



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:26 PM UTC

PDB ID : 1RUS / pdb_00001rus
Title : CRYSTAL STRUCTURE OF THE BINARY COMPLEX OF RIBULOSE-1,
5-BISPHOSPHATE CARBOXYLASE AND ITS PRODUCT, 3-PHOSPHO-
D-GLYCERATE
Authors : Lundqvist, T.; Schneider, G.
Deposited on : 1991-10-10
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

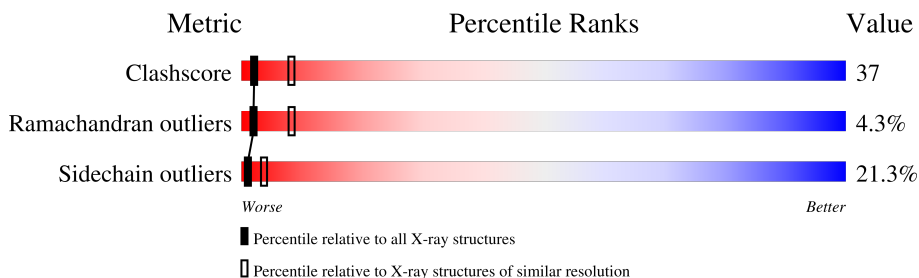
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)

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	490	
1	B	490	

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
2	3PG	A	500	-	X	X	-
2	3PG	B	500	-	X	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6677 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.

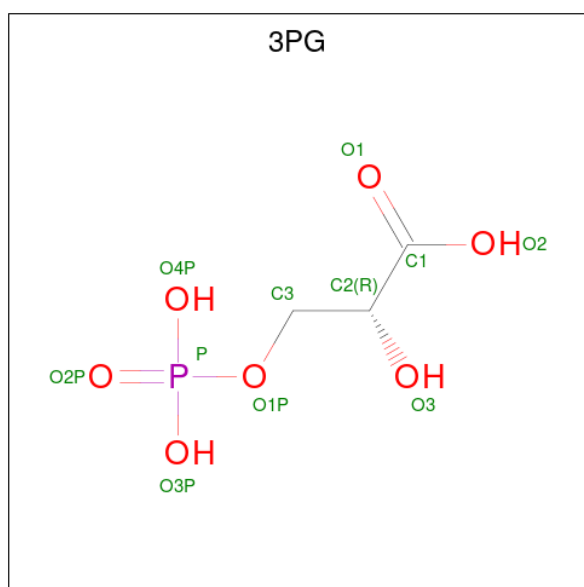
- Molecule 1 is a protein called RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	7	0	0
			3337	2115	589	617	16			
1	B	435	Total	C	N	O	S	10	0	0
			3318	2105	584	613	16			

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 3-PHOSPHOGLYCERIC ACID (CCD ID: 3PG) (formula: $C_3H_7O_7P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			11	3	7	1		

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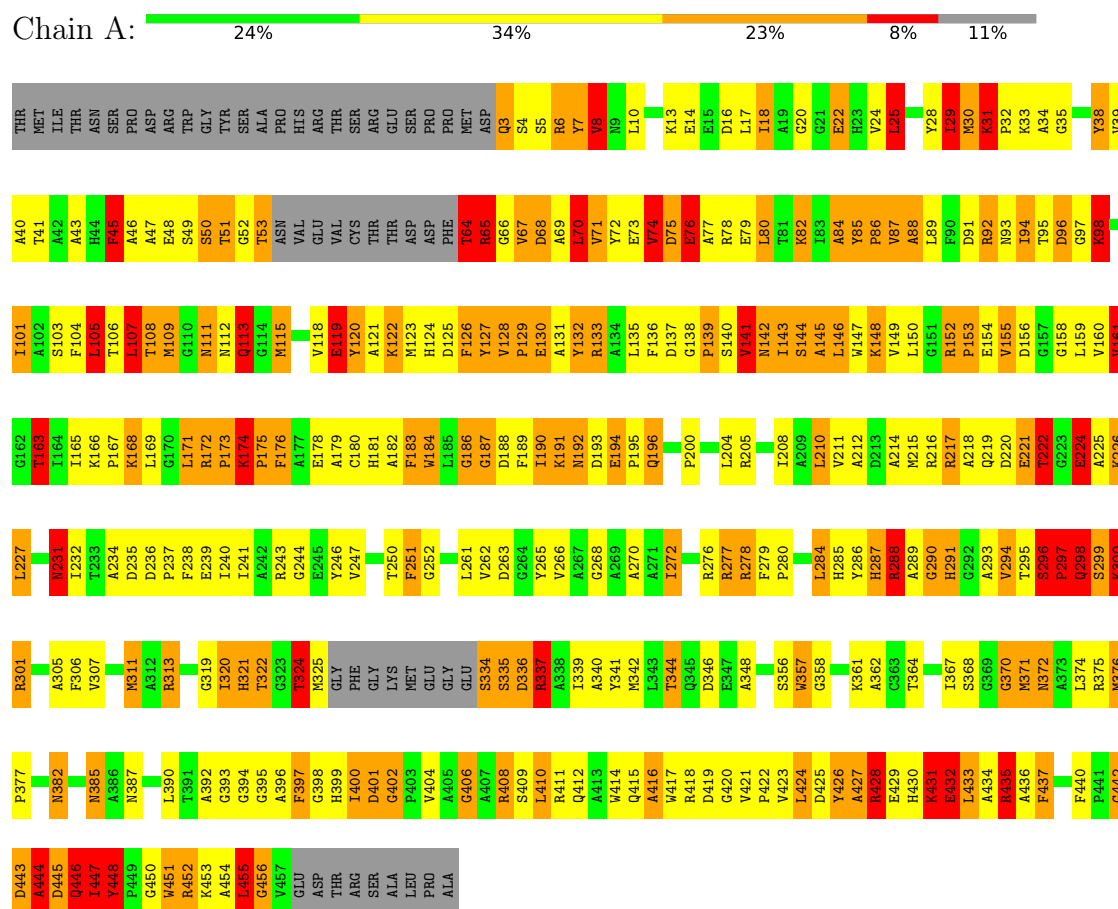
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			11	3	7	1		

3 Residue-property plots

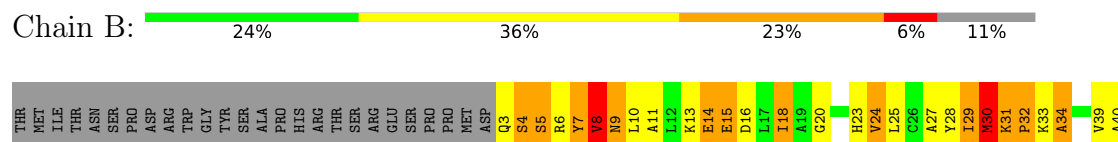
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

- Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)



- Molecule 1: RUBISCO (RIBULOSE-1,5-BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE)





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)	10.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.203 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6677	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3PG

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	1.33	8/3417 (0.2%)	2.88	377/4629 (8.1%)
1	B	1.44	13/3398 (0.4%)	2.96	405/4604 (8.8%)
All	All	1.39	21/6815 (0.3%)	2.92	782/9233 (8.5%)

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 (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	110	GLY	C-N	-7.48	1.24	1.33
1	B	288	ARG	CD-NE	7.27	1.56	1.46
1	B	288	ARG	NE-CZ	6.75	1.40	1.33
1	A	322	THR	N-CA	6.64	1.55	1.46
1	A	163	THR	CA-CB	6.57	1.63	1.53
1	A	265	TYR	C-N	-6.54	1.27	1.34
1	A	297	PRO	C-N	-6.22	1.25	1.33
1	A	287	HIS	C-N	-6.14	1.25	1.33
1	B	189	PHE	C-N	-5.97	1.25	1.33
1	B	195	PRO	N-CD	-5.83	1.39	1.47
1	A	210	LEU	C-N	5.79	1.41	1.33
1	B	111	ASN	C-N	-5.77	1.26	1.33
1	B	194	GLU	CA-C	5.70	1.60	1.52
1	B	382	ASN	N-CA	5.40	1.52	1.46
1	B	357	TRP	NE1-CE2	-5.28	1.31	1.37
1	B	115	MET	N-CA	-5.21	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	SER	CA-C	5.21	1.59	1.52
1	A	357	TRP	NE1-CE2	-5.19	1.31	1.37
1	B	193	ASP	N-CA	5.14	1.52	1.45
1	B	378	GLY	N-CA	5.09	1.52	1.45
1	B	24	VAL	C-N	-5.01	1.26	1.33

