



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:54 AM UTC

PDB ID : 1PVD / pdb_00001pvd
Title : CRYSTAL STRUCTURE OF THE THIAMIN DIPHOSPHATE DEPENDENT ENZYME PYRUVATE DECARBOXYLASE FROM THE YEAST SACCHAROMYCES CEREVISIAE AT 2.3 ANGSTROMS RESOLUTION
Authors : Furey, W.; Arjunan, P.
Deposited on : 1995-04-20
Resolution : 2.30 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

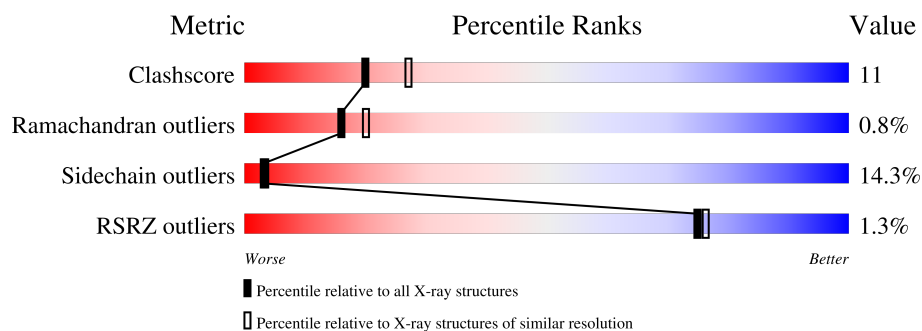
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	555	2% 44% 36% 13% • •
1	B	555	2% 43% 38% 12% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8753 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 PYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			
1	B	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			

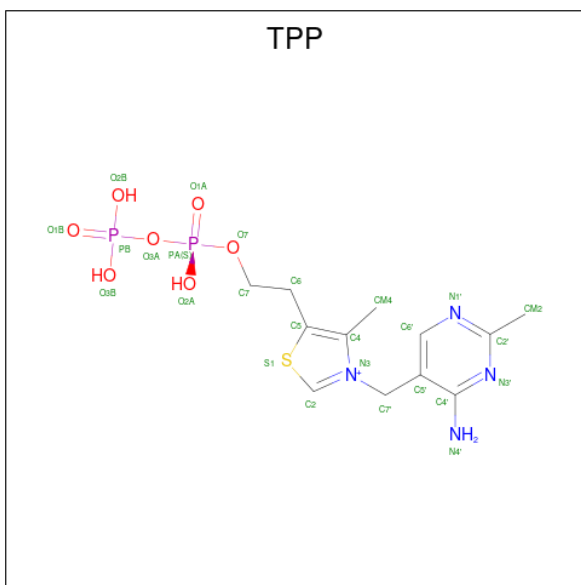
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	ARG	conflict	UNP P06169
A	143	ALA	CYS	conflict	UNP P06169
A	206	ALA	VAL	conflict	UNP P06169
A	208	VAL	ALA	conflict	UNP P06169
A	538	ILE	VAL	conflict	UNP P06169
A	551	LYS	GLU	conflict	UNP P06169
B	55	ALA	ARG	conflict	UNP P06169
B	143	ALA	CYS	conflict	UNP P06169
B	206	ALA	VAL	conflict	UNP P06169
B	208	VAL	ALA	conflict	UNP P06169
B	538	ILE	VAL	conflict	UNP P06169
B	551	LYS	GLU	conflict	UNP P06169

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
3	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

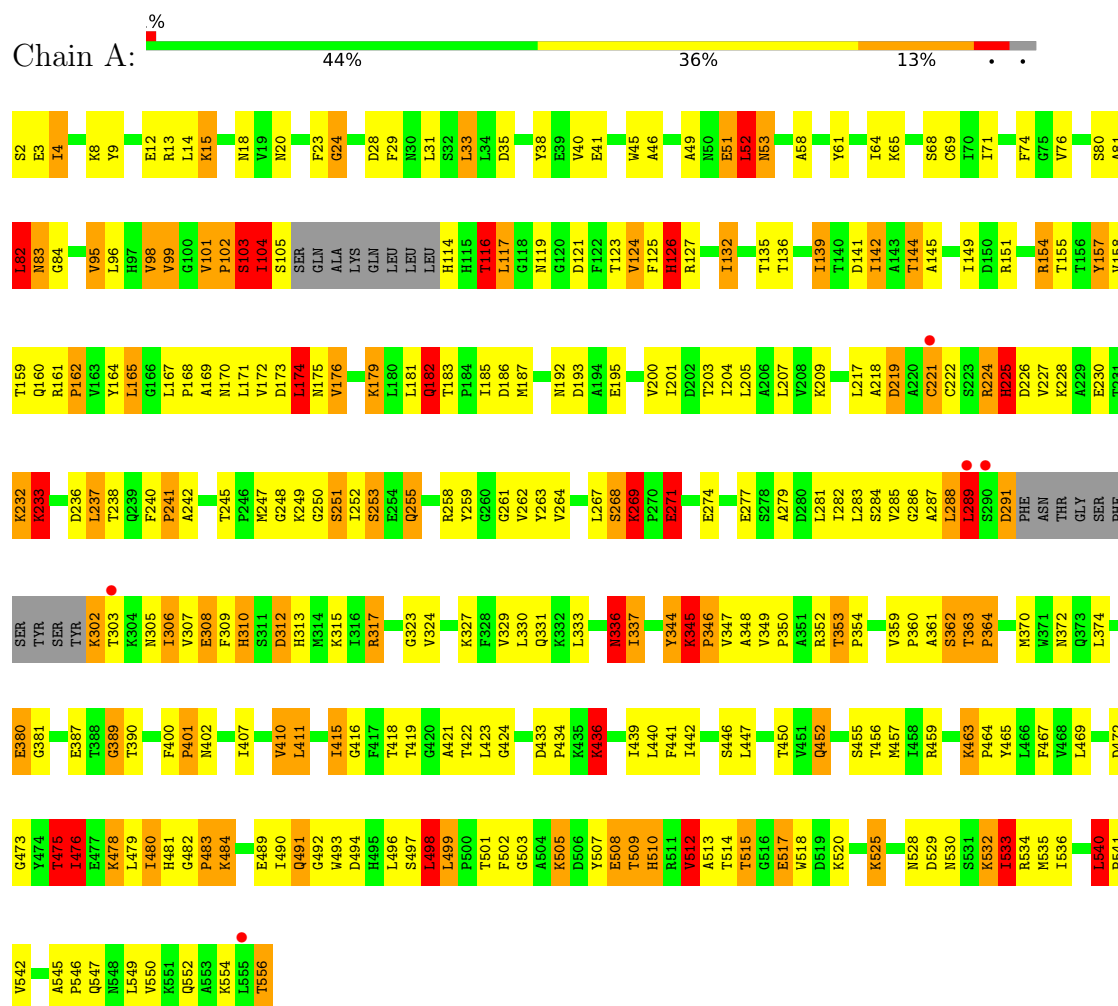
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	235	Total O 235 235	0	0
4	B	204	Total O 204 204	0	0

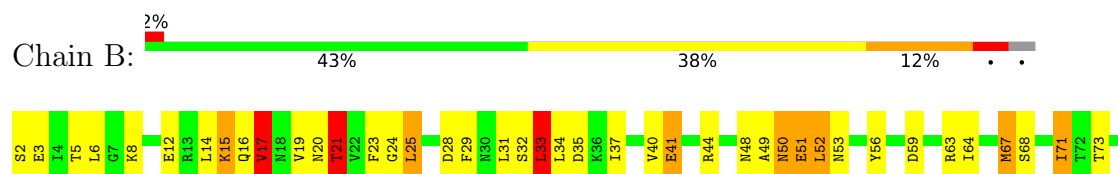
3 Residue-property plots

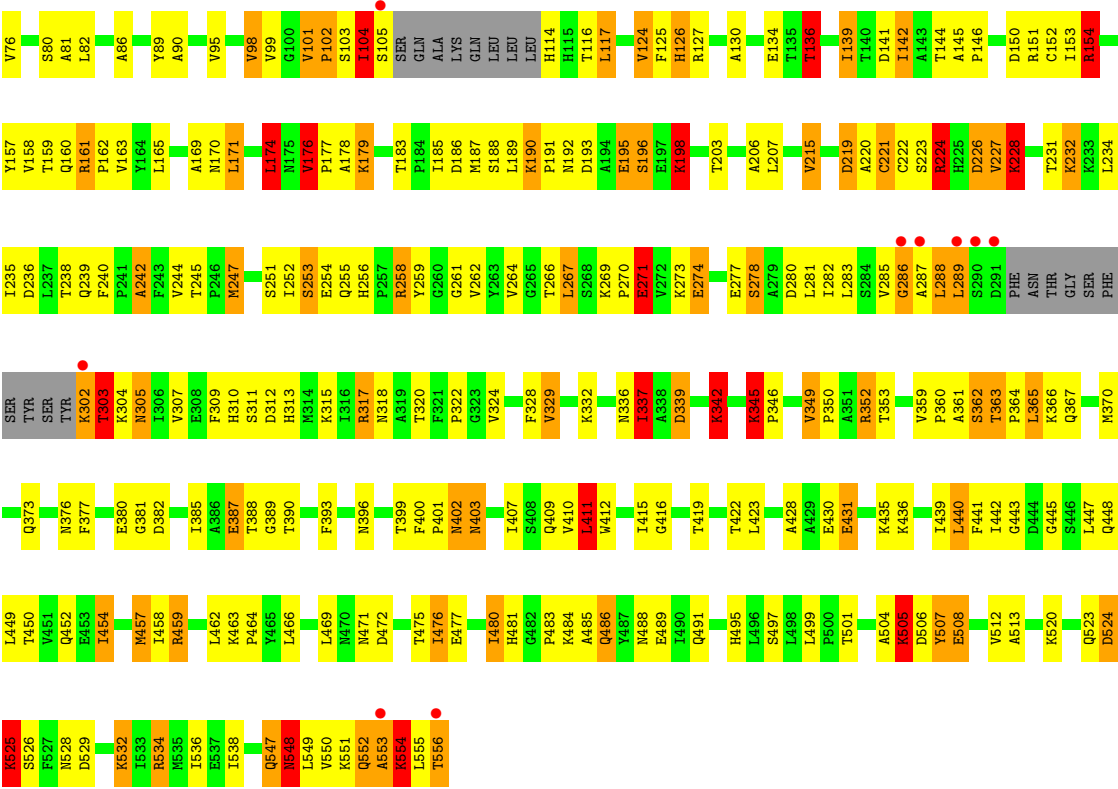
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PYRUVATE DECARBOXYLASE



• Molecule 1: PYRUVATE DECARBOXYLASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.06Å 74.75Å 120.32Å 90.00° 116.58° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (10.00-2.30) 91.8 (10.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	GPRLSA, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available) 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.6	EDS
L-test for twinning ¹	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	12/4215 (0.3%)	2.61	355/5728 (6.2%)
1	B	1.35	7/4215 (0.2%)	2.63	363/5728 (6.3%)
All	All	1.37	19/8430 (0.2%)	2.62	718/11456 (6.3%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	ILE	C-O	7.67	1.33	1.24
1	A	416	GLY	N-CA	7.14	1.55	1.45
1	B	89	TYR	N-CA	6.46	1.54	1.46
1	B	471	ASN	CB-CG	6.40	1.68	1.52
1	A	24	GLY	N-CA	6.11	1.53	1.44
1	A	176	VAL	C-O	5.97	1.29	1.24
1	A	49	ALA	N-CA	5.94	1.54	1.46
1	A	76	VAL	C-O	5.73	1.30	1.24
1	A	176	VAL	N-CA	5.73	1.51	1.46
1	B	440	LEU	N-CA	5.61	1.52	1.45
1	A	535	MET	N-CA	5.60	1.52	1.46
1	A	204	ILE	N-CA	5.53	1.53	1.46
1	A	205	LEU	N-CA	5.29	1.52	1.46
1	B	253	SER	CB-OG	5.22	1.52	1.42
1	B	345	LYS	N-CA	5.19	1.52	1.45
1	A	360	PRO	C-N	-5.14	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	101	VAL	C-O	5.07	1.30	1.24
1	B	459	ARG	CZ-NH1	5.04	1.39	1.32
1	A	132	ILE	CA-CB	5.02	1.61	1.54

