121.54
1	A	391	THR	CB-CA-C	5.82	119.83	110.16
1	A	217	ARG	N-CA-C	-5.82	104.85	111.14
1	A	37	GLY	N-CA-C	5.82	126.97	113.18
1	B	277	ARG	CB-CA-C	5.82	122.00	110.42
1	A	64	THR	N-CA-CB	5.81	122.56	112.27
1	B	337	ARG	CA-C-O	5.81	127.09	120.00
1	A	296	SER	N-CA-CB	5.79	121.09	109.28
1	A	445	ASP	N-CA-C	-5.79	98.48	110.80
1	A	279	PHE	O-C-N	5.78	126.68	121.42
1	A	432	GLU	CG-CD-OE1	-5.78	105.10	118.40
1	A	226	LYS	N-CA-CB	-5.78	101.38	110.69
1	A	197	GLY	N-CA-C	-5.77	99.50	113.18
1	A	198	ASN	CB-CG-OD1	5.77	132.34	120.80
1	A	334	SER	CA-C-N	5.77	128.90	120.71
1	A	334	SER	C-N-CA	5.77	128.90	120.71
1	B	372	ASN	CA-C-O	-5.77	114.62	121.66
1	A	18	ILE	N-CA-C	5.76	116.54	110.72
1	B	330	MET	N-CA-CB	5.76	120.22	110.49
1	A	269	ALA	N-CA-C	5.75	119.11	111.75
1	A	242	ALA	N-CA-C	5.75	117.63	111.36
1	A	254	ASN	O-C-N	5.75	129.47	121.83
1	A	129	PRO	CA-N-CD	-5.74	103.96	112.00
1	B	133	ARG	NH1-CZ-NH2	-5.74	111.83	119.30
1	A	160	VAL	CA-CB-CG1	5.74	120.16	110.40
1	B	430	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	81	THR	CB-CA-C	5.74	119.49	110.19
1	A	422	PRO	N-CA-CB	-5.74	97.22	103.25
1	A	51	THR	CA-CB-CG2	5.73	120.25	110.50
1	B	53	THR	CA-CB-CG2	5.73	120.24	110.50
1	B	16	ASP	CA-C-N	5.73	128.23	120.44
1	B	16	ASP	C-N-CA	5.73	128.23	120.44
1	B	219	GLN	OE1-CD-NE2	5.73	128.33	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	SER	CA-CB-OG	5.73	122.55	111.10
1	A	188	ASP	CA-C-O	5.72	128.89	120.42
1	A	194	GLU	CA-C-N	5.72	126.99	119.84
1	A	194	GLU	C-N-CA	5.72	126.99	119.84
1	A	247	VAL	N-CA-CB	5.72	116.85	110.62
1	B	369	GLY	CA-C-N	5.72	132.61	121.41
1	B	369	GLY	C-N-CA	5.72	132.61	121.41
1	B	426	TYR	CB-CA-C	5.71	121.20	110.63
1	B	243	ARG	CA-C-N	5.71	132.59	121.41
1	B	243	ARG	C-N-CA	5.71	132.59	121.41
1	B	214	ALA	CA-C-O	-5.71	112.35	120.51
1	B	316	GLY	N-CA-C	5.70	126.69	113.18
1	A	274	THR	CA-CB-CG2	5.70	120.19	110.50
1	A	64	THR	CB-CA-C	5.70	120.36	111.70
1	B	222	THR	O-C-N	-5.70	115.59	122.48
1	A	203	PRO	CA-C-O	5.70	127.91	120.85
1	A	278	ARG	CG-CD-NE	5.69	124.52	112.00
1	B	69	ALA	CB-CA-C	5.69	118.99	109.89
1	B	17	LEU	CA-C-N	5.68	127.81	120.70
1	B	17	LEU	C-N-CA	5.68	127.81	120.70
1	A	273	THR	CB-CA-C	5.68	121.58	110.67
1	B	200	PRO	O-C-N	-5.67	115.14	122.23
1	A	311	MET	CB-CG-SD	-5.67	95.70	112.70
1	A	112	ASN	N-CA-CB	5.66	119.28	110.44
1	B	455	LEU	CB-CA-C	5.66	121.05	109.67
1	B	29	ILE	N-CA-C	-5.66	98.99	107.37
1	B	277	ARG	CA-C-N	5.66	134.03	121.80
1	B	277	ARG	C-N-CA	5.66	134.03	121.80
1	B	295	THR	N-CA-CB	5.66	118.96	110.53
1	A	121	ALA	CB-CA-C	5.65	118.26	110.34
1	A	388	VAL	O-C-N	5.65	129.64	122.57
1	A	412	GLN	N-CA-C	-5.65	104.82	110.97
1	B	138	GLY	CA-C-O	-5.64	113.45	121.52
1	B	304	THR	CA-CB-CG2	5.64	120.10	110.50
1	A	102	ALA	CA-C-O	5.64	126.72	120.63
1	A	291	HIS	CA-C-N	5.64	132.47	121.41
1	A	291	HIS	C-N-CA	5.64	132.47	121.41
1	A	234	ALA	O-C-N	5.64	129.71	123.33
1	A	90	PHE	CA-C-O	-5.63	114.33	120.81
1	A	13	LYS	N-CA-CB	5.63	118.24	109.97
1	A	239	GLU	N-CA-CB	5.63	118.46	110.13
1	B	8	VAL	N-CA-C	-5.63	100.92	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	GLY	N-CA-C	5.62	125.41	114.16
1	B	415	GLN	CB-CG-CD	5.62	122.16	112.60
1	B	155	VAL	N-CA-CB	5.62	119.47	111.82
1	A	152	ARG	NE-CZ-NH2	5.62	124.26	119.20
1	B	176	PHE	O-C-N	5.62	127.87	122.03
1	B	232	ILE	CA-C-N	5.62	128.74	120.82
1	B	232	ILE	C-N-CA	5.62	128.74	120.82
1	A	392	ALA	O-C-N	5.62	129.97	123.17
1	A	139	PRO	N-CA-C	-5.62	102.45	111.38
1	A	318	SER	O-C-N	5.62	128.16	122.09
1	B	86	PRO	CB-CA-C	5.62	120.83	111.56
1	B	195	PRO	N-CA-C	5.61	120.92	113.57
1	A	381	GLU	CB-CG-CD	-5.61	103.06	112.60
1	B	266	VAL	CA-C-N	5.61	131.28	121.52
1	B	266	VAL	C-N-CA	5.61	131.28	121.52
1	A	220	ASP	CA-C-N	5.61	132.25	121.54
1	A	220	ASP	C-N-CA	5.61	132.25	121.54
1	B	245	GLU	CA-CB-CG	5.60	125.31	114.10
1	B	449	PRO	N-CA-C	5.60	119.66	111.03
1	A	330	MET	CA-C-N	5.60	132.24	121.54
1	A	330	MET	C-N-CA	5.60	132.24	121.54
1	B	172	ARG	NH1-CZ-NH2	-5.60	112.02	119.30
1	A	4	SER	N-CA-CB	5.60	119.95	110.49
1	A	437	PHE	N-CA-C	-5.60	104.57	111.40
1	B	68	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	219	GLN	CA-CB-CG	5.59	125.28	114.10
1	A	334	SER	CA-C-O	5.59	128.50	120.51
1	B	91	ASP	CA-C-N	5.59	131.58	122.81
1	B	91	ASP	C-N-CA	5.59	131.58	122.81
1	B	329	LYS	CA-C-N	5.58	132.19	121.54
1	B	329	LYS	C-N-CA	5.58	132.19	121.54
1	A	4	SER	N-CA-C	-5.58	98.92	110.80
1	A	419	ASP	O-C-N	-5.58	116.21	122.12
1	B	278	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	A	15	GLU	CA-C-N	5.56	130.09	120.58
1	A	15	GLU	C-N-CA	5.56	130.09	120.58
1	B	93	ASN	OD1-CG-ND2	5.56	128.16	122.60
1	B	48	GLU	N-CA-CB	5.56	120.12	110.39
1	B	146	LEU	CA-C-N	5.56	129.99	120.71
1	B	146	LEU	C-N-CA	5.56	129.99	120.71
1	A	208	ILE	CA-C-N	5.56	128.18	120.29
1	A	208	ILE	C-N-CA	5.56	128.18	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	PHE	CA-C-N	5.56	125.39	119.28
1	A	440	PHE	C-N-CA	5.56	125.39	119.28
1	A	323	GLY	CA-C-N	5.54	132.12	121.54
1	A	323	GLY	C-N-CA	5.54	132.12	121.54
1	A	415	GLN	CB-CG-CD	-5.54	103.18	112.60
1	B	282	ASN	CB-CA-C	5.54	121.12	109.65
1	B	80	LEU	O-C-N	5.54	130.21	123.01
1	B	217	ARG	NE-CZ-NH2	5.54	124.18	119.20
1	A	141	VAL	CA-CB-CG2	5.53	119.81	110.40
1	A	344	THR	N-CA-CB	-5.53	102.38	110.40
1	B	401	ASP	CB-CA-C	5.53	120.07	110.72
1	B	144	SER	CA-CB-OG	-5.53	100.04	111.10
1	A	382	ASN	CB-CA-C	5.53	121.54	109.99
1	A	16	ASP	N-CA-C	-5.52	104.90	111.69
1	A	211	VAL	CA-C-N	5.52	128.70	120.31
1	A	211	VAL	C-N-CA	5.52	128.70	120.31
1	B	36	TYR	N-CA-CB	-5.51	102.23	110.17
1	B	101	ILE	O-C-N	5.51	127.22	121.87
1	A	440	PHE	N-CA-C	5.51	118.99	108.97
1	B	130	GLU	CA-C-O	5.50	126.35	120.24
1	B	318	SER	CA-C-O	-5.50	113.64	119.97
1	A	452	ARG	CD-NE-CZ	5.50	132.10	124.40
1	B	133	ARG	CB-CG-CD	5.50	123.94	111.30
1	B	229	SER	CA-C-O	-5.49	114.70	120.58
1	B	330	MET	CA-C-N	5.49	131.85	121.69
1	B	330	MET	C-N-CA	5.49	131.85	121.69
1	B	152	ARG	CG-CD-NE	5.49	124.08	112.00
1	B	16	ASP	N-CA-C	-5.48	105.32	112.23
1	B	113	GLN	OE1-CD-NE2	-5.47	117.12	122.60
1	B	446	GLN	N-CA-CB	5.47	119.73	110.49
1	A	331	GLU	CA-CB-CG	5.46	125.03	114.10
1	B	347	GLU	O-C-N	5.46	129.92	123.36
1	A	3	GLN	CA-C-O	5.46	128.32	120.51
1	A	15	GLU	N-CA-C	5.46	119.20	112.54
1	A	9	ASN	N-CA-CB	5.46	119.72	110.49
1	A	282	ASN	OD1-CG-ND2	-5.46	117.14	122.60
1	B	279	PHE	CA-CB-CG	5.46	119.26	113.80
1	B	330	MET	CA-C-O	5.46	128.32	120.51
1	B	448	TYR	CA-C-N	5.46	125.73	119.83
1	B	448	TYR	C-N-CA	5.46	125.73	119.83
1	A	272	ILE	O-C-N	5.46	127.26	121.91
1	A	136	PHE	N-CA-CB	5.46	119.72	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	GLU	CB-CA-C	-5.46	100.04	109.86
1	B	315	GLN	CB-CA-C	-5.46	102.31	110.88
1	B	326	GLY	CA-C-O	5.46	130.06	120.57
1	A	285	HIS	CA-C-N	-5.45	115.27	122.85
1	A	285	HIS	C-N-CA	-5.45	115.27	122.85
1	B	241	ILE	CA-C-N	5.45	131.98	121.18
1	B	241	ILE	C-N-CA	5.45	131.98	121.18
1	B	412	GLN	CG-CD-NE2	-5.45	108.22	116.40
1	B	303	TYR	CB-CA-C	-5.45	98.08	110.07
1	A	46	ALA	O-C-N	5.45	128.97	122.27
1	A	457	VAL	CB-CA-C	5.44	120.22	111.29
1	A	409	SER	N-CA-CB	5.44	117.85	109.91
1	B	225	ALA	CA-C-O	5.44	127.72	121.47
1	B	159	LEU	O-C-N	5.43	129.71	123.02
1	A	298	GLN	CB-CG-CD	5.43	121.83	112.60
1	B	293	ALA	N-CA-C	-5.43	105.05	110.97
1	A	246	TYR	N-CA-CB	5.43	118.17	110.13
1	B	294	VAL	CB-CA-C	5.43	116.80	110.88
1	A	127	TYR	CB-CG-CD2	5.43	128.94	120.80
1	A	33	LYS	N-CA-C	-5.42	102.85	110.50
1	A	383	LEU	N-CA-C	-5.42	99.25	110.80
1	B	419	ASP	CB-CA-C	5.41	120.38	110.36
1	A	370	GLY	CA-C-N	5.41	131.30	123.13
1	A	370	GLY	C-N-CA	5.41	131.30	123.13
1	B	181	HIS	CB-CA-C	-5.41	102.62	110.96
1	B	18	ILE	CB-CG1-CD1	5.41	125.16	113.80
1	B	266	VAL	CA-C-O	-5.41	114.02	120.78
1	B	381	GLU	CG-CD-OE1	5.41	130.84	118.40
1	A	17	LEU	CB-CA-C	5.41	119.44	110.90
1	A	133	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	A	251	PHE	CA-C-N	5.41	132.00	121.41
1	A	251	PHE	C-N-CA	5.41	132.00	121.41
1	B	282	ASN	CA-C-N	5.41	129.56	121.72
1	B	282	ASN	C-N-CA	5.41	129.56	121.72
1	B	417	TRP	N-CA-C	5.41	117.25	111.36
1	A	396	ALA	N-CA-C	-5.40	105.43	112.23
1	B	258	VAL	CA-C-N	-5.40	114.84	122.94
1	B	258	VAL	C-N-CA	-5.40	114.84	122.94