All (782) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	ASP	CA-CB-CG	24.39	136.99	112.60
1	B	429	GLU	CA-CB-CG	24.17	162.44	114.10
1	B	418	ARG	CD-NE-CZ	22.51	155.92	124.40
1	A	188	ASP	CA-CB-CG	18.40	131.00	112.60
1	A	321	HIS	CB-CA-C	17.17	130.92	109.80
1	B	45	PHE	CA-CB-CG	16.94	130.74	113.80
1	B	23	HIS	CA-CB-CG	16.34	130.14	113.80
1	A	67	VAL	N-CA-C	-15.76	98.74	113.71
1	A	428	ARG	CD-NE-CZ	15.66	146.32	124.40
1	B	445	ASP	CA-CB-CG	15.61	128.21	112.60
1	B	91	ASP	CA-CB-CG	15.26	127.86	112.60
1	B	93	ASN	CA-CB-CG	15.22	127.82	112.60
1	A	126	PHE	CA-CB-CG	15.02	128.82	113.80
1	B	126	PHE	CA-CB-CG	14.71	128.51	113.80
1	A	216	ARG	NE-CZ-NH1	14.62	136.12	121.50
1	A	152	ARG	O-C-N	14.58	131.64	121.14
1	A	430	HIS	CA-CB-CG	-14.56	99.24	113.80
1	A	173	PRO	CA-C-N	14.23	135.63	119.83
1	A	173	PRO	C-N-CA	14.23	135.63	119.83
1	B	399	HIS	CA-CB-CG	13.94	127.74	113.80
1	B	418	ARG	NE-CZ-NH1	13.80	135.30	121.50
1	A	418	ARG	CD-NE-CZ	13.60	143.44	124.40
1	A	130	GLU	CB-CG-CD	13.56	135.65	112.60
1	A	440	PHE	CA-CB-CG	13.56	127.36	113.80
1	A	224	GLU	CB-CG-CD	13.29	135.20	112.60
1	B	118	VAL	CA-C-N	12.83	138.07	120.63
1	B	118	VAL	C-N-CA	12.83	138.07	120.63
1	A	112	ASN	CA-C-O	12.82	133.77	119.15
1	B	152	ARG	NE-CZ-NH2	12.78	130.70	119.20
1	A	67	VAL	CB-CA-C	12.65	122.52	110.63
1	B	67	VAL	N-CA-CB	12.49	131.84	111.23
1	A	97	GLY	CA-C-N	11.92	137.64	120.95
1	A	97	GLY	C-N-CA	11.92	137.64	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	ARG	CD-NE-CZ	11.88	141.03	124.40
1	A	8	VAL	CA-C-O	-11.86	108.29	120.27
1	A	52	GLY	CA-C-N	11.47	142.35	121.70
1	A	52	GLY	C-N-CA	11.47	142.35	121.70
1	A	137	ASP	CA-C-N	11.37	139.72	121.87
1	A	137	ASP	C-N-CA	11.37	139.72	121.87
1	B	24	VAL	CA-C-O	-11.22	108.06	120.85
1	A	437	PHE	CA-C-N	11.19	140.72	121.14
1	A	437	PHE	C-N-CA	11.19	140.72	121.14
1	A	419	ASP	CA-CB-CG	11.18	123.78	112.60
1	A	76	GLU	CB-CG-CD	11.10	131.48	112.60
1	A	212	ALA	CA-C-N	11.10	135.54	120.44
1	A	212	ALA	C-N-CA	11.10	135.54	120.44
1	A	144	SER	CA-CB-OG	11.09	133.28	111.10
1	A	432	GLU	CA-CB-CG	11.09	136.28	114.10
1	B	139	PRO	CB-CA-C	10.79	125.05	111.12
1	B	438	GLU	CA-C-O	-10.77	109.00	120.42
1	A	111	ASN	CA-CB-CG	10.69	123.29	112.60
1	A	171	LEU	O-C-N	-10.68	110.67	123.27
1	B	73	GLU	CA-C-O	10.58	132.89	119.98
1	B	110	GLY	CA-C-N	10.53	134.80	120.38
1	B	110	GLY	C-N-CA	10.53	134.80	120.38
1	A	454	ALA	CA-C-N	10.52	141.62	121.54
1	A	454	ALA	C-N-CA	10.52	141.62	121.54
1	B	111	ASN	CA-C-N	10.49	134.33	120.28
1	B	111	ASN	C-N-CA	10.49	134.33	120.28
1	B	146	LEU	N-CA-C	-10.47	98.63	111.40
1	A	132	TYR	CA-C-O	-10.47	109.81	120.80
1	B	29	ILE	CB-CA-C	10.33	125.55	111.19
1	B	39	VAL	CA-C-N	10.33	133.87	120.44
1	B	39	VAL	C-N-CA	10.33	133.87	120.44
1	B	108	THR	CA-C-N	10.32	138.07	122.17
1	B	108	THR	C-N-CA	10.32	138.07	122.17
1	B	428	ARG	NE-CZ-NH2	10.29	128.46	119.20
1	B	447	ILE	CB-CA-C	10.28	123.37	111.55
1	B	221	GLU	CB-CG-CD	10.27	130.06	112.60
1	A	92	ARG	CA-C-O	-10.25	109.17	121.06
1	B	114	GLY	CA-C-O	10.25	130.32	120.89
1	B	18	ILE	CA-C-N	10.21	134.32	120.54
1	B	18	ILE	C-N-CA	10.21	134.32	120.54
1	B	205	ARG	NE-CZ-NH2	10.19	128.37	119.20
1	A	186	GLY	CA-C-N	10.17	136.71	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	GLY	C-N-CA	10.17	136.71	121.05
1	B	207	THR	CA-CB-OG1	-10.12	94.42	109.60
1	A	455	LEU	CA-C-N	10.07	141.14	121.41
1	A	455	LEU	C-N-CA	10.07	141.14	121.41
1	A	73	GLU	CA-C-O	10.06	132.02	120.75
1	A	112	ASN	N-CA-C	-10.05	101.02	113.38
1	A	76	GLU	CA-C-N	10.02	133.88	120.65
1	A	76	GLU	C-N-CA	10.02	133.88	120.65
1	A	409	SER	CA-C-N	10.02	134.06	120.44
1	A	409	SER	C-N-CA	10.02	134.06	120.44
1	A	221	GLU	CA-C-O	9.94	131.01	119.18
1	A	86	PRO	CA-C-O	-9.92	110.32	121.43
1	A	175	PRO	CA-C-N	9.85	133.65	120.65
1	A	175	PRO	C-N-CA	9.85	133.65	120.65
1	B	408	ARG	CA-C-N	9.85	135.28	120.31
1	B	408	ARG	C-N-CA	9.85	135.28	120.31
1	B	95	THR	CA-C-N	9.81	137.10	120.71
1	B	95	THR	C-N-CA	9.81	137.10	120.71
1	B	212	ALA	CA-C-N	9.80	134.21	120.29
1	B	212	ALA	C-N-CA	9.80	134.21	120.29
1	B	137	ASP	CA-CB-CG	9.77	122.37	112.60
1	A	149	VAL	N-CA-C	-9.76	101.86	110.74
1	B	95	THR	O-C-N	-9.70	111.90	122.38
1	A	138	GLY	O-C-N	9.69	131.46	121.77
1	A	428	ARG	NE-CZ-NH1	9.67	131.17	121.50
1	B	148	LYS	CA-C-O	-9.64	109.20	120.10
1	A	418	ARG	NE-CZ-NH2	-9.63	110.54	119.20
1	B	205	ARG	CA-C-N	9.60	133.50	120.44
1	B	205	ARG	C-N-CA	9.60	133.50	120.44
1	A	217	ARG	CA-C-O	-9.59	110.75	120.82
1	B	48	GLU	CA-C-O	-9.59	106.80	120.51
1	A	216	ARG	NE-CZ-NH2	-9.58	110.58	119.20
1	B	216	ARG	CD-NE-CZ	9.55	137.77	124.40
1	B	409	SER	CA-C-N	9.53	136.62	120.71
1	B	409	SER	C-N-CA	9.53	136.62	120.71
1	B	105	LEU	CA-C-O	-9.53	110.32	120.42
1	A	84	ALA	CA-C-N	9.50	138.98	122.06
1	A	84	ALA	C-N-CA	9.50	138.98	122.06
1	A	417	TRP	CA-C-N	9.50	133.19	120.65
1	A	417	TRP	C-N-CA	9.50	133.19	120.65
1	B	15	GLU	CA-C-N	9.47	132.75	120.44
1	B	15	GLU	C-N-CA	9.47	132.75	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ALA	CA-C-O	9.41	130.76	120.32
1	B	41	THR	CA-C-N	9.34	136.56	120.58
1	B	41	THR	C-N-CA	9.34	136.56	120.58
1	B	114	GLY	O-C-N	-9.34	114.96	122.99
1	A	226	LYS	CB-CG-CD	9.24	132.54	111.30
1	A	143	ILE	CA-C-N	9.23	133.03	120.38
1	A	143	ILE	C-N-CA	9.23	133.03	120.38
1	B	25	LEU	CA-C-O	-9.17	110.99	120.71
1	B	40	ALA	CA-C-N	9.16	133.47	120.28
1	B	40	ALA	C-N-CA	9.16	133.47	120.28
1	A	6	ARG	NE-CZ-NH2	-9.13	110.99	119.20
1	A	24	VAL	O-C-N	-9.11	112.27	122.83
1	A	430	HIS	CA-C-O	9.10	132.03	120.57
1	A	89	LEU	CA-C-N	9.03	134.39	121.02
1	A	89	LEU	C-N-CA	9.03	134.39	121.02
1	B	219	GLN	OE1-CD-NE2	-9.03	113.57	122.60
1	B	118	VAL	CA-C-O	9.02	128.25	120.22
1	B	408	ARG	NH1-CZ-NH2	8.95	130.93	119.30
1	A	138	GLY	CA-C-O	-8.88	108.82	121.52
1	A	452	ARG	N-CA-C	-8.88	101.56	111.14
1	B	68	ASP	CA-C-O	-8.87	110.93	121.05
1	A	98	LYS	CA-C-O	8.83	130.97	120.81
1	B	104	PHE	CA-CB-CG	-8.80	105.00	113.80
1	A	163	THR	N-CA-CB	8.79	125.12	111.22
1	B	97	GLY	CA-C-N	8.75	135.92	121.39
1	B	97	GLY	C-N-CA	8.75	135.92	121.39
1	A	211	VAL	N-CA-CB	8.75	122.44	110.54
1	B	16	ASP	CA-CB-CG	8.74	121.34	112.60
1	A	147	TRP	CA-C-O	-8.70	111.86	121.00
1	A	158	GLY	CA-C-N	8.67	133.09	120.95
1	A	158	GLY	C-N-CA	8.67	133.09	120.95
1	A	76	GLU	CG-CD-OE1	8.65	138.30	118.40
1	B	100	MET	CA-C-N	8.65	132.70	120.42
1	B	100	MET	C-N-CA	8.65	132.70	120.42
1	B	224	GLU	CA-C-O	-8.64	111.33	121.44
1	B	110	GLY	CA-C-O	8.62	135.56	120.57
1	B	408	ARG	NE-CZ-NH2	-8.60	111.46	119.20
1	B	443	ASP	CA-CB-CG	8.56	121.16	112.60
1	B	395	GLY	N-CA-C	-8.55	92.92	113.18
1	A	160	VAL	N-CA-CB	8.55	122.67	111.90
1	A	189	PHE	O-C-N	-8.53	113.15	123.30
1	A	180	CYS	CA-C-O	8.50	129.74	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	222	THR	N-CA-CB	-8.50	98.08	110.40
1	A	152	ARG	NE-CZ-NH2	8.47	126.82	119.20
1	B	203	PRO	CA-C-N	8.47	131.62	120.28
1	B	203	PRO	C-N-CA	8.47	131.62	120.28
1	B	40	ALA	CA-C-O	8.46	129.71	120.82
1	A	444	ALA	CA-C-O	-8.45	108.43	120.51
1	A	418	ARG	NE-CZ-NH1	8.42	129.92	121.50
1	B	166	LYS	CB-CA-C	8.42	121.59	108.63
1	A	428	ARG	CG-CD-NE	8.38	130.44	112.00
1	A	287	HIS	O-C-N	-8.36	113.25	123.04
1	A	226	LYS	CA-CB-CG	8.33	130.76	114.10
1	B	96	ASP	CA-CB-CG	8.29	120.89	112.60
1	A	183	PHE	N-CA-CB	8.28	122.02	110.01
1	B	412	GLN	OE1-CD-NE2	-8.26	114.34	122.60
1	B	418	ARG	NH1-CZ-NH2	-8.25	108.57	119.30
1	A	51	THR	CA-C-O	-8.24	109.86	119.59
1	A	147	TRP	N-CA-CB	8.23	121.93	109.91
1	B	155	VAL	N-CA-CB	8.23	122.14	112.35
1	B	391	THR	CA-C-N	8.22	133.85	120.94
1	B	391	THR	C-N-CA	8.22	133.85	120.94
1	B	129	PRO	CA-C-N	8.21	131.80	120.63
1	B	129	PRO	C-N-CA	8.21	131.80	120.63
1	A	48	GLU	CA-C-N	8.20	131.93	120.29
1	A	48	GLU	C-N-CA	8.20	131.93	120.29
1	A	422	PRO	CB-CA-C	8.20	122.11	111.21
1	B	94	ILE	CA-CB-CG1	8.18	124.31	110.40
1	B	205	ARG	CA-CB-CG	8.18	130.46	114.10
1	A	53	THR	CA-C-O	-8.17	106.92	120.80
1	B	95	THR	CA-C-O	8.13	129.65	120.71
1	B	219	GLN	N-CA-CB	8.12	122.86	110.28
1	A	18	ILE	CA-C-N	8.08	135.28	121.14
1	A	18	ILE	C-N-CA	8.08	135.28	121.14
1	A	219	GLN	CB-CG-CD	8.06	126.30	112.60
1	B	219	GLN	CG-CD-NE2	8.04	128.46	116.40
1	A	429	GLU	CB-CG-CD	8.03	126.26	112.60
1	B	44	HIS	N-CA-C	-8.02	102.13	111.03
1	B	130	GLU	CB-CG-CD	8.01	126.22	112.60
1	B	150	LEU	CA-C-N	8.01	137.10	121.41
1	B	150	LEU	C-N-CA	8.01	137.10	121.41
1	B	80	LEU	N-CA-C	7.99	121.45	108.34
1	A	183	PHE	CA-C-O	-7.98	112.44	120.82
1	A	73	GLU	CA-CB-CG	7.98	130.06	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	445	ASP	CA-C-N	7.96	130.95	120.28
1	B	445	ASP	C-N-CA	7.96	130.95	120.28
1	A	161	VAL	CB-CA-C	7.94	120.57	110.96
1	A	426	TYR	CA-C-N	7.94	130.92	120.28
1	A	426	TYR	C-N-CA	7.94	130.92	120.28
1	B	82	LYS	CG-CD-CE	7.94	129.56	111.30
1	B	73	GLU	O-C-N	-7.94	113.42	123.26
1	A	35	GLY	N-CA-C	7.93	124.13	114.69
1	A	321	HIS	CA-CB-CG	7.93	121.73	113.80
1	B	431	LYS	N-CA-C	7.91	119.99	111.36
1	A	156	ASP	CA-CB-CG	7.88	120.48	112.60
1	B	133	ARG	NE-CZ-NH2	7.88	126.29	119.20
1	A	158	GLY	N-CA-C	7.82	126.29	112.53
1	B	76	GLU	CB-CG-CD	7.82	125.89	112.60
1	B	110	GLY	N-CA-C	7.81	131.70	113.18
1	B	220	ASP	CA-C-N	7.81	133.75	120.71
1	B	220	ASP	C-N-CA	7.81	133.75	120.71
1	B	439	SER	CA-C-O	-7.79	111.02	119.97
1	A	422	PRO	N-CA-C	-7.78	98.98	111.19
1	A	38	TYR	N-CA-CB	7.77	121.49	110.07
1	A	451	TRP	N-CA-CB	-7.76	98.28	110.22
1	B	288	ARG	CD-NE-CZ	7.74	135.24	124.40
1	A	410	LEU	N-CA-C	-7.72	102.80	111.14
1	B	403	PRO	N-CA-C	7.72	123.68	113.57
1	A	172	ARG	NE-CZ-NH1	7.71	129.21	121.50
1	B	436	ALA	N-CA-C	-7.69	102.58	110.97
1	A	125	ASP	CA-C-O	-7.66	113.08	121.28
1	B	430	HIS	CA-CB-CG	-7.66	106.14	113.80
1	A	139	PRO	CB-CA-C	7.64	121.01	111.23
1	A	415	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	A	179	ALA	CA-C-N	7.62	130.35	120.44
1	A	179	ALA	C-N-CA	7.62	130.35	120.44
1	B	89	LEU	CA-C-O	7.61	128.74	119.38
1	B	88	ALA	CA-C-N	7.61	133.42	120.72
1	B	88	ALA	C-N-CA	7.61	133.42	120.72
1	B	164	ILE	N-CA-CB	7.60	119.00	110.72
1	A	141	VAL	CA-C-O	-7.58	113.87	121.45
1	B	324	THR	O-C-N	7.57	129.21	121.79
1	A	127	TYR	CA-C-N	7.57	135.57	123.46
1	A	127	TYR	C-N-CA	7.57	135.57	123.46
1	B	440	PHE	O-C-N	7.57	128.18	121.37
1	A	219	GLN	CA-C-N	7.56	131.17	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	GLN	C-N-CA	7.56	131.17	120.28
1	A	174	LYS	O-C-N	7.54	125.47	120.27
1	A	64	THR	CA-CB-CG2	7.51	123.27	110.50
1	A	220	ASP	O-C-N	-7.51	113.44	122.22
1	A	425	ASP	CB-CA-C	7.50	124.43	110.70
1	B	7	TYR	N-CA-C	7.46	121.96	113.01
1	B	135	LEU	CA-C-O	-7.46	110.64	119.15
1	A	68	ASP	CA-CB-CG	7.41	120.01	112.60
1	A	77	ALA	N-CA-C	7.38	119.02	110.97
1	B	421	VAL	O-C-N	7.38	129.51	121.10
1	B	214	ALA	CA-C-N	7.37	132.82	120.88
1	B	214	ALA	C-N-CA	7.37	132.82	120.88
1	B	130	GLU	CA-C-O	7.36	128.48	120.90
1	A	28	TYR	CA-CB-CG	7.36	127.14	113.90
1	A	404	VAL	N-CA-C	-7.36	102.98	111.00
1	A	108	THR	N-CA-C	7.33	118.91	111.07
