



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:47 PM UTC

PDB ID : 1PYD / pdb_00001pyd
Title : CATALYTIC CENTERS IN THE THIAMIN DIPHOSPHATE DEPENDENT
ENZYME PYRUVATE DECARBOXYLASE AT 2.4 ANGSTROMS RESO-
LUTION
Authors : Furey, W.; Dyda, F.
Deposited on : 1993-03-23
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

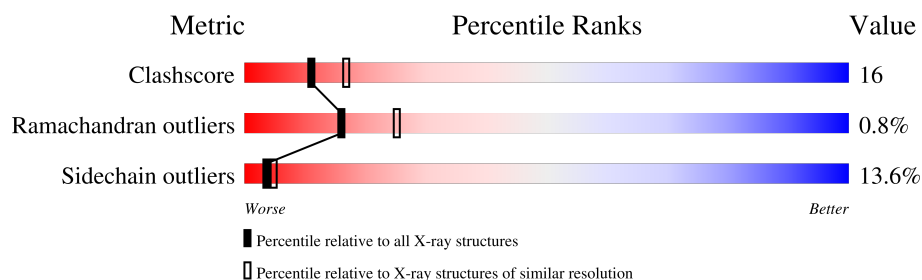
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	556	
1	B	556	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8316 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			

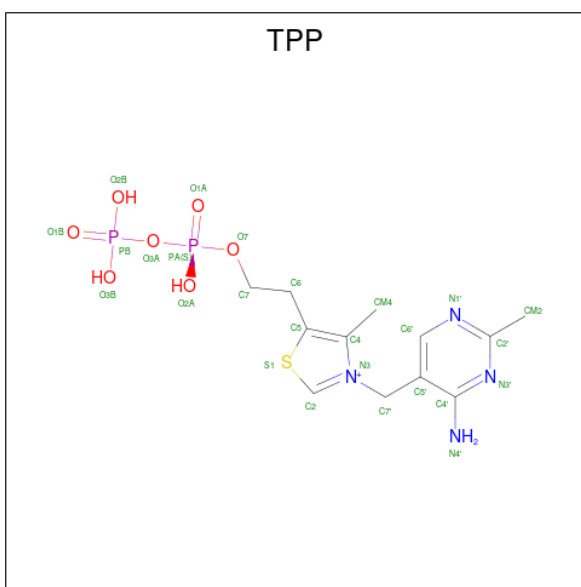
There are 12 discrepancies between the modelled and reference sequences:

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		

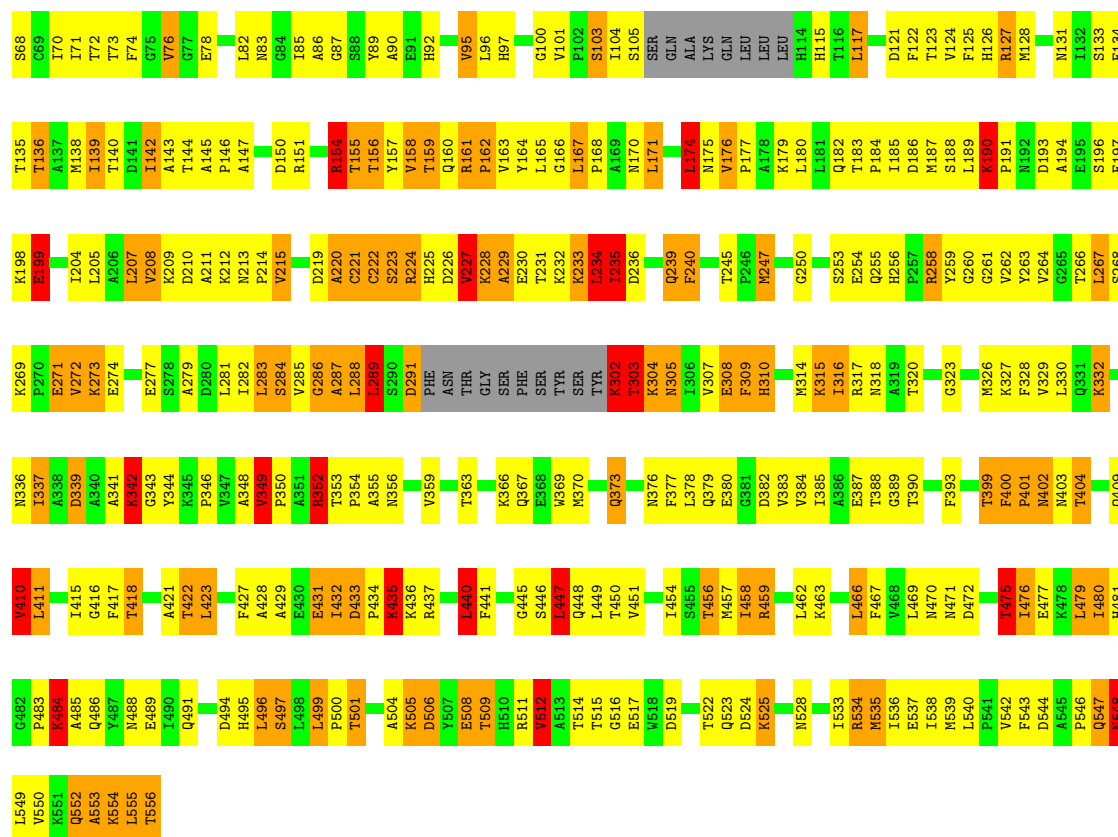
- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.95Å 74.67Å 119.95Å 90.00° 116.39° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA, X-PLOR	Depositor
R, R_{free}	0.197 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8316	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: TPP, MG

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	1.38	6/4215 (0.1%)	2.86	456/5728 (8.0%)
1	B	1.36	10/4215 (0.2%)	2.89	494/5728 (8.6%)
All	All	1.37	16/8430 (0.2%)	2.88	950/11456 (8.3%)

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	A	0	1
1	B	0	1
All	All	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	LEU	C-N	-6.27	1.29	1.33
1	B	384	VAL	N-CA	5.86	1.53	1.46
1	A	456	THR	CA-CB	5.79	1.62	1.53
1	B	446	SER	C-N	-5.75	1.26	1.33
1	B	429	ALA	N-CA	5.67	1.53	1.46
1	A	101	VAL	N-CA	5.66	1.51	1.46
1	B	310	HIS	N-CA	5.51	1.52	1.45
1	B	491	GLN	CA-C	5.51	1.60	1.52
1	B	436	LYS	CA-CB	-5.50	1.45	1.53
1	B	553	ALA	C-O	5.26	1.30	1.24
1	B	215	VAL	N-CA	5.21	1.52	1.46
1	A	316	ILE	N-CA	5.17	1.52	1.46
1	B	332	LYS	C-O	5.12	1.30	1.24
1	A	235	ILE	CA-CB	5.11	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	485	ALA	C-N	-5.07	1.27	1.34
1	A	205	LEU	N-CA	5.06	1.52	1.46