All (718) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	459	ARG	CD-NE-CZ	18.57	150.40	124.40
1	A	101	VAL	N-CA-CB	-17.52	99.74	111.83
1	A	114	HIS	CA-CB-CG	17.07	130.87	113.80
1	B	403	ASN	OD1-CG-ND2	15.90	138.50	122.60
1	A	176	VAL	N-CA-CB	-15.04	95.33	111.87
1	B	459	ARG	CA-CB-CG	13.28	140.66	114.10
1	B	227	VAL	N-CA-CB	-11.99	96.57	112.16
1	A	533	ILE	CB-CA-C	-11.93	94.82	111.28
1	B	285	VAL	CA-C-O	11.68	135.38	120.78
1	B	286	GLY	O-C-N	11.62	133.50	122.92
1	B	258	ARG	NE-CZ-NH2	-11.53	108.83	119.20
1	A	176	VAL	CB-CA-C	11.37	122.17	109.89
1	B	534	ARG	NE-CZ-NH1	-11.33	110.17	121.50
1	A	528	ASN	CA-CB-CG	-11.12	101.48	112.60
1	A	18	ASN	N-CA-C	11.06	126.66	111.39
1	A	424	GLY	CA-C-O	-10.82	109.19	120.66
1	A	102	PRO	CA-C-N	10.80	142.16	121.54
1	A	102	PRO	C-N-CA	10.80	142.16	121.54
1	B	17	VAL	CA-CB-CG1	10.80	128.75	110.40
1	A	95	VAL	CA-C-O	-10.79	109.06	120.39
1	A	141	ASP	CA-C-O	-10.75	108.39	120.32
1	A	546	PRO	CB-CA-C	10.71	124.42	111.46
1	B	176	VAL	N-CA-CB	-10.68	100.12	111.87
1	A	288	LEU	N-CA-C	-10.41	100.64	113.97
1	B	228	LYS	CA-C-O	-10.32	109.98	120.82
1	A	415	ILE	CA-C-O	-10.26	107.96	120.78
1	B	342	LYS	N-CA-CB	10.20	127.73	110.49
1	B	403	ASN	N-CA-CB	-10.14	96.73	111.84
1	B	20	ASN	OD1-CG-ND2	-10.11	112.49	122.60
1	A	515	THR	N-CA-CB	-10.11	94.88	109.94
1	A	533	ILE	CA-CB-CG2	10.02	127.54	110.50
1	B	71	ILE	CA-C-O	-10.01	109.88	120.39
1	A	317	ARG	CD-NE-CZ	9.97	138.35	124.40
1	B	227	VAL	CB-CA-C	9.94	123.78	111.65
1	A	317	ARG	NE-CZ-NH2	-9.86	110.33	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	526	SER	CA-CB-OG	-9.86	91.39	111.10
1	A	195	GLU	CA-C-O	-9.80	110.03	120.42
1	A	127	ARG	CD-NE-CZ	-9.77	110.72	124.40
1	B	176	VAL	CB-CA-C	9.57	120.22	109.89
1	A	410	VAL	N-CA-C	9.32	119.36	110.42
1	A	23	PHE	CA-CB-CG	-9.27	104.53	113.80
1	B	345	LYS	CB-CA-C	9.23	119.31	110.17
1	B	17	VAL	N-CA-CB	-9.19	96.64	112.08
1	B	141	ASP	CA-C-O	-9.17	110.14	120.32
1	B	459	ARG	NE-CZ-NH1	9.14	130.64	121.50
1	B	136	THR	N-CA-CB	-9.12	95.81	111.69
1	B	151	ARG	NE-CZ-NH2	-9.12	111.00	119.20
1	B	336	ASN	CB-CA-C	-9.10	92.96	109.15
1	B	171	LEU	N-CA-C	9.07	122.15	111.71
1	A	501	THR	CA-CB-CG2	9.06	125.91	110.50
1	B	401	PRO	N-CA-C	-9.04	98.56	111.22
1	A	400	PHE	CA-CB-CG	9.01	122.81	113.80
1	A	237	LEU	N-CA-CB	-8.91	96.58	110.30
1	A	472	ASP	N-CA-C	8.90	122.14	111.02
1	A	525	LYS	CA-C-O	-8.85	111.04	120.42
1	A	269	LYS	N-CA-C	-8.84	98.60	109.83
1	B	51	GLU	CB-CG-CD	8.84	127.62	112.60
1	A	45	TRP	CA-C-O	-8.83	110.54	120.43
1	A	418	THR	N-CA-C	8.81	121.84	111.71
1	B	547	GLN	OE1-CD-NE2	8.76	131.35	122.60
1	A	287	ALA	CA-C-N	8.72	136.42	122.11
1	A	287	ALA	C-N-CA	8.72	136.42	122.11
1	A	3	GLU	CA-C-O	-8.64	111.04	121.06
1	A	441	PHE	CA-CB-CG	-8.63	105.17	113.80
1	A	157	TYR	CA-C-O	-8.62	111.77	120.82
1	B	407	ILE	CA-C-N	8.57	135.40	121.86
1	B	407	ILE	C-N-CA	8.57	135.40	121.86
1	B	236	ASP	O-C-N	8.44	132.09	122.22
1	A	95	VAL	O-C-N	8.42	132.36	123.26
1	A	175	ASN	CA-CB-CG	-8.42	104.18	112.60
1	A	317	ARG	NE-CZ-NH1	8.39	129.89	121.50
1	B	486	GLN	CA-C-O	-8.38	111.58	120.63
1	B	349	VAL	N-CA-CB	-8.37	99.50	111.21
1	A	124	VAL	CA-C-O	-8.36	112.57	121.27
1	B	274	GLU	CA-CB-CG	8.34	130.78	114.10
1	A	344	TYR	CA-C-O	8.33	130.39	120.81
1	A	360	PRO	CA-C-N	8.31	134.01	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	PRO	C-N-CA	8.31	134.01	120.63
1	B	50	ASN	CA-CB-CG	8.29	120.89	112.60
1	A	82	LEU	N-CA-C	8.25	121.31	111.33
1	A	168	PRO	CA-C-O	-8.25	112.04	121.36
1	A	219	ASP	CA-CB-CG	8.22	120.82	112.60
1	B	127	ARG	NE-CZ-NH2	8.18	126.56	119.20
1	B	342	LYS	CA-CB-CG	8.17	130.45	114.10
1	B	178	ALA	CA-C-N	8.16	131.55	120.38
1	B	178	ALA	C-N-CA	8.16	131.55	120.38
1	B	524	ASP	CA-C-N	8.15	131.55	120.54
1	B	524	ASP	C-N-CA	8.15	131.55	120.54
1	B	475	THR	CA-C-O	-8.14	112.27	120.82
1	A	226	ASP	CA-CB-CG	8.14	120.74	112.60
1	A	127	ARG	O-C-N	8.12	130.73	122.12
1	A	331	GLN	OE1-CD-NE2	-8.12	114.48	122.60
1	A	514	THR	CA-C-O	8.10	130.56	121.40
1	B	403	ASN	CA-CB-CG	-8.09	104.51	112.60
1	B	339	ASP	CA-CB-CG	8.09	120.69	112.60
1	B	261	GLY	CA-C-N	8.07	133.50	122.93
1	B	261	GLY	C-N-CA	8.07	133.50	122.93
1	A	46	ALA	CA-C-O	-8.05	111.89	120.42
1	A	262	VAL	CA-C-O	8.03	129.34	120.59
1	A	374	LEU	N-CA-C	7.98	121.97	111.75
1	A	515	THR	OG1-CB-CG2	7.97	125.24	109.30
1	A	456	THR	CA-CB-OG1	-7.96	97.66	109.60
1	B	439	ILE	CA-C-N	-7.95	110.33	122.81
1	B	439	ILE	C-N-CA	-7.95	110.33	122.81
1	B	161	ARG	NE-CZ-NH2	-7.94	112.05	119.20
1	A	259	TYR	CA-C-O	-7.93	111.65	120.69
1	B	6	LEU	CA-C-O	-7.89	111.18	120.10
1	B	459	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	B	277	GLU	CA-C-N	7.85	134.03	120.68
1	B	277	GLU	C-N-CA	7.85	134.03	120.68
1	B	534	ARG	NE-CZ-NH2	7.85	126.26	119.20
1	A	245	THR	N-CA-C	-7.84	100.90	110.31
1	A	514	THR	CA-C-N	7.84	131.13	120.54
1	A	514	THR	C-N-CA	7.84	131.13	120.54
1	B	245	THR	N-CA-C	-7.81	100.94	110.31
1	B	486	GLN	CB-CG-CD	7.81	125.87	112.60
1	A	489	GLU	CA-C-O	-7.79	112.13	121.56
1	A	8	LYS	CA-C-N	7.79	131.05	120.54
1	A	8	LYS	C-N-CA	7.79	131.05	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	525	LYS	O-C-N	7.79	131.03	122.15
1	B	125	PHE	CA-C-O	7.79	128.90	120.10
1	B	508	GLU	CA-C-O	-7.72	111.33	120.60
1	B	525	LYS	CB-CG-CD	7.72	129.05	111.30
1	A	258	ARG	NE-CZ-NH1	7.71	129.21	121.50
1	B	144	THR	CA-CB-OG1	-7.71	98.04	109.60
1	B	258	ARG	CD-NE-CZ	7.70	135.18	124.40
1	B	125	PHE	CA-C-N	7.69	130.44	120.44
1	B	125	PHE	C-N-CA	7.69	130.44	120.44
1	A	217	LEU	CA-C-O	-7.68	112.34	120.40
1	A	225	HIS	CA-CB-CG	-7.66	106.14	113.80
1	B	203	THR	CA-CB-OG1	-7.65	98.12	109.60
1	B	158	VAL	CA-C-O	-7.64	112.75	120.85
1	B	227	VAL	CA-C-N	7.61	130.33	120.44
1	B	227	VAL	C-N-CA	7.61	130.33	120.44
1	B	98	VAL	CA-C-N	-7.60	113.77	123.19
1	B	98	VAL	C-N-CA	-7.60	113.77	123.19
1	A	157	TYR	O-C-N	7.59	129.89	122.07
1	A	241	PRO	CB-CA-C	7.58	121.23	111.46
1	A	533	ILE	N-CA-CB	7.57	125.21	110.45
1	B	550	VAL	N-CA-C	-7.55	103.17	110.42
1	A	173	ASP	O-C-N	7.51	131.73	122.34
1	B	25	LEU	CA-CB-CG	7.51	142.58	116.30
1	A	503	GLY	CA-C-O	-7.50	109.69	119.44
1	B	151	ARG	CD-NE-CZ	7.48	134.88	124.40
1	B	513	ALA	O-C-N	7.48	129.86	121.93
1	B	269	LYS	N-CA-C	-7.47	99.11	109.71
1	A	289	LEU	N-CA-C	7.46	126.70	110.80
1	A	151	ARG	NE-CZ-NH2	7.46	125.92	119.20
1	A	227	VAL	N-CA-CB	-7.45	98.93	111.23
1	A	441	PHE	CA-C-O	-7.44	112.58	120.40
1	A	552	GLN	N-CA-C	-7.44	101.94	111.02
1	B	548	ASN	CA-C-O	-7.43	111.70	120.10
1	A	141	ASP	CA-CB-CG	7.43	120.03	112.60
1	A	174	LEU	CA-C-N	7.43	132.04	121.42
1	A	174	LEU	C-N-CA	7.43	132.04	121.42
1	B	475	THR	N-CA-CB	7.42	120.78	110.01
1	B	17	VAL	CB-CA-C	7.42	123.83	111.37
1	B	380	GLU	CB-CG-CD	7.41	125.19	112.60
1	A	503	GLY	O-C-N	7.39	131.49	122.32
1	A	442	ILE	CA-C-O	-7.35	112.75	121.28
1	B	367	GLN	O-C-N	-7.33	114.46	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	PHE	CA-CB-CG	7.33	121.13	113.80
1	A	480	ILE	CA-C-O	-7.32	113.42	120.30
1	A	154	ARG	NE-CZ-NH1	-7.31	114.19	121.50
1	B	389	GLY	CA-C-N	7.30	130.06	120.28
1	B	389	GLY	C-N-CA	7.30	130.06	120.28
1	A	151	ARG	NH1-CZ-NH2	-7.26	109.87	119.30
1	A	264	VAL	N-CA-C	-7.24	94.28	109.34
1	B	454	ILE	N-CA-C	-7.22	103.25	110.62
1	B	222	CYS	N-CA-C	-7.21	103.45	111.82
1	A	162	PRO	CA-C-O	7.19	129.53	121.34
1	B	255	GLN	N-CA-C	-7.18	104.08	112.92
1	B	136	THR	OG1-CB-CG2	7.18	123.66	109.30
1	B	21	THR	CA-CB-CG2	7.15	122.66	110.50
1	B	489	GLU	CB-CG-CD	7.14	124.73	112.60
1	B	76	VAL	N-CA-C	7.13	117.89	110.62
1	A	237	LEU	CB-CA-C	7.12	124.91	110.38
1	B	376	ASN	CA-CB-CG	-7.10	105.50	112.60
1	B	21	THR	CB-CA-C	7.08	122.13	109.38
1	B	258	ARG	NE-CZ-NH1	7.07	128.57	121.50
1	B	445	GLY	CA-C-N	7.06	130.32	120.29