1	B	113	GLN	O-C-N	7.30	129.89	122.08
1	A	432	GLU	CB-CG-CD	7.29	125.00	112.60
1	A	217	ARG	NH1-CZ-NH2	7.29	128.78	119.30
1	A	92	ARG	CA-C-N	7.29	131.06	120.71
1	A	92	ARG	C-N-CA	7.29	131.06	120.71
1	B	28	TYR	CA-CB-CG	7.27	126.99	113.90
1	B	189	PHE	CA-CB-CG	7.26	121.06	113.80
1	B	11	ALA	O-C-N	7.25	130.76	122.20
1	B	43	ALA	N-CA-C	-7.23	102.80	111.69
1	B	112	ASN	CA-CB-CG	7.23	119.83	112.60
1	A	437	PHE	CA-CB-CG	-7.21	106.59	113.80
1	B	405	ALA	CA-C-N	7.21	127.80	119.94
1	B	405	ALA	C-N-CA	7.21	127.80	119.94
1	A	142	ASN	CA-C-N	7.20	132.10	120.30
1	A	142	ASN	C-N-CA	7.20	132.10	120.30
1	A	112	ASN	CB-CA-C	7.19	122.17	109.65
1	B	152	ARG	NE-CZ-NH1	-7.19	114.31	121.50
1	A	67	VAL	CA-C-O	7.17	127.23	119.35
1	A	174	LYS	CA-CB-CG	7.16	128.41	114.10
1	A	7	TYR	N-CA-C	7.14	120.86	112.72
1	A	95	THR	N-CA-C	7.13	120.09	111.40
1	B	446	GLN	CA-C-O	-7.11	113.01	120.55
1	A	112	ASN	O-C-N	-7.10	113.12	122.42
1	B	137	ASP	CA-C-O	-7.08	113.40	120.70
1	A	166	LYS	O-C-N	-7.08	113.92	121.42
1	B	393	GLY	O-C-N	7.07	131.90	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	324	THR	CB-CA-C	-7.07	101.49	112.31
1	B	155	VAL	O-C-N	7.06	129.56	122.71
1	B	48	GLU	N-CA-CB	7.04	122.40	110.49
1	B	31	LYS	CA-CB-CG	7.04	128.18	114.10
1	A	401	ASP	CA-CB-CG	7.04	119.64	112.60
1	A	211	VAL	N-CA-C	-7.03	103.45	110.62
1	A	178	GLU	CA-C-O	-7.02	113.45	120.82
1	A	85	TYR	CA-C-O	7.02	126.05	119.59
1	B	115	MET	CA-C-O	7.01	128.84	121.06
1	A	147	TRP	N-CA-C	-7.01	103.33	110.97
1	B	44	HIS	CA-CB-CG	7.01	120.81	113.80
1	B	403	PRO	CA-C-N	6.99	130.35	120.42
1	B	403	PRO	C-N-CA	6.99	130.35	120.42
1	A	126	PHE	N-CA-C	6.99	119.87	108.55
1	A	91	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	217	ARG	CA-C-N	6.96	129.60	120.28
1	B	217	ARG	C-N-CA	6.96	129.60	120.28
1	B	429	GLU	CA-C-O	6.95	127.99	119.79
1	B	89	LEU	CA-C-N	6.91	131.63	122.30
1	B	89	LEU	C-N-CA	6.91	131.63	122.30
1	B	413	ALA	CA-C-N	6.90	130.01	120.63
1	B	413	ALA	C-N-CA	6.90	130.01	120.63
1	B	132	TYR	N-CA-C	6.89	120.91	112.23
1	A	129	PRO	CB-CA-C	6.89	120.11	110.60
1	B	115	MET	CB-CA-C	6.89	121.88	110.03
1	A	428	ARG	NH1-CZ-NH2	-6.88	110.35	119.30
1	B	226	LYS	CA-CB-CG	6.86	127.82	114.10
1	A	8	VAL	O-C-N	6.84	130.30	123.18
1	A	189	PHE	N-CA-C	6.84	120.05	108.90
1	B	44	HIS	CB-CA-C	6.83	121.54	110.95
1	A	456	GLY	CA-C-O	6.83	132.45	120.57
1	B	45	PHE	CA-C-N	6.83	129.31	120.44
1	B	45	PHE	C-N-CA	6.83	129.31	120.44
1	A	148	LYS	CA-C-N	6.82	129.20	120.88
1	A	148	LYS	C-N-CA	6.82	129.20	120.88
1	A	146	LEU	CA-C-N	6.81	129.64	120.65
1	A	146	LEU	C-N-CA	6.81	129.64	120.65
1	B	166	LYS	CA-CB-CG	-6.81	100.48	114.10
1	A	105	LEU	CA-C-O	-6.81	113.20	120.42
1	B	206	ASP	CA-C-O	-6.80	113.69	120.70
1	A	231	ASN	O-C-N	6.80	131.04	123.01
1	B	447	ILE	CA-CB-CG2	6.79	122.03	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ARG	NH1-CZ-NH2	-6.78	110.48	119.30
1	A	31	LYS	O-C-N	6.77	127.88	121.38
1	B	136	PHE	CA-C-N	6.76	129.64	120.44
1	B	136	PHE	C-N-CA	6.76	129.64	120.44
1	A	91	ASP	CB-CA-C	6.76	123.64	109.65
1	B	207	THR	O-C-N	-6.75	114.80	122.09
1	A	137	ASP	N-CA-CB	-6.74	100.07	109.91
1	B	215	MET	N-CA-CB	6.74	119.97	110.07
1	B	31	LYS	O-C-N	6.73	129.06	121.32
1	A	431	LYS	CA-C-N	6.72	129.96	120.28
1	A	431	LYS	C-N-CA	6.72	129.96	120.28
1	A	96	ASP	O-C-N	6.71	130.04	122.32
1	B	81	THR	CA-C-O	-6.71	113.11	120.36
1	B	164	ILE	CA-C-N	-6.71	111.85	120.98
1	B	164	ILE	C-N-CA	-6.71	111.85	120.98
1	A	372	ASN	CA-CB-CG	6.71	119.31	112.60
1	B	418	ARG	CA-C-N	6.71	131.92	120.72
1	B	418	ARG	C-N-CA	6.71	131.92	120.72
1	B	165	ILE	CA-C-O	-6.70	113.40	121.04
1	B	70	LEU	N-CA-C	6.70	119.44	108.52
1	A	414	TRP	N-CA-CB	6.69	119.68	109.98
1	B	29	ILE	CA-C-N	6.69	133.33	122.29
1	B	29	ILE	C-N-CA	6.69	133.33	122.29
1	B	75	ASP	N-CA-C	-6.68	96.56	110.80
1	B	434	ALA	CA-C-N	6.67	132.81	121.14
1	B	434	ALA	C-N-CA	6.67	132.81	121.14
1	A	155	VAL	CA-C-O	-6.66	113.45	120.57
1	A	29	ILE	CA-C-O	6.65	129.09	120.78
1	B	435	ARG	CA-C-N	6.65	129.43	120.65
1	B	435	ARG	C-N-CA	6.65	129.43	120.65
1	B	86	PRO	O-C-N	-6.64	114.78	123.01
1	A	433	LEU	O-C-N	6.63	129.71	122.15
1	B	435	ARG	NE-CZ-NH2	6.63	125.17	119.20
1	A	189	PHE	N-CA-CB	-6.63	99.54	110.68
1	B	394	GLY	CA-C-O	6.63	132.11	120.57
1	B	422	PRO	N-CA-C	6.63	124.06	113.12
1	B	99	ALA	CA-C-O	6.61	129.53	121.87
1	B	27	ALA	O-C-N	-6.60	115.58	123.31
1	A	133	ARG	CA-C-N	6.59	131.14	120.60
1	A	133	ARG	C-N-CA	6.59	131.14	120.60
1	A	88	ALA	CA-C-N	6.57	129.09	120.28
1	A	88	ALA	C-N-CA	6.57	129.09	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ALA	N-CA-C	-6.57	103.61	111.69
1	B	397	PHE	CA-C-N	6.55	134.25	121.41
1	B	397	PHE	C-N-CA	6.55	134.25	121.41
1	A	13	LYS	CA-C-O	-6.55	112.89	120.49
1	A	400	ILE	CA-C-N	6.54	133.17	121.66
1	A	400	ILE	C-N-CA	6.54	133.17	121.66
1	B	203	PRO	CA-C-O	6.53	128.79	121.34
1	A	130	GLU	CB-CA-C	-6.52	99.60	110.68
1	B	136	PHE	CA-CB-CG	-6.51	107.29	113.80
1	A	132	TYR	N-CA-CB	6.50	119.62	110.07
1	A	324	THR	O-C-N	6.49	128.15	121.79
1	B	152	ARG	CD-NE-CZ	-6.49	115.32	124.40
1	B	80	LEU	N-CA-CB	-6.48	100.59	110.77
1	B	436	ALA	CA-C-N	6.48	129.26	120.38
1	B	436	ALA	C-N-CA	6.48	129.26	120.38
1	B	439	SER	N-CA-C	6.47	119.32	111.82
1	B	9	ASN	N-CA-CB	6.46	121.41	110.49
1	B	423	VAL	CA-C-O	-6.46	112.71	120.78
1	B	85	TYR	CA-C-O	-6.45	114.55	119.32
1	B	90	PHE	CB-CA-C	6.45	120.99	110.22
1	B	29	ILE	CA-CB-CG2	6.45	121.46	110.50
1	A	144	SER	CB-CA-C	6.45	121.64	110.68
1	A	48	GLU	CA-C-O	6.44	127.38	119.97
1	A	222	THR	CB-CA-C	6.44	119.32	109.34
1	B	81	THR	CA-C-N	6.43	132.64	122.74
1	B	81	THR	C-N-CA	6.43	132.64	122.74
1	B	399	HIS	CA-C-O	6.41	128.33	121.16
1	B	42	ALA	O-C-N	6.40	130.55	122.23
1	A	120	TYR	CA-C-O	-6.40	114.17	121.40
1	B	82	LYS	N-CA-C	-6.39	97.96	108.76
1	B	401	ASP	CA-CB-CG	6.39	118.99	112.60
1	B	443	ASP	N-CA-C	-6.37	103.86	111.69
1	A	79	GLU	CA-CB-CG	6.36	126.83	114.10
1	A	216	ARG	CG-CD-NE	6.36	125.99	112.00
1	A	402	GLY	CA-C-N	6.36	126.91	120.04
1	A	402	GLY	C-N-CA	6.36	126.91	120.04
1	B	73	GLU	CA-CB-CG	6.35	126.79	114.10
1	A	77	ALA	CA-C-O	6.34	127.66	121.00
1	B	98	LYS	N-CA-C	6.33	119.84	110.48
1	B	13	LYS	O-C-N	6.32	130.58	123.19
1	B	211	VAL	N-CA-C	-6.32	102.97	111.44
1	B	29	ILE	N-CA-C	-6.31	98.03	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	GLU	CA-C-N	6.30	129.89	120.31
1	A	14	GLU	C-N-CA	6.30	129.89	120.31
1	B	52	GLY	CA-C-N	6.30	133.05	121.70
1	B	52	GLY	C-N-CA	6.30	133.05	121.70
1	A	80	LEU	N-CA-C	6.29	118.96	108.20
1	B	79	GLU	CB-CG-CD	6.29	123.29	112.60
1	B	164	ILE	CA-C-O	-6.29	113.60	120.71
1	B	219	GLN	CA-C-O	-6.28	112.75	119.97
1	B	96	ASP	CA-C-N	6.27	132.89	121.85
1	B	96	ASP	C-N-CA	6.27	132.89	121.85
1	B	110	GLY	O-C-N	-6.25	114.57	122.70
1	A	107	LEU	CA-C-N	6.25	128.56	120.44
1	A	107	LEU	C-N-CA	6.25	128.56	120.44
1	A	93	ASN	CA-C-O	-6.25	114.32	121.19
1	A	136	PHE	CA-C-N	6.25	128.90	120.65
1	A	136	PHE	C-N-CA	6.25	128.90	120.65
1	A	133	ARG	CD-NE-CZ	-6.23	115.67	124.40
1	A	296	SER	N-CA-C	6.23	123.57	109.81
1	A	184	TRP	CA-C-N	6.22	133.63	122.06
1	A	184	TRP	C-N-CA	6.22	133.63	122.06
1	A	133	ARG	NH1-CZ-NH2	6.22	127.38	119.30
1	B	86	PRO	CA-C-N	6.22	131.07	121.19
1	B	86	PRO	C-N-CA	6.22	131.07	121.19
1	B	23	HIS	CA-C-O	-6.21	112.56	120.14
1	A	128	VAL	CA-CB-CG1	6.20	120.94	110.40
1	A	28	TYR	CA-C-N	6.20	133.12	121.97
1	A	28	TYR	C-N-CA	6.20	133.12	121.97
1	A	25	LEU	CA-CB-CG	6.20	137.99	116.30
1	B	115	MET	CA-C-N	6.20	133.55	121.41
1	B	115	MET	C-N-CA	6.20	133.55	121.41
1	B	79	GLU	CG-CD-OE1	6.19	132.63	118.40
1	B	428	ARG	CG-CD-NE	6.19	125.61	112.00
1	B	158	GLY	CA-C-N	6.18	129.53	120.82
1	B	158	GLY	C-N-CA	6.18	129.53	120.82
1	B	141	VAL	N-CA-CB	-6.18	103.14	112.35
1	B	291	HIS	CA-CB-CG	6.17	119.97	113.80
1	A	126	PHE	O-C-N	-6.17	116.45	123.48
1	A	38	TYR	CA-C-O	-6.16	114.33	120.80
1	A	412	GLN	CA-C-N	6.16	129.67	120.31
1	A	412	GLN	C-N-CA	6.16	129.67	120.31
1	B	141	VAL	CB-CA-C	6.16	120.19	110.52
1	A	442	GLY	N-CA-C	-6.16	105.04	112.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	50	SER	N-CA-C	6.15	123.90	110.80
1	A	107	LEU	CB-CA-C	6.14	120.46	110.95
1	B	123	MET	N-CA-C	-6.13	99.28	109.46
1	B	395	GLY	O-C-N	6.13	130.67	122.70
1	B	430	HIS	N-CA-C	6.13	118.52	108.52
1	B	435	ARG	N-CA-C	6.12	120.47	112.89
1	B	440	PHE	N-CA-CB	6.12	120.20	111.21
1	B	78	ARG	CA-C-O	6.11	126.42	119.27
1	B	207	THR	CA-CB-CG2	6.11	120.88	110.50
1	B	204	LEU	CA-C-N	6.11	128.96	120.29
1	B	204	LEU	C-N-CA	6.11	128.96	120.29
1	B	121	ALA	CA-C-O	-6.10	111.97	120.21
1	A	86	PRO	O-C-N	6.09	130.73	122.99
1	A	65	ARG	N-CA-CB	6.09	120.78	110.49
1	A	428	ARG	CB-CA-C	6.08	120.53	110.81
1	A	394	GLY	O-C-N	6.07	130.59	122.27
1	A	152	ARG	CA-C-O	-6.07	115.68	121.08
1	B	419	ASP	CA-CB-CG	-6.06	106.54	112.60
1	A	417	TRP	CA-C-O	6.05	127.18	120.82
1	B	209	ALA	CA-C-N	6.05	131.73	121.14
1	B	209	ALA	C-N-CA	6.05	131.73	121.14
1	B	113	GLN	N-CA-CB	6.05	119.01	109.82
1	B	204	LEU	CA-C-O	-6.04	114.15	120.55
1	A	429	GLU	CG-CD-OE1	6.04	132.29	118.40
1	B	208	ILE	CA-C-N	6.03	128.36	120.28
1	B	208	ILE	C-N-CA	6.03	128.36	120.28
1	B	5	SER	N-CA-C	6.03	123.64	110.80
1	A	414	TRP	N-CA-C	-6.01	104.36	111.03
1	B	82	LYS	CA-C-N	6.01	131.29	122.94
1	B	82	LYS	C-N-CA	6.01	131.29	122.94
1	B	412	GLN	CA-C-O	-6.01	114.19	120.92
1	B	453	LYS	O-C-N	6.00	130.57	122.59
1	B	420	GLY	N-CA-C	-5.98	106.68	115.72
1	B	424	LEU	O-C-N	5.98	129.62	122.27
1	A	87	VAL	CA-C-O	-5.96	112.45	119.85
1	B	83	ILE	CA-C-N	5.96	131.97	123.14
1	B	83	ILE	C-N-CA	5.96	131.97	123.14
1	A	321	HIS	N-CA-C	-5.96	101.82	110.64
1	A	296	SER	CA-C-N	5.95	127.28	119.84
1	A	296	SER	C-N-CA	5.95	127.28	119.84
1	B	417	TRP	O-C-N	5.95	128.28	122.09
1	A	128	VAL	CA-C-O	5.94	125.33	119.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ALA	N-CA-C	-5.94	104.73	111.14
1	A	17	LEU	O-C-N	5.94	128.18	122.07
1	A	73	GLU	O-C-N	-5.93	117.28	123.56
1	B	433	LEU	N-CA-CB	5.92	118.89	110.13
1	B	66	GLY	O-C-N	5.92	132.47	123.00
1	A	176	PHE	N-CA-CB	5.92	118.55	109.91
1	A	6	ARG	NH1-CZ-NH2	5.91	126.98	119.30
1	B	7	TYR	CA-C-N	5.91	131.54	122.68
1	B	7	TYR	C-N-CA	5.91	131.54	122.68
1	B	104	PHE	CA-C-N	5.90	128.67	120.29
1	B	104	PHE	C-N-CA	5.90	128.67	120.29
1	B	24	VAL	N-CA-C	-5.89	101.12	108.89
1	B	32	PRO	CA-C-O	-5.87	114.56	122.08
1	B	404	VAL	CA-C-O	5.87	127.07	120.85
1	B	103	SER	CA-C-N	5.86	128.14	120.28
1	B	103	SER	C-N-CA	5.86	128.14	120.28
1	B	452	ARG	N-CA-CB	5.86	118.68	109.94
1	B	215	MET	O-C-N	5.86	128.91	122.11
1	A	45	PHE	CB-CA-C	5.86	122.33	110.38
1	A	222	THR	OG1-CB-CG2	5.86	121.01	109.30
1	B	206	ASP	CA-C-N	5.86	128.40	120.44
1	B	206	ASP	C-N-CA	5.86	128.40	120.44
1	A	420	GLY	CA-C-O	5.85	125.62	119.07
1	B	49	SER	CA-CB-OG	-5.85	99.40	111.10
1	A	181	HIS	N-CA-C	-5.84	103.89	111.02
1	B	166	LYS	CB-CG-CD	5.83	124.72	111.30
1	A	299	SER	N-CA-C	-5.83	98.38	110.80
1	A	95	THR	CA-CB-OG1	-5.83	100.86	109.60
1	B	130	GLU	CG-CD-OE1	5.83	131.81	118.40
