



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:37 AM UTC

PDB ID : 4ALD / pdb_00004ald
Title : HUMAN MUSCLE FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE COM-
PLEXED WITH FRUCTOSE 1,6-BISPHOSPHATE
Authors : Dalby, A.R.; Dauter, Z.; Littlechild, J.A.
Deposited on : 1998-07-26
Resolution : 2.80 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

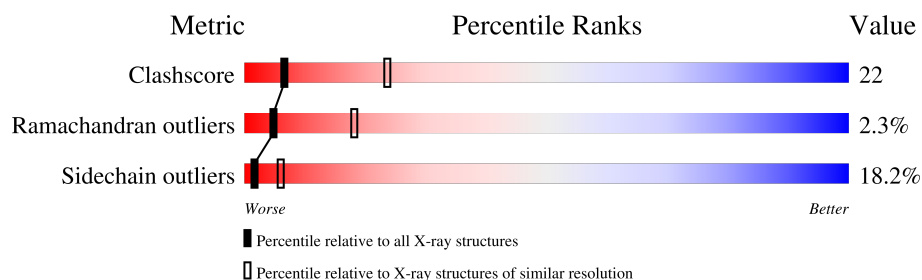
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	363	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FP	A	364	-	X	X	-

2 Entry composition [i](#)

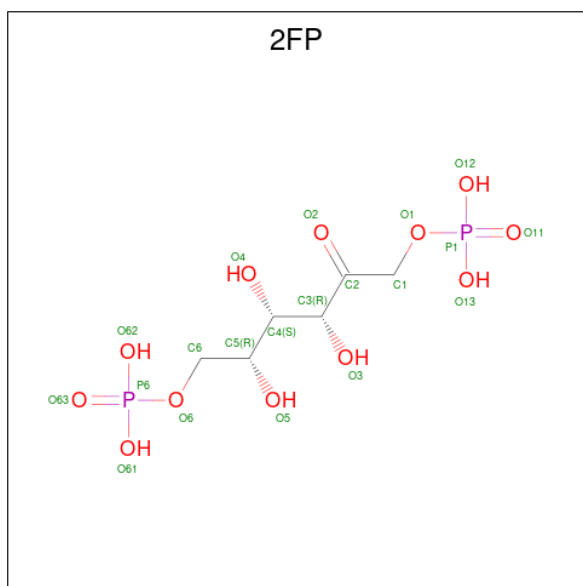
There are 2 unique types of molecules in this entry. The entry contains 2783 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 FRUCTOSE-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2763	1741	486	525	11			

- Molecule 2 is 1,6-FRUCTOSE DIPHOSPHATE (LINEAR FORM) (CCD ID: 2FP) (formula: $C_6H_{14}O_{12}P_2$).