1	B	215	MET	CA-C-O	-5.39	112.58	120.13
1	B	228	PHE	N-CA-C	5.39	118.27	109.59
1	B	371	MET	CA-C-O	-5.39	114.39	120.43
1	A	36	TYR	CA-CB-CG	-5.39	104.20	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	THR	CA-CB-OG1	-5.38	101.53	109.60
1	A	233	THR	O-C-N	5.38	129.32	123.13
1	B	249	GLU	CA-CB-CG	5.38	124.85	114.10
1	A	118	VAL	CA-C-O	-5.38	114.06	120.78
1	A	219	GLN	CA-C-O	5.38	126.18	119.78
1	A	390	LEU	N-CA-C	-5.37	100.14	108.90
1	B	165	ILE	CB-CG1-CD1	5.37	125.09	113.80
1	B	222	THR	N-CA-CB	-5.37	103.20	110.67
1	B	321	HIS	CA-C-O	-5.37	115.96	121.87
1	A	138	GLY	CA-C-O	-5.37	113.84	121.52
1	A	252	GLY	N-CA-C	5.37	125.90	113.18
1	B	175	PRO	N-CA-CB	5.37	109.38	103.26
1	B	343	LEU	CA-CB-CG	5.36	135.07	116.30
1	A	251	PHE	N-CA-C	-5.36	106.00	112.54
1	A	12	LEU	CB-CA-C	5.36	119.72	110.77
1	A	87	VAL	O-C-N	5.36	129.16	121.82
1	A	297	PRO	N-CA-C	5.36	123.50	112.47
1	A	65	ARG	N-CA-CB	-5.35	102.61	111.49
1	A	80	LEU	N-CA-C	5.35	117.35	108.20
1	A	157	GLY	CA-C-N	5.35	131.89	121.41
1	A	157	GLY	C-N-CA	5.35	131.89	121.41
1	B	136	PHE	CB-CA-C	5.35	119.38	109.54
1	B	163	THR	CA-CB-OG1	-5.35	101.58	109.60
1	A	105	LEU	CB-CA-C	5.34	119.66	110.79
1	B	362	ALA	CB-CA-C	5.34	120.63	109.68
1	A	58	CYS	CB-CA-C	-5.34	101.34	110.95
1	A	139	PRO	O-C-N	5.34	129.63	123.06
1	B	341	TYR	O-C-N	5.34	129.58	122.43
1	B	315	GLN	N-CA-CB	5.33	117.73	110.01
1	A	217	ARG	CA-C-N	5.32	127.94	120.28
1	A	217	ARG	C-N-CA	5.32	127.94	120.28
1	A	444	ALA	CA-C-N	5.32	131.70	121.54
1	A	444	ALA	C-N-CA	5.32	131.70	121.54
1	B	294	VAL	N-CA-C	5.32	119.64	113.42
1	A	432	GLU	CG-CD-OE2	5.31	130.62	118.40
1	A	122	LYS	N-CA-CB	5.31	119.60	110.68
1	B	121	ALA	CB-CA-C	5.31	117.77	110.34
1	B	251	PHE	N-CA-C	-5.31	106.31	112.89
1	B	458	GLU	CA-C-N	5.30	131.24	121.70
1	B	458	GLU	C-N-CA	5.30	131.24	121.70
1	B	360	MET	CB-CA-C	5.30	118.88	110.19
1	A	143	ILE	CA-CB-CG2	5.30	119.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	SER	N-CA-C	5.30	118.81	111.55
1	A	366	ILE	N-CA-CB	5.30	118.56	112.15
1	B	179	ALA	N-CA-CB	5.30	118.78	110.46
1	B	402	GLY	CA-C-N	5.29	126.45	119.84
1	B	402	GLY	C-N-CA	5.29	126.45	119.84
1	B	203	PRO	N-CA-C	5.29	119.39	111.14
1	A	199	GLN	CA-C-O	-5.28	115.20	120.64
1	A	205	ARG	CA-C-O	-5.28	115.26	121.07
1	A	306	PHE	CA-CB-CG	-5.28	108.52	113.80
1	A	350	GLY	O-C-N	5.28	127.05	121.77
1	B	133	ARG	CA-C-O	5.28	126.36	120.82
1	A	455	LEU	CA-C-N	5.28	131.75	121.41
1	A	455	LEU	C-N-CA	5.28	131.75	121.41
1	A	215	MET	CA-CB-CG	-5.27	103.55	114.10
1	B	155	VAL	N-CA-C	-5.27	99.97	107.77
1	A	229	SER	CB-CA-C	-5.27	102.45	111.41
1	A	226	LYS	CA-CB-CG	5.27	124.64	114.10
1	A	337	ARG	NH1-CZ-NH2	-5.27	112.45	119.30
1	B	387	ASN	N-CA-CB	-5.26	102.18	110.49
1	A	96	ASP	CB-CG-OD2	-5.26	106.31	118.40
1	A	44	HIS	CA-C-N	5.25	131.18	121.52
1	A	44	HIS	C-N-CA	5.25	131.18	121.52
1	A	14	GLU	N-CA-C	5.25	117.68	111.33
1	A	163	THR	CA-C-N	5.25	130.43	122.98
1	A	163	THR	C-N-CA	5.25	130.43	122.98
1	A	261	LEU	CB-CA-C	5.25	118.80	109.72
1	A	406	GLY	O-C-N	-5.25	117.15	122.19
1	A	316	GLY	CA-C-O	-5.24	111.45	120.57
1	A	152	ARG	CA-CB-CG	5.24	124.58	114.10
1	B	240	ILE	O-C-N	5.24	127.04	121.91
1	B	264	GLY	O-C-N	5.24	129.50	122.48
1	A	365	PRO	N-CA-C	-5.23	102.98	111.14
1	A	230	ALA	N-CA-C	5.23	117.27	108.96
1	A	97	GLY	N-CA-C	5.22	121.95	114.64
1	B	38	TYR	CA-CB-CG	-5.22	104.50	113.90
1	A	447	ILE	CB-CG1-CD1	5.22	124.76	113.80
1	B	222	THR	CA-CB-CG2	5.22	119.37	110.50
1	A	142	ASN	CB-CG-ND2	-5.22	108.58	116.40
1	A	428	ARG	CA-C-N	5.22	127.27	120.28
1	A	428	ARG	C-N-CA	5.22	127.27	120.28
1	B	38	TYR	N-CA-C	-5.22	104.51	111.24
1	B	163	THR	CA-C-O	5.21	127.03	121.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ILE	CA-CB-CG1	-5.21	101.55	110.40
1	B	192	ASN	CB-CA-C	-5.21	100.06	110.42
1	A	361	LYS	CA-C-N	-5.20	113.34	121.87
1	A	361	LYS	C-N-CA	-5.20	113.34	121.87
1	A	363	CYS	N-CA-C	-5.20	99.93	108.41
1	A	130	GLU	CG-CD-OE2	5.20	130.35	118.40
1	B	313	ARG	N-CA-CB	5.20	117.55	110.01
1	B	128	VAL	O-C-N	-5.19	116.74	121.41
1	B	123	MET	CA-CB-CG	-5.19	103.72	114.10
1	A	276	ARG	O-C-N	5.19	127.49	122.09
1	B	89	LEU	CA-C-N	5.19	129.50	120.68
1	B	89	LEU	C-N-CA	5.19	129.50	120.68
1	A	288	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	B	411	ARG	CD-NE-CZ	-5.18	117.15	124.40
1	B	3	GLN	CB-CA-C	-5.17	100.12	110.42
1	B	341	TYR	CA-CB-CG	5.17	123.21	113.90
1	A	205	ARG	CA-CB-CG	-5.17	103.76	114.10
1	B	354	ARG	N-CA-CB	5.17	118.69	110.16
1	B	49	SER	CA-C-O	5.17	124.73	119.05
1	B	78	ARG	N-CA-CB	5.17	118.01	110.88
1	B	248	LEU	CA-C-O	-5.17	113.69	119.79
1	A	65	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	A	429	GLU	N-CA-C	5.17	116.91	111.28
1	B	77	ALA	N-CA-C	5.17	118.84	112.54
1	B	168	LYS	O-C-N	5.17	128.45	122.20
1	B	166	LYS	N-CA-C	-5.16	102.14	109.62
1	B	243	ARG	N-CA-C	-5.16	99.81	110.80
1	A	81	THR	CA-CB-CG2	5.16	119.27	110.50
1	A	84	ALA	CB-CA-C	-5.16	102.53	110.78
1	B	125	ASP	CA-C-N	5.15	132.26	123.03
1	B	125	ASP	C-N-CA	5.15	132.26	123.03
1	A	310	LYS	CB-CA-C	5.15	118.97	110.88
1	B	250	THR	CA-CB-CG2	5.15	119.26	110.50
1	B	374	LEU	CA-C-O	5.15	125.30	119.27
1	A	290	GLY	N-CA-C	5.15	125.38	113.18
1	A	411	ARG	CA-CB-CG	-5.15	103.80	114.10
1	A	120	TYR	O-C-N	5.15	129.44	122.59
1	A	243	ARG	NH1-CZ-NH2	-5.15	112.61	119.30
1	A	102	ALA	O-C-N	-5.14	116.67	122.12
1	A	90	PHE	O-C-N	5.14	129.25	122.93
1	A	132	TYR	CA-C-O	-5.14	115.41	120.80
1	B	75	ASP	N-CA-C	-5.14	99.92	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	79	GLU	N-CA-CB	5.13	119.17	110.49
1	B	101	ILE	CA-C-O	-5.13	115.61	120.95
1	B	389	ILE	N-CA-C	-5.13	101.02	109.12
1	A	148	LYS	CA-C-O	-5.13	112.64	119.10
1	B	154	GLU	CA-C-O	-5.12	113.18	120.51
1	A	137	ASP	CA-CB-CG	-5.12	107.48	112.60
1	B	13	LYS	CG-CD-CE	5.12	123.08	111.30
1	B	134	ALA	N-CA-CB	-5.12	103.15	110.57
1	B	249	GLU	CB-CG-CD	5.12	121.30	112.60
1	B	448	TYR	O-C-N	5.12	125.98	121.37
1	A	183	PHE	CA-CB-CG	5.12	118.92	113.80
1	B	104	PHE	N-CA-C	-5.11	104.98	111.11
1	A	58	CYS	N-CA-CB	5.11	120.15	111.57
1	A	137	ASP	CB-CA-C	5.10	120.57	110.42
1	A	7	TYR	CA-C-N	5.09	130.04	122.71
1	A	7	TYR	C-N-CA	5.09	130.04	122.71
1	A	160	VAL	O-C-N	5.09	129.69	122.97
1	B	276	ARG	N-CA-C	-5.09	99.95	110.80
1	A	30	MET	N-CA-C	5.09	116.71	108.41
1	A	144	SER	CB-CA-C	-5.09	100.30	110.42
1	B	412	GLN	CB-CG-CD	-5.09	103.95	112.60
1	B	12	LEU	N-CA-C	-5.08	102.33	109.96
1	A	29	ILE	CB-CA-C	5.08	119.63	111.29
1	B	428	ARG	NH1-CZ-NH2	-5.08	112.69	119.30
1	B	169	LEU	CA-C-O	-5.07	114.51	120.60
1	A	44	HIS	CB-CA-C	5.07	121.30	110.21
1	A	196	GLN	CA-C-O	5.07	125.94	120.32
1	A	434	ALA	N-CA-C	-5.07	105.65	111.07
1	A	136	PHE	N-CA-C	-5.06	100.01	110.80
1	A	288	ARG	O-C-N	-5.06	115.86	122.59
1	A	333	GLU	O-C-N	-5.06	115.86	122.59
1	B	96	ASP	O-C-N	5.06	129.19	122.26
1	B	73	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	100	MET	N-CA-CB	-5.05	102.00	111.13
1	B	44	HIS	CA-C-O	-5.04	115.71	120.90
1	A	193	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	268	GLY	CA-C-N	5.04	127.73	120.38
1	A	268	GLY	C-N-CA	5.04	127.73	120.38
1	B	59	THR	CA-CB-CG2	5.04	119.06	110.50
1	B	190	ILE	N-CA-CB	5.04	118.88	111.52
1	A	253	GLU	CB-CG-CD	5.04	121.16	112.60
1	A	405	ALA	N-CA-C	-5.04	106.98	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	PRO	N-CA-CB	-5.04	97.96	103.25
1	B	295	THR	CA-CB-CG2	5.04	119.06	110.50
1	B	37	GLY	N-CA-C	-5.03	106.10	112.54
1	B	423	VAL	CA-C-O	-5.03	114.49	120.78
1	A	415	GLN	OE1-CD-NE2	5.03	127.63	122.60
1	B	341	TYR	CA-C-O	-5.03	113.20	119.38
1	A	418	ARG	CG-CD-NE	5.02	123.05	112.00
1	B	399	HIS	CA-C-O	5.02	126.72	121.19
1	A	383	LEU	CB-CA-C	5.01	120.40	110.42
1	B	365	PRO	O-C-N	-5.01	117.52	122.98
1	A	4	SER	CA-C-N	5.01	131.11	121.54
1	A	4	SER	C-N-CA	5.01	131.11	121.54
1	B	103	SER	CA-CB-OG	-5.01	101.08	111.10
1	A	325	MET	N-CA-CB	5.01	117.48	110.12
1	B	26	CYS	CA-C-O	-5.01	115.58	121.44
1	A	146	LEU	O-C-N	-5.00	116.62	122.03
1	B	98	LYS	CA-C-O	-5.00	115.72	121.47
1	B	261	LEU	CB-CA-C	5.00	118.00	109.75
1	B	13	LYS	CA-C-N	5.00	127.23	120.38
1	B	13	LYS	C-N-CA	5.00	127.23	120.38
1	B	176	PHE	N-CA-C	-5.00	105.52	110.97
1	B	331	GLU	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	457	VAL	Mainchain