1	B	47	ALA	N-CA-C	-5.82	104.56	111.03
1	A	418	ARG	O-C-N	5.81	128.08	122.03
1	A	220	ASP	CA-CB-CG	5.81	118.41	112.60
1	A	94	ILE	CA-C-O	5.80	126.51	120.25
1	A	163	THR	CB-CA-C	-5.80	98.94	111.11
1	B	126	PHE	O-C-N	5.79	129.85	123.25
1	B	446	GLN	CA-C-N	-5.79	115.52	122.35
1	B	446	GLN	C-N-CA	-5.79	115.52	122.35
1	A	174	LYS	N-CA-CB	5.79	115.89	110.39
1	A	101	ILE	CA-C-O	-5.78	114.00	120.25
1	A	145	ALA	N-CA-CB	-5.78	101.31	110.28
1	B	24	VAL	N-CA-CB	5.78	116.83	110.53
1	B	52	GLY	CA-C-O	5.78	130.63	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	GLU	N-CA-C	5.77	118.31	111.33
1	B	259	ALA	N-CA-C	-5.77	101.15	110.32
1	A	456	GLY	O-C-N	-5.77	115.20	122.70
1	B	30	MET	N-CA-CB	5.77	122.25	111.53
1	A	101	ILE	CA-CB-CG2	5.76	120.29	110.50
1	B	164	ILE	O-C-N	5.75	129.51	122.95
1	B	401	ASP	CB-CG-OD1	5.74	131.60	118.40
1	A	448	TYR	CB-CA-C	-5.73	100.28	111.29
1	A	448	TYR	CA-CB-CG	5.73	124.21	113.90
1	A	155	VAL	N-CA-CB	-5.72	104.12	110.99
1	B	78	ARG	CD-NE-CZ	-5.72	116.39	124.40
1	A	194	GLU	O-C-N	-5.72	114.74	121.32
1	B	211	VAL	CA-C-O	5.72	126.43	120.25
1	A	153	PRO	CB-CA-C	5.71	118.80	111.21
1	B	449	PRO	CA-C-O	-5.71	114.52	121.03
1	B	159	LEU	N-CA-C	5.71	118.60	110.10
1	B	437	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	146	LEU	CA-C-O	-5.70	114.45	120.55
1	A	448	TYR	N-CA-C	5.70	120.35	108.39
1	B	161	VAL	CA-C-N	5.69	127.24	122.17
1	B	161	VAL	C-N-CA	5.69	127.24	122.17
1	B	218	ALA	CA-C-O	-5.68	114.52	120.55
1	A	226	LYS	CA-C-N	5.68	131.17	122.93
1	A	226	LYS	C-N-CA	5.68	131.17	122.93
1	A	454	ALA	CA-C-O	5.68	126.36	119.38
1	A	397	PHE	CA-CB-CG	-5.67	108.13	113.80
1	A	451	TRP	CB-CG-CD2	-5.66	118.88	126.80
1	B	84	ALA	CA-C-N	5.66	129.48	121.61
1	B	84	ALA	C-N-CA	5.66	129.48	121.61
1	A	113	GLN	CG-CD-NE2	5.66	124.89	116.40
1	B	276	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	A	24	VAL	CA-C-O	-5.66	113.84	121.02
1	B	70	LEU	CA-C-N	5.65	129.66	121.18
1	B	70	LEU	C-N-CA	5.65	129.66	121.18
1	A	49	SER	CA-C-N	5.65	132.33	121.54
1	A	49	SER	C-N-CA	5.65	132.33	121.54
1	B	164	ILE	N-CA-C	-5.64	100.45	108.58
1	A	182	ALA	CA-C-O	-5.64	114.42	121.02
1	A	455	LEU	N-CA-CB	5.64	120.02	110.49
1	A	152	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
1	B	76	GLU	O-C-N	5.63	129.88	122.33
1	B	120	TYR	CA-C-O	5.63	127.06	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	HIS	CB-CA-C	-5.63	101.77	111.23
1	B	429	GLU	O-C-N	-5.63	114.79	122.33
1	A	433	LEU	N-CA-C	-5.63	105.23	111.36
1	B	225	ALA	N-CA-C	-5.63	100.51	109.96
1	B	98	LYS	CA-C-O	-5.62	115.00	121.47
1	B	224	GLU	CA-C-N	5.62	130.40	122.09
1	B	224	GLU	C-N-CA	5.62	130.40	122.09
1	A	41	THR	CA-CB-OG1	-5.61	101.19	109.60
1	B	220	ASP	N-CA-C	5.60	119.28	112.23
1	B	354	ARG	NE-CZ-NH2	5.60	124.24	119.20
1	B	105	LEU	CA-C-N	5.59	128.23	120.29
1	B	105	LEU	C-N-CA	5.59	128.23	120.29
1	B	113	GLN	N-CA-C	-5.59	104.20	111.02
1	B	424	LEU	N-CA-C	-5.59	105.34	111.82
1	B	439	SER	CB-CA-C	-5.59	99.94	110.67
1	B	336	ASP	N-CA-C	5.58	117.17	111.14
1	A	442	GLY	O-C-N	5.58	127.55	122.19
1	A	416	ALA	CA-C-O	-5.58	114.64	120.55
1	A	92	ARG	NE-CZ-NH1	-5.57	115.93	121.50
1	B	221	GLU	CG-CD-OE1	5.56	131.19	118.40
1	B	46	ALA	CA-C-N	5.56	128.19	120.63
1	B	46	ALA	C-N-CA	5.56	128.19	120.63
1	A	75	ASP	N-CA-CB	5.55	120.58	111.58
1	B	14	GLU	CG-CD-OE2	-5.55	105.63	118.40
1	A	416	ALA	N-CA-C	-5.54	105.24	111.28
1	B	75	ASP	CA-C-N	5.54	130.09	120.68
1	B	75	ASP	C-N-CA	5.54	130.09	120.68
1	A	52	GLY	O-C-N	-5.53	115.52	122.70
1	A	79	GLU	CB-CG-CD	5.53	122.00	112.60
1	B	8	VAL	CA-C-N	5.53	132.09	121.54
1	B	8	VAL	C-N-CA	5.53	132.09	121.54
1	B	437	PHE	O-C-N	5.52	127.97	122.12
1	A	133	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	B	39	VAL	N-CA-C	5.51	120.81	109.34
1	A	22	GLU	CG-CD-OE1	5.51	131.07	118.40
1	A	52	GLY	CA-C-O	5.51	130.16	120.57
1	A	178	GLU	N-CA-C	-5.51	105.18	111.07
1	A	29	ILE	CA-CB-CG2	5.50	119.86	110.50
1	A	370	GLY	O-C-N	5.50	129.86	122.70
1	A	427	ALA	N-CA-CB	5.50	118.20	110.12
1	B	438	GLU	N-CA-CB	5.49	118.28	110.16
1	B	297	PRO	N-CA-C	-5.48	108.40	114.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	TRP	O-C-N	5.48	127.73	122.03
1	A	153	PRO	N-CA-C	-5.48	102.59	111.19
1	A	385	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	394	GLY	N-CA-C	-5.47	106.20	115.34
1	B	167	PRO	O-C-N	5.47	131.50	121.10
1	A	428	ARG	CB-CG-CD	5.47	123.88	111.30
1	B	85	TYR	N-CA-CB	-5.47	103.07	110.23
1	B	28	TYR	N-CA-C	5.46	117.98	109.52
1	A	68	ASP	N-CA-CB	-5.44	101.97	109.97
1	A	66	GLY	N-CA-C	-5.44	100.29	113.18
1	B	119	GLU	N-CA-C	5.43	117.06	111.03
1	A	29	ILE	CA-C-N	5.43	130.80	122.93
1	A	29	ILE	C-N-CA	5.43	130.80	122.93
1	B	108	THR	N-CA-C	5.43	119.90	113.28
1	A	25	LEU	CB-CA-C	5.43	119.74	109.37
1	B	28	TYR	N-CA-CB	-5.43	102.11	111.55
1	B	94	ILE	CA-C-N	5.43	129.25	121.71
1	B	94	ILE	C-N-CA	5.43	129.25	121.71
1	A	7	TYR	N-CA-CB	-5.42	102.62	110.70
1	B	141	VAL	CA-CB-CG1	5.42	119.61	110.40
1	B	227	LEU	N-CA-C	5.42	118.23	109.40
1	B	122	LYS	CA-C-O	-5.42	114.43	120.66
1	B	288	ARG	NH1-CZ-NH2	-5.42	112.26	119.30
1	B	410	LEU	N-CA-C	-5.42	104.79	111.40
1	A	411	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	B	40	ALA	N-CA-CB	-5.41	102.17	110.01
1	B	116	GLY	N-CA-C	-5.41	100.37	113.18
1	B	437	PHE	CA-C-O	-5.38	114.82	120.63
1	A	24	VAL	N-CA-C	-5.38	100.69	108.87
1	B	203	PRO	O-C-N	-5.38	116.52	123.03
1	A	14	GLU	O-C-N	-5.38	116.07	122.20
1	B	194	GLU	CA-C-N	5.38	126.56	119.84
1	B	194	GLU	C-N-CA	5.38	126.56	119.84
1	B	402	GLY	CA-C-N	5.37	124.89	119.19
1	B	402	GLY	C-N-CA	5.37	124.89	119.19
1	B	133	ARG	CA-CB-CG	5.37	124.83	114.10
1	B	104	PHE	N-CA-C	-5.36	105.43	111.28
1	A	215	MET	N-CA-C	-5.36	105.13	110.97
1	A	71	VAL	O-C-N	5.36	130.12	122.62
1	B	215	MET	CA-C-O	-5.35	115.19	120.80
1	A	98	LYS	CA-C-N	5.34	131.11	121.06
1	A	98	LYS	C-N-CA	5.34	131.11	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	452	ARG	O-C-N	5.34	127.64	122.09
1	A	91	ASP	N-CA-CB	-5.34	102.62	110.26
1	A	404	VAL	O-C-N	5.34	128.89	121.84
1	B	268	GLY	CA-C-N	5.33	127.68	120.38
1	B	268	GLY	C-N-CA	5.33	127.68	120.38
1	A	95	THR	CA-C-O	5.32	126.25	120.55
1	A	131	ALA	N-CA-CB	-5.32	102.29	110.01
1	A	337	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	141	VAL	N-CA-CB	-5.32	101.10	112.00
1	B	31	LYS	CG-CD-CE	5.32	123.53	111.30
1	B	414	TRP	CA-C-N	5.32	127.94	120.28
1	B	414	TRP	C-N-CA	5.32	127.94	120.28
1	B	215	MET	CA-C-N	5.31	127.40	120.28
1	B	215	MET	C-N-CA	5.31	127.40	120.28
1	A	70	LEU	CA-C-N	5.31	130.53	123.10
1	A	70	LEU	C-N-CA	5.31	130.53	123.10
1	B	20	GLY	CA-C-O	5.30	126.28	120.66
1	A	412	GLN	CA-CB-CG	-5.29	103.51	114.10
1	A	422	PRO	CA-C-O	-5.29	114.96	121.31
1	B	216	ARG	CA-CB-CG	5.29	124.69	114.10
1	A	296	SER	N-CA-CB	-5.29	100.96	110.37
1	B	213	ASP	CA-C-N	5.29	129.55	120.72
1	B	213	ASP	C-N-CA	5.29	129.55	120.72
1	A	227	LEU	N-CA-C	5.28	118.09	109.59
1	A	3	GLN	O-C-N	5.28	131.44	123.00
1	A	172	ARG	CA-CB-CG	-5.27	103.55	114.10
1	A	108	THR	N-CA-CB	-5.27	102.37	110.01
1	B	165	ILE	CB-CA-C	5.25	119.15	111.33
1	A	313	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	13	LYS	CA-CB-CG	5.25	124.59	114.10
1	B	20	GLY	O-C-N	-5.24	117.10	122.19
1	B	415	GLN	OE1-CD-NE2	5.24	127.84	122.60
1	A	98	LYS	O-C-N	-5.24	116.48	122.93
1	B	142	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	124	HIS	CA-C-O	-5.23	113.38	118.97
1	A	216	ARG	CA-CB-CG	-5.23	103.64	114.10
1	B	240	ILE	N-CA-C	-5.23	105.62	110.53
1	B	121	ALA	CB-CA-C	5.22	118.67	109.80
1	B	87	VAL	O-C-N	5.22	129.40	122.31
1	B	455	LEU	N-CA-C	-5.21	105.69	111.36
1	A	129	PRO	O-C-N	-5.20	116.79	123.14
1	A	160	VAL	CA-CB-CG2	5.20	119.24	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ALA	N-CA-C	5.20	116.63	111.07
1	B	429	GLU	CA-C-N	5.20	130.33	123.05
1	B	429	GLU	C-N-CA	5.20	130.33	123.05
1	B	93	ASN	CA-C-N	5.20	128.87	121.02
1	B	93	ASN	C-N-CA	5.20	128.87	121.02
1	B	80	LEU	CA-C-O	5.19	125.74	120.24
1	A	406	GLY	CA-C-N	5.19	127.96	120.38
1	A	406	GLY	C-N-CA	5.19	127.96	120.38
1	A	425	ASP	CA-C-N	5.19	127.66	120.29
1	A	425	ASP	C-N-CA	5.19	127.66	120.29
1	A	284	LEU	CA-C-N	5.17	130.01	122.41
1	A	284	LEU	C-N-CA	5.17	130.01	122.41
1	B	443	ASP	N-CA-CB	5.17	117.91	110.20
1	B	256	SER	O-C-N	5.17	128.54	122.34
1	A	172	ARG	CD-NE-CZ	5.17	131.63	124.40
1	A	251	PHE	N-CA-C	-5.16	106.98	113.28
1	B	297	PRO	O-C-N	5.16	130.84	122.47
1	B	71	VAL	N-CA-CB	-5.16	105.09	110.82
1	A	130	GLU	N-CA-CB	5.16	117.80	110.06
1	A	174	LYS	CA-C-O	-5.16	114.39	119.13
1	A	71	VAL	N-CA-C	-5.16	99.53	106.85
1	A	451	TRP	CA-C-N	5.16	127.45	120.44
1	A	451	TRP	C-N-CA	5.16	127.45	120.44
1	A	232	ILE	N-CA-C	-5.15	107.69	112.43
1	A	212	ALA	CB-CA-C	5.15	119.34	110.79
1	A	187	GLY	N-CA-C	5.14	121.12	112.85
1	B	127	TYR	CB-CA-C	5.13	118.99	109.70
1	B	23	HIS	CA-C-N	5.13	128.74	121.66
1	B	23	HIS	C-N-CA	5.13	128.74	121.66
1	B	73	GLU	CB-CA-C	5.12	117.52	110.34
1	A	92	ARG	CA-CB-CG	5.12	124.35	114.10
1	A	288	ARG	CA-C-N	5.12	127.40	120.38
1	A	288	ARG	C-N-CA	5.12	127.40	120.38
1	A	94	ILE	CA-C-N	5.12	129.26	120.71
1	A	94	ILE	C-N-CA	5.12	129.26	120.71
1	A	217	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	174	LYS	CB-CA-C	-5.11	105.54	113.57
1	B	9	ASN	CB-CG-ND2	5.11	124.07	116.40
1	B	428	ARG	CB-CG-CD	5.11	123.04	111.30
1	A	415	GLN	CB-CG-CD	5.09	121.25	112.60
1	B	431	LYS	CA-C-O	-5.09	115.03	120.42
1	A	214	ALA	O-C-N	-5.09	116.73	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	B	115	MET	N-CA-CB	-5.09	103.09	111.69
1	A	74	VAL	O-C-N	5.08	128.59	123.00
1	A	276	ARG	NE-CZ-NH2	5.08	123.78	119.20
1	A	139	PRO	O-C-N	-5.08	116.72	123.01
1	B	428	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	182	ALA	O-C-N	5.07	128.33	122.20
1	A	137	ASP	CA-C-O	5.07	126.32	121.00
1	B	47	ALA	CA-C-O	-5.07	115.68	120.90
1	A	337	ARG	N-CA-C	-5.06	107.27	113.50
1	B	337	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	B	436	ALA	N-CA-CB	5.05	117.28	109.91
1	A	225	ALA	N-CA-C	-5.04	102.24	110.20
1	A	238	PHE	CA-CB-CG	-5.03	108.77	113.80
1	A	76	GLU	OE1-CD-OE2	-5.03	110.83	122.90
1	A	424	LEU	CB-CA-C	5.03	119.94	110.63
1	A	22	GLU	CA-CB-CG	5.03	124.15	114.10
1	B	411	ARG	CA-C-N	5.03	128.36	120.82
1	B	411	ARG	C-N-CA	5.03	128.36	120.82
1	A	435	ARG	CA-C-N	5.03	132.34	121.64
1	A	435	ARG	C-N-CA	5.03	132.34	121.64
1	A	447	ILE	CA-C-N	5.02	129.34	123.16
1	A	447	ILE	C-N-CA	5.02	129.34	123.16
1	A	82	LYS	CB-CA-C	-5.02	100.52	109.71
1	B	13	LYS	CG-CD-CE	-5.02	99.75	111.30
1	B	128	VAL	N-CA-CB	5.02	117.71	111.39
1	A	129	PRO	CA-C-N	5.01	127.25	120.38
1	A	129	PRO	C-N-CA	5.01	127.25	120.38
1	A	184	TRP	N-CA-C	5.01	121.48	110.80
1	B	431	LYS	CA-C-N	5.01	127.50	120.28
1	B	431	LYS	C-N-CA	5.01	127.50	120.28
1	A	430	HIS	N-CA-C	5.01	117.76	107.69
1	A	137	ASP	CB-CA-C	5.00	118.67	110.96
1	B	53	THR	CB-CA-C	5.00	120.11	109.10
1	B	163	THR	O-C-N	5.00	128.41	123.46