All (950) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	CD-NE-CZ	22.66	156.13	124.40
1	A	101	VAL	N-CA-CB	-19.95	94.71	111.67
1	B	65	LYS	CB-CG-CD	17.33	151.16	111.30
1	B	400	PHE	CA-CB-CG	16.77	130.57	113.80
1	A	219	ASP	CA-CB-CG	16.58	129.18	112.60
1	B	459	ARG	CD-NE-CZ	16.05	146.88	124.40
1	B	285	VAL	CA-C-O	14.77	139.25	120.78
1	A	552	GLN	OE1-CD-NE2	-14.17	108.43	122.60
1	A	226	ASP	CA-CB-CG	14.16	126.76	112.60
1	A	176	VAL	N-CA-CB	-14.01	96.65	111.64
1	A	141	ASP	CA-CB-CG	13.89	126.49	112.60
1	B	427	PHE	CA-CB-CG	13.66	127.46	113.80
1	A	291	ASP	CA-CB-CG	13.40	126.00	112.60
1	B	445	GLY	CA-C-N	13.02	137.73	120.28
1	B	445	GLY	C-N-CA	13.02	137.73	120.28
1	A	288	LEU	N-CA-C	-12.38	92.36	110.06
1	B	227	VAL	CB-CA-C	12.11	126.21	111.20
1	A	528	ASN	CA-CB-CG	-12.02	100.58	112.60
1	A	32	SER	CA-C-N	11.87	140.54	120.71
1	A	32	SER	C-N-CA	11.87	140.54	120.71
1	A	44	ARG	CD-NE-CZ	11.54	140.56	124.40
1	B	436	LYS	CB-CA-C	11.48	129.12	110.29
1	A	287	ALA	CA-C-O	11.24	133.75	121.16
1	B	337	ILE	N-CA-C	11.16	122.00	110.62
1	B	83	ASN	OD1-CG-ND2	11.09	133.69	122.60
1	B	402	ASN	OD1-CG-ND2	-11.01	111.59	122.60
1	A	415	ILE	CA-C-O	-10.92	108.74	120.64
1	A	209	LYS	CA-CB-CG	10.89	135.88	114.10
1	A	264	VAL	N-CA-C	-10.80	93.62	108.96
1	B	175	ASN	OD1-CG-ND2	-10.63	111.97	122.60
1	B	459	ARG	NE-CZ-NH2	-10.55	109.71	119.20
1	A	255	GLN	CA-C-N	10.54	134.79	120.67
1	A	255	GLN	C-N-CA	10.54	134.79	120.67
1	A	476	ILE	CA-C-O	-10.45	109.77	120.85
1	B	433	ASP	CA-CB-CG	10.44	123.04	112.60
1	A	264	VAL	CA-C-O	-10.42	110.62	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	THR	CA-C-N	10.37	133.93	120.44
1	B	456	THR	C-N-CA	10.37	133.93	120.44
1	A	304	LYS	CA-C-N	10.35	136.53	122.77
1	A	304	LYS	C-N-CA	10.35	136.53	122.77
1	B	287	ALA	N-CA-CB	-10.26	93.15	110.49
1	B	459	ARG	NE-CZ-NH1	10.23	131.73	121.50
1	A	179	LYS	CA-CB-CG	10.22	134.54	114.10
1	B	277	GLU	CB-CG-CD	10.12	129.81	112.60
1	B	336	ASN	OD1-CG-ND2	-10.00	112.60	122.60
1	B	332	LYS	CB-CA-C	10.00	129.87	110.67
1	B	484	LYS	CG-CD-CE	9.98	134.26	111.30
1	B	421	ALA	CA-C-N	9.94	133.60	120.28
1	B	421	ALA	C-N-CA	9.94	133.60	120.28
1	A	533	ILE	CA-CB-CG2	9.83	127.20	110.50
1	B	282	ILE	O-C-N	9.82	133.81	123.20
1	A	533	ILE	N-CA-CB	9.67	125.22	110.13
1	B	155	THR	CA-CB-OG1	-9.66	95.11	109.60
1	B	176	VAL	CB-CA-C	9.56	118.70	109.33
1	B	253	SER	CB-CA-C	9.50	124.50	110.26
1	A	245	THR	N-CA-C	-9.47	97.99	110.40
1	B	83	ASN	CA-CB-CG	-9.44	103.16	112.60
1	B	370	MET	N-CA-C	9.42	121.15	111.07
1	B	286	GLY	O-C-N	9.41	132.27	122.96
1	B	175	ASN	CA-CB-CG	9.34	121.94	112.60
1	A	305	ASN	CA-CB-CG	9.32	121.92	112.60
1	A	25	LEU	O-C-N	9.28	128.47	121.88
1	A	400	PHE	CA-CB-CG	9.27	123.07	113.80
1	B	404	THR	CA-C-O	-9.27	110.28	120.38
1	A	263	TYR	CA-C-N	9.25	135.62	122.77
1	A	263	TYR	C-N-CA	9.25	135.62	122.77
1	B	100	GLY	O-C-N	9.21	129.16	123.35
1	B	264	VAL	CA-C-N	9.17	129.93	121.31
1	B	264	VAL	C-N-CA	9.17	129.93	121.31
1	A	467	PHE	CA-CB-CG	9.16	122.96	113.80
1	B	349	VAL	N-CA-CB	-9.15	98.40	111.21
1	B	40	VAL	CA-C-O	9.14	130.56	120.59
1	B	231	THR	CA-CB-CG2	9.12	126.01	110.50
1	B	176	VAL	N-CA-CB	-9.12	101.89	111.64
1	B	86	ALA	CA-C-N	9.06	130.00	119.94
1	B	86	ALA	C-N-CA	9.06	130.00	119.94
1	A	148	GLU	CA-C-N	9.05	132.15	120.56
1	A	148	GLU	C-N-CA	9.05	132.15	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	HIS	N-CA-CB	9.04	125.76	110.49
1	A	285	VAL	N-CA-C	9.01	120.58	106.88
1	A	255	GLN	O-C-N	-8.98	111.56	122.34
1	B	344	TYR	O-C-N	8.98	133.42	123.27
1	A	480	ILE	CB-CA-C	8.98	119.45	110.65
1	A	97	HIS	CA-C-N	8.96	134.21	122.93
1	A	97	HIS	C-N-CA	8.96	134.21	122.93
1	B	222	CYS	N-CA-C	-8.93	101.63	111.36
1	B	23	PHE	CA-CB-CG	-8.93	104.87	113.80
1	A	263	TYR	CA-C-O	8.92	129.84	120.30
1	A	344	TYR	CA-C-O	8.90	131.13	121.16
1	B	282	ILE	CA-C-O	-8.89	110.94	120.36
1	A	195	GLU	CA-C-O	-8.87	111.15	120.55
1	A	41	GLU	CA-CB-CG	8.85	131.81	114.10
1	B	410	VAL	N-CA-C	8.84	120.70	110.62
1	B	486	GLN	CB-CG-CD	8.83	127.61	112.60
1	B	519	ASP	N-CA-C	8.82	120.89	111.28
1	A	462	LEU	CA-C-O	-8.80	111.02	121.05
1	B	175	ASN	CB-CG-ND2	8.77	129.55	116.40
1	B	194	ALA	N-CA-C	8.74	120.81	111.28
1	A	547	GLN	CA-C-N	8.73	132.34	120.38
1	A	547	GLN	C-N-CA	8.73	132.34	120.38
1	B	475	THR	CA-C-O	-8.71	109.95	119.97
1	A	502	PHE	CA-CB-CG	8.70	122.50	113.80
1	B	435	LYS	CB-CG-CD	8.70	131.31	111.30
1	A	530	ASN	OD1-CG-ND2	8.69	131.29	122.60
1	B	272	VAL	N-CA-C	-8.63	102.44	110.82
1	A	459	ARG	NH1-CZ-NH2	8.61	130.49	119.30
1	B	417	PHE	CA-C-N	8.60	132.17	120.38
1	B	417	PHE	C-N-CA	8.60	132.17	120.38
1	A	251	SER	CA-CB-OG	-8.56	93.98	111.10
1	A	309	PHE	CA-CB-CG	8.56	122.36	113.80
1	A	176	VAL	CB-CA-C	8.55	117.71	109.33
1	B	302	LYS	CA-CB-CG	8.49	131.09	114.10
1	B	491	GLN	N-CA-C	-8.49	97.22	109.96
1	A	165	LEU	CA-C-N	8.48	129.77	121.62
1	A	165	LEU	C-N-CA	8.48	129.77	121.62
1	A	161	ARG	NE-CZ-NH1	8.48	129.98	121.50
1	A	552	GLN	CG-CD-OE1	8.48	137.76	120.80
1	B	11	PHE	CA-C-N	8.47	131.96	120.44
1	B	11	PHE	C-N-CA	8.47	131.96	120.44
1	B	285	VAL	CA-C-N	8.46	131.85	122.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	VAL	C-N-CA	8.46	131.85	122.55
1	B	486	GLN	OE1-CD-NE2	-8.45	114.15	122.60
1	B	309	PHE	CA-C-O	-8.40	111.27	120.43
1	A	380	GLU	CB-CG-CD	8.39	126.86	112.60
1	A	19	VAL	N-CA-CB	8.39	121.89	111.41
1	B	239	GLN	OE1-CD-NE2	-8.38	114.22	122.60
1	B	35	ASP	CA-CB-CG	8.35	120.95	112.60
1	A	442	ILE	CA-C-N	8.32	128.25	120.34
1	A	442	ILE	C-N-CA	8.32	128.25	120.34
1	A	338	ALA	O-C-N	8.27	130.88	122.12
1	B	121	ASP	N-CA-CB	8.24	123.85	110.42
1	B	259	TYR	CA-C-O	-8.23	111.21	120.43
1	B	25	LEU	O-C-N	8.23	128.88	121.80
1	B	534	ARG	CD-NE-CZ	8.22	135.91	124.40
1	B	215	VAL	CA-C-O	-8.22	112.57	121.28
1	A	290	SER	N-CA-C	-8.21	100.38	111.96
1	B	115	HIS	CA-CB-CG	8.20	122.00	113.80
1	B	415	ILE	O-C-N	8.18	131.53	122.61
1	A	306	ILE	O-C-N	8.17	131.86	123.20
1	B	284	SER	CB-CA-C	8.17	125.03	111.31
1	A	141	ASP	CA-C-O	-8.16	110.81	120.60
1	B	37	ILE	O-C-N	8.13	129.86	121.89
1	B	534	ARG	NE-CZ-NH2	8.12	126.51	119.20
1	B	506	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	12	GLU	CG-CD-OE1	-8.09	99.80	118.40
1	B	436	LYS	CA-CB-CG	8.09	130.28	114.10
1	A	494	ASP	CA-C-N	8.09	131.46	120.54
1	A	494	ASP	C-N-CA	8.09	131.46	120.54
1	B	258	ARG	NE-CZ-NH2	-8.08	111.93	119.20
1	A	389	GLY	N-CA-C	-8.06	99.97	110.29
1	A	554	LYS	CA-C-N	8.02	134.12	120.72
1	A	554	LYS	C-N-CA	8.02	134.12	120.72
1	B	266	THR	CA-CB-OG1	-8.02	97.56	109.60
1	B	524	ASP	CA-C-N	8.01	131.36	120.38
1	B	524	ASP	C-N-CA	8.01	131.36	120.38
1	A	318	ASN	OD1-CG-ND2	-8.00	114.60	122.60
1	A	287	ALA	CA-C-N	8.00	135.66	122.62
1	A	287	ALA	C-N-CA	8.00	135.66	122.62
1	B	485	ALA	CA-C-N	7.96	131.75	120.28
1	B	485	ALA	C-N-CA	7.96	131.75	120.28
1	A	23	PHE	CA-CB-CG	-7.96	105.84	113.80
1	B	553	ALA	CB-CA-C	-7.96	97.53	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	LYS	N-CA-C	-7.92	97.86	109.50
1	A	533	ILE	CB-CA-C	-7.92	99.23	111.26
1	B	432	ILE	CA-C-O	-7.91	111.55	120.96
1	B	267	LEU	O-C-N	7.90	132.59	122.39
1	A	372	ASN	N-CA-C	-7.89	102.27	111.03
1	B	556	THR	CA-C-O	7.85	134.15	120.80
1	B	467	PHE	CA-C-O	-7.85	111.88	120.43
1	B	273	LYS	CA-CB-CG	7.84	129.78	114.10
1	A	405	TYR	CA-CB-CG	7.83	128.00	113.90
1	B	423	LEU	CB-CA-C	7.83	123.27	110.90
1	B	193	ASP	N-CA-C	-7.82	98.23	109.96
1	A	304	LYS	N-CA-C	7.81	127.44	110.80
1	B	534	ARG	NE-CZ-NH1	-7.79	113.71	121.50
1	B	115	HIS	N-CA-C	-7.77	94.25	110.80
1	B	524	ASP	CB-CG-OD2	7.76	136.25	118.40
1	B	509	THR	CA-CB-OG1	-7.75	97.98	109.60
1	B	401	PRO	N-CA-C	-7.73	100.40	111.22
1	B	411	LEU	CA-C-O	-7.72	110.66	120.31
1	A	424	GLY	CA-C-N	7.71	130.61	120.28
1	A	424	GLY	C-N-CA	7.71	130.61	120.28
1	B	26	PRO	CB-CA-C	-7.71	100.85	110.95
1	B	135	THR	CA-CB-CG2	7.70	123.60	110.50
1	B	227	VAL	N-CA-CB	-7.70	102.32	112.26
1	A	147	ALA	CA-C-N	7.70	130.92	120.38
1	A	147	ALA	C-N-CA	7.70	130.92	120.38
1	A	288	LEU	CA-C-O	7.69	130.40	121.78
1	A	255	GLN	CA-C-O	7.69	128.56	119.56
1	A	540	LEU	N-CA-CB	-7.69	97.19	110.72