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	3502	0	3376	284	0
1	B	3498	0	3376	257	0
2	A	18	0	8	3	0
2	B	18	0	7	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	3	0	0	2	0
4	B	3	0	0	1	0
All	All	7044	0	6767	518	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 38.

All (518) 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:234:ALA:HB3	1:B:240:ILE:HG13	1.25	1.11
1:B:321:HIS:HB3	2:B:700:RUB:O6P	1.56	1.05
1:A:167:PRO:HD3	1:B:59:THR:HG21	1.41	1.01
1:A:285:HIS:HE2	1:A:321:HIS:HE2	1.05	0.94
1:B:322:THR:HG22	1:B:323:GLY:H	1.34	0.92
1:A:457:VAL:CG1	1:A:458:GLU:H	1.81	0.92
1:B:165:ILE:HG12	1:B:176:PHE:HE1	1.32	0.90
1:A:456:GLY:O	1:A:457:VAL:HB	1.70	0.89
1:B:124:HIS:O	1:B:125:ASP:HB2	1.70	0.87
1:A:99:ALA:HB1	1:A:132:TYR:HE1	1.40	0.86
1:B:208:ILE:HD12	1:B:247:VAL:HG22	1.57	0.85
1:B:222:THR:HG22	1:B:224:GLU:HB2	1.57	0.85
1:A:321:HIS:HB3	2:A:600:RUB:O6P	1.75	0.85
1:B:123:MET:HE3	1:B:307:VAL:HG11	1.60	0.83
1:A:356:SER:O	1:A:358:GLY:N	2.12	0.83
1:B:286:TYR:HB3	1:B:320:ILE:HG12	1.63	0.81
1:A:239:GLU:HG3	1:B:95:THR:HB	1.64	0.79
1:A:170:GLY:HA3	1:B:64:THR:HG23	1.63	0.79
1:A:325:MET:HE1	1:A:371:MET:HE3	1.65	0.78
1:A:357:TRP:H	1:A:357:TRP:CD1	2.01	0.78
1:A:415:GLN:HG2	1:A:418:ARG:HH21	1.49	0.78
1:B:33:LYS:HG2	1:B:119:GLU:HB2	1.66	0.78
2:B:700:RUB:O3	4:B:701:FMT:O2	2.03	0.77
1:A:129:PRO:O	1:A:133:ARG:HB2	1.83	0.77
1:B:374:LEU:HD11	1:B:437:PHE:HA	1.68	0.76
1:B:74:VAL:HA	1:B:80:LEU:O	1.86	0.76
1:A:67:VAL:HG13	1:A:89:LEU:HD12	1.65	0.76
1:B:169:LEU:HD11	1:B:195:PRO:HB2	1.66	0.76
1:A:308:HIS:HA	1:A:311:MET:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:SER:HB3	1:B:298:GLN:OE1	1.86	0.75
1:A:12:LEU:HD13	1:A:17:LEU:HD11	1.69	0.75
1:A:306:PHE:HZ	1:A:342:MET:HE3	1.52	0.74
1:A:400:ILE:HD11	1:A:435:ARG:HG2	1.70	0.74
1:B:181:HIS:CD2	1:B:217:ARG:HH21	2.05	0.73
1:A:437:PHE:HD1	1:A:444:ALA:HB1	1.51	0.73
1:A:89:LEU:HD23	1:A:107:LEU:HD22	1.70	0.73
1:A:194:GLU:OE1	1:A:195:PRO:HD3	1.89	0.72
1:B:341:TYR:HB3	1:B:345:GLN:HG2	1.72	0.72
1:A:75:ASP:HB3	1:A:78:ARG:HG2	1.71	0.72
1:B:276:ARG:HG3	1:B:277:ARG:H	1.54	0.71
1:B:309:CYS:O	1:B:312:ALA:HB3	1.89	0.71
1:A:161:VAL:HG11	1:A:410:LEU:HD11	1.73	0.70
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.74	0.70
1:A:94:ILE:HG21	1:B:204:LEU:HD12	1.73	0.70
1:B:231:ASN:HB2	1:B:261:LEU:HD23	1.74	0.70
1:B:263:ASP:HA	1:B:287:HIS:O	1.92	0.70
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.26	0.70
1:A:233:THR:OG1	1:A:262:VAL:HA	1.92	0.69
1:A:285:HIS:CD2	1:A:321:HIS:HE2	2.09	0.69
1:B:3:GLN:O	1:B:4:SER:HB2	1.91	0.69
1:B:164:ILE:CD1	2:B:700:RUB:O3P	2.40	0.69
1:A:168:LYS:O	1:A:196:GLN:NE2	2.26	0.69
1:A:28:TYR:CE2	1:A:83:ILE:HD12	2.28	0.69
1:A:286:TYR:OH	1:A:308:HIS:HE1	1.75	0.69
1:A:373:ALA:HB3	1:A:374:LEU:HD22	1.76	0.68
1:A:74:VAL:HA	1:A:80:LEU:O	1.92	0.68
1:A:311:MET:O	1:A:315:GLN:HG3	1.93	0.68
1:B:3:GLN:HE21	1:B:40:ALA:HB1	1.59	0.68
1:A:176:PHE:HE2	1:A:211:VAL:HG21	1.59	0.68
1:A:200:PRO:HD2	1:B:88:ALA:O	1.94	0.68
1:A:313:ARG:CG	1:A:313:ARG:HH11	2.07	0.68
1:A:357:TRP:HE3	1:A:360:MET:HE2	1.59	0.68
1:A:313:ARG:HH11	1:A:313:ARG:HG3	1.59	0.67
1:A:214:ALA:HA	1:A:217:ARG:HH11	1.59	0.67
1:B:344:THR:HA	1:B:362:ALA:CB	2.25	0.67
1:A:165:ILE:HG21	1:A:176:PHE:CD1	2.30	0.66
1:B:165:ILE:HG12	1:B:176:PHE:CE1	2.23	0.66
1:A:217:ARG:O	1:A:221:GLU:HG3	1.95	0.66
1:B:115:MET:O	1:B:118:VAL:HG22	1.95	0.66
1:A:109:MET:HE2	1:A:109:MET:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ALA:HA	1:A:217:ARG:NH1	2.11	0.66
1:B:276:ARG:O	1:B:278:ARG:N	2.29	0.66
1:A:219:GLN:HE22	1:A:257:HIS:CE1	2.14	0.66
1:A:99:ALA:HB1	1:A:132:TYR:CE1	2.28	0.65
1:B:385:ASN:ND2	1:B:387:ASN:HB2	2.11	0.65
1:B:251:PHE:O	1:B:254:ASN:HB2	1.95	0.65
1:B:194:GLU:HB2	1:B:195:PRO:HD3	1.78	0.65
1:B:344:THR:HA	1:B:362:ALA:HB1	1.76	0.65
1:A:276:ARG:HD2	1:A:276:ARG:O	1.96	0.65
1:A:310:LYS:O	1:A:313:ARG:HB3	1.96	0.65
1:B:143:ILE:HD11	1:B:160:VAL:HG23	1.78	0.65
1:A:321:HIS:CB	2:A:600:RUB:O6P	2.43	0.65
1:B:45:PHE:HD2	1:B:118:VAL:HG11	1.62	0.65
1:A:165:ILE:HD11	1:A:180:CYS:SG	2.37	0.65
1:A:310:LYS:HD3	1:A:357:TRP:CZ2	2.32	0.65
1:B:399:HIS:HD2	1:B:401:ASP:H	1.45	0.65
1:A:14:GLU:HG2	1:A:18:ILE:HD12	1.78	0.64
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.78	0.64
1:B:194:GLU:HG2	1:B:287:HIS:CE1	2.31	0.64
1:A:167:PRO:HG2	1:A:171:LEU:HD13	1.79	0.64
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.79	0.64
1:B:268:GLY:O	1:B:270:ALA:N	2.30	0.64
1:B:55:VAL:O	1:B:56:GLU:HB2	1.97	0.64
1:B:385:ASN:HD22	1:B:387:ASN:H	1.44	0.64
1:B:44:HIS:O	1:B:47:ALA:HB3	1.98	0.64
1:B:152:ARG:NH2	1:B:159:LEU:O	2.31	0.64
1:A:28:TYR:HE2	1:A:83:ILE:HD12	1.62	0.64
1:B:150:LEU:HD13	1:B:152:ARG:NH1	2.12	0.64
1:A:457:VAL:HG12	1:A:458:GLU:H	1.62	0.63
1:B:167:PRO:HD2	1:B:171:LEU:HG	1.79	0.63
1:A:437:PHE:CD1	1:A:444:ALA:HB1	2.34	0.63
1:A:45:PHE:HA	1:A:115:MET:HE1	1.81	0.63
1:A:262:VAL:HG11	1:A:272:ILE:HD13	1.80	0.63
1:A:357:TRP:CE3	1:A:360:MET:HE2	2.34	0.63
1:B:93:ASN:OD1	1:B:100:MET:HE2	1.98	0.63
1:A:7:TYR:HE2	1:A:47:ALA:HA	1.62	0.62
1:A:80:LEU:HD21	1:A:82:LYS:HD2	1.80	0.62
1:A:310:LYS:HD3	1:A:357:TRP:HZ2	1.63	0.62
1:B:123:MET:HE3	1:B:307:VAL:CG1	2.29	0.62
1:A:49:SER:HB3	1:A:107:LEU:O	1.99	0.62
1:A:165:ILE:HG13	1:A:176:PHE:CE1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:NZ	1:A:355:GLN:HG2	2.15	0.62
1:A:9:ASN:ND2	1:A:12:LEU:HG	2.15	0.62
1:B:202:ALA:H	1:B:203:PRO:HD3	1.64	0.62
1:A:75:ASP:HB3	1:A:78:ARG:CG	2.30	0.62
1:A:219:GLN:HE22	1:A:257:HIS:HE1	1.48	0.62
1:A:286:TYR:OH	1:A:308:HIS:CE1	2.52	0.62
1:A:432:GLU:O	1:A:436:ALA:HB2	2.00	0.62
1:A:175:PRO:HB3	1:B:60:THR:HG21	1.80	0.61
1:A:310:LYS:HZ3	1:A:355:GLN:HG2	1.64	0.61
1:B:390:LEU:HD23	1:B:391:THR:N	2.14	0.61
1:A:33:LYS:HG2	1:A:119:GLU:OE1	2.00	0.61
1:A:193:ASP:HA	4:A:601:FMT:O2	1.99	0.61
1:A:266:VAL:O	1:A:267:ALA:HB2	2.00	0.61
1:A:374:LEU:HD21	1:A:436:ALA:O	2.01	0.61
1:A:421:VAL:HG23	1:A:421:VAL:O	2.01	0.61
1:B:62:ASP:O	1:B:63:PHE:HB2	1.99	0.61
1:B:63:PHE:HA	1:B:65:ARG:HH11	1.65	0.61
1:A:143:ILE:HB	1:A:364:THR:OG1	2.01	0.60
1:B:109:MET:CE	1:B:123:MET:HE2	2.31	0.60
1:A:147:TRP:CZ2	1:A:387:ASN:HB3	2.36	0.60
1:B:202:ALA:N	1:B:203:PRO:HD3	2.15	0.60
1:B:215:MET:O	1:B:219:GLN:HG3	2.02	0.60
1:B:285:HIS:CD2	1:B:366:ILE:HD12	2.36	0.60
1:B:217:ARG:O	1:B:221:GLU:HG3	2.02	0.60
1:B:288:ARG:O	1:B:289:ALA:HB3	2.00	0.60
1:B:401:ASP:OD2	1:B:435:ARG:HD3	2.02	0.60
1:A:173:PRO:HB3	1:A:207:THR:OG1	2.02	0.60
1:A:123:MET:HE2	1:A:126:PHE:HB3	1.84	0.59
1:B:294:VAL:HG13	1:B:302:GLY:HA3	1.82	0.59
1:A:458:GLU:O	1:A:459:ASP:HB2	2.02	0.59
1:B:385:ASN:HD22	1:B:386:ALA:N	1.99	0.59
1:A:29:ILE:HG13	1:A:124:HIS:CD2	2.37	0.59
1:A:130:GLU:CD	1:A:133:ARG:HH12	2.09	0.59
1:B:415:GLN:O	1:B:416:ALA:C	2.42	0.59
1:B:181:HIS:CG	1:B:217:ARG:HH21	2.20	0.59
1:B:234:ALA:CB	1:B:240:ILE:HG13	2.16	0.59
1:A:14:GLU:HG2	1:A:18:ILE:CD1	2.32	0.59
1:A:55:VAL:O	1:A:57:VAL:HG22	2.03	0.59
1:A:113:GLN:HB2	1:B:290:GLY:HA2	1.83	0.59
1:B:152:ARG:HG3	1:B:153:PRO:HD2	1.84	0.59
1:A:457:VAL:HG13	1:A:458:GLU:H	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:PHE:CZ	1:B:310:LYS:HG2	2.37	0.59
1:A:309:CYS:HB3	1:A:343:LEU:HD21	1.84	0.59
1:B:131:ALA:O	1:B:135:LEU:HD22	2.01	0.59
1:A:427:ALA:HB3	1:A:455:LEU:HD21	1.84	0.59
1:A:347:GLU:O	1:A:347:GLU:HG3	2.03	0.59
1:B:274:THR:O	1:B:278:ARG:HB3	2.03	0.58
1:A:453:LYS:HD2	1:A:454:ALA:N	2.18	0.58
1:A:162:GLY:N	1:A:390:LEU:O	2.32	0.58
1:B:329:LYS:HG2	1:B:333:GLU:OE1	2.04	0.58
1:A:14:GLU:OE1	1:A:82:LYS:NZ	2.37	0.58
1:A:169:LEU:O	1:B:51:THR:HG22	2.03	0.58
1:A:301:ARG:HB2	1:A:301:ARG:NH1	2.19	0.58
1:A:237:PRO:O	1:A:241:ILE:HG13	2.03	0.58
1:B:184:TRP:CE2	1:B:190:ILE:HG13	2.38	0.58