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	111	ASN	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	3337	0	3245	268	2
1	B	3318	0	3222	256	0
2	A	11	0	4	8	0
2	B	11	0	4	5	0
All	All	6677	0	6475	492	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 37.

All (492) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:GLN:O	1:A:231:ASN:ND2	1.67	1.28
1:A:288:ARG:HD3	1:A:291:HIS:NE2	1.52	1.23
1:B:3:GLN:NE2	1:B:44:HIS:HA	1.50	1.22
1:B:321:HIS:HB3	2:B:500:3PG:O4P	1.41	1.17
1:B:335:SER:O	1:B:339:ILE:CG1	1.93	1.14
1:A:263:ASP:OD1	1:A:289:ALA:HB2	1.49	1.13
1:B:335:SER:O	1:B:339:ILE:HG13	0.97	1.12
1:B:335:SER:C	1:B:339:ILE:HG13	1.74	1.11
1:A:194:GLU:HG3	1:A:195:PRO:HD3	1.17	1.11
1:A:334:SER:O	1:A:335:SER:HB3	1.53	1.08
1:A:293:ALA:O	1:A:299:SER:CB	2.03	1.06
1:B:324:THR:HG22	1:B:325:MET:H	1.19	1.06
1:B:32:PRO:HB3	1:B:41:THR:HG21	1.36	1.06
1:A:194:GLU:HG3	1:A:195:PRO:CD	1.85	1.05
1:A:293:ALA:HB2	1:B:301:ARG:HB2	1.40	1.03
1:A:194:GLU:CG	1:A:195:PRO:HD3	1.91	0.99
1:B:324:THR:CG2	1:B:325:MET:N	2.28	0.96
1:B:93:ASN:HD22	1:B:96:ASP:HB2	1.32	0.94
1:A:293:ALA:O	1:A:299:SER:OG	1.86	0.94
1:A:376:MET:HB3	1:A:377:PRO:HD3	1.49	0.93
1:A:105:LEU:HD23	1:A:109:MET:HE3	1.51	0.92
1:B:324:THR:HG22	1:B:325:MET:N	1.80	0.91
1:A:324:THR:HG23	1:A:368:SER:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:HIS:CD2	1:A:291:HIS:H	1.60	0.91
1:B:321:HIS:CB	2:B:500:3PG:O4P	2.18	0.90
1:A:65:ARG:HG3	1:A:67:VAL:HG23	1.53	0.89
1:A:278:ARG:HE	1:A:278:ARG:HA	1.39	0.87
1:B:222:THR:HG23	1:B:224:GLU:HB2	1.56	0.87
1:A:288:ARG:HD3	1:A:291:HIS:CE1	2.10	0.86
1:A:291:HIS:CD2	1:A:291:HIS:N	2.41	0.86
1:B:241:ILE:HG12	1:B:278:ARG:HG2	1.58	0.85
1:A:289:ALA:O	1:B:111:ASN:N	2.10	0.84
1:A:344:THR:HA	1:A:362:ALA:HB1	1.58	0.84
1:A:123:MET:HE3	1:A:307:VAL:HG11	1.58	0.84
1:A:163:THR:HG23	1:A:397:PHE:CE1	2.12	0.84
1:B:3:GLN:OE1	1:B:47:ALA:CB	2.26	0.83
1:B:291:HIS:CD2	1:B:295:THR:HG21	2.14	0.83
1:A:163:THR:HG23	1:A:397:PHE:HE1	1.42	0.82
1:A:263:ASP:OD1	1:A:289:ALA:CB	2.28	0.81
1:B:372:ASN:HD22	1:B:374:LEU:H	1.29	0.80
1:A:293:ALA:HB2	1:B:301:ARG:CB	2.11	0.80
1:A:401:ASP:OD2	1:A:435:ARG:HG2	1.84	0.78
1:B:3:GLN:NE2	1:B:44:HIS:CA	2.43	0.78
1:A:218:ALA:O	1:A:222:THR:HB	1.84	0.77
1:B:3:GLN:HE21	1:B:44:HIS:HA	1.49	0.77
1:B:376:MET:HB3	1:B:377:PRO:HD3	1.67	0.77
1:A:263:ASP:CG	1:A:289:ALA:HB2	2.10	0.77
1:B:128:VAL:HG23	1:B:133:ARG:HB2	1.67	0.76
1:A:53:THR:HA	1:B:167:PRO:HB3	1.68	0.76
1:B:162:GLY:HA2	1:B:189:PHE:O	1.85	0.76
1:B:174:LYS:HB3	1:B:175:PRO:HD3	1.67	0.76
1:B:274:THR:O	1:B:278:ARG:HB3	1.86	0.75
1:A:392:ALA:HB1	1:A:396:ALA:HB3	1.68	0.75
1:B:399:HIS:CE1	1:B:401:ASP:HB2	2.22	0.75
1:A:285:HIS:NE2	1:A:321:HIS:CD2	2.55	0.74
1:B:31:LYS:O	1:B:119:GLU:HB2	1.85	0.74
1:B:96:ASP:HB3	1:B:98:LYS:HG3	1.71	0.73
1:A:167:PRO:HB3	1:B:53:THR:HG22	1.69	0.73
1:B:74:VAL:HA	1:B:80:LEU:O	1.87	0.73
1:A:299:SER:C	1:A:301:ARG:H	1.97	0.73
1:B:30:MET:HG2	1:B:31:LYS:N	2.03	0.73
1:B:3:GLN:HE21	1:B:44:HIS:CB	2.01	0.72
1:A:334:SER:O	1:A:335:SER:CB	2.30	0.72
1:B:372:ASN:ND2	1:B:374:LEU:HB2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:GLY:O	1:B:457:VAL:HB	1.88	0.72
1:B:116:GLY:O	1:B:117:ASP:HB3	1.89	0.72
1:A:268:GLY:HA3	1:B:268:GLY:HA3	1.70	0.72
1:A:385:ASN:HD22	1:A:387:ASN:H	1.37	0.72
1:B:376:MET:HB3	1:B:377:PRO:CD	2.20	0.71
1:A:107:LEU:HD13	1:B:195:PRO:HB3	1.72	0.71
1:A:370:GLY:HA3	1:A:396:ALA:HB2	1.72	0.71
1:A:368:SER:CB	2:A:500:3PG:O2P	2.38	0.71
1:B:14:GLU:O	1:B:18:ILE:HG13	1.90	0.71
1:A:400:ILE:HD11	1:A:435:ARG:HG3	1.71	0.71
1:B:290:GLY:O	1:B:292:GLY:N	2.23	0.71
1:A:174:LYS:HB3	1:A:175:PRO:HD3	1.72	0.71
1:B:321:HIS:ND1	2:B:500:3PG:O4P	2.23	0.71
1:A:45:PHE:HB2	1:A:115:MET:HE1	1.71	0.70
1:A:168:LYS:HE3	1:A:193:ASP:OD1	1.91	0.70
1:B:183:PHE:HB3	1:B:190:ILE:HD11	1.72	0.70
1:B:234:ALA:HB3	1:B:240:ILE:HG13	1.73	0.70
1:A:321:HIS:HB3	2:A:500:3PG:O3P	1.91	0.70
1:A:152:ARG:HB3	1:A:153:PRO:HD2	1.73	0.69
1:A:296:SER:CB	1:A:297:PRO:HD2	2.22	0.69
1:A:286:TYR:HB3	1:A:320:ILE:HG13	1.74	0.69
1:B:3:GLN:OE1	1:B:47:ALA:HB2	1.91	0.69
1:A:191:LYS:O	1:A:191:LYS:HG3	1.92	0.69
1:A:293:ALA:HA	1:B:301:ARG:HD3	1.75	0.69
1:B:192:ASN:ND2	1:B:196:GLN:OE1	2.24	0.69
1:B:285:HIS:HE2	1:B:321:HIS:CD2	2.10	0.69
1:A:278:ARG:CG	1:A:279:PHE:CE1	2.76	0.69
1:A:96:ASP:HB3	1:A:98:LYS:HB2	1.74	0.68
1:B:335:SER:C	1:B:339:ILE:CG1	2.54	0.68
1:A:70:LEU:H	1:A:70:LEU:HD12	1.58	0.68
1:A:431:LYS:O	1:A:434:ALA:HB3	1.94	0.68
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.59	0.68
1:A:167:PRO:HB3	1:B:53:THR:HA	1.76	0.68
1:B:32:PRO:CB	1:B:41:THR:HG21	2.21	0.68
1:A:237:PRO:O	1:A:241:ILE:HG13	1.94	0.67
1:A:295:THR:HG23	1:A:305:ALA:N	2.08	0.67
1:A:376:MET:HB3	1:A:377:PRO:CD	2.25	0.67
1:A:278:ARG:HG3	1:A:279:PHE:CE1	2.29	0.66
1:A:342:MET:HA	1:A:348:ALA:CB	2.26	0.66
1:B:321:HIS:CG	2:B:500:3PG:O4P	2.48	0.66
1:A:370:GLY:CA	1:A:396:ALA:HB2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:HD3	1:B:278:ARG:O	1.94	0.66
1:A:235:ASP:O	1:B:270:ALA:HA	1.95	0.66
1:B:374:LEU:HD11	1:B:437:PHE:HA	1.77	0.66
1:A:293:ALA:O	1:A:299:SER:HB3	1.92	0.66
1:A:296:SER:C	1:A:298:GLN:H	2.04	0.65
1:A:289:ALA:O	1:B:111:ASN:CA	2.44	0.65
1:A:368:SER:HB3	2:A:500:3PG:O2P	1.96	0.65
1:A:65:ARG:HD2	1:A:65:ARG:O	1.96	0.65
1:A:288:ARG:CD	1:A:291:HIS:CE1	2.79	0.65
1:A:291:HIS:HB2	1:A:295:THR:HB	1.79	0.64
1:A:294:VAL:HG12	1:A:295:THR:N	2.12	0.64
1:A:392:ALA:HB3	1:A:397:PHE:CZ	2.32	0.64
1:A:142:ASN:OD1	1:A:144:SER:HB3	1.98	0.64
1:A:423:VAL:HG13	1:A:433:LEU:HD21	1.80	0.64
1:A:368:SER:HB2	2:A:500:3PG:O2P	1.97	0.64
1:B:93:ASN:HD22	1:B:96:ASP:CB	2.08	0.64
1:B:174:LYS:CB	1:B:175:PRO:HD3	2.28	0.64
1:A:217:ARG:O	1:A:221:GLU:HG3	1.97	0.64
1:A:291:HIS:CB	1:A:295:THR:HB	2.28	0.63
1:B:165:ILE:HG12	1:B:190:ILE:HG23	1.79	0.63
1:B:215:MET:O	1:B:219:GLN:HG3	1.98	0.63
1:A:222:THR:HG22	1:A:224:GLU:H	1.64	0.63
1:B:399:HIS:ND1	1:B:401:ASP:HB2	2.14	0.63
1:B:376:MET:HG3	1:B:380:PHE:CE2	2.33	0.63
1:A:107:LEU:HD13	1:B:195:PRO:CB	2.28	0.63
1:A:382:ASN:C	1:A:382:ASN:HD22	2.06	0.62
1:B:239:GLU:OE1	1:B:243:ARG:NE	2.32	0.62
1:A:167:PRO:HB3	1:B:53:THR:CG2	2.30	0.62
1:A:120:TYR:HB2	1:A:300:LYS:HB2	1.80	0.62
1:B:336:ASP:HA	1:B:339:ILE:HB	1.80	0.62
1:A:53:THR:CA	1:B:167:PRO:HB3	2.30	0.62
1:A:53:THR:O	1:B:166:LYS:HG2	2.00	0.62
1:B:178:GLU:OE1	1:B:217:ARG:NH2	2.26	0.62
1:A:278:ARG:HG3	1:A:279:PHE:CD1	2.34	0.61
1:B:3:GLN:HE22	1:B:44:HIS:HA	1.59	0.61
1:A:340:ALA:O	1:A:344:THR:OG1	2.19	0.61
1:B:67:VAL:O	1:B:89:LEU:HD21	2.01	0.61
1:A:150:LEU:HG	1:A:227:LEU:HD11	1.83	0.61
1:A:424:LEU:HD13	1:A:437:PHE:CZ	2.34	0.61
1:B:371:MET:HB3	1:B:376:MET:HE1	1.82	0.61
1:A:278:ARG:HG2	1:A:279:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLY:C	1:A:395:GLY:H	2.08	0.60
1:B:247:VAL:O	1:B:251:PHE:HD1	1.84	0.60
1:B:159:LEU:HD22	1:B:380:PHE:HZ	1.66	0.60
1:A:70:LEU:HD12	1:A:70:LEU:N	2.17	0.60
1:B:110:GLY:O	1:B:113:GLN:HB2	2.01	0.60
1:B:4:SER:O	1:B:6:ARG:N	2.35	0.60
1:A:122:LYS:NZ	1:A:294:VAL:O	2.35	0.60
1:A:270:ALA:HA	1:B:235:ASP:O	2.01	0.60
1:B:324:THR:O	1:B:325:MET:O	2.20	0.59
1:B:447:ILE:HD12	1:B:447:ILE:O	2.02	0.59
1:A:443:ASP:O	1:A:447:ILE:HG13	2.03	0.59
1:A:293:ALA:CB	1:B:301:ARG:HB2	2.25	0.59
1:A:46:ALA:O	1:A:50:SER:HB2	2.02	0.59
1:B:129:PRO:HG2	1:B:132:TYR:HB3	1.83	0.59
1:B:168:LYS:HE2	1:B:193:ASP:OD2	2.02	0.59
1:A:442:GLY:O	1:A:446:GLN:NE2	2.30	0.59
1:B:241:ILE:O	1:B:245:GLU:HG3	2.03	0.59
1:B:424:LEU:HD21	1:B:451:TRP:HA	1.85	0.58
1:A:167:PRO:CB	1:B:53:THR:HG22	2.31	0.58
1:A:270:ALA:HB3	1:B:270:ALA:HB3	1.85	0.58
1:A:120:TYR:CB	1:A:300:LYS:HB2	2.33	0.58
1:B:457:VAL:HG12	1:B:457:VAL:O	2.02	0.58
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.18	0.58
1:B:32:PRO:HB3	1:B:41:THR:CG2	2.22	0.58
1:A:397:PHE:HE2	1:A:410:LEU:CD1	2.16	0.58
1:B:3:GLN:HE21	1:B:44:HIS:HB2	1.67	0.57
1:B:424:LEU:HD23	1:B:454:ALA:HB3	1.85	0.57
1:B:393:GLY:O	1:B:397:PHE:HB2	2.03	0.57
1:B:424:LEU:HD11	1:B:448:TYR:HB3	1.86	0.57
1:A:234:ALA:HB3	1:A:240:ILE:HG12	1.85	0.57
1:B:372:ASN:OD1	1:B:443:ASP:OD2	2.22	0.57
1:A:431:LYS:HE3	1:A:432:GLU:OE1	2.05	0.57
1:B:335:SER:C	1:B:339:ILE:CD1	2.78	0.57
1:A:174:LYS:HB3	1:A:175:PRO:CD	2.35	0.57
1:B:101:ILE:HD11	1:B:311:MET:CG	2.35	0.57
1:A:297:PRO:O	1:A:298:GLN:CB	2.51	0.57
1:A:65:ARG:HG3	1:A:67:VAL:CG2	2.30	0.56
1:B:164:ILE:HD12	1:B:164:ILE:N	2.19	0.56
1:B:288:ARG:HD2	1:B:321:HIS:HB2	1.87	0.56
1:A:8:VAL:HG21	1:A:39:VAL:HG13	1.85	0.56
1:B:30:MET:HA	1:B:120:TYR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NE	1:A:291:HIS:CE1	2.73	0.56
1:A:109:MET:SD	1:A:123:MET:HE2	2.46	0.56
1:A:278:ARG:HA	1:A:278:ARG:NE	2.15	0.56
1:A:444:ALA:O	1:A:445:ASP:C	2.49	0.56
1:A:96:ASP:OD1	1:A:277:ARG:NH1	2.37	0.56
1:A:445:ASP:O	1:A:446:GLN:C	2.48	0.56
1:A:143:ILE:O	1:A:146:LEU:HB2	2.06	0.55
1:B:447:ILE:O	1:B:449:PRO:HD3	2.05	0.55
1:A:167:PRO:HG3	1:B:53:THR:HG22	1.89	0.55
1:A:204:LEU:HD22	1:B:94:ILE:HD13	1.89	0.55
1:B:400:ILE:HG22	1:B:439:SER:OG	2.06	0.55
1:A:7:TYR:CD2	1:A:47:ALA:HB2	2.42	0.55
1:A:7:TYR:CE2	1:A:47:ALA:HB2	2.41	0.55
1:A:38:TYR:HE2	1:A:74:VAL:HG22	1.72	0.55
1:A:299:SER:C	1:A:301:ARG:N	2.63	0.55
1:B:364:THR:HG22	1:B:365:PRO:O	2.07	0.55
1:B:447:ILE:HG13	1:B:448:TYR:CD2	2.42	0.55
1:B:44:HIS:CE1	1:B:115:MET:HE2	2.42	0.55
1:B:241:ILE:HG12	1:B:278:ARG:CG	2.35	0.55
1:B:321:HIS:HB3	2:B:500:3PG:P	2.46	0.54
1:B:270:ALA:O	1:B:274:THR:OG1	2.18	0.54
1:B:423:VAL:HG13	1:B:433:LEU:HD21	1.89	0.54
1:A:74:VAL:HA	1:A:80:LEU:O	2.06	0.54
1:A:443:ASP:HA	1:A:446:GLN:HG3	1.89	0.54
1:A:382:ASN:C	1:A:382:ASN:ND2	2.65	0.54
1:B:291:HIS:O	1:B:293:ALA:N	2.41	0.54
1:A:64:THR:HG22	1:A:68:ASP:OD1	2.08	0.53
1:B:142:ASN:OD1	1:B:142:ASN:C	2.51	0.53
1:B:272:ILE:HG21	1:B:315:GLN:NE2	2.23	0.53
1:B:296:SER:CB	1:B:299:SER:HB2	2.37	0.53
1:A:297:PRO:HG2	1:B:301:ARG:NH2	2.23	0.53
1:B:288:ARG:HB3	1:B:308:HIS:HE1	1.74	0.53
1:B:336:ASP:HA	1:B:339:ILE:HD12	1.90	0.53
1:A:168:LYS:O	1:A:196:GLN:NE2	2.40	0.53
1:A:186:GLY:HA2	1:A:408:ARG:HD2	1.90	0.53
2:A:500:3PG:O3	1:B:111:ASN:ND2	2.39	0.53
1:A:337:ARG:HE	1:A:341:TYR:HE1	1.55	0.53
1:B:336:ASP:O	1:B:337:ARG:C	2.49	0.53
1:B:412:GLN:OE1	1:B:432:GLU:HB2	2.09	0.53
1:A:296:SER:HB3	1:A:299:SER:H	1.73	0.53
1:A:424:LEU:O	1:A:428:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:VAL:HG13	1:B:302:GLY:HA3	1.91	0.53
1:B:372:ASN:HD21	1:B:374:LEU:HB2	1.74	0.53
1:A:290:GLY:HA3	1:B:110:GLY:O	2.09	0.52
1:A:397:PHE:HE2	1:A:410:LEU:HD12	1.74	0.52
1:A:104:PHE:O	1:A:108:THR:HB	2.08	0.52
1:A:450:GLY:O	1:A:453:LYS:HB3	2.09	0.52
1:B:128:VAL:CG2	1:B:133:ARG:HB2	2.37	0.52
1:A:200:PRO:HD2	1:B:88:ALA:O	2.10	0.52
1:A:392:ALA:HB1	1:A:396:ALA:CB	2.37	0.52
1:A:399:HIS:CE1	1:A:435:ARG:HB3	2.45	0.52
1:A:143:ILE:HD12	1:A:364:THR:HG21	1.92	0.52
1:A:451:TRP:CZ2	1:A:452:ARG:HG3	2.45	0.51
1:B:3:GLN:NE2	1:B:44:HIS:CB	2.67	0.51
1:B:3:GLN:HE22	1:B:47:ALA:HB3	1.76	0.51