1	A	305	ASN	CB-CA-C	-7.68	97.74	110.19
1	A	364	PRO	CB-CA-C	7.67	121.35	111.46
1	B	494	ASP	CA-C-N	7.67	130.88	120.38
1	B	494	ASP	C-N-CA	7.67	130.88	120.38
1	A	104	ILE	N-CA-CB	7.64	123.84	111.23
1	B	528	ASN	OD1-CG-ND2	7.64	130.24	122.60
1	A	359	VAL	CB-CA-C	7.62	118.12	109.89
1	A	474	TYR	CA-C-O	-7.61	112.82	122.63
1	A	493	TRP	O-C-N	7.61	132.74	123.16
1	A	185	ILE	O-C-N	7.60	131.25	122.81
1	A	4	ILE	CA-CB-CG2	7.59	123.41	110.50
1	A	491	GLN	OE1-CD-NE2	-7.58	115.02	122.60
1	B	59	ASP	CA-CB-CG	7.57	120.17	112.60
1	B	226	ASP	CA-CB-CG	7.57	120.17	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	VAL	CB-CA-C	7.57	121.71	110.97
1	B	547	GLN	CA-C-O	-7.55	112.46	120.92
1	A	119	ASN	N-CA-C	7.55	123.41	113.30
1	A	325	GLN	CB-CG-CD	7.54	125.42	112.60
1	A	193	ASP	N-CA-C	-7.53	98.88	110.10
1	A	316	ILE	CA-C-O	-7.53	112.67	120.27
1	A	373	GLN	CA-C-N	7.53	130.70	120.54
1	A	373	GLN	C-N-CA	7.53	130.70	120.54
1	A	418	THR	N-CA-C	7.52	121.56	112.38
1	B	44	ARG	CA-C-N	7.49	132.58	122.84
1	B	44	ARG	C-N-CA	7.49	132.58	122.84
1	B	50	ASN	CA-CB-CG	7.49	120.09	112.60
1	A	142	ILE	N-CA-CB	7.49	124.32	110.77
1	B	422	THR	N-CA-CB	7.46	121.09	110.12
1	A	115	HIS	N-CA-CB	7.44	123.07	110.49
1	A	415	ILE	N-CA-C	7.44	121.43	111.17
1	A	230	GLU	O-C-N	7.43	130.92	122.22
1	B	307	VAL	CA-C-N	-7.41	112.91	122.77
1	B	307	VAL	C-N-CA	-7.41	112.91	122.77
1	A	526	SER	CA-CB-OG	-7.40	96.30	111.10
1	A	323	GLY	CA-C-O	-7.39	111.58	119.27
1	B	250	GLY	N-CA-C	-7.39	105.31	114.92
1	A	102	PRO	CA-C-O	7.39	129.71	121.36
1	A	312	ASP	O-C-N	7.38	132.19	122.15
1	A	514	THR	CA-C-O	7.37	129.61	121.06
1	B	454	ILE	N-CA-C	-7.36	103.12	110.62
1	B	470	ASN	O-C-N	7.35	131.75	122.93
1	B	185	ILE	N-CA-C	-7.33	100.05	109.80
1	B	376	ASN	CA-C-O	-7.32	111.15	119.79
1	A	542	VAL	CA-CB-CG1	7.30	122.82	110.40
1	B	533	ILE	CA-C-O	-7.30	112.43	121.11
1	A	45	TRP	CA-C-O	-7.29	112.30	120.32
1	B	353	THR	O-C-N	7.29	129.59	121.43
1	A	456	THR	CA-CB-OG1	-7.28	98.67	109.60
1	A	83	ASN	OD1-CG-ND2	7.27	129.87	122.60
1	A	533	ILE	N-CA-C	-7.26	100.22	109.58
1	B	95	VAL	CA-C-O	-7.25	112.77	120.53
1	A	173	ASP	CA-CB-CG	-7.24	105.36	112.60
1	A	485	ALA	CA-C-O	-7.24	112.43	120.69
1	A	321	PHE	O-C-N	7.24	128.14	121.04
1	A	427	PHE	CA-CB-CG	7.24	121.04	113.80
1	A	410	VAL	N-CA-C	7.23	118.00	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	219	ASP	CA-CB-CG	7.23	119.83	112.60
1	A	529	ASP	CB-CA-C	7.23	122.23	109.72
1	B	21	THR	CB-CA-C	7.23	123.18	109.37
1	A	309	PHE	CA-C-O	-7.23	112.37	120.32
1	A	472	ASP	N-CA-C	7.22	121.21	111.24
1	A	121	ASP	CA-C-O	7.22	128.31	120.58
1	A	509	THR	CA-C-O	-7.21	113.02	121.46
1	A	468	VAL	O-C-N	-7.20	114.68	123.10
1	A	337	ILE	N-CA-C	7.19	117.32	110.42
1	B	274	GLU	CA-CB-CG	7.18	128.46	114.10
1	A	363	THR	CA-CB-OG1	-7.18	98.83	109.60
1	A	448	GLN	N-CA-C	7.17	119.95	111.71
1	A	510	HIS	O-C-N	7.16	131.50	123.48
1	A	233	LYS	N-CA-C	-7.16	103.41	111.14
1	B	402	ASN	CA-C-O	-7.15	113.76	121.56
1	A	493	TRP	CA-C-O	-7.15	113.08	121.16
1	B	209	LYS	N-CA-CB	-7.14	98.53	110.39
1	B	310	HIS	CA-C-O	-7.14	113.08	121.44
1	B	536	ILE	CA-C-O	-7.14	113.32	120.31
1	A	441	PHE	N-CA-CB	7.13	122.45	110.69
1	B	42	GLY	CA-C-O	7.12	127.05	119.07
1	B	235	ILE	CB-CA-C	7.12	121.75	112.14
1	B	258	ARG	NE-CZ-NH1	7.11	128.61	121.50
1	A	312	ASP	CA-C-O	-7.11	112.12	119.51
1	B	235	ILE	CA-CB-CG2	7.09	122.55	110.50
1	A	489	GLU	CA-C-N	7.06	132.72	122.69
1	A	489	GLU	C-N-CA	7.06	132.72	122.69
1	B	151	ARG	CD-NE-CZ	7.05	134.28	124.40
1	B	124	VAL	N-CA-C	7.03	117.12	110.30
1	B	369	TRP	N-CA-C	-7.03	103.70	111.36
1	A	84	GLY	CA-C-N	7.02	130.08	120.46
1	A	84	GLY	C-N-CA	7.02	130.08	120.46
1	A	174	LEU	CA-C-N	7.02	131.46	121.42
1	A	174	LEU	C-N-CA	7.02	131.46	121.42
1	A	73	THR	OG1-CB-CG2	7.01	123.32	109.30
1	B	457	MET	N-CA-C	-7.01	103.57	111.07
1	B	254	GLU	CA-C-O	-6.99	109.96	119.12
1	A	102	PRO	CA-C-N	6.99	134.90	121.54
1	A	102	PRO	C-N-CA	6.99	134.90	121.54
1	A	389	GLY	CA-C-O	-6.97	114.79	120.79
1	B	472	ASP	N-CA-C	6.96	121.14	111.74
1	A	493	TRP	N-CA-CB	6.96	121.98	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	THR	N-CA-C	-6.96	101.96	110.31
1	B	253	SER	N-CA-C	-6.95	99.38	109.59
1	A	230	GLU	CA-C-O	-6.94	112.25	120.10
1	A	525	LYS	N-CA-CB	6.94	120.43	110.16
1	B	186	ASP	N-CA-C	-6.94	98.63	109.25
1	A	36	LYS	CA-C-O	-6.92	112.28	120.10
1	A	317	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	A	511	ARG	NE-CZ-NH1	6.92	128.42	121.50
1	B	341	ALA	CA-C-O	-6.92	111.27	119.15
1	A	467	PHE	CA-C-O	-6.91	112.97	120.36
1	B	501	THR	CA-CB-OG1	-6.91	99.24	109.60
1	A	287	ALA	O-C-N	-6.88	114.50	122.89
1	B	279	ALA	N-CA-CB	6.88	120.07	110.17
1	A	531	SER	CA-CB-OG	-6.86	97.37	111.10
1	B	127	ARG	CA-C-O	-6.86	113.28	120.55
1	B	151	ARG	NE-CZ-NH2	-6.85	113.04	119.20
1	A	407	ILE	N-CA-CB	6.84	121.13	111.82
1	A	488	ASN	OD1-CG-ND2	6.84	129.44	122.60
1	A	455	SER	CA-C-N	6.83	130.69	120.31
1	A	455	SER	C-N-CA	6.83	130.69	120.31
1	B	65	LYS	CA-CB-CG	6.83	127.76	114.10
1	B	514	THR	CA-C-N	6.83	129.32	120.44
1	B	514	THR	C-N-CA	6.83	129.32	120.44
1	A	185	ILE	CA-C-O	-6.82	113.07	120.85
1	B	273	LYS	CA-C-N	6.82	129.75	120.54
1	B	273	LYS	C-N-CA	6.82	129.75	120.54
1	A	361	ALA	CA-C-N	6.82	130.68	120.31
1	A	361	ALA	C-N-CA	6.82	130.68	120.31
1	B	304	LYS	CB-CG-CD	6.82	126.98	111.30
1	A	488	ASN	N-CA-CB	6.82	120.51	110.56
1	B	383	VAL	CA-C-N	-6.82	114.74	123.19
1	B	383	VAL	C-N-CA	-6.82	114.74	123.19
1	B	308	GLU	CA-C-O	-6.81	113.07	120.36
1	A	287	ALA	N-CA-C	6.81	120.36	110.28
1	A	397	GLN	OE1-CD-NE2	-6.81	115.79	122.60
1	A	11	PHE	CA-CB-CG	-6.80	107.00	113.80
1	B	171	LEU	CA-C-N	6.79	131.75	120.62
1	B	171	LEU	C-N-CA	6.79	131.75	120.62
1	A	18	ASN	N-CA-C	6.79	120.77	111.54
1	B	415	ILE	CA-C-N	-6.79	115.36	123.44
1	B	415	ILE	C-N-CA	-6.79	115.36	123.44
1	B	170	ASN	CA-C-O	-6.79	113.22	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ALA	CA-C-N	6.77	132.72	122.56
1	A	504	ALA	C-N-CA	6.77	132.72	122.56
1	B	37	ILE	CA-C-O	-6.75	114.03	121.05
1	A	252	ILE	CB-CA-C	6.75	121.07	110.81
1	A	502	PHE	CA-C-N	6.75	130.84	121.26
1	A	502	PHE	C-N-CA	6.75	130.84	121.26
1	B	175	ASN	CA-C-O	6.73	129.44	121.36
1	A	307	VAL	N-CA-C	-6.71	98.19	107.99
1	A	86	ALA	N-CA-CB	6.71	119.99	110.12
1	A	473	GLY	CA-C-N	6.71	131.98	122.05
1	A	473	GLY	C-N-CA	6.71	131.98	122.05
1	A	491	GLN	CA-C-O	-6.71	113.27	120.92
1	B	267	LEU	CA-C-O	-6.71	111.31	119.43
1	B	160	GLN	N-CA-C	-6.71	102.13	111.52
1	A	384	VAL	O-C-N	6.70	130.30	123.20
1	A	534	ARG	CD-NE-CZ	6.70	133.78	124.40
1	B	399	THR	N-CA-CB	6.70	121.42	110.17
1	A	247	MET	N-CA-CB	6.69	121.50	110.39
1	A	353	THR	CA-CB-OG1	-6.69	99.57	109.60
1	B	65	LYS	N-CA-C	6.68	119.57	111.82
1	B	320	THR	CA-CB-OG1	-6.68	99.57	109.60
1	B	196	SER	O-C-N	6.68	129.31	122.09
1	A	515	THR	OG1-CB-CG2	6.67	122.64	109.30
1	A	144	THR	N-CA-CB	-6.66	100.74	110.53
1	B	255	GLN	CA-C-O	6.66	127.35	119.56
1	A	512	VAL	CA-C-O	-6.65	113.18	120.43
1	A	173	ASP	O-C-N	6.65	131.13	122.42
1	A	209	LYS	N-CA-CB	6.65	120.46	110.22
1	A	328	PHE	CA-CB-CG	6.65	120.45	113.80
1	A	245	THR	CA-CB-OG1	-6.65	99.63	109.60
1	A	505	LYS	CA-C-O	6.64	130.05	120.16
1	B	208	VAL	O-C-N	6.64	129.30	121.80
1	A	282	ILE	CA-C-O	-6.63	113.43	120.39
1	B	82	LEU	N-CA-C	6.62	119.34	111.33
1	A	203	THR	CA-CB-OG1	-6.62	99.67	109.60
1	B	271	GLU	CA-C-N	6.62	130.21	120.74
1	B	271	GLU	C-N-CA	6.62	130.21	120.74
1	B	24	GLY	N-CA-C	6.62	119.24	111.63
1	A	472	ASP	N-CA-CB	-6.62	101.20	111.65
1	A	265	GLY	O-C-N	6.59	131.27	122.70
1	B	329	VAL	N-CA-C	-6.59	104.09	110.42
1	A	515	THR	N-CA-CB	-6.58	99.05	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	LYS	CA-C-O	-6.57	112.18	120.20
1	A	256	HIS	CA-CB-CG	-6.57	107.23	113.80
1	A	303	THR	CB-CA-C	6.56	119.91	110.79
1	A	391	SER	CA-C-O	-6.56	113.94	120.82
1	B	158	VAL	N-CA-C	6.56	119.25	111.05
1	B	117	LEU	N-CA-CB	-6.55	100.37	110.46
1	A	251	SER	CA-C-O	6.55	127.50	119.97
1	B	315	LYS	O-C-N	6.54	131.65	123.28
1	B	134	GLU	CA-C-O	6.53	127.50	119.79
1	B	477	GLU	N-CA-C	6.52	119.38	111.82
1	A	259	TYR	CA-C-O	-6.51	113.03	120.58