1	B	445	GLY	C-N-CA	7.06	130.32	120.29
1	A	103	SER	CA-C-O	-7.06	110.42	120.51
1	A	337	ILE	CA-C-O	-7.06	113.93	121.27
1	B	254	GLU	N-CA-C	7.06	121.48	113.01
1	B	259	TYR	CA-C-O	-7.06	112.69	120.81
1	B	285	VAL	CA-C-N	7.05	132.20	122.04
1	B	285	VAL	C-N-CA	7.05	132.20	122.04
1	B	309	PHE	CA-C-O	-7.04	112.58	120.54
1	B	190	LYS	N-CA-C	-7.04	101.20	109.93
1	A	463	LYS	N-CA-C	7.03	122.54	110.02
1	B	525	LYS	CG-CD-CE	7.03	127.47	111.30
1	A	459	ARG	NH1-CZ-NH2	7.02	128.43	119.30
1	A	127	ARG	CA-C-O	-7.02	113.11	120.55
1	A	494	ASP	OD1-CG-OD2	-7.00	106.09	122.90
1	B	285	VAL	N-CA-C	-7.00	94.78	109.34
1	A	261	GLY	CA-C-O	7.00	127.85	121.76
1	A	419	THR	N-CA-C	-6.98	103.75	111.36
1	A	225	HIS	N-CA-C	6.98	120.75	112.93
1	B	277	GLU	CB-CG-CD	6.97	124.45	112.60
1	B	236	ASP	CA-C-O	-6.97	112.23	120.10
1	A	532	LYS	CA-C-O	-6.96	114.00	121.38
1	A	203	THR	CA-CB-OG1	-6.96	99.16	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	317	ARG	O-C-N	6.93	130.07	121.33
1	A	251	SER	CA-C-O	-6.93	113.20	120.55
1	A	285	VAL	N-CA-C	6.93	117.84	107.51
1	B	195	GLU	CB-CG-CD	6.93	124.37	112.60
1	B	73	THR	CA-CB-OG1	-6.92	99.22	109.60
1	B	264	VAL	CA-C-N	6.92	131.28	120.00
1	B	264	VAL	C-N-CA	6.92	131.28	120.00
1	B	428	ALA	CA-C-N	6.92	129.55	120.28
1	B	428	ALA	C-N-CA	6.92	129.55	120.28
1	B	309	PHE	O-C-N	6.91	131.10	123.22
1	B	280	ASP	CA-CB-CG	6.89	119.49	112.60
1	B	402	ASN	OD1-CG-ND2	6.87	129.47	122.60
1	A	175	ASN	O-C-N	6.86	131.11	123.01
1	A	282	ILE	CA-C-O	-6.86	113.21	120.48
1	A	263	TYR	CA-C-O	6.86	127.67	120.54
1	B	245	THR	O-C-N	6.85	127.50	120.99
1	A	542	VAL	CA-C-O	-6.85	113.83	120.95
1	B	19	VAL	N-CA-C	-6.84	96.47	106.88
1	B	536	ILE	CA-C-O	-6.84	112.95	120.48
1	A	490	ILE	CA-C-O	-6.82	114.95	121.64
1	B	320	THR	CA-CB-OG1	-6.82	99.37	109.60
1	A	98	VAL	CA-C-O	-6.82	113.00	120.71
1	A	452	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	A	167	LEU	CA-C-N	6.76	126.80	119.90
1	A	167	LEU	C-N-CA	6.76	126.80	119.90
1	A	363	THR	O-C-N	6.75	127.82	121.27
1	A	472	ASP	N-CA-CB	-6.75	99.59	111.40
1	A	291	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	499	LEU	O-C-N	6.73	125.70	120.38
1	B	41	GLU	CB-CA-C	-6.73	100.47	110.16
1	A	84	GLY	CA-C-N	6.72	129.02	120.56
1	A	84	GLY	C-N-CA	6.72	129.02	120.56
1	A	185	ILE	O-C-N	6.71	129.98	122.67
1	B	480	ILE	O-C-N	6.71	129.04	122.07
1	A	309	PHE	CA-C-O	-6.70	113.19	120.36
1	A	288	LEU	CA-C-O	6.70	126.14	118.97
1	A	463	LYS	CB-CG-CD	6.70	126.71	111.30
1	A	546	PRO	CA-C-N	6.70	131.84	121.19
1	A	546	PRO	C-N-CA	6.70	131.84	121.19
1	B	196	SER	O-C-N	6.69	129.78	122.15
1	A	45	TRP	O-C-N	6.69	130.82	123.13
1	B	484	LYS	CB-CA-C	6.68	121.83	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ILE	CA-C-O	-6.66	113.79	120.85
1	A	513	ALA	O-C-N	6.65	129.04	122.19
1	B	126	HIS	CA-C-N	6.65	129.19	120.28
1	B	126	HIS	C-N-CA	6.65	129.19	120.28
1	A	441	PHE	CA-C-N	-6.65	112.12	122.69
1	A	441	PHE	C-N-CA	-6.65	112.12	122.69
1	A	497	SER	CA-CB-OG	-6.65	97.80	111.10
1	B	151	ARG	NE-CZ-NH1	6.64	128.15	121.50
1	A	515	THR	CB-CA-C	6.63	121.42	110.81
1	A	116	THR	OG1-CB-CG2	-6.62	96.06	109.30
1	B	310	HIS	N-CA-CB	6.61	123.20	111.69
1	A	116	THR	CA-CB-OG1	6.57	119.46	109.60
1	A	407	ILE	N-CA-CB	6.57	120.51	112.10
1	A	359	VAL	CB-CA-C	6.56	116.97	109.89
1	B	422	THR	N-CA-CB	6.55	119.76	110.12
1	A	439	ILE	CA-CB-CG2	6.55	121.63	110.50
1	B	305	ASN	CA-CB-CG	6.54	119.14	112.60
1	A	264	VAL	CA-C-O	-6.54	112.61	120.78
1	B	264	VAL	CA-C-O	6.53	128.94	120.78
1	A	307	VAL	CA-C-O	-6.51	113.58	120.48
1	B	339	ASP	CB-CA-C	6.51	123.16	110.67
1	A	380	GLU	CB-CG-CD	6.50	123.65	112.60
1	A	126	HIS	CA-C-N	6.49	128.98	120.28
1	A	126	HIS	C-N-CA	6.49	128.98	120.28
1	A	306	ILE	O-C-N	6.49	130.08	123.20
1	B	491	GLN	OE1-CD-NE2	-6.49	116.11	122.60
1	A	227	VAL	CB-CA-C	6.48	121.92	111.29
1	A	436	LYS	N-CA-CB	-6.48	100.04	109.83
1	A	238	THR	CA-CB-CG2	6.48	121.51	110.50
1	B	491	GLN	N-CA-C	-6.48	99.97	110.20
1	A	289	LEU	N-CA-CB	-6.47	99.55	110.49
1	B	195	GLU	N-CA-C	6.46	117.99	111.07
1	B	17	VAL	CA-C-N	6.45	131.77	122.35
1	B	17	VAL	C-N-CA	6.45	131.77	122.35
1	B	497	SER	CA-C-N	6.45	129.76	120.79
1	B	497	SER	C-N-CA	6.45	129.76	120.79
1	A	135	THR	CA-C-O	-6.45	114.55	121.45
1	B	430	GLU	CA-C-N	6.45	130.11	120.31
1	B	430	GLU	C-N-CA	6.45	130.11	120.31
1	B	289	LEU	CB-CA-C	6.45	120.58	111.74
1	B	6	LEU	O-C-N	6.45	129.76	122.22
1	B	488	ASN	CA-CB-CG	-6.44	106.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	THR	CA-CB-OG1	-6.43	99.95	109.60
1	B	56	TYR	N-CA-C	-6.43	103.40	111.11
1	B	367	GLN	CA-C-O	6.42	127.77	120.90
1	A	33	LEU	CA-C-O	-6.41	114.09	120.70
1	A	491	GLN	OE1-CD-NE2	-6.41	116.19	122.60
1	A	185	ILE	CA-C-O	-6.40	113.75	121.04
1	A	529	ASP	N-CA-CB	-6.39	100.01	110.43
1	A	512	VAL	CB-CA-C	6.39	120.37	110.28
1	A	286	GLY	O-C-N	6.38	129.81	122.34
1	B	206	ALA	CA-C-N	6.38	129.35	120.29
1	B	206	ALA	C-N-CA	6.38	129.35	120.29
1	A	28	ASP	CA-C-O	-6.37	113.75	120.63
1	A	227	VAL	N-CA-C	6.37	122.58	109.34
1	B	457	MET	N-CA-C	-6.37	104.27	111.14
1	A	271	GLU	CA-CB-CG	6.35	126.80	114.10
1	B	353	THR	O-C-N	6.35	127.84	121.30
1	B	116	THR	N-CA-CB	6.35	121.48	111.20
1	A	530	ASN	OD1-CG-ND2	6.35	128.95	122.60
1	B	385	ILE	CA-C-O	-6.34	113.75	120.48
1	A	261	GLY	N-CA-C	6.34	119.97	110.97
1	A	415	ILE	N-CA-C	6.33	122.51	109.34
1	B	362	SER	CA-C-N	6.33	129.15	120.67
1	B	362	SER	C-N-CA	6.33	129.15	120.67
1	B	480	ILE	CB-CA-C	6.32	117.37	111.30
1	A	505	LYS	CB-CG-CD	6.32	125.83	111.30
1	B	448	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	A	76	VAL	O-C-N	6.30	127.98	121.87
1	B	158	VAL	N-CA-C	6.29	117.07	110.72
1	B	486	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	A	144	THR	N-CA-CB	-6.27	101.31	110.53
1	A	510	HIS	CA-CB-CG	6.27	120.07	113.80
1	B	361	ALA	O-C-N	6.26	130.47	122.33
1	A	494	ASP	CB-CG-OD2	6.26	132.79	118.40
1	B	380	GLU	O-C-N	6.26	130.71	122.95
1	A	498	LEU	CA-C-O	-6.25	114.26	120.70
1	B	439	ILE	O-C-N	6.24	130.00	123.26
1	B	5	THR	CA-CB-OG1	-6.24	100.25	109.60
1	A	249	LYS	O-C-N	6.23	130.68	122.95
1	A	119	ASN	N-CA-C	6.23	120.92	112.88
1	B	486	GLN	CG-CD-NE2	6.23	125.74	116.40
1	B	380	GLU	CB-CA-C	-6.23	100.18	109.90
1	B	317	ARG	CA-CB-CG	6.22	126.54	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ASN	CB-CG-ND2	-6.22	107.07	116.40
1	B	337	ILE	CA-C-O	-6.21	113.02	120.78
1	A	167	LEU	N-CA-CB	-6.21	99.88	110.43
1	B	532	LYS	CG-CD-CE	6.21	125.57	111.30
1	A	149	ILE	N-CA-C	-6.19	104.48	110.42
1	A	144	THR	CA-CB-CG2	6.19	121.02	110.50
1	B	192	ASN	CA-CB-CG	6.18	118.78	112.60
1	B	485	ALA	CA-C-N	6.18	128.84	120.38
1	B	485	ALA	C-N-CA	6.18	128.84	120.38
1	A	195	GLU	N-CA-CB	6.17	119.30	110.16
1	B	363	THR	O-C-N	6.16	127.44	121.28
1	B	302	LYS	CA-CB-CG	6.16	126.42	114.10
1	A	361	ALA	CA-C-N	6.16	131.92	121.14
1	A	361	ALA	C-N-CA	6.16	131.92	121.14
1	A	533	ILE	O-C-N	6.16	129.16	122.57
1	B	399	THR	CA-C-O	-6.15	113.59	120.54
1	A	155	THR	CA-CB-OG1	-6.14	100.38	109.60
1	A	345	LYS	O-C-N	6.14	127.33	120.83
1	A	102	PRO	CA-C-O	6.13	128.67	121.56
1	A	418	THR	CA-CB-OG1	-6.13	100.41	109.60
1	B	508	GLU	O-C-N	6.12	130.74	123.33
1	B	101	VAL	N-CA-C	6.08	114.59	107.84
1	B	411	LEU	CA-C-O	-6.08	114.41	120.80
1	A	164	TYR	O-C-N	6.07	130.43	123.27
1	A	348	ALA	CA-C-O	-6.07	114.37	121.16
1	B	416	GLY	O-C-N	6.06	129.11	122.56
1	A	40	VAL	CB-CA-C	6.06	119.81	110.96
1	A	142	ILE	CB-CA-C	-6.05	102.46	112.26
1	B	311	SER	CA-C-O	-6.04	114.10	120.63
1	B	477	GLU	OE1-CD-OE2	6.03	137.37	122.90
1	B	464	PRO	CA-C-O	-6.02	114.38	122.08
1	B	532	LYS	CB-CG-CD	6.01	125.13	111.30
1	B	329	VAL	CA-CB-CG1	6.01	120.61	110.40
1	B	215	VAL	N-CA-CB	-6.00	101.61	111.45