1:B:428:ARG:O	1:B:429:GLU:HB2	2.04	0.58
1:A:183:PHE:CZ	1:A:187:GLY:HA3	2.38	0.57
1:A:195:PRO:HB3	1:B:107:LEU:CD1	2.34	0.57
1:A:376:MET:CB	1:A:377:PRO:HD3	2.34	0.57
1:B:133:ARG:HD3	1:B:356:SER:O	2.04	0.57
1:A:7:TYR:OH	1:A:51:THR:HB	2.03	0.57
1:A:191:LYS:CB	1:A:229:SER:HB3	2.35	0.57
1:A:6:ARG:HD3	1:A:7:TYR:CE1	2.39	0.57
1:B:276:ARG:HG3	1:B:277:ARG:N	2.20	0.57
1:B:428:ARG:NH2	1:B:454:ALA:HB1	2.19	0.57
1:B:398:GLY:HA3	1:B:440:PHE:CZ	2.40	0.57
1:A:311:MET:HA	1:A:314:LEU:HD12	1.87	0.57
1:A:167:PRO:HD3	1:B:59:THR:CG2	2.27	0.57
1:B:42:ALA:HB1	1:B:71:VAL:HG21	1.87	0.57
1:A:421:VAL:O	1:A:422:PRO:O	2.22	0.56
1:A:409:SER:HB2	1:A:436:ALA:HB2	1.88	0.56
1:B:62:ASP:H	1:B:65:ARG:HD2	1.69	0.56
1:A:349:GLN:OE1	1:A:354:ARG:HB2	2.04	0.56
1:B:192:ASN:ND2	1:B:196:GLN:OE1	2.38	0.56
1:B:171:LEU:CD1	1:B:176:PHE:HA	2.35	0.56
1:A:285:HIS:HE2	1:A:321:HIS:CE1	2.24	0.56
1:B:191:LYS:O	1:B:229:SER:O	2.24	0.55
1:A:6:ARG:HD3	1:A:7:TYR:HE1	1.71	0.55
1:A:294:VAL:O	1:A:299:SER:HB3	2.06	0.55
1:A:320:ILE:HG22	1:A:363:CYS:SG	2.46	0.55
1:B:67:VAL:O	1:B:89:LEU:HD11	2.06	0.55
1:A:437:PHE:HD1	1:A:444:ALA:CB	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:SER:OG	2:B:700:RUB:O1P	2.24	0.55
1:A:423:VAL:HG11	1:A:448:TYR:CD2	2.41	0.55
1:A:127:TYR:CE2	1:A:129:PRO:HD3	2.42	0.55
1:B:309:CYS:HB3	1:B:343:LEU:HD21	1.89	0.55
1:A:224:GLU:OE1	1:A:411:ARG:NH2	2.39	0.54
1:A:364:THR:HG22	1:A:365:PRO:O	2.06	0.54
1:A:380:PHE:CZ	1:A:414:TRP:HB2	2.42	0.54
1:A:427:ALA:CB	1:A:455:LEU:HD21	2.36	0.54
1:B:288:ARG:O	1:B:289:ALA:CB	2.56	0.54
1:A:373:ALA:CB	1:A:436:ALA:HB1	2.37	0.54
1:A:435:ARG:HG3	1:A:435:ARG:HH11	1.72	0.54
1:A:385:ASN:HB2	1:A:387:ASN:ND2	2.21	0.54
1:A:400:ILE:HD11	1:A:435:ARG:CG	2.38	0.54
1:B:231:ASN:HB2	1:B:261:LEU:CD2	2.37	0.54
1:B:396:ALA:HA	1:B:406:GLY:HA3	1.88	0.54
1:B:399:HIS:CD2	1:B:401:ASP:H	2.23	0.54
1:A:5:SER:O	1:A:6:ARG:HB3	2.07	0.54
1:A:147:TRP:HZ2	1:A:387:ASN:HB3	1.73	0.54
1:A:374:LEU:HG	1:A:444:ALA:HB2	1.89	0.54
1:A:3:GLN:HE22	1:A:6:ARG:HD2	1.74	0.53
1:A:192:ASN:ND2	1:A:228:PHE:HZ	2.06	0.53
1:B:202:ALA:N	1:B:203:PRO:CD	2.72	0.53
1:A:88:ALA:O	1:B:200:PRO:HD2	2.07	0.53
1:B:376:MET:HG2	1:B:380:PHE:CE2	2.43	0.53
1:B:399:HIS:HA	1:B:439:SER:OG	2.09	0.53
1:B:3:GLN:O	1:B:4:SER:CB	2.55	0.53
1:B:341:TYR:HB3	1:B:345:GLN:CG	2.39	0.53
1:A:262:VAL:CG1	1:A:272:ILE:HD13	2.38	0.53
1:B:72:TYR:HD2	1:B:84:ALA:HB2	1.73	0.53
1:A:341:TYR:O	1:A:345:GLN:HB3	2.09	0.53
1:A:261:LEU:HD11	1:A:287:HIS:HB3	1.90	0.52
1:A:405:ALA:HB1	1:A:432:GLU:HB3	1.92	0.52
1:B:96:ASP:OD2	1:B:277:ARG:NH1	2.42	0.52
1:B:152:ARG:CG	1:B:153:PRO:HD2	2.40	0.52
1:A:6:ARG:HD3	1:A:68:ASP:OD2	2.09	0.52
1:A:25:LEU:HB2	1:A:127:TYR:HB3	1.91	0.52
1:A:325:MET:HB3	1:A:379:PHE:HE1	1.74	0.52
1:A:146:LEU:HD22	1:A:283:PHE:CD2	2.44	0.52
1:A:445:ASP:OD2	1:A:452:ARG:NH2	2.42	0.52
1:B:164:ILE:HD11	2:B:700:RUB:O3P	2.10	0.52
1:A:123:MET:CE	1:A:126:PHE:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ALA:O	1:A:434:ALA:HB2	2.09	0.52
1:A:376:MET:CE	1:A:390:LEU:HD22	2.40	0.51
1:B:184:TRP:NE1	1:B:190:ILE:HG12	2.24	0.51
1:B:311:MET:O	1:B:315:GLN:HG3	2.10	0.51
1:B:341:TYR:O	1:B:345:GLN:HB2	2.10	0.51
1:A:440:PHE:O	1:A:444:ALA:HB3	2.09	0.51
1:B:339:ILE:O	1:B:343:LEU:HG	2.10	0.51
1:B:385:ASN:ND2	1:B:387:ASN:H	2.08	0.51
1:A:210:LEU:O	1:A:211:VAL:C	2.52	0.51
1:A:428:ARG:HG2	1:A:455:LEU:HD12	1.91	0.51
1:A:168:LYS:HE3	1:A:195:PRO:HG2	1.93	0.51
1:A:193:ASP:OD1	4:A:601:FMT:O2	2.29	0.51
1:B:284:LEU:HD13	1:B:317:ALA:HA	1.92	0.51
1:A:140:SER:O	1:A:141:VAL:HG23	2.11	0.51
1:B:275:ALA:C	1:B:276:ARG:O	2.52	0.51
1:B:322:THR:HG22	1:B:323:GLY:N	2.15	0.51
1:B:428:ARG:O	1:B:429:GLU:CB	2.58	0.51
1:B:374:LEU:HD21	1:B:437:PHE:CD1	2.46	0.51
1:B:6:ARG:NH1	1:B:65:ARG:HA	2.26	0.51
1:B:191:LYS:O	1:B:192:ASN:HB2	2.11	0.51
1:A:168:LYS:HG3	1:A:193:ASP:HB3	1.93	0.50
1:A:456:GLY:O	1:A:457:VAL:CB	2.51	0.50
1:B:213:ASP:O	1:B:215:MET:N	2.44	0.50
1:B:439:SER:O	1:B:441:PRO:HD3	2.11	0.50
1:A:50:SER:OG	1:A:69:ALA:HB3	2.12	0.50
1:B:349:GLN:NE2	1:B:350:GLY:O	2.44	0.50
1:A:10:LEU:HD21	1:A:71:VAL:HG23	1.93	0.50
1:B:321:HIS:HA	1:B:366:ILE:HB	1.92	0.50
1:A:228:PHE:O	1:A:258:VAL:HA	2.12	0.50
1:B:436:ALA:O	1:B:439:SER:HB2	2.11	0.50
1:A:284:LEU:N	1:A:318:SER:HB2	2.27	0.50
1:A:94:ILE:HD12	1:A:94:ILE:C	2.36	0.50
1:A:239:GLU:O	1:A:240:ILE:C	2.52	0.50
1:B:29:ILE:HA	1:B:79:GLU:O	2.11	0.50
1:B:165:ILE:N	1:B:165:ILE:HD12	2.26	0.50
1:B:86:PRO:HB2	1:B:89:LEU:HD13	1.94	0.50
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.47	0.49
1:A:57:VAL:HB	1:B:166:LYS:HB3	1.94	0.49
1:B:377:PRO:HG2	1:B:448:TYR:OH	2.12	0.49
1:B:22:GLU:O	1:B:87:VAL:HG23	2.11	0.49
1:B:322:THR:CG2	1:B:323:GLY:H	2.08	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:C	1:A:172:ARG:O	2.53	0.49
1:A:200:PRO:HG2	1:B:88:ALA:HB1	1.94	0.49
1:A:142:ASN:O	1:A:143:ILE:C	2.54	0.49
1:A:161:VAL:HG11	1:A:410:LEU:CD1	2.41	0.49
1:A:174:LYS:N	1:A:175:PRO:HD2	2.28	0.49
1:A:196:GLN:O	1:A:231:ASN:ND2	2.46	0.49
1:B:171:LEU:HD13	1:B:176:PHE:HA	1.94	0.49
1:A:399:HIS:ND1	1:A:405:ALA:HB3	2.28	0.49
1:B:85:TYR:O	1:B:86:PRO:C	2.55	0.49
1:B:150:LEU:HD21	1:B:227:LEU:HD22	1.94	0.49
1:A:88:ALA:HB1	1:B:200:PRO:HG2	1.94	0.49
1:B:268:GLY:O	1:B:269:ALA:C	2.55	0.49
1:A:29:ILE:HG13	1:A:124:HIS:NE2	2.27	0.48
1:A:184:TRP:CE2	1:A:190:ILE:HD12	2.48	0.48
1:B:385:ASN:ND2	1:B:385:ASN:C	2.71	0.48
1:A:409:SER:HB2	1:A:432:GLU:O	2.13	0.48
1:B:313:ARG:NH2	1:B:360:MET:O	2.37	0.48
1:A:12:LEU:HD13	1:A:17:LEU:CD1	2.41	0.48
1:A:176:PHE:HE2	1:A:211:VAL:CG2	2.24	0.48
1:B:399:HIS:HD2	1:B:401:ASP:N	2.10	0.48
1:A:173:PRO:O	1:A:210:LEU:HD23	2.13	0.48
1:A:184:TRP:CD1	1:A:226:LYS:HG3	2.49	0.48
1:A:299:SER:HB2	1:B:301:ARG:HD3	1.95	0.48
1:B:95:THR:HG22	1:B:96:ASP:N	2.29	0.48
1:B:254:ASN:O	1:B:257:HIS:HB2	2.14	0.48
1:A:101:ILE:O	1:A:105:LEU:HB2	2.14	0.48
1:B:184:TRP:CE2	1:B:190:ILE:CG1	2.97	0.48
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.95	0.48
1:B:326:GLY:O	1:B:327:PHE:HB2	2.14	0.48
1:B:165:ILE:HD12	1:B:165:ILE:H	1.79	0.47
1:B:194:GLU:HG2	1:B:287:HIS:HE1	1.79	0.47
1:B:376:MET:HE2	1:B:413:ALA:HB3	1.96	0.47
1:A:67:VAL:HG12	1:A:67:VAL:O	2.13	0.47
1:A:290:GLY:HA2	1:B:110:GLY:O	2.14	0.47
1:B:414:TRP:O	1:B:417:TRP:N	2.47	0.47
1:A:377:PRO:HA	1:A:380:PHE:CD2	2.49	0.47
1:A:284:LEU:H	1:A:318:SER:HB2	1.78	0.47
1:A:376:MET:HE2	1:A:410:LEU:HD13	1.97	0.47
1:A:411:ARG:O	1:A:411:ARG:HG2	2.14	0.47
1:B:452:ARG:HB2	1:B:458:GLU:O	2.15	0.47
1:B:231:ASN:CB	1:B:261:LEU:HD23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:GLN:NE2	1:B:426:TYR:OH	2.47	0.47
1:A:247:VAL:HG23	1:A:251:PHE:CD1	2.50	0.47
1:A:346:ASP:O	1:A:347:GLU:HB2	2.15	0.47
1:A:424:LEU:H	1:A:424:LEU:HG	1.42	0.47
1:B:90:PHE:HE1	1:B:104:PHE:HA	1.79	0.47
1:A:427:ALA:CB	1:A:437:PHE:HE2	2.28	0.47
1:B:141:VAL:O	1:B:318:SER:HB3	2.14	0.47
1:A:294:VAL:HG23	1:A:295:THR:H	1.79	0.47
1:A:373:ALA:HB2	1:A:409:SER:OG	2.15	0.47
1:B:174:LYS:HB3	1:B:175:PRO:CD	2.45	0.47
1:B:184:TRP:CH2	1:B:215:MET:HE3	2.50	0.47
1:A:194:GLU:N	1:A:195:PRO:HD3	2.31	0.46
1:A:203:PRO:O	1:A:204:LEU:C	2.57	0.46
1:B:33:LYS:HG2	1:B:119:GLU:HG3	1.97	0.46
1:B:33:LYS:HG2	1:B:119:GLU:CB	2.40	0.46
1:B:322:THR:O	1:B:323:GLY:O	2.34	0.46
1:A:128:VAL:H	1:A:355:GLN:HE22	1.63	0.46
1:B:4:SER:HB3	1:B:6:ARG:H	1.81	0.46
1:B:422:PRO:O	1:B:424:LEU:N	2.46	0.46
1:A:122:LYS:HE3	1:A:303:TYR:O	2.15	0.46
1:A:385:ASN:HB2	1:A:387:ASN:HD21	1.79	0.46
1:A:385:ASN:ND2	1:A:387:ASN:HD22	2.13	0.46
1:A:133:ARG:HH11	1:A:133:ARG:HD3	1.45	0.46
1:B:173:PRO:O	1:B:176:PHE:HB3	2.16	0.46
1:B:377:PRO:HD3	1:B:413:ALA:HB1	1.98	0.46
1:A:109:MET:HA	1:A:109:MET:CE	2.38	0.46
1:B:189:PHE:HD1	1:B:227:LEU:HB3	1.81	0.45
1:B:305:ALA:O	1:B:306:PHE:C	2.57	0.45