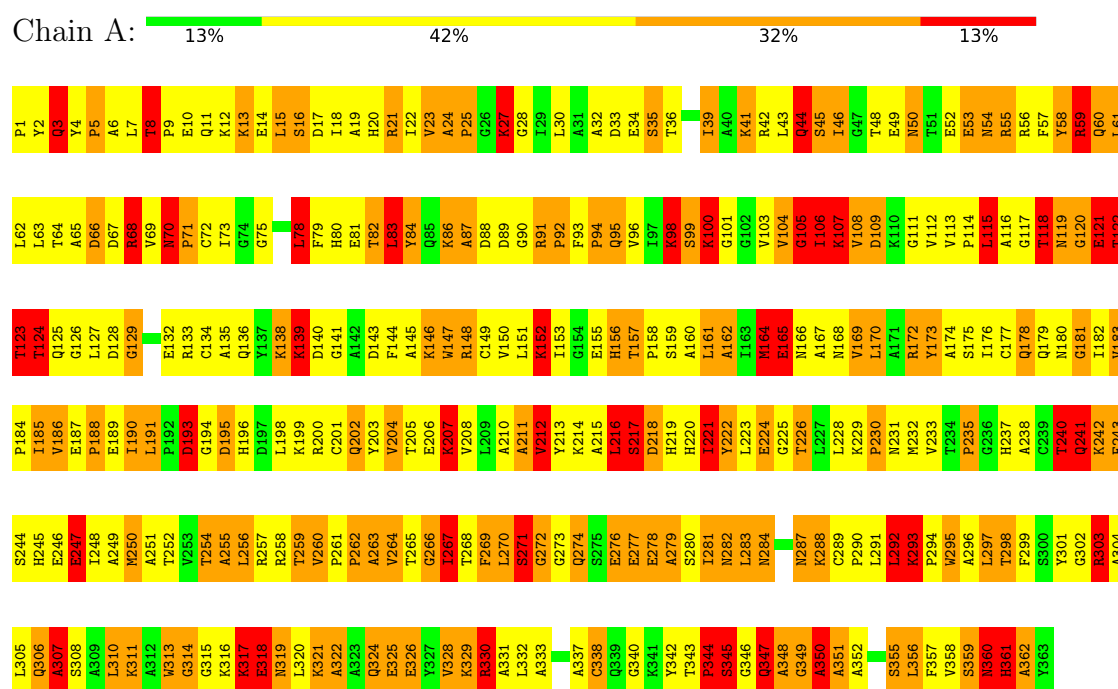
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: FRUCTOSE-BISPHOSPHATE ALDOLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	96.50Å 96.50Å 166.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.56 – 2.80	Depositor
% Data completeness (in resolution range)	93.7 (19.56-2.80)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.202 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2783	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2FP

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	1.80	33/2817 (1.2%)	3.82	602/3818 (15.8%)

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	59

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	VAL	C-N	-8.78	1.26	1.33
1	A	157	THR	C-O	-7.43	1.16	1.24
1	A	128	ASP	C-N	-7.31	1.24	1.33
1	A	24	ALA	N-CA	6.97	1.55	1.45
1	A	59	ARG	NE-CZ	-6.79	1.25	1.33
1	A	152	LYS	C-O	-6.53	1.16	1.23
1	A	219	HIS	CE1-NE2	-6.44	1.26	1.32
1	A	258	ARG	CD-NE	6.35	1.55	1.46
1	A	189	GLU	C-N	6.24	1.41	1.33
1	A	59	ARG	CD-NE	-6.16	1.37	1.46
1	A	343	THR	C-O	-5.91	1.20	1.25
1	A	272	GLY	C-O	5.87	1.31	1.23
1	A	126	GLY	N-CA	-5.87	1.36	1.45
1	A	54	ASN	C-O	5.79	1.30	1.24
1	A	80	HIS	ND1-CE1	5.77	1.38	1.32
1	A	113	VAL	CA-C	5.71	1.58	1.52
1	A	298	THR	C-O	-5.61	1.17	1.24
1	A	122	THR	CB-OG1	-5.60	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLU	N-CA	-5.55	1.39	1.46
1	A	293	LYS	C-O	-5.54	1.17	1.24
1	A	359	SER	C-O	5.50	1.30	1.24
1	A	203	TYR	C-O	-5.42	1.17	1.24
1	A	148	ARG	CD-NE	-5.39	1.38	1.46
1	A	262	PRO	C-O	-5.23	1.17	1.24
1	A	272	GLY	N-CA	-5.20	1.37	1.45
1	A	199	LYS	C-N	-5.18	1.26	1.33
1	A	129	GLY	N-CA	-5.16	1.38	1.45
1	A	128	ASP	N-CA	5.14	1.52	1.46
1	A	211	ALA	N-CA	-5.09	1.40	1.46
1	A	216	LEU	C-N	5.07	1.41	1.33
1	A	213	TYR	C-O	5.02	1.30	1.24
1	A	221	ILE	C-O	-5.00	1.17	1.24
1	A	218	ASP	N-CA	-5.00	1.40	1.46