1	B	16	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	B	422	THR	N-CA-C	-5.99	104.75	111.28
1	B	68	SER	O-C-N	5.98	129.98	123.10
1	A	277	GLU	N-CA-C	5.98	118.58	111.71
1	B	102	PRO	CA-C-O	5.98	128.50	121.56
1	B	526	SER	O-C-N	5.97	128.45	122.12
1	A	499	LEU	CB-CA-C	5.97	124.36	113.49
1	B	342	LYS	CB-CG-CD	5.97	125.03	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	227	VAL	CG1-CB-CG2	5.95	123.89	110.80
1	B	253	SER	CB-CA-C	5.95	119.18	110.26
1	B	390	THR	N-CA-CB	5.95	118.86	110.12
1	A	222	CYS	N-CA-C	-5.94	104.74	112.23
1	B	215	VAL	CA-CB-CG1	5.93	120.49	110.40
1	A	478	LYS	N-CA-CB	5.93	119.36	110.22
1	B	163	VAL	CA-C-O	5.93	127.29	120.76
1	B	396	ASN	CA-CB-CG	-5.92	106.68	112.60
1	B	32	SER	CA-C-O	-5.92	113.16	119.97
1	A	226	ASP	N-CA-C	5.92	123.40	110.80
1	B	304	LYS	N-CA-C	-5.91	105.90	113.23
1	B	102	PRO	CB-CA-C	5.91	118.80	111.23
1	B	472	ASP	CA-C-O	-5.91	114.65	122.03
1	A	182	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	236	ASP	CA-C-N	5.89	130.70	120.68
1	A	236	ASP	C-N-CA	5.89	130.70	120.68
1	B	484	LYS	CA-C-O	5.88	127.07	119.95
1	B	193	ASP	N-CA-C	-5.88	101.20	109.96
1	B	189	LEU	O-C-N	5.87	130.03	122.81
1	B	554	LYS	CA-C-O	5.87	126.97	120.63
1	A	69	CYS	CA-C-O	-5.87	113.56	120.60
1	B	48	ASN	O-C-N	5.87	129.48	122.79
1	A	498	LEU	O-C-N	5.87	128.42	122.09
1	B	203	THR	CA-C-O	-5.87	114.66	120.70
1	B	495	HIS	N-CA-C	5.86	118.14	111.11
1	B	307	VAL	CA-C-O	-5.86	113.80	120.66
1	A	83	ASN	OD1-CG-ND2	-5.86	116.75	122.60
1	B	251	SER	CB-CA-C	-5.85	98.08	110.31
1	A	525	LYS	N-CA-CB	5.85	118.82	110.16
1	B	523	GLN	N-CA-CB	5.84	119.23	110.53
1	A	169	ALA	CA-C-O	-5.84	113.26	119.97
1	A	195	GLU	CB-CG-CD	5.83	122.51	112.60
1	B	227	VAL	N-CA-C	5.83	117.79	112.43
1	B	52	LEU	N-CA-C	-5.82	104.85	111.14
1	B	174	LEU	CB-CA-C	5.82	120.17	109.46
1	A	421	ALA	CA-C-N	5.82	128.08	120.28
1	A	421	ALA	C-N-CA	5.82	128.08	120.28
1	B	324	VAL	CA-C-N	5.82	130.15	121.72
1	B	324	VAL	C-N-CA	5.82	130.15	121.72
1	B	431	GLU	CB-CG-CD	5.82	122.48	112.60
1	A	336	ASN	CB-CG-ND2	-5.81	107.68	116.40
1	A	482	GLY	CA-C-N	5.81	126.21	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	482	GLY	C-N-CA	5.81	126.21	119.47
1	A	159	THR	CA-C-O	-5.80	112.11	119.31
1	B	409	GLN	CB-CA-C	5.80	120.73	111.91
1	A	9	TYR	N-CA-C	-5.80	104.15	111.11
1	B	452	GLN	N-CA-CB	5.79	119.30	110.14
1	B	512	VAL	CB-CA-C	5.79	118.78	110.33
1	A	457	MET	N-CA-C	-5.79	105.05	111.36
1	B	81	ALA	CA-C-O	-5.79	111.70	119.11
1	A	492	GLY	CA-C-O	-5.79	115.57	120.89
1	A	96	LEU	CA-C-O	-5.78	114.13	120.43
1	A	489	GLU	O-C-N	5.77	130.55	123.10
1	A	354	PRO	CB-CA-C	-5.77	103.42	110.98
1	A	329	VAL	CA-C-O	-5.77	115.06	121.17
1	A	51	GLU	CA-C-O	-5.76	113.59	120.10
1	B	23	PHE	CA-CB-CG	-5.76	108.04	113.80
1	B	33	LEU	N-CA-C	-5.76	104.63	111.03
1	A	287	ALA	N-CA-C	5.76	118.91	109.76
1	A	195	GLU	CA-CB-CG	5.74	125.57	114.10
1	B	367	GLN	CA-C-N	5.74	128.28	120.54
1	B	367	GLN	C-N-CA	5.74	128.28	120.54
1	A	4	ILE	CA-C-O	-5.73	115.82	121.67
1	A	52	LEU	CA-C-N	5.73	127.96	120.28
1	A	52	LEU	C-N-CA	5.73	127.96	120.28
1	A	200	VAL	CA-C-N	5.73	127.78	120.56
1	A	200	VAL	C-N-CA	5.73	127.78	120.56
1	B	450	THR	CA-C-N	5.73	128.61	120.53
1	B	450	THR	C-N-CA	5.73	128.61	120.53
1	B	513	ALA	CA-C-O	-5.72	111.28	118.43
1	A	323	GLY	CA-C-O	-5.72	112.87	119.10
1	A	142	ILE	N-CA-CB	5.72	121.12	110.77
1	A	518	TRP	CA-C-O	5.71	127.35	121.07
1	B	17	VAL	O-C-N	-5.71	116.60	122.14
1	B	322	PRO	CB-CA-C	-5.71	104.45	111.64
1	B	393	PHE	N-CA-C	-5.71	104.97	111.14
1	A	389	GLY	N-CA-C	-5.70	102.73	110.43
1	B	385	ILE	O-C-N	5.70	129.17	123.18
1	A	116	THR	CA-C-N	5.70	133.34	121.94
1	A	116	THR	C-N-CA	5.70	133.34	121.94
1	B	28	ASP	N-CA-C	5.70	118.23	111.33
1	B	53	ASN	CA-C-O	-5.70	114.51	120.55
1	A	121	ASP	CA-C-O	5.69	126.67	120.58
1	B	170	ASN	CB-CG-ND2	5.69	124.93	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ILE	O-C-N	5.68	127.48	121.91
1	A	549	LEU	CB-CA-C	5.67	120.20	110.79
1	B	73	THR	OG1-CB-CG2	5.67	120.64	109.30
1	B	40	VAL	CA-C-O	5.67	127.31	120.74
1	B	150	ASP	CA-C-N	5.66	127.80	120.44
1	B	150	ASP	C-N-CA	5.66	127.80	120.44
1	B	336	ASN	O-C-N	5.66	129.05	122.25
1	B	484	LYS	CG-CD-CE	5.66	124.31	111.30
1	A	127	ARG	CB-CA-C	-5.65	101.40	110.79
1	A	201	ILE	CA-C-N	5.65	127.79	120.44
1	A	201	ILE	C-N-CA	5.65	127.79	120.44
1	B	463	LYS	N-CA-C	5.65	119.49	110.73
1	B	63	ARG	CD-NE-CZ	-5.65	116.49	124.40
1	A	193	ASP	N-CA-C	-5.63	101.57	109.96
1	B	53	ASN	O-C-N	5.63	128.09	122.12
1	B	373	GLN	N-CA-C	5.63	119.41	112.54
1	B	86	ALA	CA-C-N	5.63	127.37	120.22
1	B	86	ALA	C-N-CA	5.63	127.37	120.22
1	A	310	HIS	CA-C-O	-5.63	114.85	121.44
1	B	277	GLU	CA-C-O	5.63	126.37	119.05
1	A	465	TYR	CA-C-O	-5.62	114.69	120.54
1	A	224	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	A	224	ARG	N-CA-CB	5.61	118.86	110.22
1	B	551	LYS	N-CA-C	5.61	119.30	112.23
1	A	464	PRO	CB-CA-C	-5.60	103.61	110.95
1	A	104	ILE	N-CA-CB	5.60	120.47	111.23
1	A	69	CYS	O-C-N	5.59	130.09	123.33
1	A	362	SER	CB-CA-C	-5.59	98.31	109.99
1	B	332	LYS	CB-CA-C	5.58	120.34	110.85
1	A	284	SER	CA-CB-OG	-5.57	99.95	111.10
1	B	19	VAL	O-C-N	5.57	130.34	122.59
1	B	20	ASN	CB-CG-ND2	5.57	124.75	116.40
1	B	419	THR	CA-C-O	-5.57	114.52	120.42
1	A	540	LEU	N-CA-CB	-5.56	100.34	110.63
1	B	407	ILE	CA-C-O	-5.56	114.66	120.27
1	B	114	HIS	N-CA-CB	5.56	119.94	110.50
1	B	130	ALA	CA-C-O	-5.55	113.82	120.10
1	B	365	LEU	CB-CA-C	5.55	118.77	109.89
1	A	308	GLU	CA-C-O	-5.55	114.33	120.38
1	B	71	ILE	O-C-N	5.55	129.25	123.26
1	A	307	VAL	N-CA-C	-5.54	100.41	108.17
1	A	312	ASP	CB-CG-OD1	5.54	131.15	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLU	CB-CG-CD	5.54	122.02	112.60
1	B	219	ASP	N-CA-CB	-5.54	102.50	110.87
1	B	328	PHE	CA-C-O	-5.54	113.60	119.97
1	A	483	PRO	O-C-N	5.54	128.87	122.17
1	B	196	SER	CA-C-O	-5.54	114.55	120.42
1	A	99	VAL	CA-CB-CG2	5.53	119.80	110.40
1	B	484	LYS	CA-C-N	5.53	128.69	120.95
1	B	484	LYS	C-N-CA	5.53	128.69	120.95
1	B	538	ILE	CA-CB-CG1	5.53	119.80	110.40
1	A	493	TRP	O-C-N	5.52	130.22	123.10
1	A	13	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	B	19	VAL	CA-C-O	-5.51	114.41	120.97
1	B	528	ASN	O-C-N	5.50	130.47	122.43
1	B	382	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	476	ILE	O-C-N	5.49	127.49	121.83
1	A	96	LEU	O-C-N	5.49	129.47	123.27
1	A	101	VAL	CA-C-O	5.49	127.87	120.90
1	B	82	LEU	N-CA-C	5.49	118.78	111.75
1	B	277	GLU	CB-CA-C	5.49	121.36	110.17
1	B	472	ASP	N-CA-C	5.48	118.68	111.28
1	B	159	THR	CA-CB-OG1	-5.47	101.39	109.60
1	B	259	TYR	O-C-N	5.47	129.66	122.93
1	A	192	ASN	CA-CB-CG	5.47	118.07	112.60
1	A	353	THR	O-C-N	5.47	125.86	121.38
1	A	534	ARG	O-C-N	5.47	129.61	123.27
1	B	256	HIS	O-C-N	5.47	126.75	121.28
1	A	467	PHE	CA-C-O	-5.47	114.31	120.43
1	B	32	SER	O-C-N	5.46	128.99	122.27
1	B	271	GLU	N-CA-CB	5.46	118.24	110.16
1	A	58	ALA	N-CA-C	-5.46	105.33	111.28
1	B	161	ARG	CA-CB-CG	-5.46	103.19	114.10
1	A	233	LYS	CA-C-N	5.45	127.59	120.28
1	A	233	LYS	C-N-CA	5.45	127.59	120.28
1	A	352	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	A	473	GLY	O-C-N	-5.44	117.39	123.10
1	A	258	ARG	NH1-CZ-NH2	-5.44	112.23	119.30
1	A	324	VAL	O-C-N	5.44	128.60	122.68
1	A	20	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	263	TYR	CB-CA-C	5.43	119.48	110.78
1	A	509	THR	N-CA-C	-5.43	101.10	109.52
1	A	475	THR	CA-C-O	-5.43	113.97	120.10
1	A	480	ILE	O-C-N	5.42	127.71	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	329	VAL	N-CA-CB	5.42	117.91	110.54
1	A	33	LEU	N-CA-C	-5.42	105.29	111.14
1	B	185	ILE	N-CA-C	-5.42	101.84	109.21
1	A	74	PHE	CB-CA-C	5.42	117.24	109.71
1	A	331	GLN	CA-C-O	-5.42	114.81	120.55
1	B	277	GLU	OE1-CD-OE2	-5.41	109.91	122.90
1	B	251	SER	CA-C-N	5.40	130.50	122.99