1	A	437	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	B	446	SER	N-CA-CB	6.50	119.68	110.12
1	B	402	ASN	CB-CG-ND2	6.49	126.14	116.40
1	A	459	ARG	NE-CZ-NH1	-6.49	115.01	121.50
1	B	508	GLU	O-C-N	6.48	131.17	123.33
1	A	2	SER	N-CA-CB	6.48	121.51	110.50
1	B	445	GLY	O-C-N	-6.48	115.96	122.18
1	B	121	ASP	N-CA-C	-6.47	98.17	108.73
1	A	469	LEU	N-CA-CB	6.47	119.62	110.24
1	A	318	ASN	CB-CG-ND2	6.47	126.10	116.40
1	A	303	THR	CA-CB-CG2	6.46	121.48	110.50
1	A	368	GLU	CB-CG-CD	6.46	123.58	112.60
1	A	156	THR	CA-C-O	6.45	127.80	120.90
1	B	504	ALA	CA-C-N	6.45	134.73	122.60
1	B	504	ALA	C-N-CA	6.45	134.73	122.60
1	A	307	VAL	CA-C-O	-6.44	113.57	120.59
1	A	171	LEU	N-CA-C	6.43	120.23	112.38
1	A	527	PHE	CA-CB-CG	-6.43	107.36	113.80
1	B	78	GLU	O-C-N	6.43	128.70	122.07
1	B	35	ASP	CA-C-O	-6.43	112.84	120.10
1	B	387	GLU	N-CA-C	6.42	119.98	110.48
1	B	437	ARG	O-C-N	6.42	130.25	123.06
1	B	332	LYS	N-CA-CB	-6.40	100.36	110.28
1	A	44	ARG	NE-CZ-NH2	6.40	124.96	119.20
1	B	96	LEU	O-C-N	6.40	130.61	122.93
1	A	179	LYS	N-CA-CB	-6.39	100.48	110.06
1	B	51	GLU	CA-CB-CG	6.38	126.87	114.10
1	B	25	LEU	CA-CB-CG	6.38	138.63	116.30
1	A	12	GLU	OE1-CD-OE2	6.38	138.21	122.90
1	B	548	ASN	CA-CB-CG	6.38	118.98	112.60
1	B	180	LEU	CA-C-O	-6.38	111.78	119.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	85	ILE	CA-C-O	-6.37	114.33	120.95
1	A	418	THR	CA-CB-OG1	-6.36	100.06	109.60
1	B	318	ASN	CA-C-N	6.36	130.94	121.72
1	B	318	ASN	C-N-CA	6.36	130.94	121.72
1	B	390	THR	CA-C-N	6.34	129.11	120.54
1	B	390	THR	C-N-CA	6.34	129.11	120.54
1	B	5	THR	CA-CB-OG1	-6.34	100.09	109.60
1	A	419	THR	N-CA-C	-6.34	104.45	111.36
1	B	34	LEU	CB-CA-C	6.34	121.45	110.68
1	A	322	PRO	CA-C-O	-6.33	113.72	121.31
1	B	260	GLY	CA-C-O	-6.33	113.28	119.04
1	B	348	ALA	CA-C-O	6.33	128.09	120.81
1	B	496	LEU	CB-CA-C	6.32	122.54	110.27
1	B	285	VAL	N-CA-C	-6.31	96.21	109.34
1	A	469	LEU	CA-C-N	-6.31	113.78	122.30
1	A	469	LEU	C-N-CA	-6.31	113.78	122.30
1	B	377	PHE	CA-C-N	6.31	129.67	120.71
1	B	377	PHE	C-N-CA	6.31	129.67	120.71
1	A	383	VAL	N-CA-CB	6.30	119.61	111.67
1	B	143	ALA	N-CA-C	-6.30	103.94	111.69
1	B	535	MET	CA-C-O	-6.30	113.33	120.32
1	B	227	VAL	CA-C-O	6.29	125.96	119.35
1	A	508	GLU	CG-CD-OE2	-6.29	103.93	118.40
1	B	285	VAL	O-C-N	-6.29	114.70	122.57
1	B	72	THR	CA-CB-OG1	-6.29	100.17	109.60
1	B	266	THR	CA-CB-CG2	6.28	121.17	110.50
1	A	205	LEU	N-CA-CB	-6.28	100.64	110.06
1	A	56	TYR	CA-CB-CG	6.28	125.19	113.90
1	B	143	ALA	N-CA-CB	6.27	119.55	110.20
1	A	288	LEU	CA-C-N	6.27	129.66	120.82
1	A	288	LEU	C-N-CA	6.27	129.66	120.82
1	B	323	GLY	N-CA-C	6.27	124.01	115.30
1	A	332	LYS	CA-C-O	-6.27	114.25	120.70
1	B	495	HIS	CA-C-O	-6.26	113.86	120.63
1	B	504	ALA	CA-C-O	6.26	128.01	120.81
1	B	459	ARG	CA-CB-CG	6.26	126.63	114.10
1	B	135	THR	CA-CB-OG1	-6.25	100.22	109.60
1	B	31	LEU	N-CA-C	6.25	118.89	111.33
1	A	305	ASN	N-CA-CB	6.24	120.59	110.42
1	B	52	LEU	CA-C-O	6.24	127.37	120.82
1	A	95	VAL	CA-C-O	-6.24	113.86	120.53
1	A	280	ASP	CA-C-N	6.23	132.23	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ASP	C-N-CA	6.23	132.23	121.64
1	A	491	GLN	O-C-N	6.23	130.67	122.95
1	A	49	ALA	CB-CA-C	6.22	121.67	109.72
1	A	488	ASN	CA-CB-CG	6.22	118.82	112.60
1	A	409	GLN	OE1-CD-NE2	-6.22	116.38	122.60
1	B	182	GLN	CB-CG-CD	6.22	123.17	112.60
1	A	20	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	65	LYS	CG-CD-CE	6.21	125.58	111.30
1	B	528	ASN	CA-CB-CG	-6.21	106.39	112.60
1	B	19	VAL	CA-C-O	-6.20	113.78	121.04
1	B	5	THR	CA-CB-CG2	6.20	121.04	110.50
1	B	512	VAL	N-CA-CB	-6.20	101.27	111.44
1	B	539	MET	CG-SD-CE	6.20	114.53	100.90
1	B	210	ASP	CA-C-O	-6.20	112.33	119.14
1	B	258	ARG	CB-CA-C	-6.18	100.27	110.72
1	A	429	ALA	CA-C-O	6.18	127.31	120.63
1	B	346	PRO	N-CA-C	6.18	120.96	110.95
1	B	11	PHE	O-C-N	-6.18	115.57	122.12
1	B	554	LYS	O-C-N	6.18	130.80	122.59
1	B	512	VAL	CB-CA-C	6.17	120.01	110.50
1	B	140	THR	CA-CB-OG1	-6.17	100.35	109.60
1	B	427	PHE	N-CA-C	-6.17	104.64	111.36
1	B	367	GLN	CA-C-O	6.14	127.27	120.63
1	A	498	LEU	O-C-N	6.14	128.72	122.09
1	A	392	ALA	CA-C-N	6.13	128.78	120.44
1	A	392	ALA	C-N-CA	6.13	128.78	120.44
1	B	539	MET	CB-CA-C	6.13	120.58	110.78
1	B	261	GLY	N-CA-C	6.12	119.66	110.97
1	A	533	ILE	O-C-N	6.11	129.27	122.61
1	B	164	TYR	CA-C-O	-6.11	113.60	120.32
1	A	135	THR	CA-CB-OG1	-6.10	100.45	109.60
1	B	73	THR	CA-CB-OG1	-6.10	100.45	109.60
1	A	538	ILE	CA-C-O	-6.09	114.01	120.53
1	B	535	MET	O-C-N	6.09	130.44	123.31
1	B	431	GLU	CG-CD-OE1	6.09	132.40	118.40
1	A	28	ASP	CA-C-O	-6.08	111.81	120.51
1	B	55	ALA	CA-C-N	6.08	128.75	120.54
1	B	55	ALA	C-N-CA	6.08	128.75	120.54
1	A	417	PHE	CA-C-N	6.08	130.33	120.60
1	A	417	PHE	C-N-CA	6.08	130.33	120.60
1	B	236	ASP	CA-CB-CG	6.08	118.68	112.60
1	A	469	LEU	CA-C-O	-6.08	114.42	120.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	N-CA-CB	6.07	118.92	110.17
1	B	415	ILE	CA-C-O	-6.07	114.73	121.23
1	A	235	ILE	N-CA-CB	6.07	118.34	110.57
1	A	498	LEU	CA-C-O	-6.07	114.45	120.70
1	B	96	LEU	CB-CA-C	-6.07	100.80	110.81
1	B	435	LYS	CA-CB-CG	6.06	126.22	114.10
1	A	119	ASN	N-CA-CB	-6.05	101.47	110.61
1	B	174	LEU	CB-CA-C	6.05	119.76	109.53
1	B	136	THR	N-CA-CB	-6.05	101.02	111.55
1	A	501	THR	CA-CB-OG1	-6.05	100.53	109.60
1	A	305	ASN	OD1-CG-ND2	6.04	128.65	122.60
1	A	338	ALA	CA-C-O	-6.04	114.10	120.63
1	B	304	LYS	N-CA-C	-6.04	105.40	112.89
1	A	532	LYS	CA-C-O	-6.04	114.99	121.45
1	B	421	ALA	O-C-N	-6.03	115.33	122.20
1	A	208	VAL	CB-CA-C	6.03	119.68	111.97
1	A	178	ALA	CA-C-O	6.02	126.90	120.10
1	B	53	ASN	O-C-N	6.02	128.52	122.08
1	B	204	ILE	CB-CA-C	6.02	119.67	111.97
1	A	366	LYS	N-CA-C	-6.02	99.99	109.50
1	B	186	ASP	CA-C-O	-6.01	113.52	120.49
1	B	329	VAL	N-CA-CB	6.01	117.58	110.55
1	B	86	ALA	CA-C-O	6.00	126.91	120.55
1	A	306	ILE	CA-C-N	-6.00	115.22	122.90
1	A	306	ILE	C-N-CA	-6.00	115.22	122.90
1	B	139	ILE	CA-C-N	6.00	130.98	121.44
1	B	139	ILE	C-N-CA	6.00	130.98	121.44
1	A	372	ASN	CA-C-N	5.98	132.97	121.54
1	A	372	ASN	C-N-CA	5.98	132.97	121.54
1	A	415	ILE	CA-CB-CG2	-5.98	100.33	110.50
1	B	343	GLY	CA-C-N	-5.97	114.48	122.72
1	B	343	GLY	C-N-CA	-5.97	114.48	122.72
1	A	478	LYS	N-CA-CB	5.97	118.89	110.12
1	A	402	ASN	OD1-CG-ND2	-5.97	116.63	122.60
1	B	157	TYR	CA-CB-CG	-5.97	103.16	113.90
1	B	316	ILE	CB-CA-C	5.96	118.74	110.99
1	B	373	GLN	CA-C-N	5.95	128.26	120.28
1	B	373	GLN	C-N-CA	5.95	128.26	120.28
1	B	83	ASN	CA-C-O	5.95	126.73	120.42
1	A	468	VAL	CA-C-O	5.95	126.89	120.53
1	B	177	PRO	CA-C-O	-5.94	115.03	121.27
1	B	221	CYS	O-C-N	5.94	130.66	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	VAL	CA-C-N	5.94	128.16	120.44
1	A	124	VAL	C-N-CA	5.94	128.16	120.44
1	A	271	GLU	CB-CG-CD	5.94	122.69	112.60
1	A	438	VAL	CB-CA-C	5.93	118.70	110.99
1	A	512	VAL	N-CA-CB	-5.92	101.98	111.58
1	B	448	GLN	OE1-CD-NE2	-5.91	116.69	122.60
1	B	68	SER	O-C-N	5.91	129.31	122.99
1	B	187	MET	CA-C-O	5.91	126.35	119.32
1	B	436	LYS	CA-C-O	5.90	127.34	120.49
1	A	99	VAL	CB-CA-C	5.90	118.39	110.42
1	B	125	PHE	CA-C-N	5.90	128.51	120.54
1	B	125	PHE	C-N-CA	5.90	128.51	120.54
1	B	47	GLY	CA-C-O	-5.90	110.30	120.57
1	B	127	ARG	N-CA-CB	5.90	118.79	110.12
1	B	196	SER	N-CA-C	-5.90	104.77	111.14
1	A	142	ILE	CB-CA-C	-5.89	102.71	112.26
1	B	432	ILE	N-CA-C	-5.89	105.11	110.82
1	B	471	ASN	CA-C-O	5.89	125.63	119.51
1	B	488	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	B	495	HIS	O-C-N	5.88	128.35	122.12
1	A	127	ARG	CD-NE-CZ	-5.87	116.18	124.40
1	B	515	THR	OG1-CB-CG2	5.87	121.05	109.30
1	B	78	GLU	CA-C-O	-5.87	114.66	120.82
1	B	138	MET	N-CA-CB	5.87	119.80	110.65
1	A	19	VAL	CA-C-O	-5.87	113.94	120.74
1	B	373	GLN	N-CA-C	5.87	119.54	112.38
1	B	190	LYS	N-CA-CB	-5.86	102.12	110.04
1	B	273	LYS	N-CA-CB	5.86	118.73	109.82
1	B	523	GLN	OE1-CD-NE2	-5.86	116.74	122.60
1	A	258	ARG	CB-CA-C	5.86	119.87	110.09
1	A	496	LEU	CB-CA-C	5.86	121.47	110.63
1	B	303	THR	CA-C-O	5.86	128.89	120.51
1	B	355	ALA	CA-C-O	-5.86	115.11	121.44
1	B	456	THR	CA-C-O	5.86	126.76	120.55