1:B:153:PRO:HD2	1:B:157:GLY:HA2	1.93	0.51
1:B:169:LEU:HD13	1:B:196:GLN:HG2	1.91	0.51
1:B:164:ILE:HD12	1:B:164:ILE:H	1.74	0.51
1:A:168:LYS:HE2	1:A:194:GLU:HG2	1.91	0.51
1:B:101:ILE:HD11	1:B:311:MET:HG3	1.92	0.51
1:A:45:PHE:CB	1:A:115:MET:HE1	2.40	0.51
1:A:374:LEU:HB3	1:A:448:TYR:CE2	2.45	0.51
1:B:164:ILE:HD11	1:B:391:THR:HG23	1.91	0.51
1:A:247:VAL:O	1:A:251:PHE:HD2	1.94	0.51
1:A:285:HIS:NE2	1:A:321:HIS:NE2	2.59	0.51
1:A:321:HIS:CB	2:A:500:3PG:O3P	2.58	0.51
1:B:222:THR:CG2	1:B:224:GLU:HB2	2.35	0.51
1:B:385:ASN:HB2	1:B:387:ASN:ND2	2.26	0.51
1:A:194:GLU:HG3	1:A:195:PRO:CG	2.37	0.51
1:A:296:SER:CB	1:A:297:PRO:CD	2.86	0.51
1:B:87:VAL:O	1:B:92:ARG:NH2	2.43	0.51
1:A:285:HIS:NE2	1:A:321:HIS:HD2	2.09	0.50
1:B:341:TYR:O	1:B:345:GLN:HB2	2.11	0.50
1:A:344:THR:HA	1:A:362:ALA:CB	2.37	0.50
1:A:376:MET:HA	1:A:376:MET:CE	2.41	0.50
1:B:342:MET:HA	1:B:348:ALA:CB	2.41	0.50
1:A:72:TYR:CZ	1:A:82:LYS:HB3	2.46	0.50
1:A:87:VAL:HG11	1:A:132:TYR:HB2	1.93	0.50
1:A:96:ASP:HB3	1:A:98:LYS:H	1.77	0.50
1:B:30:MET:HB2	1:B:121:ALA:HB2	1.92	0.50
1:A:165:ILE:HG21	1:A:176:PHE:CE2	2.47	0.50
1:B:6:ARG:HG2	1:B:7:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ARG:HA	1:B:246:TYR:CE1	2.47	0.50
1:B:261:LEU:CD1	1:B:287:HIS:HB2	2.41	0.50
1:A:183:PHE:CE1	1:A:187:GLY:HA3	2.47	0.50
1:A:88:ALA:O	1:B:200:PRO:HD2	2.12	0.50
1:B:174:LYS:HB3	1:B:175:PRO:CD	2.39	0.50
1:B:443:ASP:O	1:B:447:ILE:N	2.39	0.49
1:A:306:PHE:HA	1:A:339:ILE:HG12	1.94	0.49
1:A:370:GLY:H	1:A:371:MET:HE3	1.77	0.49
1:A:141:VAL:HG13	1:A:145:ALA:CB	2.42	0.49
1:A:235:ASP:OD2	1:B:101:ILE:HG22	2.12	0.49
1:A:30:MET:HG2	1:A:31:LYS:N	2.27	0.49
1:A:169:LEU:HD11	1:A:195:PRO:HB2	1.93	0.49
1:B:6:ARG:HG2	1:B:7:TYR:CD2	2.46	0.49
1:B:444:ALA:O	1:B:445:ASP:C	2.55	0.49
1:A:433:LEU:O	1:A:436:ALA:HB3	2.12	0.49
1:B:261:LEU:HD11	1:B:287:HIS:HB2	1.93	0.49
1:A:50:SER:OG	1:A:69:ALA:CB	2.61	0.49
1:A:243:ARG:O	1:A:244:GLY:C	2.55	0.49
1:B:265:TYR:CE1	1:B:291:HIS:HA	2.48	0.49
1:A:437:PHE:HB3	1:A:451:TRP:CE3	2.48	0.49
1:A:119:GLU:O	1:A:301:ARG:NH2	2.46	0.49
1:A:261:LEU:HA	1:A:285:HIS:O	2.12	0.49
1:B:109:MET:HE1	1:B:123:MET:HE1	1.93	0.49
1:A:123:MET:HE3	1:A:307:VAL:CG1	2.35	0.49
1:A:262:VAL:CG1	1:A:272:ILE:HD13	2.43	0.49
1:B:247:VAL:O	1:B:251:PHE:CD1	2.65	0.49
1:A:6:ARG:HE	1:A:64:THR:CG2	2.25	0.48
1:A:416:ALA:HB2	1:A:426:TYR:CG	2.48	0.48
1:B:116:GLY:O	1:B:117:ASP:CB	2.60	0.48
1:A:8:VAL:HA	1:A:71:VAL:HB	1.93	0.48
1:A:452:ARG:O	1:A:455:LEU:HA	2.13	0.48
1:A:159:LEU:HD21	1:A:161:VAL:HG23	1.95	0.48
1:B:243:ARG:O	1:B:247:VAL:HG23	2.13	0.48
1:B:324:THR:HG23	1:B:325:MET:N	2.26	0.48
1:A:70:LEU:H	1:A:70:LEU:CD1	2.26	0.48
1:A:167:PRO:CG	1:B:53:THR:HG22	2.44	0.48
1:A:111:ASN:HB2	1:B:289:ALA:HA	1.96	0.48
1:B:447:ILE:HG13	1:B:448:TYR:CE2	2.49	0.48
1:B:376:MET:HA	1:B:376:MET:HE2	1.93	0.48
1:A:29:ILE:HD12	1:A:80:LEU:HD12	1.95	0.48
1:A:96:ASP:OD1	1:A:277:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:O	1:A:301:ARG:N	2.46	0.48
1:B:307:VAL:O	1:B:311:MET:HB2	2.14	0.48
1:A:296:SER:C	1:A:298:GLN:N	2.67	0.48
1:B:185:LEU:O	1:B:408:ARG:NH2	2.47	0.48
1:B:292:GLY:HA2	1:B:295:THR:HG22	1.96	0.48
1:A:447:ILE:HB	1:A:448:TYR:CD2	2.49	0.47
1:B:218:ALA:O	1:B:222:THR:HB	2.15	0.47
1:A:222:THR:CG2	1:A:224:GLU:H	2.27	0.47
1:A:297:PRO:O	1:A:298:GLN:HB2	2.13	0.47
1:B:8:VAL:HG23	1:B:43:ALA:HB2	1.97	0.47
1:B:50:SER:HB3	1:B:69:ALA:CB	2.45	0.47
1:B:109:MET:HE1	1:B:123:MET:CE	2.45	0.47
1:A:96:ASP:CB	1:A:98:LYS:HB2	2.43	0.47
1:A:65:ARG:O	1:A:65:ARG:CD	2.62	0.47
1:A:183:PHE:HE2	1:A:397:PHE:CE1	2.33	0.47
1:B:371:MET:SD	1:B:376:MET:HE2	2.55	0.46
1:A:6:ARG:HH21	1:A:64:THR:HG23	1.80	0.46
1:A:38:TYR:CE2	1:A:74:VAL:HG13	2.51	0.46
1:B:30:MET:HB2	1:B:121:ALA:CB	2.45	0.46
1:B:400:ILE:HG12	1:B:400:ILE:O	2.15	0.46
1:A:236:ASP:O	1:A:239:GLU:HB3	2.15	0.46
1:B:166:LYS:HG2	1:B:167:PRO:HA	1.97	0.46
1:A:130:GLU:O	1:A:130:GLU:HG2	2.14	0.46
1:A:205:ARG:HA	1:A:246:TYR:CE2	2.50	0.46
1:B:344:THR:HA	1:B:362:ALA:HB1	1.97	0.46
1:B:372:ASN:ND2	1:B:374:LEU:H	2.06	0.46
1:B:411:ARG:O	1:B:414:TRP:HB3	2.16	0.46
1:A:16:ASP:O	1:A:20:GLY:N	2.49	0.46
1:A:94:ILE:HD12	1:B:205:ARG:NH1	2.31	0.46
1:A:371:MET:HB2	1:A:376:MET:HE3	1.96	0.46
1:B:306:PHE:HZ	1:B:342:MET:HE3	1.80	0.46
1:A:431:LYS:HB2	1:A:432:GLU:OE1	2.15	0.46
1:A:6:ARG:NH2	1:A:64:THR:HG23	2.31	0.46
1:A:289:ALA:O	1:B:111:ASN:HA	2.14	0.46
1:B:81:THR:HG22	1:B:83:ILE:HD11	1.98	0.46
1:B:254:ASN:O	1:B:257:HIS:HB2	2.16	0.46
1:A:18:ILE:HG23	1:A:127:TYR:CZ	2.50	0.46
1:A:427:ALA:O	1:A:434:ALA:HB2	2.16	0.45
1:B:50:SER:HB3	1:B:69:ALA:HB2	1.98	0.45
1:B:400:ILE:HD13	1:B:435:ARG:NH2	2.31	0.45
1:A:25:LEU:HD12	1:A:84:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:O	1:A:243:ARG:HG3	2.15	0.45
1:A:246:TYR:O	1:A:250:THR:OG1	2.29	0.45
1:A:75:ASP:OD1	1:A:78:ARG:NH1	2.49	0.45
1:B:276:ARG:HB2	1:B:284:LEU:CD1	2.46	0.45
1:A:295:THR:HG23	1:A:305:ALA:CA	2.46	0.45
1:B:169:LEU:HD11	1:B:196:GLN:HA	1.97	0.45
1:B:174:LYS:CB	1:B:175:PRO:CD	2.94	0.45
1:A:113:GLN:OE1	1:A:121:ALA:O	2.35	0.45
1:A:455:LEU:HA	1:A:455:LEU:HD12	1.75	0.45
1:B:33:LYS:O	1:B:34:ALA:C	2.60	0.45
1:B:7:TYR:O	1:B:70:LEU:HA	2.16	0.45
1:B:168:LYS:HG3	1:B:193:ASP:CG	2.42	0.45
1:B:448:TYR:O	1:B:451:TRP:HB3	2.16	0.45
1:A:294:VAL:CG1	1:A:295:THR:N	2.78	0.45
1:B:272:ILE:HG21	1:B:315:GLN:HE21	1.82	0.45
1:B:168:LYS:HG2	1:B:169:LEU:HD22	1.99	0.45
1:B:209:ALA:HA	1:B:250:THR:HG21	1.99	0.45
1:B:295:THR:O	1:B:296:SER:C	2.58	0.45
1:B:276:ARG:HB2	1:B:284:LEU:HD12	1.99	0.45
1:B:162:GLY:CA	1:B:189:PHE:O	2.61	0.44
1:A:291:HIS:H	1:A:291:HIS:HD2	1.47	0.44
1:A:431:LYS:H	1:A:431:LYS:HG3	1.39	0.44
1:A:38:TYR:HE2	1:A:74:VAL:CG2	2.30	0.44
1:A:295:THR:CG2	1:A:305:ALA:HB2	2.46	0.44
1:A:337:ARG:NE	1:A:341:TYR:HE1	2.15	0.44
1:A:357:TRP:O	1:A:358:GLY:C	2.59	0.44
1:A:367:ILE:HG22	1:A:390:LEU:HD12	1.98	0.44
1:A:437:PHE:HB3	1:A:451:TRP:CZ3	2.52	0.44
1:B:343:LEU:HB3	1:B:363:CYS:O	2.17	0.44
1:B:375:ARG:O	1:B:376:MET:C	2.61	0.44
1:A:191:LYS:HE2	1:A:192:ASN:O	2.18	0.44
1:A:101:ILE:HD12	1:A:101:ILE:HA	1.97	0.44
1:B:101:ILE:HD11	1:B:311:MET:HG2	1.98	0.44
1:B:231:ASN:HD21	1:B:233:THR:HB	1.82	0.44
1:A:294:VAL:HG12	1:A:295:THR:H	1.81	0.44
1:A:51:THR:HG22	1:B:169:LEU:O	2.18	0.43
1:A:128:VAL:HA	1:A:129:PRO:HD3	1.71	0.43
1:A:208:ILE:HG21	1:A:247:VAL:HG22	2.00	0.43
1:A:421:VAL:CG1	1:A:426:TYR:HB2	2.48	0.43
1:B:193:ASP:O	1:B:194:GLU:C	2.60	0.43
1:A:76:GLU:H	1:A:76:GLU:HG2	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:N	1:B:115:MET:HE1	2.33	0.43
1:B:273:THR:HG22	1:B:273:THR:O	2.18	0.43
1:B:322:THR:HG21	1:B:365:PRO:HB3	2.01	0.43
1:B:376:MET:CB	1:B:377:PRO:CD	2.89	0.43
1:B:104:PHE:CD2	1:B:104:PHE:C	2.96	0.43
1:B:165:ILE:HD13	1:B:165:ILE:HA	1.94	0.43
1:B:444:ALA:O	1:B:448:TYR:N	2.50	0.43
1:A:80:LEU:HD21	1:A:82:LYS:HE3	2.01	0.43
1:A:172:ARG:HB3	1:A:173:PRO:HD2	2.00	0.43
1:B:93:ASN:ND2	1:B:96:ASP:HB2	2.16	0.43
1:B:138:GLY:HA2	1:B:313:ARG:O	2.18	0.43
1:B:336:ASP:HA	1:B:339:ILE:CB	2.47	0.43
1:A:98:LYS:HG3	1:A:135:LEU:O	2.19	0.43
1:A:191:LYS:HD2	1:A:285:HIS:HE1	1.82	0.43
1:B:195:PRO:O	1:B:196:GLN:C	2.61	0.43
1:B:436:ALA:O	1:B:439:SER:N	2.51	0.43
1:A:65:ARG:O	1:A:65:ARG:CG	2.66	0.43
1:A:163:THR:HG23	1:A:397:PHE:CD1	2.52	0.43
1:B:120:TYR:HB2	1:B:300:LYS:O	2.18	0.43
1:A:288:ARG:NE	1:A:291:HIS:HE1	2.17	0.43
1:A:101:ILE:HD11	1:A:311:MET:HG2	2.01	0.42
1:B:45:PHE:CA	1:B:115:MET:HE1	2.49	0.42
1:B:296:SER:HA	1:B:297:PRO:HD3	1.62	0.42
1:A:222:THR:HG23	1:A:224:GLU:HG3	2.01	0.42
1:A:337:ARG:HD2	1:A:382:ASN:HD21	1.84	0.42
1:B:159:LEU:HD12	1:B:160:VAL:N	2.34	0.42
1:A:168:LYS:HB2	1:A:193:ASP:OD1	2.19	0.42
1:A:337:ARG:O	1:A:337:ARG:HG2	2.18	0.42
1:B:379:PHE:O	1:B:383:LEU:HB3	2.19	0.42
2:A:500:3PG:O3	1:B:111:ASN:OD1	2.34	0.42
1:B:109:MET:SD	1:B:123:MET:HE2	2.59	0.42
1:A:45:PHE:CA	1:A:115:MET:HE1	2.50	0.42
1:A:397:PHE:O	1:A:398:GLY:C	2.63	0.42
1:B:184:TRP:CG	1:B:226:LYS:HD3	2.55	0.42
1:A:150:LEU:CG	1:A:227:LEU:HD11	2.48	0.42
1:B:374:LEU:HD22	1:B:448:TYR:CD2	2.55	0.42
1:B:451:TRP:O	1:B:455:LEU:HB2	2.19	0.42
1:A:8:VAL:HG21	1:A:39:VAL:CG1	2.50	0.42
1:A:320:ILE:O	1:A:321:HIS:C	2.63	0.42
1:A:402:GLY:O	1:A:406:GLY:N	2.52	0.42
1:B:261:LEU:HD11	1:B:287:HIS:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:THR:O	1:B:277:ARG:HG3	2.19	0.42
1:A:50:SER:HB3	1:A:51:THR:H	1.59	0.42
1:A:103:SER:O	1:A:104:PHE:C	2.62	0.42
1:B:367:ILE:HG12	1:B:379:PHE:HZ	1.85	0.42
1:A:152:ARG:HB3	1:A:153:PRO:CD	2.48	0.42
1:B:372:ASN:OD1	1:B:375:ARG:NH1	2.52	0.42
1:B:103:SER:O	1:B:107:LEU:HB2	2.20	0.41
1:B:168:LYS:HG3	1:B:193:ASP:OD2	2.19	0.41
1:B:372:ASN:O	1:B:376:MET:HE3	2.20	0.41
1:B:424:LEU:HD23	1:B:454:ALA:CB	2.50	0.41
1:A:399:HIS:HE1	1:A:435:ARG:HB3	1.85	0.41
1:B:3:GLN:HE21	1:B:44:HIS:CG	2.38	0.41
1:B:334:SER:O	1:B:338:ALA:HB3	2.20	0.41
1:A:300:LYS:H	1:A:300:LYS:HG2	1.48	0.41
1:B:41:THR:HG22	1:B:118:VAL:HG22	2.03	0.41
1:B:291:HIS:NE2	1:B:295:THR:HG21	2.34	0.41
1:A:191:LYS:HD2	1:A:285:HIS:CE1	2.55	0.41
2:A:500:3PG:HO3	1:B:111:ASN:CG	2.28	0.41
1:B:433:LEU:HD12	1:B:433:LEU:HA	1.97	0.41
1:B:286:TYR:C	1:B:286:TYR:CD1	2.98	0.41
1:A:45:PHE:HA	1:A:115:MET:HE1	2.02	0.41
1:B:24:VAL:HG21	1:B:90:PHE:CE1	2.56	0.41
1:A:25:LEU:HD22	1:A:127:TYR:HD1	1.86	0.41
1:A:31:LYS:HA	1:A:32:PRO:HD3	1.88	0.41
1:A:85:TYR:O	1:A:86:PRO:C	2.60	0.41
1:A:126:PHE:CD1	1:A:307:VAL:HG13	2.56	0.41
1:A:319:GLY:HA2	1:A:364:THR:O	2.20	0.41
1:B:152:ARG:HB3	1:B:153:PRO:CD	2.51	0.41
1:B:183:PHE:C	1:B:185:LEU:H	2.29	0.41
1:B:336:ASP:HA	1:B:339:ILE:CG1	2.51	0.41
1:B:456:GLY:O	1:B:457:VAL:CB	2.63	0.41
1:A:31:LYS:O	1:A:119:GLU:HB2	2.20	0.41
1:A:143:ILE:HB	1:A:364:THR:OG1	2.20	0.41
1:A:148:LYS:HB2	1:A:154:GLU:HG2	2.03	0.41
1:A:261:LEU:HD11	1:A:287:HIS:HB2	2.02	0.41
1:B:244:GLY:HA3	1:B:279:PHE:CZ	2.56	0.41
1:A:139:PRO:HD3	1:A:313:ARG:O	2.21	0.40
1:B:159:LEU:HD12	1:B:160:VAL:H	1.86	0.40
1:B:184:TRP:HB3	1:B:226:LYS:HD3	2.03	0.40
1:B:201:PHE:CD2	1:B:201:PHE:C	2.99	0.40
1:A:336:ASP:HA	1:A:339:ILE:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:NE	1:A:341:TYR:CE1	2.88	0.40
1:A:434:ALA:O	1:A:437:PHE:HB2	2.21	0.40
1:B:41:THR:HG23	1:B:117:ASP:O	2.21	0.40
1:B:45:PHE:HA	1:B:115:MET:HE1	2.03	0.40
1:B:109:MET:HE2	1:B:109:MET:HB2	1.86	0.40
1:B:128:VAL:C	1:B:129:PRO:O	2.64	0.40
1:B:286:TYR:HB2	1:B:317:ALA:HB1	2.04	0.40
1:A:146:LEU:HD22	1:A:227:LEU:HD22	2.03	0.40
1:A:165:ILE:HD11	1:A:190:ILE:HG21	2.02	0.40
1:A:289:ALA:O	1:B:110:GLY:C	2.63	0.40
1:A:307:VAL:O	1:A:311:MET:HB2	2.22	0.40
1:B:265:TYR:CZ	1:B:291:HIS:HA	2.56	0.40
1:B:366:ILE:HD13	1:B:366:ILE:HG21	1.85	0.40
1:A:64:THR:HA	1:A:68:ASP:CG	2.47	0.40
1:A:140:SER:OG	1:A:280:PRO:O	2.37	0.40
1:A:278:ARG:HE	1:A:278:ARG:CA	2.09	0.40
1:B:172:ARG:HE	1:B:172:ARG:HB3	1.61	0.40
1:B:193:ASP:C	1:B:195:PRO:CD	2.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ASP:OD2	1:A:408:ARG:NH2[2_646]	1.89	0.31
1:A:358:GLY:O	1:A:431:LYS:CD[2_646]	2.07	0.13