1	B	251	SER	C-N-CA	5.40	130.50	122.99
1	A	104	ILE	CA-C-O	5.40	127.53	120.78
1	B	228	LYS	O-C-N	5.39	127.62	122.07
1	A	372	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	B	19	VAL	CA-C-N	-5.39	112.60	121.92
1	B	19	VAL	C-N-CA	-5.39	112.60	121.92
1	B	37	ILE	O-C-N	5.39	127.10	121.87
1	B	382	ASP	CA-C-O	-5.39	115.62	121.87
1	B	442	ILE	CA-C-N	5.38	125.45	120.34
1	B	442	ILE	C-N-CA	5.38	125.45	120.34
1	B	232	LYS	CA-CB-CG	-5.38	103.34	114.10
1	B	480	ILE	N-CA-CB	-5.38	102.83	111.82
1	A	53	ASN	CA-C-N	5.38	127.49	120.28
1	A	53	ASN	C-N-CA	5.38	127.49	120.28
1	A	127	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	126	HIS	CA-CB-CG	5.37	119.17	113.80
1	B	399	THR	O-C-N	5.37	129.34	123.22
1	A	546	PRO	N-CA-C	-5.37	102.70	110.80
1	A	411	LEU	CB-CA-C	5.36	119.71	110.86
1	B	101	VAL	CA-C-O	5.36	127.70	120.90
1	B	245	THR	CA-C-O	-5.34	115.71	121.27
1	A	473	GLY	CA-C-N	5.34	130.46	122.23
1	A	473	GLY	C-N-CA	5.34	130.46	122.23
1	B	277	GLU	O-C-N	-5.34	115.09	122.46
1	A	249	LYS	CA-C-N	-5.34	117.09	123.44
1	A	249	LYS	C-N-CA	-5.34	117.09	123.44
1	A	253	SER	CB-CA-C	5.33	119.04	110.29
1	A	421	ALA	CA-C-O	5.33	126.39	120.63
1	B	134	GLU	N-CA-C	-5.33	105.14	111.69
1	A	493	TRP	CA-C-O	-5.33	115.12	121.56
1	B	139	ILE	CB-CA-C	5.33	118.47	111.33
1	A	161	ARG	CA-C-N	5.32	125.24	119.76
1	A	161	ARG	C-N-CA	5.32	125.24	119.76
1	A	507	TYR	O-C-N	5.32	128.69	122.99
1	A	510	HIS	O-C-N	5.32	129.44	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	PHE	CA-C-N	-5.32	113.59	122.21
1	B	309	PHE	C-N-CA	-5.32	113.59	122.21
1	B	235	ILE	CA-C-O	-5.32	115.53	121.17
1	B	349	VAL	CB-CA-C	5.32	121.04	111.36
1	A	186	ASP	CA-CB-CG	-5.32	107.28	112.60
1	B	475	THR	CA-CB-OG1	-5.31	101.63	109.60
1	A	123	THR	CA-CB-OG1	-5.30	101.65	109.60
1	B	443	GLY	N-CA-C	-5.30	105.31	112.14
1	B	17	VAL	CA-C-O	5.29	125.89	119.54
1	B	231	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	336	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	542	VAL	O-C-N	5.29	127.00	121.87
1	A	255	GLN	OE1-CD-NE2	-5.28	117.32	122.60
1	A	29	PHE	CA-C-O	-5.28	113.72	119.95
1	A	345	LYS	CB-CG-CD	5.28	123.44	111.30
1	A	230	GLU	N-CA-CB	5.28	117.87	110.12
1	B	416	GLY	N-CA-C	-5.28	107.72	114.37
1	A	99	VAL	CB-CA-C	5.27	118.44	110.63
1	A	467	PHE	CA-CB-CG	5.27	119.07	113.80
1	B	183	THR	CA-CB-CG2	5.27	119.46	110.50
1	B	336	ASN	N-CA-C	5.27	120.57	114.04
1	A	144	THR	CA-CB-OG1	-5.26	101.70	109.60
1	A	327	LYS	CG-CD-CE	5.26	123.40	111.30
1	B	385	ILE	CA-C-N	-5.26	115.58	122.99
1	B	385	ILE	C-N-CA	-5.26	115.58	122.99
1	B	59	ASP	CA-C-N	5.25	125.92	119.99
1	B	59	ASP	C-N-CA	5.25	125.92	119.99
1	A	312	ASP	OD1-CG-OD2	-5.25	110.31	122.90
1	B	532	LYS	CA-C-O	-5.25	115.66	121.33
1	A	241	PRO	CA-C-O	5.25	127.32	121.34
1	A	306	ILE	CA-C-N	-5.24	116.69	123.19
1	A	306	ILE	C-N-CA	-5.24	116.69	123.19
1	B	224	ARG	CA-C-O	-5.23	114.19	120.10
1	B	462	LEU	N-CA-C	-5.23	103.48	110.55
1	B	152	CYS	CA-C-O	-5.23	115.33	120.82
1	B	24	GLY	CA-C-O	-5.23	117.21	121.76
1	A	364	PRO	CA-C-N	5.23	128.27	120.95
1	A	364	PRO	C-N-CA	5.23	128.27	120.95
1	A	61	TYR	CA-C-N	5.22	127.28	120.28
1	A	61	TYR	C-N-CA	5.22	127.28	120.28
1	A	510	HIS	CA-C-O	-5.22	115.14	120.89
1	B	256	HIS	N-CA-C	-5.22	101.82	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	125	PHE	CA-C-N	5.22	127.58	120.54
1	A	125	PHE	C-N-CA	5.22	127.58	120.54
1	B	475	THR	OG1-CB-CG2	5.21	119.73	109.30
1	A	433	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	372	ASN	N-CA-CB	5.21	117.87	110.16
1	B	124	VAL	N-CA-C	5.21	115.42	110.42
1	B	317	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	A	105	SER	CB-CA-C	5.20	119.98	110.10
1	A	517	GLU	O-C-N	5.20	128.07	122.15
1	A	508	GLU	CA-C-O	-5.20	115.03	121.06
1	B	15	LYS	N-CA-C	-5.19	105.63	111.28
1	B	99	VAL	CB-CA-C	5.18	118.55	110.83
1	A	209	LYS	CA-C-O	-5.18	115.03	120.63
1	A	250	GLY	N-CA-C	-5.18	107.73	113.79
1	A	174	LEU	CB-CA-C	5.18	118.07	109.53
1	B	401	PRO	N-CD-CG	-5.18	95.44	103.20
1	A	81	ALA	N-CA-CB	-5.17	101.72	110.41
1	B	366	LYS	N-CA-CB	5.17	120.78	111.37
1	B	196	SER	CA-CB-OG	-5.17	100.76	111.10
1	B	370	MET	O-C-N	5.17	127.40	122.03
1	B	152	CYS	O-C-N	5.16	127.39	122.07
1	B	161	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	B	400	PHE	N-CA-CB	-5.16	103.79	110.03
1	B	387	GLU	CA-C-N	5.16	128.65	121.02
1	B	387	GLU	C-N-CA	5.16	128.65	121.02
1	B	336	ASN	OD1-CG-ND2	5.16	127.75	122.60
1	B	280	ASP	N-CA-C	-5.15	106.68	113.17
1	B	507	TYR	O-C-N	5.15	128.66	123.26
1	B	125	PHE	O-C-N	-5.14	116.20	122.22
1	B	471	ASN	N-CA-CB	5.14	121.84	111.60
1	B	236	ASP	CB-CA-C	-5.14	101.12	110.63
1	A	13	ARG	NH1-CZ-NH2	5.14	125.98	119.30
1	B	169	ALA	CA-C-O	-5.14	114.45	120.20
1	A	64	ILE	N-CA-C	5.13	115.41	110.74
1	A	434	PRO	CA-C-O	-5.13	111.78	118.86
1	A	149	ILE	CA-CB-CG1	-5.13	101.67	110.40
1	B	520	LYS	CA-CB-CG	-5.13	103.83	114.10
1	A	268	SER	CA-C-N	5.13	127.78	120.49
1	A	268	SER	C-N-CA	5.13	127.78	120.49
1	A	195	GLU	O-C-N	5.13	128.00	122.15
1	B	476	ILE	N-CA-CB	-5.12	104.07	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	401	PRO	N-CA-C	-5.11	101.95	112.47
1	B	491	GLN	CG-CD-NE2	5.11	124.06	116.40
1	B	29	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	63	ARG	NE-CZ-NH1	5.10	126.60	121.50
1	A	240	PHE	CA-CB-CG	5.09	118.89	113.80
1	B	219	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	441	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	160	GLN	N-CA-CB	5.09	119.64	111.91
1	B	64	ILE	N-CA-C	5.09	116.18	111.45
1	A	18	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	B	377	PHE	CA-CB-CG	5.08	118.88	113.80
1	A	233	LYS	N-CA-C	-5.08	105.74	111.28
1	A	422	THR	CA-CB-OG1	-5.08	101.98	109.60
1	A	525	LYS	CA-C-N	-5.08	112.60	120.31
1	A	525	LYS	C-N-CA	-5.08	112.60	120.31
1	A	123	THR	CA-CB-CG2	5.07	119.12	110.50
1	A	463	LYS	CA-C-N	5.07	125.05	120.03
1	A	463	LYS	C-N-CA	5.07	125.05	120.03
1	A	491	GLN	CA-C-O	-5.06	115.49	121.16
1	B	221	CYS	O-C-N	5.06	129.16	122.43
1	B	337	ILE	O-C-N	5.06	128.89	122.57
1	A	68	SER	CA-C-O	-5.06	116.04	121.45
1	B	528	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	502	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	475	THR	N-CA-C	5.05	117.52	111.71
1	B	412	TRP	CB-CA-C	5.05	118.88	110.90
1	A	363	THR	OG1-CB-CG2	5.05	119.39	109.30
1	A	312	ASP	CA-C-O	-5.04	113.53	119.48
1	A	127	ARG	N-CA-CB	5.04	117.53	110.12
1	A	183	THR	CA-C-N	5.04	125.31	119.92
1	A	183	THR	C-N-CA	5.04	125.31	119.92
1	A	352	ARG	CB-CA-C	5.03	118.80	109.54
1	B	505	LYS	N-CA-CB	-5.03	101.58	110.34
1	A	277	GLU	O-C-N	5.03	128.10	122.22
1	B	242	ALA	CA-C-O	-5.03	114.93	120.36
1	A	532	LYS	O-C-N	5.03	128.54	123.26
1	B	345	LYS	O-C-N	5.03	125.91	121.19
1	B	352	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	B	529	ASP	N-CA-CB	-5.02	102.24	110.43
1	B	198	LYS	N-CA-CB	5.02	117.29	110.01
1	A	390	THR	CA-C-O	-5.02	114.43	120.10
1	A	459	ARG	NE-CZ-NH2	-5.01	114.69	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	ARG	CG-CD-NE	-5.01	100.97	112.00
1	A	436	LYS	CD-CE-NZ	-5.01	95.86	111.90
1	B	32	SER	N-CA-CB	5.01	118.05	110.28
1	B	102	PRO	CA-C-N	5.01	128.18	120.82
1	B	102	PRO	C-N-CA	5.01	128.18	120.82
1	A	12	GLU	CA-CB-CG	5.01	124.11	114.10
1	A	387	GLU	CB-CG-CD	-5.01	104.09	112.60
1	B	303	THR	OG1-CB-CG2	5.01	119.31	109.30
1	A	370	MET	N-CA-C	5.00	117.11	111.11
1	A	498	LEU	CD1-CG-CD2	5.00	121.81	110.80
1	B	469	LEU	CA-C-O	-5.00	115.98	121.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4130	0	4151	88	0
1	B	4130	0	4151	108	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
4	A	235	0	0	8	0
4	B	204	0	0	6	0
All	All	8753	0	8334	190	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 11.