1:B:452:ARG:CB	1:B:458:GLU:O	2.64	0.45
1:A:128:VAL:H	1:A:355:GLN:NE2	2.13	0.45
1:A:195:PRO:HB3	1:B:107:LEU:HD13	1.97	0.45
1:A:412:GLN:HB3	1:A:433:LEU:CD1	2.46	0.45
1:B:101:ILE:HD12	1:B:101:ILE:HA	1.67	0.45
1:B:373:ALA:HB1	1:B:413:ALA:HB2	1.97	0.45
1:A:114:GLY:O	1:A:115:MET:C	2.60	0.45
1:A:405:ALA:O	1:A:409:SER:HB3	2.17	0.45
1:B:194:GLU:H	1:B:194:GLU:HG3	1.37	0.45
1:B:276:ARG:O	1:B:277:ARG:C	2.58	0.45
1:B:342:MET:SD	1:B:357:TRP:HZ2	2.39	0.45
1:A:30:MET:HG2	1:A:121:ALA:HB2	1.98	0.45
1:B:26:CYS:HB3	1:B:28:TYR:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:HIS:CD2	1:B:288:ARG:N	2.85	0.45
1:A:204:LEU:O	1:A:208:ILE:HB	2.16	0.45
1:A:426:TYR:HD2	1:A:433:LEU:HD12	1.82	0.45
1:B:159:LEU:O	1:B:159:LEU:HD12	2.17	0.45
1:B:199:GLN:HB3	1:B:201:PHE:CD1	2.51	0.45
1:B:423:VAL:HG11	1:B:448:TYR:CZ	2.51	0.45
1:A:218:ALA:O	1:A:222:THR:HG23	2.17	0.45
1:A:457:VAL:CG1	1:A:458:GLU:N	2.63	0.45
1:B:75:ASP:HB3	1:B:80:LEU:HB2	1.99	0.45
1:B:327:PHE:HD1	1:B:328:GLY:H	1.63	0.45
1:B:287:HIS:CD2	1:B:288:ARG:H	2.35	0.45
1:B:426:TYR:O	1:B:430:HIS:ND1	2.49	0.45
1:A:420:GLY:O	1:A:422:PRO:HD2	2.17	0.44
1:B:171:LEU:HD12	1:B:176:PHE:HA	1.98	0.44
1:A:285:HIS:NE2	1:A:321:HIS:NE2	2.34	0.44
1:A:376:MET:HB3	1:A:377:PRO:CD	2.44	0.44
1:B:212:ALA:O	1:B:215:MET:HB3	2.17	0.44
1:B:243:ARG:O	1:B:246:TYR:N	2.51	0.44
1:A:143:ILE:HA	1:A:143:ILE:HD12	1.55	0.44
1:A:176:PHE:CE2	1:A:211:VAL:CG2	3.01	0.44
1:B:430:HIS:ND1	1:B:430:HIS:N	2.65	0.44
1:B:225:ALA:HB1	1:B:257:HIS:CE1	2.52	0.44
1:A:292:GLY:O	1:A:296:SER:HB2	2.17	0.44
1:A:385:ASN:HD22	1:A:387:ASN:H	1.66	0.44
1:B:411:ARG:O	1:B:412:GLN:C	2.59	0.44
1:A:100:MET:HG3	1:A:103:SER:H	1.82	0.44
1:A:103:SER:O	1:A:104:PHE:C	2.61	0.44
1:A:164:ILE:HD11	1:A:391:THR:HG23	1.99	0.44
1:A:325:MET:HB3	1:A:379:PHE:CE1	2.51	0.44
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.99	0.44
1:B:184:TRP:CZ2	1:B:190:ILE:HG13	2.53	0.44
1:A:191:LYS:HB2	1:A:229:SER:HB3	1.99	0.44
1:A:310:LYS:HZ3	1:A:355:GLN:CG	2.30	0.44
1:B:287:HIS:HD2	1:B:288:ARG:H	1.66	0.44
1:B:72:TYR:CD2	1:B:84:ALA:HB2	2.53	0.44
1:B:95:THR:HG22	1:B:96:ASP:H	1.83	0.44
1:B:115:MET:O	1:B:115:MET:SD	2.76	0.44
1:B:138:GLY:C	1:B:316:GLY:HA2	2.42	0.44
1:A:236:ASP:O	1:A:239:GLU:N	2.50	0.44
1:A:317:ALA:O	1:A:363:CYS:HB2	2.18	0.44
1:B:75:ASP:CB	1:B:80:LEU:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:TYR:O	1:B:427:ALA:C	2.61	0.44
1:B:322:THR:O	1:B:323:GLY:C	2.61	0.43
1:B:375:ARG:HD2	1:B:443:ASP:OD2	2.18	0.43
1:B:380:PHE:CE1	1:B:386:ALA:HB1	2.53	0.43
1:B:422:PRO:HG2	1:B:425:ASP:OD2	2.18	0.43
1:B:71:VAL:HG22	1:B:83:ILE:HG12	2.00	0.43
1:B:191:LYS:HE3	1:B:192:ASN:O	2.18	0.43
1:A:13:LYS:HD2	1:A:16:ASP:OD2	2.19	0.43
1:A:178:GLU:HA	1:A:178:GLU:OE1	2.18	0.43
1:A:444:ALA:O	1:A:445:ASP:HB2	2.18	0.43
1:B:398:GLY:HA3	1:B:440:PHE:HZ	1.80	0.43
1:A:284:LEU:H	1:A:318:SER:CB	2.30	0.43
1:A:321:HIS:HA	1:A:366:ILE:O	2.19	0.43
1:B:268:GLY:O	1:B:271:ALA:N	2.39	0.43
1:B:376:MET:CE	1:B:413:ALA:HB3	2.48	0.43
1:B:163:THR:HB	1:B:183:PHE:CZ	2.54	0.43
1:B:162:GLY:N	1:B:390:LEU:O	2.51	0.43
1:A:45:PHE:CA	1:A:115:MET:HE1	2.48	0.43
1:A:165:ILE:HG21	1:A:176:PHE:HD1	1.80	0.43
1:A:270:ALA:HA	1:B:235:ASP:O	2.18	0.43
1:B:172:ARG:HB3	1:B:173:PRO:HD2	2.00	0.43
1:B:225:ALA:HB1	1:B:257:HIS:HE1	1.83	0.43
1:A:99:ALA:CB	1:A:132:TYR:CE1	3.02	0.43
1:A:185:LEU:O	1:A:404:VAL:HG13	2.18	0.43
1:A:427:ALA:HB2	1:A:437:PHE:HE2	1.84	0.43
1:A:67:VAL:O	1:A:89:LEU:HD11	2.19	0.43
1:A:142:ASN:HB2	1:A:143:ILE:H	1.70	0.43
1:A:248:LEU:HD23	1:A:258:VAL:HG11	1.99	0.43
1:B:276:ARG:HG3	1:B:276:ARG:NH1	2.34	0.43
1:A:49:SER:OG	1:A:112:ASN:ND2	2.49	0.43
1:B:107:LEU:HD12	1:B:107:LEU:HA	1.89	0.43
1:B:141:VAL:CG2	1:B:283:PHE:HA	2.49	0.43
1:A:239:GLU:CG	1:B:95:THR:HB	2.44	0.42
1:A:376:MET:HE3	1:A:390:LEU:HD22	1.99	0.42
1:B:125:ASP:OD2	1:B:351:PRO:HD2	2.19	0.42
1:B:199:GLN:HB3	1:B:200:PRO:HD2	2.01	0.42
1:B:162:GLY:HA2	1:B:189:PHE:O	2.19	0.42
1:A:3:GLN:NE2	1:A:6:ARG:HD2	2.34	0.42
1:A:374:LEU:HD22	1:A:374:LEU:H	1.84	0.42
1:B:122:LYS:HB2	1:B:300:LYS:O	2.19	0.42
1:B:376:MET:HE2	1:B:376:MET:HB3	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:SER:O	1:A:6:ARG:CB	2.65	0.42
1:A:6:ARG:NH1	1:A:65:ARG:HB3	2.34	0.42
1:B:110:GLY:C	1:B:112:ASN:H	2.27	0.42
1:A:161:VAL:CG1	1:A:390:LEU:HD23	2.49	0.42
1:A:247:VAL:HG23	1:A:251:PHE:CE1	2.54	0.42
1:B:56:GLU:HB3	1:B:57:VAL:H	1.64	0.42
1:B:184:TRP:O	1:B:226:LYS:NZ	2.51	0.42
1:B:296:SER:HA	1:B:297:PRO:HD3	1.78	0.42
1:A:30:MET:HA	1:A:120:TYR:O	2.19	0.42
1:A:265:TYR:O	1:A:267:ALA:N	2.51	0.42
1:A:357:TRP:CD1	1:A:357:TRP:N	2.79	0.42
1:B:374:LEU:HD11	1:B:437:PHE:CA	2.44	0.42
1:B:394:GLY:O	1:B:440:PHE:HZ	2.02	0.42
1:B:111:ASN:O	1:B:115:MET:HB2	2.19	0.42
1:B:277:ARG:HE	1:B:277:ARG:HB2	1.77	0.42
1:B:229:SER:HA	1:B:259:ALA:O	2.20	0.42
1:A:85:TYR:O	1:A:86:PRO:C	2.61	0.42
1:A:155:VAL:O	1:A:157:GLY:N	2.52	0.42
1:A:168:LYS:HE3	1:A:195:PRO:CG	2.50	0.42
1:A:194:GLU:N	1:A:195:PRO:CD	2.83	0.42
1:A:268:GLY:HA3	1:B:268:GLY:HA3	2.02	0.42
1:A:377:PRO:HA	1:A:380:PHE:HD2	1.85	0.42
1:B:133:ARG:O	1:B:136:PHE:HB2	2.20	0.42
1:B:230:ALA:HB3	1:B:247:VAL:HG11	2.01	0.42
1:B:306:PHE:CZ	1:B:342:MET:HG2	2.55	0.42
1:B:439:SER:C	1:B:441:PRO:HD3	2.45	0.42
1:A:101:ILE:O	1:A:104:PHE:HB3	2.20	0.41
1:B:225:ALA:O	1:B:226:LYS:HD3	2.18	0.41
1:A:239:GLU:HG3	1:B:95:THR:CB	2.41	0.41
1:A:371:MET:O	1:A:376:MET:SD	2.78	0.41
1:A:397:PHE:CE1	1:A:410:LEU:HD21	2.55	0.41
1:B:385:ASN:HD22	1:B:385:ASN:C	2.27	0.41
1:A:110:GLY:O	1:A:113:GLN:HB2	2.21	0.41
1:A:171:LEU:O	1:A:172:ARG:O	2.38	0.41
1:A:195:PRO:HB3	1:B:107:LEU:HD11	2.00	0.41
1:A:368:SER:HB3	2:A:600:RUB:O5P	2.20	0.41
1:B:273:THR:O	1:B:277:ARG:HB3	2.19	0.41
1:A:165:ILE:HG21	1:A:176:PHE:CE1	2.54	0.41
1:A:402:GLY:O	1:A:404:VAL:N	2.54	0.41
1:A:94:ILE:HG21	1:B:204:LEU:CD1	2.46	0.41
1:A:310:LYS:NZ	1:A:355:GLN:HE21	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:THR:HG23	1:A:339:ILE:HG21	2.03	0.41
1:B:365:PRO:HB2	1:B:388:VAL:HG22	2.02	0.41
1:A:204:LEU:O	1:A:205:ARG:C	2.63	0.41
1:B:275:ALA:O	1:B:276:ARG:O	2.38	0.41
1:A:6:ARG:O	1:A:6:ARG:HG2	2.21	0.41
1:A:162:GLY:HA3	1:A:189:PHE:O	2.21	0.41
1:A:310:LYS:HZ3	1:A:355:GLN:HE21	1.68	0.41
1:A:236:ASP:O	1:A:237:PRO:C	2.63	0.41
1:A:412:GLN:O	1:A:413:ALA:C	2.61	0.41
1:A:448:TYR:HD1	1:A:448:TYR:HA	1.64	0.41
1:B:53:THR:O	1:B:54:ASN:C	2.64	0.41
1:B:184:TRP:CG	1:B:226:LYS:HG3	2.56	0.41
1:B:193:ASP:OD1	1:B:194:GLU:HG3	2.21	0.41
1:B:194:GLU:CB	1:B:195:PRO:HD3	2.47	0.41
1:B:355:GLN:HG3	1:B:356:SER:N	2.36	0.41
1:A:65:ARG:O	1:A:68:ASP:HB2	2.21	0.41
1:A:91:ASP:HB3	1:A:103:SER:HB2	2.02	0.41
1:A:272:ILE:HD13	1:A:272:ILE:HA	1.82	0.41
1:B:202:ALA:H	1:B:203:PRO:CD	2.32	0.41
1:B:46:ALA:O	1:B:50:SER:OG	2.30	0.40
1:B:163:THR:HB	1:B:183:PHE:CE2	2.56	0.40
1:B:168:LYS:HG3	1:B:193:ASP:OD2	2.21	0.40
1:A:313:ARG:CG	1:A:313:ARG:NH1	2.79	0.40
1:A:452:ARG:H	1:A:452:ARG:HG2	1.70	0.40
1:B:22:GLU:OE1	1:B:86:PRO:HA	2.21	0.40
1:B:63:PHE:H	1:B:65:ARG:NE	2.18	0.40
1:B:141:VAL:HG11	1:B:281:ASP:O	2.21	0.40
1:B:213:ASP:C	1:B:215:MET:H	2.30	0.40
1:A:248:LEU:HD22	1:A:282:ASN:HD21	1.86	0.40
1:A:274:THR:OG1	1:B:237:PRO:HG3	2.22	0.40
1:A:318:SER:O	1:A:363:CYS:HA	2.22	0.40
1:A:415:GLN:CG	1:A:418:ARG:HH21	2.27	0.40
1:B:85:TYR:CZ	1:B:108:THR:HG22	2.57	0.40
1:B:367:ILE:O	1:B:391:THR:HG22	2.21	0.40
1:A:90:PHE:O	1:A:92:ARG:HD3	2.22	0.40
1:A:426:TYR:O	1:A:430:HIS:N	2.49	0.40
1:B:84:ALA:O	1:B:86:PRO:HD3	2.22	0.40
1:B:374:LEU:HD22	1:B:448:TYR:CD2	2.57	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	457/466 (98%)	330 (72%)	82 (18%)	45 (10%)	0	0
1	B	456/466 (98%)	360 (79%)	60 (13%)	36 (8%)	1	0
All	All	913/932 (98%)	690 (76%)	142 (16%)	81 (9%)	0	0