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	CD-NE-CZ	27.14	162.40	124.40
1	A	68	ARG	NE-CZ-NH2	-20.95	100.34	119.20
1	A	311	LYS	CB-CG-CD	19.85	156.95	111.30
1	A	157	THR	CA-C-O	-17.77	102.36	120.66
1	A	133	ARG	NH1-CZ-NH2	16.61	140.89	119.30
1	A	133	ARG	NE-CZ-NH2	-15.68	105.08	119.20
1	A	202	GLN	OE1-CD-NE2	-15.42	107.18	122.60
1	A	348	ALA	N-CA-C	15.21	133.11	110.30
1	A	157	THR	O-C-N	14.66	133.81	121.35
1	A	2	TYR	CA-C-N	14.00	148.28	121.54
1	A	2	TYR	C-N-CA	14.00	148.28	121.54
1	A	91	ARG	CB-CA-C	13.93	129.84	109.08
1	A	44	GLN	CA-C-O	13.71	135.09	120.55
1	A	99	SER	CA-C-O	-13.62	104.95	120.20
1	A	303	ARG	CG-CD-NE	13.50	141.69	112.00
1	A	91	ARG	NH1-CZ-NH2	13.42	136.74	119.30
1	A	165	GLU	CB-CG-CD	13.35	135.30	112.60
1	A	56	ARG	NE-CZ-NH1	13.33	134.83	121.50
1	A	17	ASP	CA-C-O	-13.30	107.00	120.70
1	A	91	ARG	NE-CZ-NH2	-13.14	107.37	119.20
1	A	59	ARG	NE-CZ-NH2	13.10	130.99	119.20
1	A	56	ARG	NE-CZ-NH2	-12.98	107.52	119.20
1	A	158	PRO	N-CA-CB	12.97	116.87	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	ARG	CD-NE-CZ	-12.78	106.52	124.40
1	A	343	THR	O-C-N	12.68	139.10	121.47
1	A	330	ARG	NE-CZ-NH2	-12.53	107.92	119.20
1	A	318	GLU	CB-CG-CD	12.52	133.89	112.60
1	A	220	HIS	CA-CB-CG	-12.26	101.54	113.80
1	A	185	ILE	O-C-N	-12.25	109.32	122.67
1	A	279	ALA	O-C-N	-12.20	109.40	122.09
1	A	44	GLN	O-C-N	-12.01	109.39	122.12
1	A	116	ALA	CA-C-O	-11.98	108.01	121.19
1	A	311	LYS	N-CA-C	-11.95	97.96	111.82
1	A	166	ASN	CA-CB-CG	-11.86	100.74	112.60
1	A	242	LYS	CB-CA-C	11.82	129.34	109.48
1	A	138	LYS	CA-C-N	11.81	136.48	120.54
1	A	138	LYS	C-N-CA	11.81	136.48	120.54
1	A	148	ARG	NE-CZ-NH2	-11.79	108.59	119.20
1	A	105	GLY	O-C-N	-11.74	113.08	123.29
1	A	107	LYS	CD-CE-NZ	11.68	149.29	111.90
1	A	179	GLN	OE1-CD-NE2	11.66	134.26	122.60
1	A	176	ILE	N-CA-C	-11.62	99.61	110.53
1	A	326	GLU	CB-CG-CD	11.60	132.32	112.60
1	A	91	ARG	CA-C-O	11.56	129.14	119.66
1	A	81	GLU	O-C-N	-11.46	108.93	122.11
1	A	122	THR	CA-C-O	-11.46	108.16	121.68
1	A	21	ARG	CD-NE-CZ	-11.25	108.64	124.40
1	A	350	ALA	CA-C-N	11.23	138.57	120.60
1	A	350	ALA	C-N-CA	11.23	138.57	120.60
1	A	245	HIS	CA-CB-CG	11.13	124.93	113.80
1	A	359	SER	CA-C-N	-10.99	106.79	123.17
1	A	359	SER	C-N-CA	-10.99	106.79	123.17
1	A	150	VAL	CA-C-O	-10.93	109.02	120.39