1	A	319	ALA	N-CA-C	5.86	119.45	110.20
1	A	282	ILE	N-CA-CB	5.85	119.49	111.41
1	B	548	ASN	N-CA-C	5.85	117.66	111.28
1	A	264	VAL	CA-CB-CG2	5.85	120.34	110.40
1	B	31	LEU	CA-C-O	-5.84	114.32	120.63
1	A	273	LYS	O-C-N	5.84	128.08	122.07
1	A	470	ASN	CB-CA-C	5.83	119.96	110.22
1	A	29	PHE	CA-C-O	-5.83	113.08	119.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	VAL	N-CA-CB	-5.82	102.62	110.54
1	A	9	TYR	CA-C-N	5.82	128.40	120.54
1	A	9	TYR	C-N-CA	5.82	128.40	120.54
1	A	259	TYR	N-CA-CB	5.82	118.67	109.71
1	B	74	PHE	CA-CB-CG	5.82	119.62	113.80
1	B	199	GLU	CA-CB-CG	5.82	125.73	114.10
1	B	556	THR	CB-CA-C	5.82	121.89	109.10
1	B	223	SER	CA-CB-OG	5.81	122.71	111.10
1	A	502	PHE	CA-C-O	5.80	126.45	119.43
1	B	421	ALA	N-CA-C	5.80	119.17	111.75
1	A	476	ILE	O-C-N	5.80	127.80	121.83
1	A	178	ALA	CA-C-N	5.79	128.32	120.38
1	A	178	ALA	C-N-CA	5.79	128.32	120.38
1	A	155	THR	CA-CB-CG2	5.79	120.34	110.50
1	A	326	MET	N-CA-C	5.79	119.44	112.38
1	A	17	VAL	CA-C-O	-5.79	113.54	120.78
1	B	47	GLY	O-C-N	5.79	130.22	122.70
1	A	390	THR	N-CA-C	-5.79	106.18	113.18
1	A	195	GLU	N-CA-CB	5.78	118.62	110.12
1	A	431	GLU	CA-C-N	5.78	127.94	120.88
1	A	431	GLU	C-N-CA	5.78	127.94	120.88
1	A	543	PHE	CA-CB-CG	-5.78	108.02	113.80
1	B	20	ASN	CA-C-O	-5.78	112.56	119.15
1	B	359	VAL	O-C-N	5.78	126.71	121.57
1	B	131	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	A	436	LYS	CA-C-N	5.78	130.64	122.09
1	A	436	LYS	C-N-CA	5.78	130.64	122.09
1	A	230	GLU	N-CA-CB	5.77	119.11	110.22
1	A	442	ILE	N-CA-C	5.77	116.79	108.48
1	B	133	SER	CA-C-O	-5.76	114.37	121.06
1	B	95	VAL	O-C-N	5.76	129.84	123.10
1	B	379	GLN	CA-C-O	5.76	128.18	121.44
1	A	512	VAL	CB-CA-C	5.75	119.37	110.28
1	A	312	ASP	CB-CG-OD2	-5.75	105.17	118.40
1	B	494	ASP	CA-CB-CG	-5.75	106.85	112.60
1	B	388	THR	CA-CB-CG2	5.74	120.27	110.50
1	B	210	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	273	LYS	CB-CA-C	5.74	119.89	110.88
1	B	330	LEU	O-C-N	5.74	128.22	122.08
1	A	552	GLN	N-CA-C	-5.72	103.86	111.24
1	B	142	ILE	O-C-N	5.71	129.19	122.17
1	B	184	PRO	CB-CA-C	5.70	118.78	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	347	VAL	N-CA-C	-5.70	100.21	108.71
1	A	32	SER	CA-CB-OG	-5.70	99.70	111.10
1	A	232	LYS	CB-CG-CD	5.70	124.41	111.30
1	B	352	ARG	N-CA-C	-5.70	102.47	110.50
1	A	553	ALA	N-CA-C	5.69	118.22	111.33
1	B	230	GLU	CA-CB-CG	5.69	125.47	114.10
1	A	31	LEU	N-CA-C	5.68	117.93	111.11
1	A	531	SER	N-CA-CB	-5.68	101.81	110.33
1	B	166	GLY	CA-C-O	-5.67	116.17	120.76
1	A	312	ASP	CB-CG-OD1	5.67	131.44	118.40
1	B	336	ASN	N-CA-C	5.67	121.76	114.56
1	B	95	VAL	CA-CB-CG1	-5.67	100.77	110.40
1	A	325	GLN	CA-C-O	-5.66	114.30	120.81
1	A	152	CYS	N-CA-CB	5.66	118.44	110.12
1	B	508	GLU	CA-C-O	-5.66	113.81	120.60
1	A	507	TYR	O-C-N	5.65	129.22	122.72
1	A	338	ALA	N-CA-CB	5.65	118.54	110.06
1	A	549	LEU	O-C-N	5.65	129.90	122.33
1	A	22	VAL	CA-C-N	5.65	133.02	122.74
1	A	22	VAL	C-N-CA	5.65	133.02	122.74
1	B	174	LEU	N-CA-CB	-5.65	101.53	110.06
1	B	346	PRO	CB-CA-C	-5.65	104.37	111.71
1	A	331	GLN	CA-C-O	5.64	126.40	120.42
1	B	230	GLU	CB-CG-CD	5.64	122.19	112.60
1	B	450	THR	CB-CA-C	5.64	120.10	110.85
1	B	170	ASN	O-C-N	5.64	128.58	122.15
1	B	382	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	262	VAL	N-CA-C	-5.64	100.30	108.36
1	B	272	VAL	N-CA-CB	5.63	118.63	110.52
1	A	103	SER	CA-C-N	5.63	132.11	121.97
1	A	103	SER	C-N-CA	5.63	132.11	121.97
1	A	520	LYS	CB-CA-C	5.63	119.82	110.81
1	A	188	SER	N-CA-CB	5.63	119.45	110.16
1	B	304	LYS	N-CA-CB	-5.63	101.22	110.40
1	A	505	LYS	CB-CG-CD	5.63	124.25	111.30
1	A	529	ASP	N-CA-CB	-5.63	101.73	110.57
1	B	428	ALA	N-CA-C	-5.63	105.06	111.14
1	B	277	GLU	N-CA-CB	5.62	118.38	110.12
1	B	416	GLY	N-CA-C	-5.62	107.21	113.79
1	A	28	ASP	O-C-N	5.62	130.06	122.59
1	A	380	GLU	CB-CA-C	5.62	119.04	109.72
1	B	463	LYS	N-CA-C	5.61	122.21	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	554	LYS	CA-CB-CG	-5.61	102.88	114.10
1	B	291	ASP	CA-C-O	-5.61	111.27	120.80
1	A	446	SER	O-C-N	5.61	129.52	122.23
1	B	548	ASN	CA-C-O	-5.60	114.61	120.55
1	A	421	ALA	O-C-N	5.60	128.06	122.12
1	B	163	VAL	CA-C-O	5.59	126.92	120.76
1	A	289	LEU	N-CA-C	5.59	118.43	110.10
1	B	97	HIS	CA-C-N	5.59	130.06	122.90
1	B	97	HIS	C-N-CA	5.59	130.06	122.90
1	B	543	PHE	CA-CB-CG	-5.59	108.21	113.80
1	A	21	THR	N-CA-CB	5.59	120.07	110.68
1	B	100	GLY	CA-C-O	-5.59	116.00	120.81
1	B	339	ASP	CB-CA-C	5.59	119.73	110.90
1	B	479	LEU	CA-C-N	5.58	128.72	123.08
1	B	479	LEU	C-N-CA	5.58	128.72	123.08
1	A	18	ASN	OD1-CG-ND2	5.58	128.18	122.60
1	B	537	GLU	CA-CB-CG	5.58	125.27	114.10
1	A	306	ILE	CA-CB-CG1	-5.58	100.91	110.40
1	A	223	SER	N-CA-C	5.58	120.21	112.90
1	B	48	ASN	OD1-CG-ND2	-5.57	117.03	122.60
1	B	240	PHE	O-C-N	5.57	129.21	121.64
1	A	525	LYS	CA-C-O	-5.56	114.52	120.42
1	B	555	LEU	CA-C-N	-5.56	111.69	121.70
1	B	555	LEU	C-N-CA	-5.56	111.69	121.70
1	B	255	GLN	CA-C-N	5.56	128.12	120.67
1	B	255	GLN	C-N-CA	5.56	128.12	120.67
1	A	239	GLN	CB-CG-CD	5.56	122.05	112.60
1	A	202	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	534	ARG	NE-CZ-NH1	5.55	127.06	121.50
1	A	44	ARG	CA-C-N	5.55	130.82	123.05
1	A	44	ARG	C-N-CA	5.55	130.82	123.05
1	A	410	VAL	CA-C-O	-5.55	115.18	120.95
1	B	528	ASN	CB-CG-OD1	-5.55	109.70	120.80
1	A	556	THR	OG1-CB-CG2	-5.54	98.22	109.30
1	A	214	PRO	CB-CA-C	5.53	118.54	110.63
1	B	422	THR	N-CA-C	-5.53	105.25	111.28
1	B	274	GLU	O-C-N	-5.53	116.34	122.09
1	A	388	THR	N-CA-C	-5.53	101.87	110.10
1	B	247	MET	CA-C-O	5.52	126.28	120.42
1	B	447	LEU	CA-C-N	5.52	127.68	120.28
1	B	447	LEU	C-N-CA	5.52	127.68	120.28
1	A	395	ILE	CA-C-N	5.52	129.43	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ILE	C-N-CA	5.52	129.43	120.60
1	B	22	VAL	CB-CA-C	5.52	118.80	110.63
1	B	469	LEU	CA-C-O	-5.52	114.37	120.60
1	B	156	THR	O-C-N	5.51	127.74	122.07
1	B	359	VAL	N-CA-CB	-5.51	106.99	111.67
1	A	341	ALA	N-CA-C	5.51	120.00	113.28
1	A	554	LYS	CB-CA-C	-5.51	102.48	110.96
1	B	277	GLU	CG-CD-OE1	5.50	131.06	118.40
1	B	459	ARG	CB-CG-CD	5.50	123.94	111.30
1	A	201	ILE	CA-C-O	-5.50	114.95	121.05
1	A	478	LYS	O-C-N	5.50	127.95	122.12
1	B	436	LYS	O-C-N	-5.49	116.27	123.02
1	A	546	PRO	CA-C-N	5.49	132.02	121.54
1	A	546	PRO	C-N-CA	5.49	132.02	121.54
1	B	302	LYS	CB-CG-CD	5.49	123.92	111.30
1	A	11	PHE	CA-C-O	5.48	126.27	119.97
1	A	32	SER	N-CA-C	5.48	118.01	111.71
1	A	206	ALA	CA-C-N	5.48	127.56	120.44
1	A	206	ALA	C-N-CA	5.48	127.56	120.44
1	A	122	PHE	CA-CB-CG	-5.48	108.32	113.80
1	B	309	PHE	CA-C-N	-5.47	114.00	122.59
1	B	309	PHE	C-N-CA	-5.47	114.00	122.59
1	B	226	ASP	N-CA-C	5.47	122.45	110.80
1	B	462	LEU	N-CA-C	-5.47	101.63	110.32
1	A	315	LYS	CA-C-N	-5.47	115.22	122.98
1	A	315	LYS	C-N-CA	-5.47	115.22	122.98
1	A	445	GLY	CA-C-N	5.46	129.93	120.58
1	A	445	GLY	C-N-CA	5.46	129.93	120.58
1	B	384	VAL	CB-CA-C	5.46	118.97	110.83
1	A	439	ILE	CA-C-O	-5.46	114.69	120.53
1	A	167	LEU	N-CA-CB	-5.45	101.43	111.03
1	A	274	GLU	O-C-N	5.45	127.98	122.09
1	B	83	ASN	CB-CG-ND2	-5.45	108.22	116.40
1	A	372	ASN	O-C-N	-5.45	116.14	122.03
1	B	469	LEU	O-C-N	5.45	129.90	122.82
1	B	205	LEU	O-C-N	5.44	127.75	122.09
1	A	482	GLY	CA-C-N	5.44	125.11	119.56
1	A	482	GLY	C-N-CA	5.44	125.11	119.56
1	B	449	LEU	CA-C-O	-5.44	113.72	119.97
1	A	121	ASP	O-C-N	-5.43	116.41	122.93
1	B	283	LEU	N-CA-C	-5.43	98.91	108.20
1	A	12	GLU	CA-CB-CG	-5.43	103.25	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ARG	CB-CG-CD	5.42	123.76	111.30
1	A	332	LYS	CA-CB-CG	-5.41	103.28	114.10
1	A	227	VAL	N-CA-C	5.40	120.58	109.34
1	B	336	ASN	CA-CB-CG	5.40	118.00	112.60
1	B	353	THR	CA-C-O	-5.40	114.42	120.25
1	B	171	LEU	N-CA-C	5.40	119.13	112.54
1	B	399	THR	CA-CB-OG1	-5.40	101.50	109.60
1	B	354	PRO	CA-C-N	5.40	128.75	120.82
1	B	354	PRO	C-N-CA	5.40	128.75	120.82
1	A	358	ALA	CA-C-O	-5.39	114.61	120.81
1	B	495	HIS	CB-CG-CD2	-5.39	124.19	131.20
1	B	229	ALA	N-CA-C	5.39	117.91	111.71
1	A	12	GLU	O-C-N	5.39	128.29	122.15
1	A	373	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	A	468	VAL	CA-CB-CG1	5.38	119.55	110.40