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	38	TYR
1	A	129	PRO
1	A	136	PHE
1	A	144	SER
1	A	156	ASP
1	A	171	LEU
1	A	252	GLY
1	A	264	GLY
1	A	266	VAL
1	A	267	ALA
1	A	288	ARG
1	A	333	GLU
1	A	357	TRP
1	A	360	MET
1	A	372	ASN
1	A	394	GLY
1	A	422	PRO
1	A	445	ASP
1	A	449	PRO
1	A	451	TRP
1	A	456	GLY
1	A	457	VAL
1	A	459	ASP
1	B	4	SER

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Mol	Chain	Res	Type
1	B	54	ASN
1	B	125	ASP
1	B	192	ASN
1	B	202	ALA
1	B	214	ALA
1	B	269	ALA
1	B	276	ARG
1	B	277	ARG
1	B	289	ALA
1	B	323	GLY
1	B	327	PHE
1	B	330	MET
1	B	335	SER
1	B	423	VAL
1	B	445	ASP
1	B	458	GLU
1	A	5	SER
1	A	157	GLY
1	A	204	LEU
1	A	326	GLY
1	A	358	GLY
1	B	3	GLN
1	B	56	GLU
1	B	58	CYS
1	B	63	PHE
1	B	393	GLY
1	B	403	PRO
1	B	429	GLU
1	A	184	TRP
1	A	221	GLU
1	A	268	GLY
1	A	347	GLU
1	A	373	ALA
1	A	418	ARG
1	B	120	TYR
1	B	373	ALA
1	A	9	ASN
1	A	55	VAL
1	A	186	GLY
1	A	403	PRO
1	B	62	ASP
1	B	246	TYR