All (190) 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:228:LYS:HD3	1:B:228:LYS:H	1.17	1.09
1:A:157:TYR:HD2	1:A:187:MET:HE2	1.24	1.00
1:A:303:THR:HG22	1:A:306:ILE:HD11	1.47	0.96
1:B:505:LYS:HE2	1:B:506:ASP:H	1.31	0.91
1:A:116:THR:HG22	4:A:935:HOH:O	1.73	0.88
1:A:157:TYR:CD2	1:A:187:MET:HE2	2.11	0.85
1:A:496:LEU:HD22	1:A:509:THR:HB	1.56	0.85
1:A:475:THR:HG22	4:A:834:HOH:O	1.77	0.83
1:A:241:PRO:HB3	1:A:349:VAL:HG12	1.62	0.82
1:A:158:VAL:HG23	1:A:187:MET:HE3	1.59	0.81
1:B:476:ILE:HG22	4:B:861:HOH:O	1.86	0.74
1:B:266:THR:HA	1:B:273:LYS:HE2	1.69	0.73
1:A:380:GLU:HG2	1:A:401:PRO:HB2	1.71	0.73
1:A:158:VAL:HG23	1:A:187:MET:CE	2.18	0.72
1:B:228:LYS:H	1:B:228:LYS:CD	2.01	0.71
1:A:415:ILE:O	1:A:446:SER:HB3	1.92	0.70
1:B:219:ASP:HB3	1:B:286:GLY:HA2	1.72	0.70
1:B:553:ALA:HA	1:B:556:THR:HG22	1.73	0.69
1:B:228:LYS:HD3	1:B:228:LYS:N	1.99	0.68
1:B:525:LYS:H	1:B:525:LYS:HE2	1.58	0.68
1:B:154:ARG:NH2	1:B:188:SER:O	2.27	0.67
1:B:345:LYS:HE3	1:B:346:PRO:HD2	1.77	0.67
1:B:476:ILE:O	1:B:480:ILE:HD12	1.95	0.66
1:B:287:ALA:HB1	1:B:288:LEU:HD12	1.78	0.66
1:B:303:THR:HB	1:B:305:ASN:H	1.61	0.65
1:B:274:GLU:O	1:B:278:SER:HB2	1.96	0.65
1:B:267:LEU:HD11	1:B:552:GLN:HA	1.77	0.65
1:B:387:GLU:HG3	1:B:388:THR:N	2.11	0.64
1:A:499:LEU:HD22	1:A:533:ILE:HD12	1.80	0.64
1:A:508:GLU:HG3	1:A:532:LYS:HD2	1.81	0.63
1:B:524:ASP:HA	1:B:525:LYS:HE2	1.81	0.62
1:A:171:LEU:HA	1:A:174:LEU:HD22	1.82	0.62
1:B:139:ILE:HG22	1:B:171:LEU:HD12	1.81	0.61
1:B:505:LYS:H	1:B:505:LYS:CD	2.14	0.60
1:A:71:ILE:HG12	1:A:98:VAL:HB	1.83	0.60
1:A:139:ILE:HG21	1:A:145:ALA:HB2	1.83	0.60
1:B:95:VAL:O	1:B:162:PRO:HA	2.01	0.60
1:B:342:LYS:HD2	1:B:342:LYS:O	2.01	0.60
1:B:554:LYS:HD2	1:B:555:LEU:HG	1.84	0.60
1:B:247:MET:HG3	1:B:410:VAL:HB	1.84	0.59
1:B:359:VAL:HB	1:B:360:PRO:HD2	1.85	0.59
1:A:219:ASP:HB2	4:A:965:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HG22	1:A:517:GLU:HB3	1.85	0.58
1:A:126:HIS:HE1	1:A:136:THR:OG1	1.85	0.58
1:B:476:ILE:HG13	1:B:549:LEU:HD21	1.85	0.58
1:A:95:VAL:O	1:A:162:PRO:HA	2.04	0.57
1:B:15:LYS:HE3	1:B:41:GLU:O	2.03	0.57
1:A:478:LYS:HB3	1:A:483:PRO:HA	1.85	0.57
1:B:142:ILE:HG21	1:B:174:LEU:HB3	1.86	0.57
1:A:247:MET:CG	1:A:410:VAL:HB	2.35	0.57
1:A:271:GLU:HB3	1:A:350:PRO:HB3	1.86	0.56
1:A:228:LYS:O	1:A:232:LYS:HG3	2.06	0.56
1:A:269:LYS:HE3	4:A:667:HOH:O	2.06	0.56
1:B:33:LEU:HD13	1:B:71:ILE:HD13	1.87	0.56
1:B:504:ALA:HA	1:B:505:LYS:HZ3	1.70	0.56
1:B:552:GLN:OE1	1:B:553:ALA:N	2.39	0.56
1:A:101:VAL:HG13	1:A:102:PRO:HD2	1.88	0.56
1:B:160:GLN:O	1:B:161:ARG:HG3	2.06	0.55
1:B:177:PRO:HB3	1:B:179:LYS:HE2	1.89	0.55
1:A:389:GLY:HA2	1:A:476:ILE:HG21	1.89	0.55
1:B:525:LYS:H	1:B:525:LYS:CD	2.20	0.55
1:B:302:LYS:O	1:B:303:THR:OG1	2.23	0.55
1:A:104:ILE:O	1:A:104:ILE:HG22	2.07	0.55
1:A:4:ILE:HD11	1:A:181:LEU:HD11	1.89	0.55
1:B:267:LEU:HD21	1:B:552:GLN:HB2	1.89	0.55
1:B:525:LYS:H	1:B:525:LYS:CE	2.19	0.55
1:B:49:ALA:O	1:B:50:ASN:HB3	2.07	0.54
1:B:228:LYS:HE2	4:B:966:HOH:O	2.07	0.54
1:A:484:LYS:HB2	1:A:484:LYS:NZ	2.22	0.54
1:B:126:HIS:HE1	1:B:136:THR:CG2	2.20	0.54
1:B:67:MET:HE1	1:B:153:ILE:HG23	1.90	0.54
1:B:288:LEU:HD12	1:B:288:LEU:H	1.71	0.54
1:B:98:VAL:HG22	1:B:165:LEU:HD23	1.90	0.53
1:B:271:GLU:HB2	1:B:350:PRO:HB3	1.91	0.53
1:B:508:GLU:HB2	1:B:534:ARG:HG2	1.91	0.52
1:A:247:MET:HG3	1:A:410:VAL:HB	1.91	0.52
1:A:233:LYS:O	1:A:237:LEU:HB2	2.09	0.52
1:A:253:SER:HB3	1:A:402:ASN:OD1	2.10	0.52
1:B:21:THR:HB	1:B:44:ARG:HG3	1.92	0.52
1:A:345:LYS:H	1:A:345:LYS:CD	2.24	0.51
1:A:281:LEU:HD13	1:A:305:ASN:HB3	1.93	0.50
1:A:463:LYS:NZ	4:A:798:HOH:O	2.38	0.50
1:A:481:HIS:HE1	1:B:35:ASP:OD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HE3	4:B:941:HOH:O	2.10	0.49
1:A:52:LEU:HD21	1:A:83:ASN:HB3	1.94	0.49
1:B:190:LYS:HG2	1:B:191:PRO:HD2	1.94	0.49
1:B:154:ARG:HG3	1:B:186:ASP:O	2.12	0.49
1:A:224:ARG:NH1	4:A:854:HOH:O	2.42	0.48
1:B:505:LYS:H	1:B:505:LYS:CE	2.26	0.48
1:A:15:LYS:HG2	4:A:895:HOH:O	2.14	0.48
1:B:21:THR:HG22	1:B:431:GLU:OE2	2.14	0.48
1:A:154:ARG:O	1:A:187:MET:HE1	2.14	0.48
1:B:17:VAL:HG22	1:B:187:MET:HE2	1.95	0.48
1:A:179:LYS:O	1:A:182:GLN:HG2	2.14	0.48
1:B:126:HIS:HE1	1:B:136:THR:HG23	1.78	0.47
1:B:232:LYS:NZ	4:B:893:HOH:O	2.47	0.47
1:B:548:ASN:O	1:B:552:GLN:HB2	2.14	0.47
1:B:157:TYR:HB2	1:B:187:MET:HE1	1.96	0.47
1:B:126:HIS:CE1	1:B:136:THR:HG23	2.49	0.47
1:A:139:ILE:HD11	1:A:165:LEU:HD21	1.96	0.47
1:A:233:LYS:HD3	1:A:233:LYS:HA	1.86	0.47
1:B:226:ASP:HB3	4:B:936:HOH:O	2.15	0.47
1:A:554:LYS:O	1:A:554:LYS:HD2	2.15	0.47
1:B:483:PRO:HG3	4:B:605:HOH:O	2.14	0.47
1:A:117:LEU:HD22	1:A:124:VAL:HG11	1.97	0.47
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.50	0.47
1:B:317:ARG:NH1	1:B:317:ARG:HG2	2.29	0.47
1:A:554:LYS:C	1:A:556:THR:H	2.23	0.46
1:A:53:ASN:OD1	1:A:450:THR:HG22	2.16	0.46
1:A:248:GLY:O	1:A:251:SER:HB2	2.16	0.46
1:A:218:ALA:HB2	1:A:252:ILE:HD11	1.98	0.45
1:A:232:LYS:HZ1	1:A:252:ILE:HG23	1.81	0.45
1:A:279:ALA:O	1:A:302:LYS:NZ	2.49	0.45
1:A:508:GLU:OE1	1:A:510:HIS:NE2	2.31	0.45
1:B:238:THR:HB	1:B:240:PHE:CE1	2.52	0.45
1:A:38:TYR:OH	1:B:486:GLN:HB3	2.16	0.45
1:A:255:GLN:HB2	1:A:402:ASN:OD1	2.17	0.45
1:A:308:GLU:HB3	1:A:310:HIS:NE2	2.31	0.45
1:A:336:ASN:ND2	1:A:336:ASN:N	2.64	0.45
1:B:190:LYS:HG2	1:B:191:PRO:CD	2.47	0.45
1:B:381:GLY:O	1:B:436:LYS:HG3	2.17	0.45
1:B:145:ALA:HB3	1:B:146:PRO:HD3	1.98	0.45
1:B:238:THR:CG2	1:B:337:ILE:HG12	2.46	0.45
1:B:302:LYS:C	1:B:303:THR:OG1	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LYS:HE2	1:B:317:ARG:O	2.17	0.45
1:B:317:ARG:HB3	1:B:318:ASN:H	1.61	0.45
1:B:171:LEU:HA	1:B:174:LEU:HD22	1.98	0.44
1:B:171:LEU:O	1:B:174:LEU:HB2	2.17	0.44
1:B:8:LYS:NZ	1:B:12:GLU:OE2	2.47	0.44
1:B:221:CYS:HA	1:B:224:ARG:HB2	2.00	0.44
1:A:312:ASP:O	1:A:313:HIS:HB3	2.18	0.44
1:A:104:ILE:HD12	1:A:170:ASN:OD1	2.18	0.44
1:A:481:HIS:HB3	1:B:31:LEU:HD13	1.99	0.44
1:B:312:ASP:O	1:B:313:HIS:HB3	2.17	0.44
1:B:51:GLU:HB2	1:B:80:SER:HB2	1.99	0.43
1:B:499:LEU:HD13	1:B:507:TYR:HB2	1.99	0.43
1:B:534:ARG:HH11	1:B:534:ARG:HD2	1.50	0.43
1:A:344:TYR:CD1	1:A:345:LYS:HE3	2.53	0.43
1:A:498:LEU:HD13	1:B:501:THR:HG21	2.00	0.43
1:B:117:LEU:HD22	1:B:124:VAL:HG11	1.99	0.43
1:B:239:GLN:O	1:B:258:ARG:HD3	2.18	0.43
1:B:449:LEU:HD12	1:B:449:LEU:N	2.33	0.43
1:A:232:LYS:NZ	1:A:252:ILE:HG23	2.33	0.43
1:A:491:GLN:H	1:B:459:ARG:NH1	2.15	0.43
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.91	0.43
1:A:82:LEU:HG	1:A:132:ILE:HD11	2.00	0.43
1:A:545:ALA:HB3	1:A:550:VAL:HG23	2.01	0.43
1:B:253:SER:HB3	1:B:402:ASN:OD1	2.18	0.43
1:A:15:LYS:HE3	1:A:41:GLU:O	2.18	0.43
1:A:308:GLU:HB3	1:A:310:HIS:HE2	1.84	0.43
1:B:454:ILE:O	1:B:457:MET:HB2	2.19	0.43
1:A:139:ILE:HG21	1:A:145:ALA:CB	2.46	0.43
1:B:505:LYS:H	1:B:505:LYS:HD3	1.84	0.43
1:B:458:ILE:HG23	1:B:505:LYS:NZ	2.34	0.43
1:B:101:VAL:HB	1:B:102:PRO:CD	2.49	0.42
1:B:242:ALA:HB1	1:B:252:ILE:HD13	2.01	0.42
1:B:90:ALA:HB1	1:B:411:LEU:HD13	2.01	0.42
1:B:104:ILE:O	1:B:105:SER:CB	2.67	0.42
1:B:480:ILE:CG1	1:B:553:ALA:HB1	2.48	0.42
1:A:540:LEU:HA	1:A:541:PRO:HD3	1.88	0.42
1:B:244:VAL:O	1:B:262:VAL:HA	2.19	0.42
1:A:154:ARG:HA	1:A:187:MET:HE1	2.02	0.42
1:A:308:GLU:HB2	1:A:315:LYS:HB3	2.01	0.42
1:A:363:THR:HA	1:A:364:PRO:HD3	1.83	0.42
1:B:302:LYS:HB3	1:B:303:THR:H	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD22	1:A:337:ILE:HD13	2.01	0.42
1:A:51:GLU:HB2	1:A:80:SER:HB2	2.02	0.41
1:A:242:ALA:HB1	1:A:252:ILE:HD13	2.02	0.41
1:A:221:CYS:O	1:A:225:HIS:HB2	2.21	0.41
1:A:269:LYS:N	1:A:269:LYS:HD3	2.34	0.41
1:A:35:ASP:OD2	1:B:481:HIS:HE1	2.03	0.41
1:B:176:VAL:HA	1:B:177:PRO:HD3	1.81	0.41
1:B:352:ARG:N	1:B:352:ARG:HD2	2.36	0.41
1:B:21:THR:CG2	1:B:44:ARG:HE	2.33	0.41
1:B:198:LYS:HD3	1:B:198:LYS:HA	1.62	0.41
1:B:363:THR:HA	1:B:364:PRO:HD3	1.82	0.41
1:A:24:GLY:HA3	1:A:71:ILE:O	2.20	0.41
3:A:557:TPP:N1'	1:B:51:GLU:OE2	2.54	0.41
1:B:552:GLN:O	1:B:554:LYS:N	2.54	0.41
1:A:157:TYR:HB3	1:A:187:MET:CE	2.51	0.41
1:A:381:GLY:O	1:A:436:LYS:HG3	2.21	0.41
1:A:452:GLN:O	1:A:455:SER:HB3	2.21	0.41
1:B:126:HIS:CE1	1:B:136:THR:CG2	3.03	0.41
1:B:480:ILE:HD11	1:B:553:ALA:HB1	2.03	0.41
1:A:302:LYS:HE3	1:A:302:LYS:HB3	1.81	0.40
1:B:552:GLN:HB3	1:B:553:ALA:H	1.73	0.40
1:A:158:VAL:HG11	4:A:723:HOH:O	2.21	0.40
1:B:388:THR:HB	1:B:415:ILE:HG22	2.02	0.40
1:B:238:THR:O	1:B:239:GLN:HB2	2.22	0.40
1:A:247:MET:HE2	1:A:410:VAL:HG12	2.04	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	531/555 (96%)	503 (95%)	25 (5%)	3 (1%)	21 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	531/555 (96%)	501 (94%)	25 (5%)	5 (1%)	14	17
All	All	1062/1110 (96%)	1004 (94%)	50 (5%)	8 (1%)	16	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	B	553	ALA
1	A	289	LEU
1	B	226	ASP
1	B	552	GLN
1	B	220	ALA
1	A	104	ILE
1	B	104	ILE