1	A	13	ARG	CB-CA-C	5.38	119.39	110.90
1	A	150	ASP	O-C-N	5.38	127.61	122.07
1	A	344	TYR	CA-C-N	5.38	132.03	122.35
1	A	344	TYR	C-N-CA	5.38	132.03	122.35
1	A	183	THR	CA-CB-OG1	-5.38	101.54	109.60
1	A	348	ALA	CA-C-O	-5.37	115.70	121.56
1	B	29	PHE	CA-C-N	-5.37	113.92	122.29
1	B	29	PHE	C-N-CA	-5.37	113.92	122.29
1	B	389	GLY	N-CA-C	-5.36	103.42	110.29
1	A	233	LYS	N-CA-CB	5.36	117.84	110.07
1	A	161	ARG	CA-C-N	5.36	125.26	119.85
1	A	161	ARG	C-N-CA	5.36	125.26	119.85
1	B	404	THR	O-C-N	5.36	129.61	123.29
1	A	525	LYS	CG-CD-CE	5.36	123.62	111.30
1	B	522	THR	N-CA-C	5.36	118.92	112.38
1	A	545	ALA	N-CA-CB	-5.35	100.84	110.37
1	B	52	LEU	N-CA-C	-5.35	105.35	111.07
1	B	539	MET	N-CA-CB	-5.35	101.55	110.37
1	B	52	LEU	CA-C-N	5.35	128.22	120.79
1	B	52	LEU	C-N-CA	5.35	128.22	120.79
1	B	346	PRO	CA-C-O	5.34	126.88	121.27
1	B	484	LYS	CB-CG-CD	5.34	123.58	111.30
1	A	536	ILE	O-C-N	5.33	127.88	122.71
1	A	336	ASN	CB-CG-ND2	-5.33	108.40	116.40
1	A	363	THR	CB-CA-C	5.33	117.65	109.60
1	B	459	ARG	N-CA-CB	5.33	117.88	109.94
1	A	475	THR	N-CA-C	5.33	117.83	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	274	GLU	N-CA-C	5.32	117.50	111.11
1	A	275	ALA	CB-CA-C	5.32	119.72	110.68
1	B	379	GLN	CG-CD-NE2	-5.32	108.42	116.40
1	B	499	LEU	CB-CA-C	5.32	120.65	110.17
1	A	459	ARG	NE-CZ-NH2	-5.32	114.41	119.20
1	A	398	THR	CA-CB-OG1	-5.31	101.63	109.60
1	A	219	ASP	CA-C-O	5.31	128.78	121.88
1	B	234	LEU	N-CA-C	-5.31	105.57	111.36
1	B	326	MET	O-C-N	5.31	128.43	122.22
1	B	211	ALA	CA-C-O	-5.31	114.71	120.81
1	B	553	ALA	CA-C-O	5.31	126.86	120.92
1	B	555	LEU	CA-C-O	-5.30	113.53	119.79
1	B	37	ILE	CB-CA-C	-5.30	105.10	112.04
1	B	128	MET	CA-C-O	-5.30	114.36	120.24
1	A	6	LEU	CA-C-N	5.29	125.81	119.94
1	A	6	LEU	C-N-CA	5.29	125.81	119.94
1	B	472	ASP	N-CA-CB	-5.29	104.14	112.13
1	A	71	ILE	CB-CA-C	5.29	118.71	110.83
1	A	99	VAL	CA-C-N	5.29	126.03	120.43
1	A	99	VAL	C-N-CA	5.29	126.03	120.43
1	B	167	LEU	CA-C-N	5.29	125.59	119.93
1	B	167	LEU	C-N-CA	5.29	125.59	119.93
1	B	458	ILE	CA-C-O	-5.29	115.57	121.17
1	A	118	GLY	CA-C-O	5.28	126.01	119.25
1	B	516	GLY	CA-C-O	-5.28	115.31	120.75
1	A	45	TRP	O-C-N	5.28	129.50	123.27
1	A	347	VAL	CB-CA-C	5.28	118.42	110.98
1	A	450	THR	N-CA-CB	-5.28	102.72	111.49
1	A	540	LEU	CA-C-N	5.28	125.04	119.76
1	A	540	LEU	C-N-CA	5.28	125.04	119.76
1	B	486	GLN	CG-CD-NE2	5.28	124.31	116.40
1	A	469	LEU	O-C-N	5.27	129.64	122.57
1	B	359	VAL	CB-CA-C	5.27	118.46	110.97
1	B	488	ASN	CB-CG-ND2	5.27	124.31	116.40
1	A	149	ILE	N-CA-C	-5.27	105.58	110.53
1	B	393	PHE	CA-CB-CG	-5.27	108.53	113.80
1	B	418	THR	N-CA-C	5.26	117.70	111.33
1	B	33	LEU	N-CA-C	-5.26	105.46	111.14
1	A	402	ASN	CB-CG-ND2	5.26	124.29	116.40
1	B	37	ILE	N-CA-CB	5.25	117.04	110.47
1	B	213	ASN	OD1-CG-ND2	-5.25	117.34	122.60
1	A	416	GLY	CA-C-O	5.25	125.65	119.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	LEU	CA-C-N	5.25	127.28	120.56
1	A	234	LEU	C-N-CA	5.25	127.28	120.56
1	B	230	GLU	CA-C-O	-5.25	114.86	120.42
1	A	6	LEU	CA-C-O	5.24	126.11	120.55
1	B	124	VAL	CB-CA-C	5.24	118.36	111.81
1	B	103	SER	CA-CB-OG	-5.24	100.62	111.10
1	A	225	HIS	CA-CB-CG	-5.24	108.56	113.80
1	B	497	SER	N-CA-CB	5.24	118.33	110.53
1	A	118	GLY	O-C-N	-5.23	115.39	122.35
1	B	388	THR	CA-C-O	5.23	126.72	120.70
1	B	53	ASN	CA-C-O	-5.23	115.32	121.07
1	B	342	LYS	CA-CB-CG	5.23	124.56	114.10
1	B	87	GLY	CA-C-O	-5.23	115.35	121.00
1	A	450	THR	N-CA-C	5.22	119.40	112.30
1	B	220	ALA	N-CA-CB	-5.22	101.66	110.49
1	A	98	VAL	N-CA-CB	5.22	117.26	110.99
1	B	411	LEU	O-C-N	5.22	129.35	122.30
1	B	76	VAL	CA-C-O	-5.21	114.96	120.64
1	A	50	ASN	CB-CG-ND2	5.21	124.21	116.40
1	B	303	THR	OG1-CB-CG2	5.21	119.72	109.30
1	B	284	SER	O-C-N	-5.21	116.47	122.87
1	A	399	THR	N-CA-CB	5.20	118.48	110.21
1	B	63	ARG	CA-C-N	5.20	127.22	120.88
1	B	63	ARG	C-N-CA	5.20	127.22	120.88
1	B	485	ALA	N-CA-C	-5.20	102.59	110.28
1	A	314	MET	N-CA-C	-5.19	101.65	109.85
1	B	186	ASP	O-C-N	5.19	129.40	123.02
1	B	245	THR	CA-CB-CG2	5.19	119.32	110.50
1	B	456	THR	N-CA-C	5.18	116.93	111.28
1	B	454	ILE	CB-CA-C	5.18	119.13	112.14
1	A	117	LEU	N-CA-CB	-5.18	103.06	110.57
1	A	203	THR	CA-C-O	-5.18	114.93	120.42
1	B	28	ASP	CA-CB-CG	-5.18	107.42	112.60
1	B	28	ASP	O-C-N	5.17	128.06	122.11
1	B	409	GLN	CB-CA-C	5.17	120.71	110.42
1	A	127	ARG	N-CA-CB	5.17	118.29	110.28
1	A	262	VAL	CA-CB-CG2	5.17	119.18	110.40
1	B	524	ASP	CA-C-O	5.16	126.64	120.70
1	B	136	THR	CA-CB-OG1	-5.16	101.86	109.60
1	B	271	GLU	CB-CG-CD	5.16	121.37	112.60
1	A	540	LEU	CB-CA-C	5.16	116.86	108.87
1	B	122	PHE	CA-CB-CG	5.16	118.96	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	304	LYS	O-C-N	-5.16	115.73	122.59
1	B	15	LYS	N-CA-C	-5.15	104.93	111.11
1	B	150	ASP	N-CA-CB	5.15	117.79	110.06
1	B	190	LYS	CA-C-N	5.15	124.91	119.76
1	B	190	LYS	C-N-CA	5.15	124.91	119.76
1	A	490	ILE	CA-C-N	5.15	128.07	120.82
1	A	490	ILE	C-N-CA	5.15	128.07	120.82
1	A	273	LYS	CA-CB-CG	5.14	124.39	114.10
1	A	420	GLY	O-C-N	5.14	127.17	122.19
1	B	64	ILE	CA-C-N	5.14	128.12	120.31
1	B	64	ILE	C-N-CA	5.14	128.12	120.31
1	B	83	ASN	CB-CA-C	5.14	119.59	110.85
1	A	126	HIS	CA-C-O	-5.14	115.40	120.90
1	A	73	THR	CA-CB-OG1	-5.13	101.90	109.60
1	B	489	GLU	CB-CG-CD	5.13	121.32	112.60
1	B	29	PHE	CB-CA-C	5.13	119.23	110.56
1	B	377	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	511	ARG	O-C-N	5.13	129.53	123.27
1	B	30	ASN	CA-C-N	5.12	127.40	120.38
1	B	30	ASN	C-N-CA	5.12	127.40	120.38
1	A	269	LYS	O-C-N	5.12	126.40	121.28
1	B	315	LYS	CB-CA-C	5.12	118.03	110.14
1	B	127	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	376	ASN	N-CA-CB	5.12	118.18	110.30
1	B	78	GLU	N-CA-CB	5.11	117.42	110.01
1	A	478	LYS	N-CA-C	-5.11	105.71	111.28
1	A	170	ASN	CA-C-O	-5.11	115.46	120.82
1	B	45	TRP	CA-C-O	-5.10	115.24	120.54
1	B	480	ILE	O-C-N	5.10	126.52	121.98
1	A	376	ASN	CA-C-N	5.09	129.29	120.58
1	A	376	ASN	C-N-CA	5.09	129.29	120.58
1	B	125	PHE	CB-CA-C	5.09	119.33	110.68
1	B	262	VAL	CA-C-N	-5.09	115.70	122.72
1	B	262	VAL	C-N-CA	-5.09	115.70	122.72
1	A	30	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	545	ALA	CB-CA-C	5.09	120.19	110.17
1	B	308	GLU	O-C-N	5.09	129.02	123.22
1	B	332	LYS	CB-CG-CD	5.08	123.00	111.30
1	B	336	ASN	CB-CG-ND2	5.08	124.03	116.40
1	A	103	SER	N-CA-CB	-5.08	101.91	110.49
1	B	378	LEU	O-C-N	5.08	129.11	122.87
1	B	259	TYR	O-C-N	5.08	128.97	123.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	56	TYR	O-C-N	5.07	127.37	122.09
1	B	182	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	440	LEU	N-CA-CB	-5.07	102.17	110.68
1	A	284	SER	N-CA-C	5.07	116.96	107.99
1	A	154	ARG	CA-C-N	5.06	127.37	120.54
1	A	154	ARG	C-N-CA	5.06	127.37	120.54
1	A	525	LYS	O-C-N	5.06	127.92	122.15
1	B	72	THR	CA-CB-CG2	5.06	119.09	110.50
1	A	99	VAL	CA-CB-CG1	5.05	118.99	110.40
1	B	20	ASN	N-CA-CB	5.05	118.06	110.53
1	B	256	HIS	ND1-CE1-NE2	-5.05	103.34	108.40
1	B	236	ASP	CB-CA-C	-5.05	102.26	110.85
1	B	289	LEU	N-CA-C	5.05	121.56	110.80
1	A	553	ALA	CB-CA-C	-5.05	102.10	110.68
1	B	32	SER	O-C-N	5.04	128.47	122.27
1	B	229	ALA	O-C-N	5.04	128.12	122.22
1	B	159	THR	N-CA-CB	-5.04	102.78	110.33
1	A	160	GLN	CA-C-N	5.03	132.67	122.45
1	A	160	GLN	C-N-CA	5.03	132.67	122.45
1	A	27	GLY	CA-C-O	5.03	126.94	121.56
1	A	317	ARG	NH1-CZ-NH2	-5.03	112.76	119.30
1	A	282	ILE	O-C-N	5.03	128.69	123.26
1	B	197	GLU	CB-CG-CD	-5.03	104.06	112.60
1	A	230	GLU	CB-CA-C	-5.02	101.34	110.63
1	A	104	ILE	CA-CB-CG1	5.02	118.94	110.40
1	B	34	LEU	O-C-N	5.02	127.44	122.12
1	B	389	GLY	CA-C-O	-5.01	116.48	120.79
1	A	202	ASP	CB-CG-OD2	-5.01	106.88	118.40
1	B	154	ARG	CG-CD-NE	-5.01	100.99	112.00
1	B	263	TYR	N-CA-CB	5.00	118.59	110.43
1	B	544	ASP	N-CA-CB	-5.00	101.91	110.16
1	A	441	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	352	ARG	Sidechain
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	144	1
1	B	4130	0	4151	136	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	3	0
3	B	26	0	16	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8316	0	8334	273	1