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Mol	Chain	Res	Type
1	B	288	ARG
1	A	263	ASP
1	A	421	VAL
1	B	99	ALA
1	B	154	GLU
1	B	326	GLY
1	A	172	ARG
1	A	297	PRO
1	B	186	GLY
1	A	67	VAL
1	B	66	GLY
1	B	86	PRO
1	A	388	VAL
1	B	247	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/354 (98%)	266 (76%)	82 (24%)	1	1
1	B	348/354 (98%)	255 (73%)	93 (27%)	0	1
All	All	696/708 (98%)	521 (75%)	175 (25%)	0	1

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	3	GLN
1	A	5	SER
1	A	6	ARG
1	A	10	LEU
1	A	12	LEU
1	A	17	LEU
1	A	29	ILE
1	A	41	THR

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Mol	Chain	Res	Type
1	A	48	GLU
1	A	51	THR
1	A	54	ASN
1	A	55	VAL
1	A	65	ARG
1	A	70	LEU
1	A	71	VAL
1	A	81	THR
1	A	82	LYS
1	A	92	ARG
1	A	93	ASN
1	A	94	ILE
1	A	106	THR
1	A	115	MET
1	A	128	VAL
1	A	135	LEU
1	A	141	VAL
1	A	144	SER
1	A	146	LEU
1	A	156	ASP
1	A	161	VAL
1	A	163	THR
1	A	169	LEU
1	A	178	GLU
1	A	191	LYS
1	A	192	ASN
1	A	194	GLU
1	A	196	GLN
1	A	204	LEU
1	A	206	ASP
1	A	210	LEU
1	A	216	ARG
1	A	219	GLN
1	A	220	ASP
1	A	224	GLU
1	A	226	LYS
1	A	237	PRO
1	A	239	GLU
1	A	254	ASN
1	A	256	SER
1	A	260	LEU
1	A	278	ARG

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Mol	Chain	Res	Type
1	A	286	TYR
1	A	294	VAL
1	A	301	ARG
1	A	311	MET
1	A	325	MET
1	A	327	PHE
1	A	329	LYS
1	A	330	MET
1	A	360	MET
1	A	363	CYS
1	A	374	LEU
1	A	376	MET
1	A	383	LEU
1	A	387	ASN
1	A	390	LEU
1	A	391	THR
1	A	397	PHE
1	A	409	SER
1	A	410	LEU
1	A	415	GLN
1	A	421	VAL
1	A	422	PRO
1	A	423	VAL
1	A	424	LEU
1	A	431	LYS
1	A	432	GLU
1	A	446	GLN
1	A	447	ILE
1	A	449	PRO
1	A	453	LYS
1	A	455	LEU
1	B	2	ASP
1	B	3	GLN
1	B	5	SER
1	B	8	VAL
1	B	10	LEU
1	B	14	GLU
1	B	15	GLU
1	B	16	ASP
1	B	25	LEU
1	B	28	TYR
1	B	29	ILE

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Mol	Chain	Res	Type
1	B	33	LYS
1	B	50	SER
1	B	53	THR
1	B	54	ASN
1	B	55	VAL
1	B	58	CYS
1	B	61	ASP
1	B	64	THR
1	B	65	ARG
1	B	71	VAL
1	B	80	LEU
1	B	86	PRO
1	B	95	THR
1	B	101	ILE
1	B	107	LEU
1	B	112	ASN
1	B	113	GLN
1	B	115	MET
1	B	120	TYR
1	B	126	PHE
1	B	130	GLU
1	B	133	ARG
1	B	135	LEU
1	B	141	VAL
1	B	146	LEU
1	B	159	LEU
1	B	163	THR
1	B	165	ILE
1	B	169	LEU
1	B	171	LEU
1	B	174	LYS
1	B	178	GLU
1	B	180	CYS
1	B	188	ASP
1	B	190	ILE
1	B	191	LYS
1	B	192	ASN
1	B	194	GLU
1	B	204	LEU
1	B	205	ARG
1	B	208	ILE
1	B	210	LEU

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Mol	Chain	Res	Type
1	B	227	LEU
1	B	229	SER
1	B	240	ILE
1	B	247	VAL
1	B	249	GLU
1	B	250	THR
1	B	253	GLU
1	B	256	SER
1	B	258	VAL
1	B	261	LEU
1	B	263	ASP
1	B	266	VAL
1	B	272	ILE
1	B	284	LEU
1	B	286	TYR
1	B	314	LEU
1	B	320	ILE
1	B	337	ARG
1	B	366	ILE
1	B	368	SER
1	B	377	PRO
1	B	381	GLU
1	B	382	ASN
1	B	388	VAL
1	B	391	THR
1	B	403	PRO
1	B	409	SER
1	B	421	VAL
1	B	424	LEU
1	B	428	ARG
1	B	430	HIS
1	B	431	LYS
1	B	435	ARG
1	B	437	PHE
1	B	443	ASP
1	B	446	GLN
1	B	452	ARG
1	B	455	LEU
1	B	457	VAL
1	B	459	ASP

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	9	ASN
1	A	44	HIS
1	A	192	ASN
1	A	196	GLN
1	A	198	ASN
1	A	219	GLN
1	A	282	ASN
1	A	287	HIS
1	A	298	GLN
1	A	308	HIS
1	A	355	GLN
1	A	385	ASN
1	A	387	ASN
1	A	415	GLN
1	B	3	GLN
1	B	181	HIS
1	B	192	ASN
1	B	196	GLN
1	B	287	HIS
1	B	315	GLN
1	B	385	ASN
1	B	399	HIS
1	B	415	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
2	RUB	A	600	3	17,17,17	3.00	9 (52%)	17,25,25	1.53	4 (23%)
2	RUB	B	700	3	17,17,17	1.57	3 (17%)	17,25,25	0.89	1 (5%)
4	FMT	B	701	3,1	2,2,2	1.68	1 (50%)	1,1,1	1.36	0
4	FMT	A	601	3,1	2,2,2	1.35	0	1,1,1	0.82	0