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	431/490 (88%)	374 (87%)	38 (9%)	19 (4%)	2 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	429/490 (88%)	365 (85%)	46 (11%)	18 (4%)	2	9
All	All	860/980 (88%)	739 (86%)	84 (10%)	37 (4%)	2	8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	298	GLN
1	A	372	ASN
1	B	4	SER
1	B	5	SER
1	B	34	ALA
1	B	50	SER
1	B	110	GLY
1	B	291	HIS
1	B	292	GLY
1	A	252	GLY
1	A	335	SER
1	A	431	LYS
1	A	455	LEU
1	B	117	ASP
1	B	335	SER
1	B	423	VAL
1	A	300	LYS
1	A	446	GLN
1	B	49	SER
1	B	184	TRP
1	A	10	LEU
1	A	34	ALA
1	A	115	MET
1	A	119	GLU
1	A	184	TRP
1	A	290	GLY
1	A	297	PRO
1	B	9	ASN
1	B	195	PRO
1	A	444	ALA
1	A	456	GLY
1	B	79	GLU
1	B	393	GLY
1	B	129	PRO
1	B	194	GLU

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Mol	Chain	Res	Type
1	A	296	SER

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	330/376 (88%)	251 (76%)	79 (24%)	1	3
1	B	327/376 (87%)	266 (81%)	61 (19%)	1	5
All	All	657/752 (87%)	517 (79%)	140 (21%)	1	4