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 16.

All (273) 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:267:LEU:HD11	1:B:552:GLN:HB2	1.47	0.93
1:B:4:ILE:HD11	1:B:8:LYS:HG2	1.56	0.86
1:B:505:LYS:H	1:B:505:LYS:HD2	1.45	0.81
1:A:345:LYS:H	1:A:345:LYS:HD3	1.45	0.81
1:A:553:ALA:O	1:A:556:THR:HG22	1.81	0.81
1:A:158:VAL:HG23	1:A:187:MET:CE	2.11	0.80
1:A:267:LEU:HD21	1:A:552:GLN:NE2	1.96	0.80
1:B:159:THR:HG22	1:B:161:ARG:HB2	1.63	0.79
1:A:132:ILE:HG22	1:B:117:LEU:HD21	1.67	0.76
1:A:12:GLU:HG2	1:A:181:LEU:HD13	1.67	0.75
1:A:287:ALA:HB1	1:A:289:LEU:HB3	1.68	0.75
1:B:476:ILE:HD12	1:B:549:LEU:HD21	1.67	0.75
1:B:126:HIS:HE1	1:B:136:THR:OG1	1.71	0.74
1:A:158:VAL:HG23	1:A:187:MET:HE3	1.71	0.72
1:B:65:LYS:HD2	1:B:432:ILE:HD11	1.71	0.72
1:A:280:ASP:HA	1:A:304:LYS:HE2	1.71	0.72
1:A:157:TYR:HD2	1:A:187:MET:HE2	1.55	0.71
1:A:327:LYS:O	1:A:331:GLN:HG3	1.90	0.71
1:B:553:ALA:O	1:B:554:LYS:C	2.33	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLU:HG2	1:B:350:PRO:HB3	1.74	0.70
1:A:473:GLY:HA2	1:A:490:ILE:HG12	1.73	0.70
1:B:476:ILE:HD12	1:B:549:LEU:CD2	2.22	0.69
1:A:505:LYS:H	1:A:505:LYS:HD3	1.57	0.69
1:A:491:GLN:HB2	1:B:459:ARG:HG2	1.75	0.67
1:A:505:LYS:H	1:A:505:LYS:CD	2.07	0.67
1:A:241:PRO:HB3	1:A:349:VAL:HG12	1.77	0.66
1:A:553:ALA:C	1:A:556:THR:HG22	2.20	0.66
1:B:525:LYS:H	1:B:525:LYS:HD2	1.61	0.66
1:A:302:LYS:HZ3	1:A:304:LYS:HD3	1.62	0.65
1:A:505:LYS:HD3	1:A:506:ASP:H	1.62	0.65
1:B:546:PRO:HB2	1:B:548:ASN:ND2	2.12	0.64
1:B:342:LYS:HD2	1:B:342:LYS:O	1.98	0.64
1:B:525:LYS:H	1:B:525:LYS:CD	2.11	0.63
1:A:4:ILE:CG1	1:A:8:LYS:HD3	2.28	0.63
1:A:157:TYR:CD2	1:A:187:MET:HE2	2.34	0.62
1:B:95:VAL:O	1:B:162:PRO:HA	2.00	0.62
1:B:21:THR:HG22	1:B:431:GLU:OE2	1.99	0.62
1:A:302:LYS:NZ	1:A:304:LYS:NZ	2.48	0.61
1:B:480:ILE:HG12	1:B:556:THR:HG23	1.82	0.61
1:B:126:HIS:CE1	1:B:136:THR:OG1	2.53	0.61
1:A:114:HIS:N	1:A:116:THR:HG1	1.99	0.61
1:A:154:ARG:HA	1:A:187:MET:HE1	1.83	0.61
1:A:369:TRP:CH2	1:A:373:GLN:HG2	2.36	0.61
1:A:212:LYS:O	1:A:345:LYS:HE2	2.00	0.61
1:B:287:ALA:HB1	1:B:288:LEU:HD12	1.82	0.61
1:A:4:ILE:HG12	1:A:8:LYS:HD3	1.82	0.61
1:B:103:SER:O	1:B:105:SER:N	2.34	0.61
1:B:288:LEU:HD12	1:B:288:LEU:H	1.65	0.61
1:B:553:ALA:HA	1:B:556:THR:HG22	1.83	0.61
1:A:104:ILE:O	1:A:104:ILE:HG22	2.00	0.60
1:B:385:ILE:HG22	1:B:418:THR:HG22	1.83	0.59
1:B:480:ILE:HG12	1:B:556:THR:CG2	2.32	0.59
1:A:79:LEU:HA	1:A:82:LEU:HD22	1.83	0.59
1:A:218:ALA:HB2	1:A:252:ILE:HD11	1.84	0.59
1:A:499:LEU:HD22	1:A:533:ILE:HD12	1.83	0.59
1:A:200:VAL:O	1:A:204:ILE:HG13	2.02	0.58
1:A:426:ALA:HA	1:A:438:VAL:HG21	1.83	0.58
1:B:235:ILE:HD11	1:B:258:ARG:HB2	1.85	0.58
1:B:555:LEU:O	1:B:555:LEU:HD12	2.04	0.58
3:A:557:TPP:N1'	1:B:51:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ASP:O	1:B:342:LYS:HG3	2.03	0.57
1:B:145:ALA:HB3	1:B:146:PRO:HD3	1.85	0.57
1:A:267:LEU:HD21	1:A:552:GLN:HE22	1.68	0.57
1:B:284:SER:C	1:B:286:GLY:H	2.13	0.57
1:A:51:GLU:HB2	1:A:80:SER:HB2	1.86	0.57
1:A:67:MET:HE1	1:A:153:ILE:HG23	1.87	0.57
1:B:190:LYS:HD2	1:B:191:PRO:HD2	1.87	0.57
1:A:71:ILE:HA	1:A:98:VAL:O	2.04	0.56
1:A:232:LYS:HE3	1:A:252:ILE:HA	1.87	0.56
1:A:262:VAL:O	1:A:272:VAL:HG11	2.05	0.56
1:A:496:LEU:HD22	1:A:509:THR:HB	1.86	0.56
1:A:95:VAL:O	1:A:162:PRO:HA	2.04	0.56
1:B:380:GLU:HG3	1:B:402:ASN:O	2.06	0.56
1:A:244:VAL:O	1:A:262:VAL:HA	2.05	0.56
1:A:345:LYS:H	1:A:345:LYS:CD	2.11	0.56
1:A:266:THR:HG22	1:A:273:LYS:HZ1	1.71	0.55
1:B:475:THR:HG21	1:B:542:VAL:O	2.06	0.55
1:B:65:LYS:HD2	1:B:432:ILE:CD1	2.37	0.55
1:A:380:GLU:HG2	1:A:401:PRO:HB2	1.89	0.55
1:B:228:LYS:HD3	1:B:229:ALA:H	1.71	0.54
1:B:233:LYS:HZ2	1:B:233:LYS:HB3	1.72	0.54
1:A:218:ALA:CB	1:A:252:ILE:HD11	2.37	0.54
1:A:152:CYS:HB3	1:A:163:VAL:HG11	1.90	0.54
1:A:13:ARG:HG3	1:A:185:ILE:HD11	1.89	0.54
1:A:139:ILE:HG21	1:A:145:ALA:HB2	1.90	0.54
1:A:415:ILE:O	1:A:446:SER:HB3	2.08	0.54
1:A:92:HIS:O	1:A:224:ARG:HG2	2.07	0.53
1:B:4:ILE:CD1	1:B:8:LYS:HG2	2.34	0.53
1:A:22:VAL:HG11	1:A:71:ILE:HD12	1.91	0.53
1:B:505:LYS:HD2	1:B:506:ASP:H	1.72	0.53
1:A:27:GLY:HA2	3:B:557:TPP:H7'1	1.91	0.53
1:A:203:THR:O	1:A:206:ALA:HB3	2.08	0.53
1:A:267:LEU:CD2	1:A:552:GLN:NE2	2.69	0.53
1:A:264:VAL:O	1:A:268:SER:OG	2.26	0.53
1:B:497:SER:C	1:B:500:PRO:HD2	2.34	0.53
1:B:440:LEU:HD12	1:B:466:LEU:HD12	1.90	0.52
1:B:221:CYS:H	1:B:287:ALA:CB	2.21	0.52
1:A:227:VAL:HG21	1:A:330:LEU:HD23	1.90	0.52
1:B:440:LEU:HD22	1:B:441:PHE:N	2.25	0.52
1:A:385:ILE:HG12	1:A:407:ILE:HD12	1.92	0.52
1:B:144:THR:O	1:B:147:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:THR:OG1	1:A:517:GLU:HG3	2.10	0.52
1:B:235:ILE:CD1	1:B:258:ARG:HB2	2.40	0.51
1:B:499:LEU:HB2	1:B:500:PRO:HD3	1.91	0.51
1:A:228:LYS:O	1:A:232:LYS:HG2	2.10	0.51
1:A:440:LEU:HD12	1:A:466:LEU:HD22	1.92	0.51
1:A:249:LYS:HE3	1:A:400:PHE:CZ	2.45	0.51
1:B:33:LEU:HD13	1:B:71:ILE:HD13	1.92	0.51
1:B:302:LYS:O	1:B:303:THR:OG1	2.26	0.51
1:B:401:PRO:HD2	1:B:404:THR:OG1	2.10	0.51
1:B:214:PRO:HG2	1:B:240:PHE:CE1	2.45	0.51
1:B:214:PRO:HG2	1:B:240:PHE:CD1	2.46	0.51
1:A:550:VAL:O	1:A:554:LYS:HB2	2.11	0.51
1:B:497:SER:O	1:B:500:PRO:HD2	2.11	0.50
1:B:123:THR:O	1:B:127:ARG:HG3	2.11	0.50
1:A:498:LEU:HD13	1:B:501:THR:HG21	1.93	0.50
1:A:302:LYS:HZ1	1:A:304:LYS:HZ3	1.60	0.50
1:B:207:LEU:CD1	1:B:305:ASN:HD21	2.24	0.50
3:A:557:TPP:H7'1	1:B:27:GLY:HA2	1.93	0.50
1:B:154:ARG:NH2	1:B:188:SER:O	2.45	0.50
1:A:471:ASN:O	1:A:542:VAL:HG22	2.11	0.50
1:B:456:THR:HA	1:B:459:ARG:HG3	1.92	0.50
1:A:71:ILE:HG12	1:A:98:VAL:HB	1.93	0.50
1:B:154:ARG:O	1:B:158:VAL:HG22	2.11	0.50
1:B:221:CYS:SG	1:B:287:ALA:HB1	2.52	0.50
1:A:35:ASP:OD2	1:B:481:HIS:HE1	1.95	0.49
1:A:511:ARG:NH2	1:A:537:GLU:OE1	2.45	0.49
1:B:207:LEU:HG	1:B:305:ASN:ND2	2.27	0.49
1:B:221:CYS:HA	1:B:224:ARG:HB2	1.94	0.49
1:A:4:ILE:HG13	1:A:8:LYS:HD3	1.93	0.49
1:B:139:ILE:HG22	1:B:171:LEU:CD1	2.43	0.49
1:B:547:GLN:O	1:B:550:VAL:HB	2.13	0.49
1:A:148:GLU:OE2	1:A:151:ARG:NH1	2.46	0.49
1:A:222:CYS:O	1:A:227:VAL:HG13	2.13	0.49
1:B:155:THR:O	1:B:159:THR:HB	2.13	0.49
1:B:302:LYS:HE2	1:B:302:LYS:HA	1.94	0.49
1:A:13:ARG:HD3	1:A:181:LEU:CD2	2.43	0.49
1:A:302:LYS:CE	1:A:304:LYS:HZ2	2.26	0.49
1:A:499:LEU:HD22	1:A:533:ILE:CD1	2.43	0.49
1:A:273:LYS:HD2	1:A:277:GLU:CD	2.38	0.48
1:B:221:CYS:SG	1:B:288:LEU:CD1	3.01	0.48
1:B:483:PRO:C	1:B:484:LYS:HG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLU:HB2	1:A:400:PHE:O	2.13	0.48
1:A:243:PHE:HA	1:A:261:GLY:O	2.14	0.48
1:B:549:LEU:O	1:B:553:ALA:HB2	2.14	0.48
1:A:6:LEU:O	1:A:9:TYR:HB3	2.14	0.47
1:A:142:ILE:HD12	1:A:142:ILE:H	1.79	0.47
1:A:273:LYS:HD2	1:A:277:GLU:OE1	2.14	0.47
1:B:509:THR:HA	1:B:535:MET:O	2.15	0.47
1:B:458:ILE:HG23	1:B:505:LYS:NZ	2.30	0.47
1:B:271:GLU:CG	1:B:350:PRO:HB3	2.43	0.47
1:B:505:LYS:CD	1:B:506:ASP:H	2.28	0.47
1:A:302:LYS:HZ3	1:A:304:LYS:CD	2.28	0.47
1:A:414:SER:HB2	1:B:76:VAL:HG12	1.95	0.47
1:B:411:LEU:C	1:B:411:LEU:HD23	2.40	0.47
1:B:555:LEU:O	1:B:556:THR:C	2.56	0.47
1:A:361:ALA:HA	1:A:515:THR:HG22	1.97	0.47
1:B:101:VAL:O	1:B:168:PRO:HA	2.15	0.46
1:A:302:LYS:NZ	1:A:304:LYS:HZ2	2.14	0.46
1:B:268:SER:O	1:B:269:LYS:C	2.59	0.46
1:A:209:LYS:HB2	1:A:209:LYS:HE3	1.76	0.46
1:A:117:LEU:HD22	1:A:124:VAL:HG11	1.96	0.46
1:A:317:ARG:NH1	1:A:317:ARG:HB2	2.30	0.46
1:B:21:THR:HB	1:B:44:ARG:HG3	1.97	0.46
1:B:61:TYR:OH	1:B:431:GLU:OE1	2.31	0.46
1:B:356:ASN:ND2	1:B:373:GLN:OE1	2.48	0.46
1:A:505:LYS:CD	1:A:506:ASP:H	2.29	0.46
1:B:67:MET:HE3	1:B:156:THR:HG21	1.97	0.46
1:B:435:LYS:O	1:B:435:LYS:HG3	2.15	0.46
1:A:117:LEU:HG	1:B:89:TYR:CD2	2.51	0.46
1:B:552:GLN:O	1:B:552:GLN:HG3	2.08	0.46
1:B:221:CYS:H	1:B:287:ALA:HB2	1.81	0.45
1:B:234:LEU:HD21	1:B:337:ILE:HD13	1.97	0.45
1:A:228:LYS:O	1:A:232:LYS:CG	2.65	0.45
1:B:553:ALA:O	1:B:556:THR:HG22	2.15	0.45
1:A:83:ASN:HD21	1:B:76:VAL:HA	1.82	0.45
1:A:179:LYS:O	1:A:182:GLN:HG2	2.16	0.45
1:A:289:LEU:HD12	1:A:291:ASP:OD1	2.17	0.45
1:B:512:VAL:HG22	1:B:517:GLU:HB3	1.98	0.45
1:B:302:LYS:HB3	1:B:303:THR:H	1.50	0.45
1:A:12:GLU:HG2	1:A:181:LEU:CD1	2.42	0.45
1:A:142:ILE:HD12	1:A:142:ILE:N	2.32	0.45
1:A:384:VAL:HG11	1:A:395:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:SER:HA	1:A:326:MET:HG2	1.99	0.45
1:A:435:LYS:N	1:A:435:LYS:HD2	2.32	0.45
1:B:222:CYS:HA	1:B:227:VAL:HG12	1.99	0.45
1:B:553:ALA:HA	1:B:556:THR:CG2	2.47	0.45
1:A:59:ASP:O	1:A:62:ALA:HB3	2.17	0.45
1:A:459:ARG:HH11	1:A:459:ARG:HD2	1.55	0.45
1:B:538:ILE:HG22	1:B:540:LEU:HG	1.98	0.45
1:B:553:ALA:CA	1:B:556:THR:HG22	2.47	0.45
1:A:134:GLU:HB2	1:A:161:ARG:HB3	1.99	0.44
1:A:475:THR:HB	1:A:542:VAL:O	2.17	0.44
1:A:540:LEU:HA	1:A:541:PRO:HD3	1.76	0.44
1:B:349:VAL:HA	1:B:350:PRO:HD3	1.82	0.44
1:B:546:PRO:O	1:B:547:GLN:C	2.59	0.44
1:B:458:ILE:HG23	1:B:505:LYS:HZ2	1.83	0.44
1:A:302:LYS:HD3	1:A:304:LYS:HD3	1.98	0.44
1:A:365:LEU:HD13	1:A:538:ILE:HG23	1.98	0.44
1:B:315:LYS:HE2	1:B:317:ARG:O	2.16	0.44
1:A:249:LYS:HE2	1:A:395:ILE:O	2.18	0.44
1:A:349:VAL:HG23	1:A:352:ARG:HH21	1.83	0.44
1:A:515:THR:HG22	1:A:516:GLY:N	2.32	0.44
1:B:422:THR:OG1	1:B:440:LEU:HG	2.18	0.44
1:A:176:VAL:HA	1:A:177:PRO:HD3	1.93	0.44
1:A:147:ALA:O	1:A:150:ASP:HB2	2.18	0.43
1:A:467:PHE:HB3	1:A:538:ILE:HD11	2.00	0.43
1:A:365:LEU:HD11	1:A:512:VAL:HG13	2.00	0.43
1:B:220:ALA:HB3	1:B:288:LEU:HD13	1.99	0.43
1:B:190:LYS:CD	1:B:191:PRO:HD2	2.48	0.43
1:B:139:ILE:HD11	1:B:165:LEU:HD11	2.00	0.43
1:B:475:THR:CG2	1:B:542:VAL:O	2.66	0.43
1:A:101:VAL:O	1:A:102:PRO:C	2.61	0.43
1:B:308:GLU:HB3	1:B:310:HIS:NE2	2.33	0.43
1:B:352:ARG:NH1	1:B:352:ARG:HG3	2.33	0.43
1:A:315:LYS:HA	1:A:319:ALA:O	2.19	0.43
1:B:221:CYS:SG	1:B:288:LEU:HD11	2.59	0.43
1:A:365:LEU:HD13	1:A:538:ILE:CG2	2.49	0.43
1:B:90:ALA:HB1	1:B:411:LEU:HD22	2.01	0.42
1:B:555:LEU:O	1:B:556:THR:O	2.37	0.42
1:A:267:LEU:CD2	1:A:552:GLN:HE22	2.30	0.42
1:B:139:ILE:CD1	1:B:165:LEU:HD11	2.50	0.42
1:A:267:LEU:HD21	1:A:552:GLN:HE21	1.77	0.42
1:B:221:CYS:SG	1:B:288:LEU:HD12	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:CG2	1:A:352:ARG:HH21	2.33	0.42
1:A:416:GLY:HA3	1:A:450:THR:HG23	2.02	0.42
1:B:496:LEU:HD22	1:B:509:THR:HB	2.01	0.42
1:A:469:LEU:CD2	1:A:538:ILE:HD12	2.49	0.42
1:A:135:THR:O	1:A:163:VAL:HG13	2.19	0.42
1:A:314:MET:HE3	1:A:314:MET:HB3	1.75	0.42
1:A:72:THR:O	1:A:99:VAL:HA	2.20	0.42
1:B:14:LEU:HD12	1:B:14:LEU:HA	1.96	0.42
1:A:336:ASN:ND2	1:A:336:ASN:N	2.68	0.41
1:A:553:ALA:O	1:A:556:THR:CG2	2.60	0.41
1:B:508:GLU:HB2	1:B:534:ARG:HG2	2.00	0.41
1:B:400:PHE:HA	1:B:401:PRO:HD3	1.84	0.41
1:A:3:GLU:O	1:A:4:ILE:HD12	2.21	0.41
1:A:304:LYS:HB3	1:A:305:ASN:H	1.61	0.41
1:A:345:LYS:HE3	1:A:345:LYS:O	2.20	0.41
1:B:247:MET:HG3	1:B:410:VAL:HB	2.03	0.41
1:B:440:LEU:HD22	1:B:440:LEU:C	2.45	0.41
1:A:360:PRO:HG2	1:A:363:THR:OG1	2.20	0.41
1:A:67:MET:HE3	1:A:156:THR:HB	2.03	0.41
1:A:138:MET:HE2	1:A:138:MET:HB2	1.90	0.41
1:A:214:PRO:HD2	1:A:344:TYR:CE1	2.55	0.41
1:A:447:LEU:HD11	1:A:451:VAL:HG23	2.02	0.41
1:B:171:LEU:O	1:B:174:LEU:HB2	2.20	0.41
3:A:557:TPP:HN42	3:A:557:TPP:C2	2.34	0.41
1:B:352:ARG:HD3	1:B:399:THR:HG21	2.02	0.41
1:B:505:LYS:H	1:B:505:LYS:CD	2.14	0.41
1:A:27:GLY:O	1:A:31:LEU:HD13	2.21	0.41
1:A:62:ALA:HB2	1:A:68:SER:OG	2.20	0.41
1:A:302:LYS:HE2	1:A:304:LYS:HZ2	1.86	0.41
1:B:239:GLN:O	1:B:258:ARG:HD3	2.21	0.41
1:B:302:LYS:C	1:B:303:THR:OG1	2.64	0.41
1:B:316:ILE:O	1:B:317:ARG:C	2.63	0.41
1:B:447:LEU:O	1:B:451:VAL:HB	2.21	0.41
1:A:266:THR:HG22	1:A:273:LYS:NZ	2.36	0.41
1:B:234:LEU:CD2	1:B:337:ILE:HD13	2.51	0.41
1:B:433:ASP:HA	1:B:434:PRO:HD3	1.96	0.41
1:A:227:VAL:HG22	1:A:227:VAL:O	2.21	0.40
1:B:92:HIS:HD2	1:B:225:HIS:HE1	1.69	0.40
1:B:284:SER:C	1:B:286:GLY:N	2.74	0.40
1:A:23:PHE:O	1:A:70:ILE:HA	2.21	0.40
1:A:35:ASP:OD2	1:B:481:HIS:CE1	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.87	0.40
1:B:269:LYS:O	1:B:272:VAL:HB	2.21	0.40
1:B:220:ALA:HB3	1:B:288:LEU:CD1	2.51	0.40
1:B:328:PHE:O	1:B:332:LYS:HB2	2.22	0.40
1:A:227:VAL:CG2	1:A:330:LEU:HD23	2.52	0.40
1:A:555:LEU:O	1:A:555:LEU:HG	2.20	0.40
1:B:272:VAL:O	1:B:273:LYS:C	2.65	0.40
1:B:309:PHE:CD2	1:B:314:MET:HE1	2.57	0.40