5.3.2 Protein sidechains [i](#)

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	447/463 (96%)	380 (85%)	67 (15%)	3	3
1	B	447/463 (96%)	386 (86%)	61 (14%)	3	4
All	All	894/926 (96%)	766 (86%)	128 (14%)	3	3

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	14	LEU
1	A	15	LYS
1	A	31	LEU
1	A	33	LEU
1	A	52	LEU
1	A	65	LYS
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	99	VAL
1	A	103	SER
1	A	116	THR
1	A	117	LEU
1	A	126	HIS
1	A	139	ILE
1	A	142	ILE
1	A	144	THR
1	A	165	LEU
1	A	172	VAL
1	A	174	LEU
1	A	176	VAL
1	A	179	LYS
1	A	182	GLN
1	A	207	LEU
1	A	221	CYS
1	A	225	HIS
1	A	232	LYS
1	A	233	LYS
1	A	267	LEU
1	A	268	SER
1	A	269	LYS
1	A	271	GLU
1	A	274	GLU
1	A	283	LEU
1	A	288	LEU
1	A	289	LEU
1	A	291	ASP
1	A	302	LYS
1	A	317	ARG
1	A	330	LEU
1	A	336	ASN
1	A	345	LYS
1	A	346	PRO
1	A	347	VAL
1	A	353	THR
1	A	362	SER
1	A	411	LEU
1	A	423	LEU
1	A	436	LYS
1	A	440	LEU
1	A	447	LEU

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Mol	Chain	Res	Type
1	A	469	LEU
1	A	475	THR
1	A	476	ILE
1	A	479	LEU
1	A	480	ILE
1	A	484	LYS
1	A	498	LEU
1	A	505	LYS
1	A	512	VAL
1	A	515	THR
1	A	520	LYS
1	A	525	LYS
1	A	533	ILE
1	A	536	ILE
1	A	540	LEU
1	A	547	GLN
1	A	556	THR
1	B	2	SER
1	B	3	GLU
1	B	14	LEU
1	B	17	VAL
1	B	21	THR
1	B	25	LEU
1	B	33	LEU
1	B	34	LEU
1	B	52	LEU
1	B	67	MET
1	B	103	SER
1	B	104	ILE
1	B	117	LEU
1	B	136	THR
1	B	142	ILE
1	B	174	LEU
1	B	176	VAL
1	B	179	LYS
1	B	195	GLU
1	B	196	SER
1	B	198	LYS
1	B	207	LEU
1	B	215	VAL
1	B	223	SER
1	B	224	ARG

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Mol	Chain	Res	Type
1	B	227	VAL
1	B	228	LYS
1	B	234	LEU
1	B	247	MET
1	B	267	LEU
1	B	270	PRO
1	B	271	GLU
1	B	278	SER
1	B	281	LEU
1	B	282	ILE
1	B	283	LEU
1	B	288	LEU
1	B	289	LEU
1	B	303	THR
1	B	329	VAL
1	B	337	ILE
1	B	339	ASP
1	B	342	LYS
1	B	345	LYS
1	B	349	VAL
1	B	362	SER
1	B	365	LEU
1	B	403	ASN
1	B	411	LEU
1	B	423	LEU
1	B	435	LYS
1	B	440	LEU
1	B	447	LEU
1	B	466	LEU
1	B	505	LYS
1	B	525	LYS
1	B	532	LYS
1	B	547	GLN
1	B	548	ASN
1	B	554	LYS
1	B	556	THR

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	20	ASN
1	A	92	HIS

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Mol	Chain	Res	Type
1	A	126	HIS
1	A	372	ASN
1	A	397	GLN
1	A	403	ASN
1	A	481	HIS
1	A	523	GLN
1	A	547	GLN
1	B	20	ASN
1	B	126	HIS
1	B	213	ASN
1	B	225	HIS
1	B	396	ASN
1	B	481	HIS
1	B	548	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TPP	B	557	2	26,27,27	1.48	4 (15%)	38,40,40	1.66	11 (28%)
3	TPP	A	557	2	26,27,27	1.19	3 (11%)	38,40,40	1.21	4 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TPP	B	557	2	-	3/17/17/17	0/2/2/2
3	TPP	A	557	2	-	5/17/17/17	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	557	TPP	C4'-N3'	3.59	1.39	1.35
3	A	557	TPP	C7'-N3	3.30	1.55	1.48
3	B	557	TPP	PB-O2B	-3.23	1.42	1.54
3	A	557	TPP	C4'-N3'	3.07	1.39	1.35
3	B	557	TPP	C7'-N3	2.96	1.54	1.48
3	B	557	TPP	PB-O1B	2.56	1.58	1.50
3	A	557	TPP	PB-O3B	-2.35	1.46	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	557	TPP	CM2-C2'-N1'	4.07	121.53	117.20
3	B	557	TPP	O3B-PB-O2B	3.47	120.80	107.80
3	A	557	TPP	C2-S1-C5	-3.23	89.08	91.22
3	B	557	TPP	O3A-PB-O1B	-2.71	96.77	111.04
3	B	557	TPP	O2B-PB-O1B	2.67	121.23	110.83
3	B	557	TPP	O3B-PB-O1B	-2.63	100.61	110.83
3	B	557	TPP	O2A-PA-O3A	-2.62	100.20	107.27
3	B	557	TPP	C7'-N3-C2	-2.58	118.10	123.48
3	B	557	TPP	C7'-N3-C4	2.57	129.17	122.36
3	B	557	TPP	C7'-C5'-C4'	2.54	127.00	122.36
3	B	557	TPP	O2A-PA-O1A	2.47	123.92	112.44
3	A	557	TPP	C5'-C4'-N4'	2.24	125.15	122.14
3	B	557	TPP	O3A-PA-O1A	2.05	116.86	110.70
3	A	557	TPP	N4'-C4'-N3'	-2.03	114.29	117.03
3	B	557	TPP	C6'-N1'-C2'	2.02	119.40	116.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