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

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	SER
1	A	8	VAL
1	A	22	GLU
1	A	25	LEU
1	A	29	ILE
1	A	30	MET
1	A	31	LYS
1	A	33	LYS
1	A	45	PHE
1	A	50	SER
1	A	64	THR
1	A	65	ARG
1	A	70	LEU
1	A	74	VAL
1	A	76	GLU
1	A	92	ARG
1	A	98	LYS
1	A	105	LEU
1	A	106	THR
1	A	107	LEU
1	A	109	MET

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	118	VAL
1	A	119	GLU
1	A	122	LYS
1	A	133	ARG
1	A	141	VAL
1	A	155	VAL
1	A	161	VAL
1	A	163	THR
1	A	168	LYS
1	A	171	LEU
1	A	174	LYS
1	A	190	ILE
1	A	191	LYS
1	A	192	ASN
1	A	196	GLN
1	A	210	LEU
1	A	222	THR
1	A	224	GLU
1	A	226	LYS
1	A	231	ASN
1	A	266	VAL
1	A	272	ILE
1	A	278	ARG
1	A	284	LEU
1	A	288	ARG
1	A	291	HIS
1	A	294	VAL
1	A	296	SER
1	A	298	GLN
1	A	300	LYS
1	A	301	ARG
1	A	311	MET
1	A	320	ILE
1	A	322	THR
1	A	324	THR
1	A	325	MET
1	A	334	SER
1	A	336	ASP
1	A	337	ARG
1	A	344	THR
1	A	356	SER

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Mol	Chain	Res	Type
1	A	361	LYS
1	A	371	MET
1	A	375	ARG
1	A	376	MET
1	A	382	ASN
1	A	408	ARG
1	A	428	ARG
1	A	431	LYS
1	A	432	GLU
1	A	435	ARG
1	A	443	ASP
1	A	445	ASP
1	A	446	GLN
1	A	447	ILE
1	A	448	TYR
1	B	8	VAL
1	B	10	LEU
1	B	15	GLU
1	B	29	ILE
1	B	30	MET
1	B	49	SER
1	B	73	GLU
1	B	76	GLU
1	B	106	THR
1	B	107	LEU
1	B	111	ASN
1	B	112	ASN
1	B	113	GLN
1	B	115	MET
1	B	117	ASP
1	B	119	GLU
1	B	130	GLU
1	B	141	VAL
1	B	163	THR
1	B	164	ILE
1	B	169	LEU
1	B	172	ARG
1	B	174	LYS
1	B	178	GLU
1	B	192	ASN
1	B	201	PHE
1	B	205	ARG

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Mol	Chain	Res	Type
1	B	222	THR
1	B	226	LYS
1	B	227	LEU
1	B	258	VAL
1	B	261	LEU
1	B	266	VAL
1	B	288	ARG
1	B	295	THR
1	B	301	ARG
1	B	320	ILE
1	B	322	THR
1	B	324	THR
1	B	325	MET
1	B	337	ARG
1	B	345	GLN
1	B	354	ARG
1	B	367	ILE
1	B	371	MET
1	B	376	MET
1	B	381	GLU
1	B	382	ASN
1	B	391	THR
1	B	400	ILE
1	B	404	VAL
1	B	422	PRO
1	B	424	LEU
1	B	431	LYS
1	B	443	ASP
1	B	446	GLN
1	B	447	ILE
1	B	452	ARG
1	B	453	LYS
1	B	455	LEU
1	B	457	VAL

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

Mol	Chain	Res	Type
1	A	93	ASN
1	A	111	ASN
1	A	291	HIS
1	A	298	GLN

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Mol	Chain	Res	Type
1	A	382	ASN
1	A	385	ASN
1	A	415	GLN
1	B	3	GLN
1	B	9	ASN
1	B	93	ASN
1	B	111	ASN
1	B	231	ASN
1	B	315	GLN
1	B	345	GLN
1	B	372	ASN
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](#)

2 ligands are modelled in this entry.

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	3PG	B	500	-	9,10,10	1.97	3 (33%)	11,14,14	2.34	4 (36%)
2	3PG	A	500	-	9,10,10	3.70	6 (66%)	11,14,14	3.50	9 (81%)

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	3PG	B	500	-	-	7/10/10/10	-
2	3PG	A	500	-	-	7/10/10/10	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	3PG	P-O1P	8.30	1.86	1.60
2	A	500	3PG	P-O2P	3.88	1.62	1.50
2	A	500	3PG	O1P-C3	3.88	1.59	1.44
2	B	500	3PG	P-O2P	3.47	1.61	1.50
2	A	500	3PG	O1-C1	2.97	1.30	1.22
2	B	500	3PG	O1-C1	2.68	1.30	1.22
2	A	500	3PG	P-O4P	2.67	1.64	1.54
2	A	500	3PG	P-O3P	2.27	1.63	1.54
2	B	500	3PG	O1P-C3	-2.06	1.36	1.44

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	3PG	O2-C1-C2	5.68	124.74	112.74
2	B	500	3PG	O1P-C3-C2	5.28	122.81	107.96
2	A	500	3PG	O1P-C3-C2	4.76	121.36	107.96
2	A	500	3PG	O3-C2-C1	-4.13	99.88	110.36
2	A	500	3PG	O1P-P-O2P	4.07	117.44	106.44
2	A	500	3PG	O3P-P-O1P	3.69	116.29	106.67
2	B	500	3PG	O2-C1-C2	3.54	120.23	112.74
2	A	500	3PG	O2-C1-O1	-2.72	117.90	124.08
2	A	500	3PG	O1-C1-C2	-2.64	117.32	122.60
2	A	500	3PG	O4P-P-O1P	2.64	113.55	106.67
2	A	500	3PG	O4P-P-O2P	-2.37	101.61	110.83
2	B	500	3PG	O2-C1-O1	-2.35	118.75	124.08
2	B	500	3PG	O4P-P-O1P	2.05	112.01	106.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	3PG	O1-C1-C2-O3
2	A	500	3PG	O2-C1-C2-O3
2	A	500	3PG	C1-C2-C3-O1P
2	A	500	3PG	O3-C2-C3-O1P
2	B	500	3PG	C2-C3-O1P-P
2	B	500	3PG	C3-O1P-P-O2P
2	B	500	3PG	C3-O1P-P-O3P
2	B	500	3PG	C3-O1P-P-O4P
2	A	500	3PG	O1-C1-C2-C3
2	A	500	3PG	O2-C1-C2-C3
2	B	500	3PG	O1-C1-C2-C3
2	B	500	3PG	O2-C1-C2-O3
2	A	500	3PG	C2-C3-O1P-P
2	B	500	3PG	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	3PG	5	0
2	A	500	3PG	8	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.