All (1) 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:317:ARG:NH1	1:B:199:GLU:OE2[2_555]	2.08	0.12

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	531/556 (96%)	490 (92%)	37 (7%)	4 (1%)	16	25
1	B	531/556 (96%)	492 (93%)	34 (6%)	5 (1%)	14	22
All	All	1062/1112 (96%)	982 (92%)	71 (7%)	9 (1%)	16	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	A	227	VAL
1	A	304	LYS
1	B	288	LEU
1	B	289	LEU

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Mol	Chain	Res	Type
1	B	104	ILE
1	A	417	PHE
1	B	303	THR
1	B	342	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	447/464 (96%)	387 (87%)	60 (13%)	4	5
1	B	447/464 (96%)	385 (86%)	62 (14%)	3	4
All	All	894/928 (96%)	772 (86%)	122 (14%)	3	5

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	14	LEU
1	A	31	LEU
1	A	33	LEU
1	A	34	LEU
1	A	52	LEU
1	A	70	ILE
1	A	82	LEU
1	A	99	VAL
1	A	102	PRO
1	A	103	SER
1	A	104	ILE
1	A	114	HIS
1	A	117	LEU
1	A	135	THR
1	A	142	ILE
1	A	144	THR
1	A	165	LEU
1	A	176	VAL

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Mol	Chain	Res	Type
1	A	179	LYS
1	A	196	SER
1	A	199	GLU
1	A	207	LEU
1	A	230	GLU
1	A	232	LYS
1	A	233	LYS
1	A	234	LEU
1	A	237	LEU
1	A	264	VAL
1	A	267	LEU
1	A	271	GLU
1	A	273	LYS
1	A	289	LEU
1	A	291	ASP
1	A	302	LYS
1	A	303	THR
1	A	304	LYS
1	A	315	LYS
1	A	330	LEU
1	A	336	ASN
1	A	345	LYS
1	A	359	VAL
1	A	362	SER
1	A	405	TYR
1	A	423	LEU
1	A	440	LEU
1	A	453	GLU
1	A	475	THR
1	A	479	LEU
1	A	480	ILE
1	A	490	ILE
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	540	LEU
1	A	555	LEU
1	B	2	SER

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Mol	Chain	Res	Type
1	B	14	LEU
1	B	21	THR
1	B	25	LEU
1	B	33	LEU
1	B	34	LEU
1	B	52	LEU
1	B	70	ILE
1	B	142	ILE
1	B	161	ARG
1	B	162	PRO
1	B	167	LEU
1	B	174	LEU
1	B	176	VAL
1	B	179	LYS
1	B	183	THR
1	B	189	LEU
1	B	190	LYS
1	B	198	LYS
1	B	199	GLU
1	B	207	LEU
1	B	208	VAL
1	B	212	LYS
1	B	215	VAL
1	B	223	SER
1	B	224	ARG
1	B	227	VAL
1	B	228	LYS
1	B	232	LYS
1	B	233	LYS
1	B	234	LEU
1	B	235	ILE
1	B	281	LEU
1	B	283	LEU
1	B	289	LEU
1	B	291	ASP
1	B	302	LYS
1	B	303	THR
1	B	304	LYS
1	B	305	ASN
1	B	327	LYS
1	B	342	LYS
1	B	349	VAL

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Mol	Chain	Res	Type
1	B	352	ARG
1	B	363	THR
1	B	366	LYS
1	B	403	ASN
1	B	410	VAL
1	B	423	LEU
1	B	435	LYS
1	B	440	LEU
1	B	447	LEU
1	B	466	LEU
1	B	475	THR
1	B	476	ILE
1	B	479	LEU
1	B	484	LYS
1	B	505	LYS
1	B	512	VAL
1	B	525	LYS
1	B	548	ASN
1	B	552	GLN

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	83	ASN
1	A	126	HIS
1	A	255	GLN
1	A	403	ASN
1	A	552	GLN
1	B	20	ASN
1	B	126	HIS
1	B	131	ASN
1	B	213	ASN
1	B	225	HIS
1	B	313	HIS
1	B	376	ASN
1	B	396	ASN
1	B	397	GLN
1	B	548	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.17	3 (11%)	38,40,40	1.99	12 (31%)
3	TPP	A	557	2	26,27,27	1.16	3 (11%)	38,40,40	1.43	7 (18%)

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	-	5/17/17/17	0/2/2/2
3	TPP	A	557	2	-	5/17/17/17	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	557	TPP	C5-C4	2.73	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	557	TPP	C2'-N3'	-2.55	1.29	1.34
3	A	557	TPP	C4'-N3'	2.26	1.38	1.35
3	A	557	TPP	C7'-N3	2.16	1.53	1.48
3	A	557	TPP	C5-C4	2.11	1.39	1.35
3	B	557	TPP	PB-O3B	-2.01	1.47	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	557	TPP	C7'-N3-C2	-5.57	111.85	123.48
3	B	557	TPP	C7'-N3-C4	5.54	137.03	122.36
3	A	557	TPP	CM2-C2'-N1'	3.24	120.66	117.20
3	A	557	TPP	O2B-PB-O1B	3.00	122.53	110.83
3	A	557	TPP	PA-O7-C7	2.86	134.87	121.26
3	B	557	TPP	S1-C2-N3	2.72	115.75	112.30
3	A	557	TPP	C7'-N3-C4	2.62	129.30	122.36
3	B	557	TPP	CM4-C4-C5	-2.62	121.05	127.75
3	B	557	TPP	CM4-C4-N3	2.50	126.34	120.57
3	A	557	TPP	S1-C2-N3	2.38	115.31	112.30
3	B	557	TPP	N1'-C2'-N3'	-2.32	121.67	125.53
3	A	557	TPP	N1'-C2'-N3'	-2.28	121.73	125.53
3	B	557	TPP	C2-S1-C5	-2.22	89.75	91.22
3	B	557	TPP	C2-N3-C4	-2.21	111.07	114.06
3	A	557	TPP	C7'-N3-C2	-2.19	118.91	123.48
3	B	557	TPP	C2'-N3'-C4'	2.18	121.44	118.10
3	B	557	TPP	O2A-PA-O3A	2.17	113.12	107.27
3	B	557	TPP	O2A-PA-O1A	2.11	122.27	112.44
3	B	557	TPP	CM2-C2'-N1'	2.10	119.43	117.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	557	TPP	C7-O7-PA-O1A
3	A	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	PB-O3A-PA-O1A
3	A	557	TPP	C7-O7-PA-O2A
3	B	557	TPP	PB-O3A-PA-O2A
3	A	557	TPP	PB-O3A-PA-O1A
3	B	557	TPP	PA-O3A-PB-O1B
3	B	557	TPP	PA-O3A-PB-O2B

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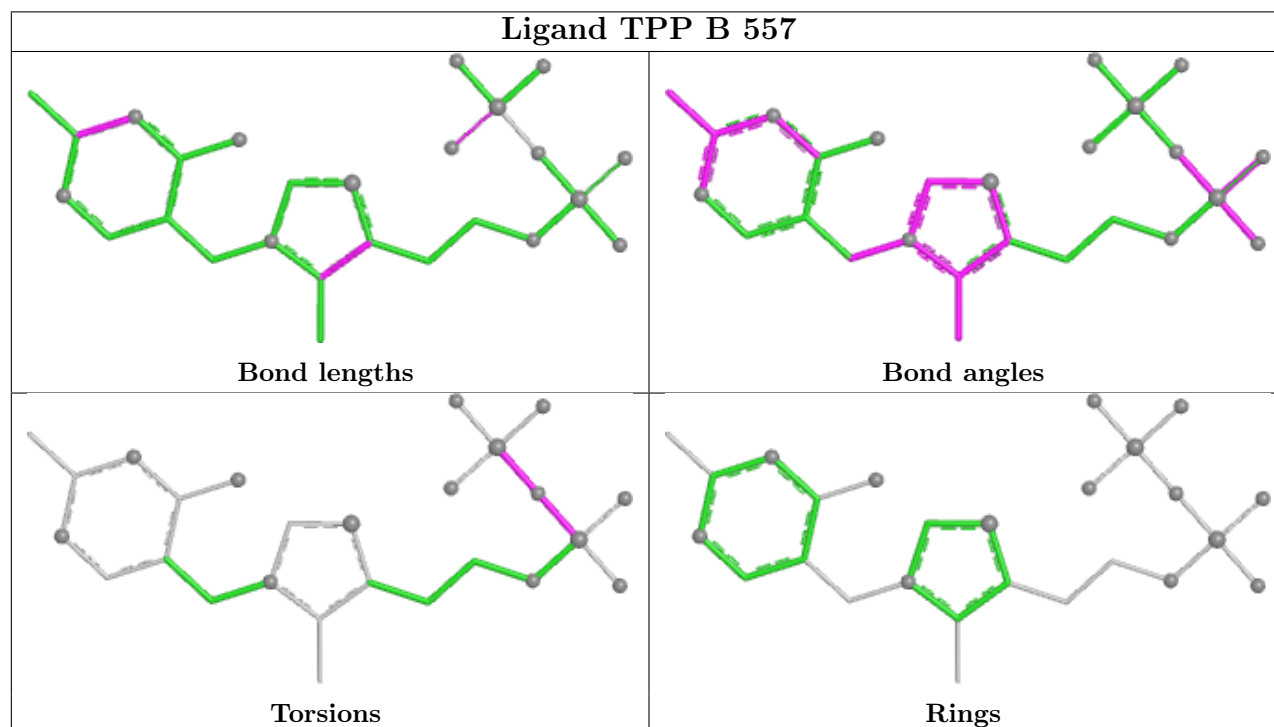
Mol	Chain	Res	Type	Atoms
3	A	557	TPP	PB-O3A-PA-O2A

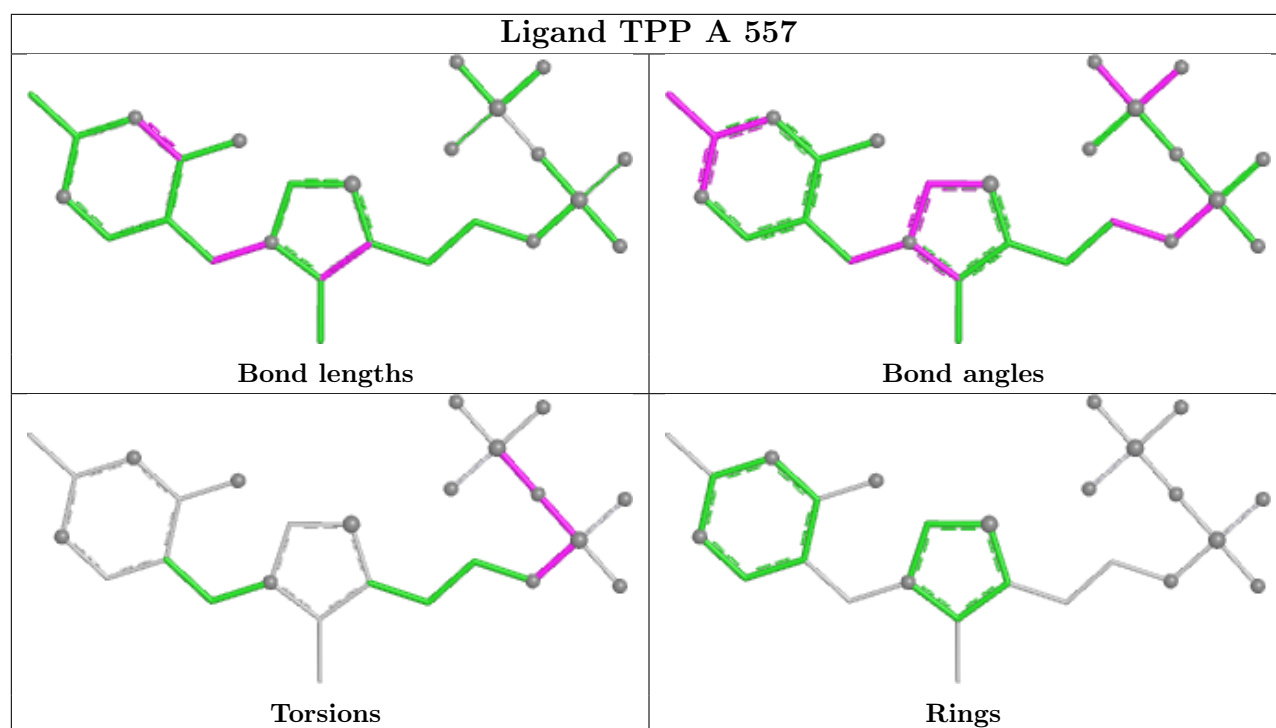
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	557	TPP	1	0
3	A	557	TPP	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.