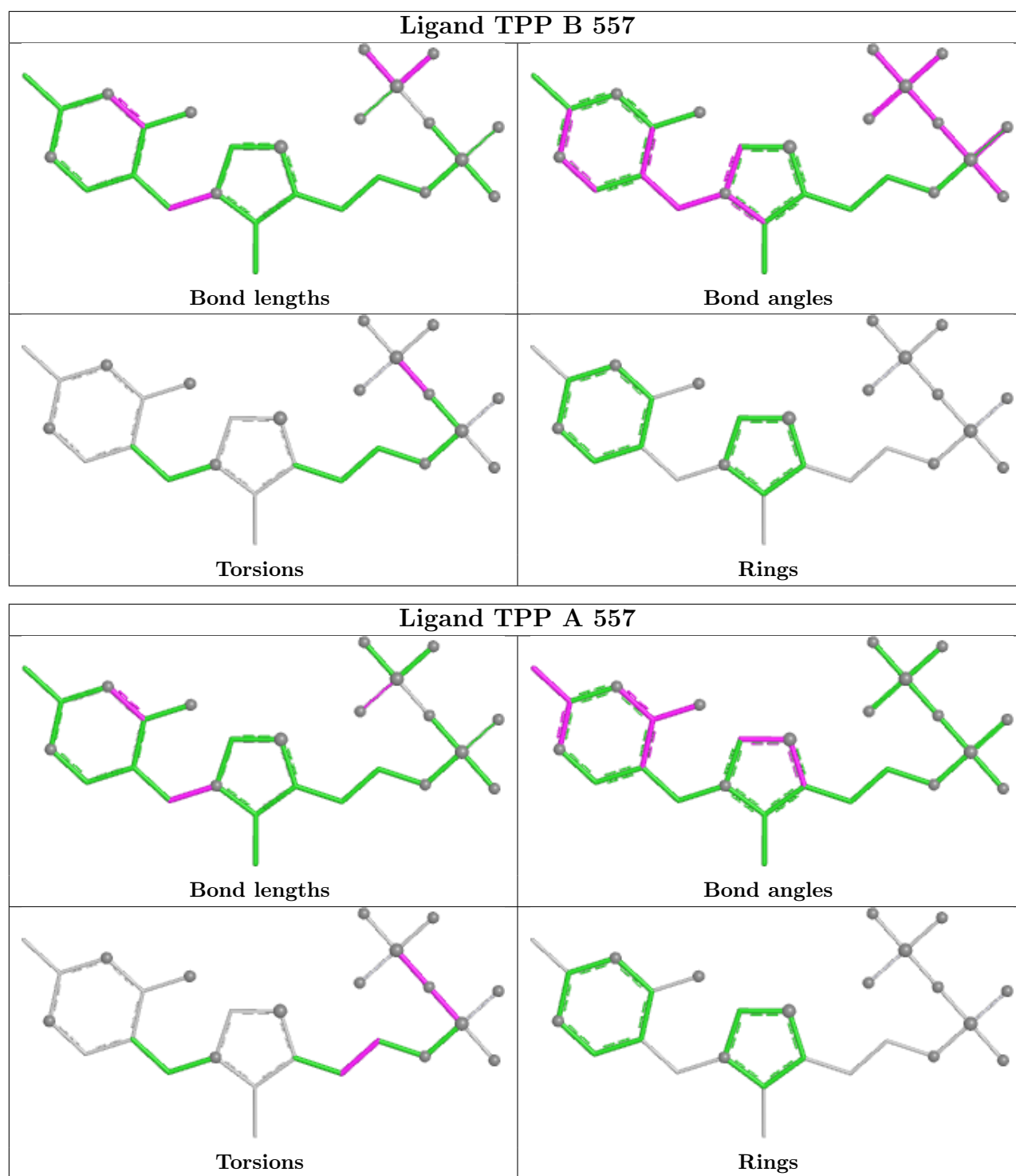
Mol	Chain	Res	Type	Atoms
3	A	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	PA-O3A-PB-O1B
3	A	557	TPP	PA-O3A-PB-O2B
3	B	557	TPP	PA-O3A-PB-O2B
3	A	557	TPP	C5-C6-C7-O7
3	A	557	TPP	PA-O3A-PB-O1B
3	A	557	TPP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	TPP	1	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	537/555 (96%)	-0.67	5 (0%) 81 82	3, 13, 33, 58	0
1	B	537/555 (96%)	-0.64	9 (1%) 69 70	3, 13, 32, 58	0
All	All	1074/1110 (96%)	-0.66	14 (1%) 75 76	3, 13, 33, 58	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	CYS	4.9
1	B	290	SER	4.7
1	B	291	ASP	4.3
1	B	287	ALA	3.8
1	B	553	ALA	3.8
1	B	289	LEU	3.1
1	A	290	SER	2.8
1	B	105	SER	2.7
1	A	303	THR	2.6
1	B	286	GLY	2.2
1	B	302	LYS	2.2
1	B	556	THR	2.2
1	A	555	LEU	2.1
1	A	289	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

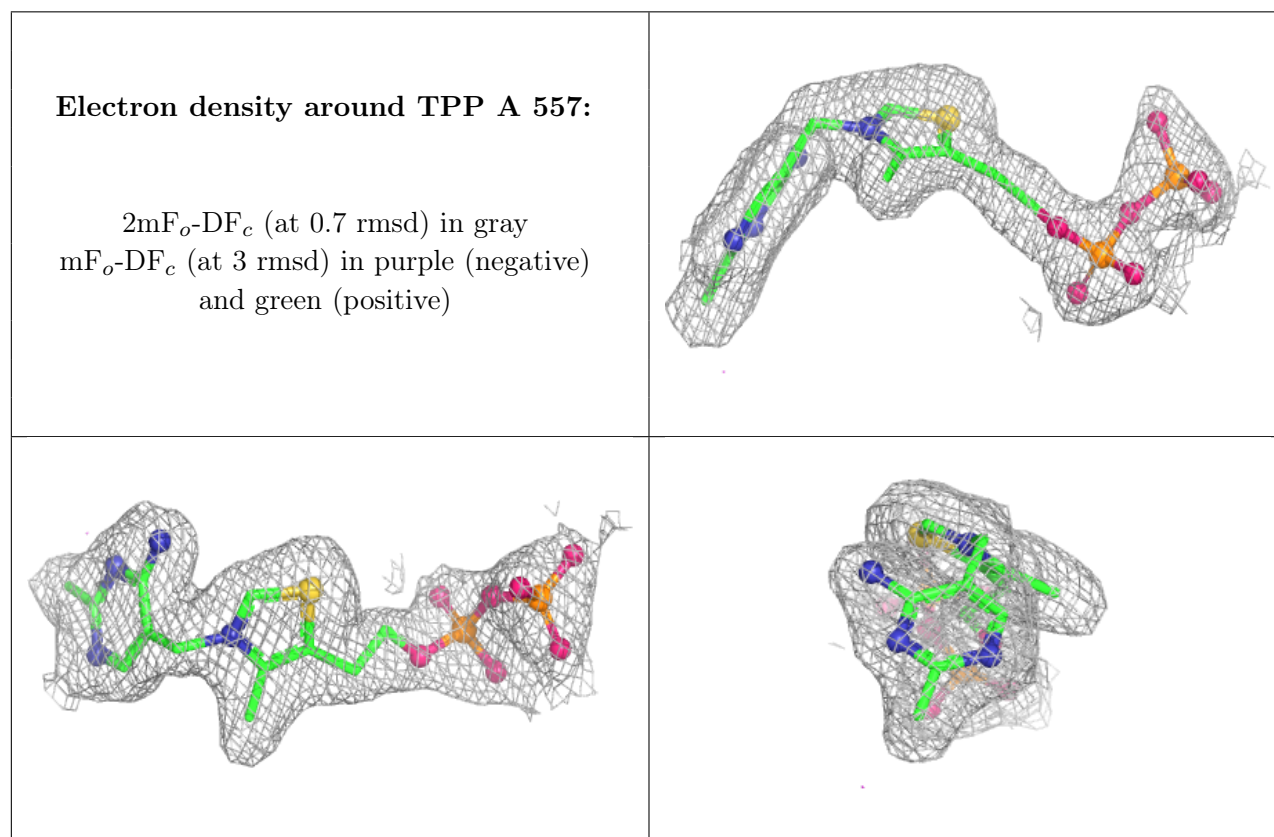
There are no oligosaccharides in this entry.

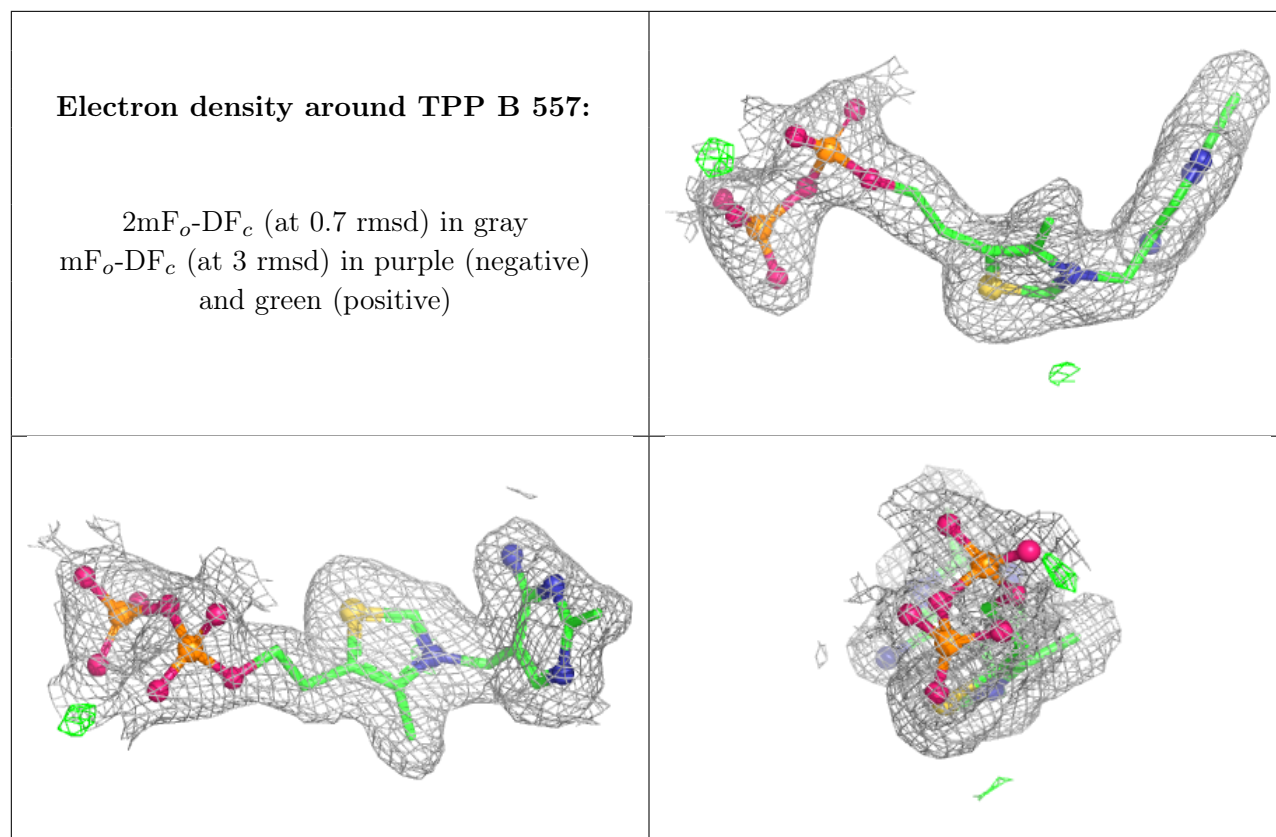
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	558	1/1	0.92	0.07	19,19,19,19	0
2	MG	B	558	1/1	0.97	0.14	13,13,13,13	0
3	TPP	A	557	26/26	0.99	0.04	2,6,8,11	0
3	TPP	B	557	26/26	0.99	0.04	2,5,10,11	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.