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
2	RUB	A	600	3	-	11/20/20/20	-
2	RUB	B	700	3	-	16/20/20/20	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	RUB	C5-C4	7.47	1.62	1.51
2	A	600	RUB	C4-C3	4.47	1.58	1.53
2	A	600	RUB	C1-C2	4.21	1.57	1.51
2	A	600	RUB	P2-O4P	3.47	1.61	1.50
2	A	600	RUB	P1-O1P	3.31	1.60	1.50
2	B	700	RUB	P1-O1P	3.31	1.60	1.50
2	B	700	RUB	P2-O4P	3.22	1.60	1.50
2	A	600	RUB	P2-O5	2.85	1.69	1.60
4	B	701	FMT	O2-C	-2.29	1.17	1.28
2	A	600	RUB	P2-O5P	2.29	1.63	1.54
2	A	600	RUB	C3-C2	2.22	1.61	1.51
2	A	600	RUB	O2-C2	2.18	1.25	1.21
2	B	700	RUB	C1-C2	2.02	1.54	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	RUB	O6P-P2-O5	2.56	113.34	106.67
2	A	600	RUB	O5-P2-O4P	2.36	112.82	106.44
2	A	600	RUB	O3P-P1-O1	2.35	112.79	106.67
2	A	600	RUB	O5-C5-C4	2.09	114.93	109.36
2	B	700	RUB	O3P-P1-O1	2.02	111.93	106.67

There are no chirality outliers.

All (27) torsion outliers are listed below:

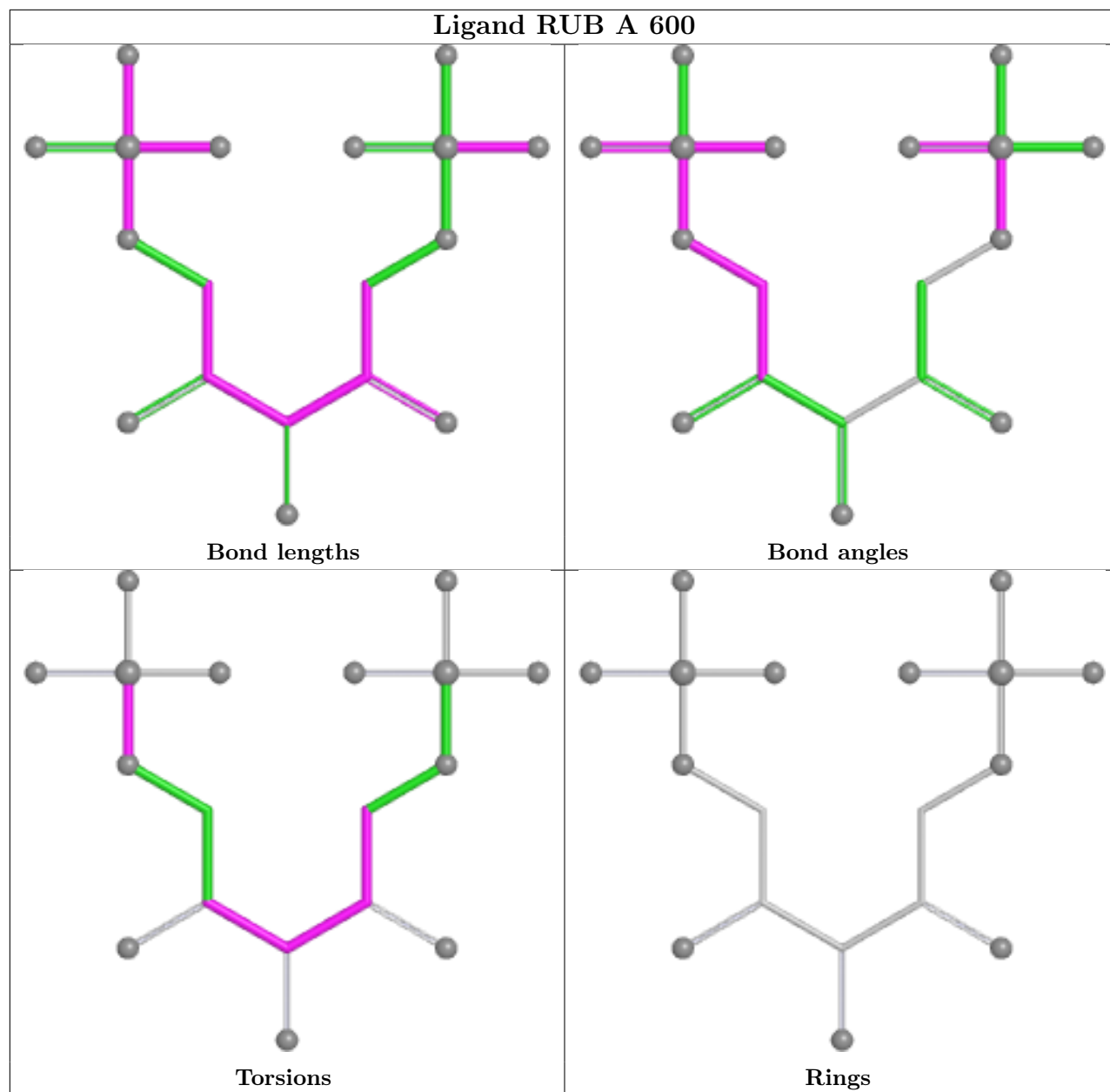
Mol	Chain	Res	Type	Atoms
2	A	600	RUB	O1-C1-C2-O2
2	A	600	RUB	O2-C2-C3-O3
2	A	600	RUB	C2-C3-C4-C5
2	A	600	RUB	C2-C3-C4-O4
2	A	600	RUB	O3-C3-C4-C5
2	A	600	RUB	O3-C3-C4-O4
2	A	600	RUB	C5-O5-P2-O4P
2	A	600	RUB	C5-O5-P2-O5P
2	A	600	RUB	C5-O5-P2-O6P
2	B	700	RUB	O1-C1-C2-C3
2	B	700	RUB	O1-C1-C2-O2
2	B	700	RUB	C2-C3-C4-C5
2	B	700	RUB	C2-C3-C4-O4
2	B	700	RUB	O3-C3-C4-C5
2	B	700	RUB	O3-C3-C4-O4
2	B	700	RUB	C3-C4-C5-O5
2	B	700	RUB	O4-C4-C5-O5
2	B	700	RUB	C1-O1-P1-O1P
2	B	700	RUB	C1-O1-P1-O2P
2	B	700	RUB	C1-O1-P1-O3P
2	B	700	RUB	C5-O5-P2-O4P
2	B	700	RUB	C5-O5-P2-O5P
2	B	700	RUB	C5-O5-P2-O6P
2	B	700	RUB	C1-C2-C3-O3
2	B	700	RUB	O2-C2-C3-O3
2	A	600	RUB	O1-C1-C2-C3
2	A	600	RUB	C1-C2-C3-O3

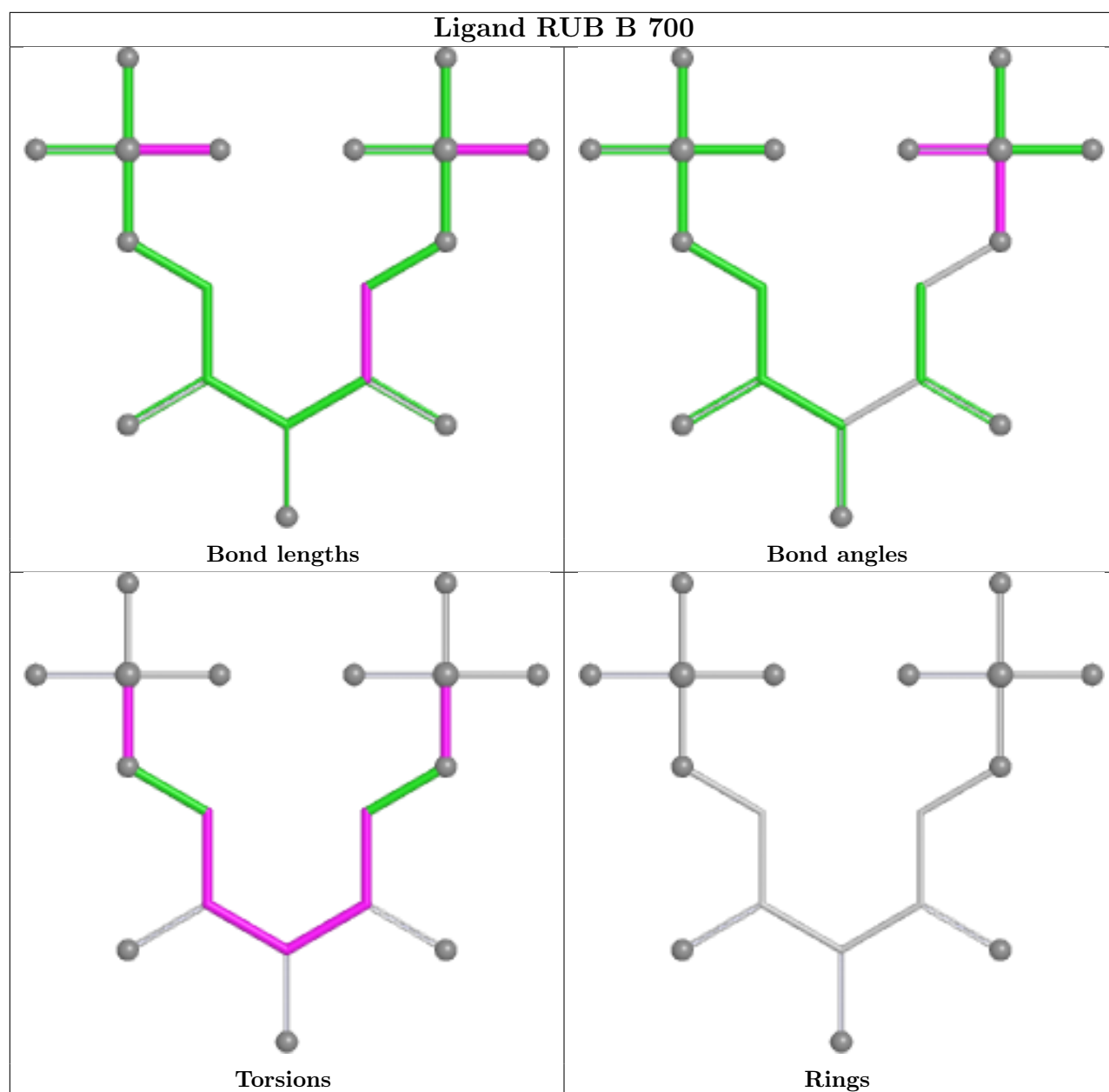
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	RUB	3	0
2	B	700	RUB	5	0
4	B	701	FMT	1	0
4	A	601	FMT	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.