1	A	123	THR	CB-CA-C	-10.93	89.82	112.44
1	A	5	PRO	CA-C-N	10.83	134.79	120.28
1	A	5	PRO	C-N-CA	10.83	134.79	120.28
1	A	127	LEU	CA-C-O	-10.81	107.54	119.97
1	A	265	THR	N-CA-C	10.68	122.92	111.28
1	A	212	VAL	O-C-N	-10.68	109.23	122.57
1	A	78	LEU	CA-C-N	10.66	135.87	120.95
1	A	78	LEU	C-N-CA	10.66	135.87	120.95
1	A	186	VAL	CA-C-O	10.55	131.82	120.53
1	A	117	GLY	CA-C-O	10.43	131.92	119.19
1	A	135	ALA	CA-C-O	-10.42	109.50	120.55
1	A	206	GLU	CA-C-O	-10.39	109.91	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LYS	O-C-N	-10.39	110.31	122.15
1	A	148	ARG	CD-NE-CZ	10.33	138.86	124.40
1	A	351	ALA	CA-C-O	10.28	131.93	119.49
1	A	281	ILE	CA-CB-CG2	10.26	127.95	110.50
1	A	332	LEU	CA-C-O	10.20	131.23	120.42
1	A	237	HIS	O-C-N	-10.16	111.35	122.12
1	A	269	PHE	N-CA-C	10.11	124.89	110.23
1	A	202	GLN	CG-CD-NE2	10.11	131.56	116.40
1	A	17	ASP	N-CA-CB	10.09	124.70	110.07
1	A	62	LEU	O-C-N	-9.91	110.85	122.15
1	A	109	ASP	CA-C-O	-9.90	109.47	121.36
1	A	161	LEU	N-CA-C	-9.88	99.54	111.69
1	A	246	GLU	CB-CG-CD	9.87	129.37	112.60
1	A	304	ALA	CA-C-O	-9.79	106.77	119.10
1	A	172	ARG	NE-CZ-NH1	-9.79	111.71	121.50
1	A	3	GLN	OE1-CD-NE2	9.78	132.38	122.60
1	A	2	TYR	O-C-N	-9.74	111.46	123.44
1	A	343	THR	CA-C-O	-9.74	109.46	119.49
1	A	271	SER	CA-C-N	9.72	140.46	121.41
1	A	271	SER	C-N-CA	9.72	140.46	121.41
1	A	95	GLN	OE1-CD-NE2	-9.71	112.89	122.60
1	A	2	TYR	CA-C-O	9.68	133.28	120.21
1	A	340	GLY	O-C-N	-9.68	113.76	122.57
1	A	43	LEU	O-C-N	-9.66	110.92	122.22
1	A	174	ALA	N-CA-CB	9.66	124.02	110.01
1	A	345	SER	CA-C-O	9.65	134.31	120.51
1	A	113	VAL	N-CA-C	-9.57	101.35	109.19
1	A	279	ALA	CA-C-N	9.51	133.02	120.28
1	A	279	ALA	C-N-CA	9.51	133.02	120.28
1	A	123	THR	N-CA-CB	9.51	126.62	110.65
1	A	347	GLN	CA-C-N	9.49	136.34	121.26
1	A	347	GLN	C-N-CA	9.49	136.34	121.26
1	A	360	ASN	CB-CA-C	9.42	127.25	111.23
1	A	318	GLU	CA-C-O	-9.41	108.51	119.61
1	A	186	VAL	O-C-N	-9.40	112.10	123.10
1	A	289	CYS	O-C-N	-9.38	112.95	121.30
1	A	115	LEU	N-CA-CB	-9.31	95.40	110.21
1	A	266	GLY	CA-C-N	-9.28	111.69	123.19
1	A	266	GLY	C-N-CA	-9.28	111.69	123.19
1	A	21	ARG	NE-CZ-NH2	-9.27	110.86	119.20
1	A	249	ALA	CA-C-N	9.25	133.02	120.44
1	A	249	ALA	C-N-CA	9.25	133.02	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLU	O-C-N	-9.21	111.54	122.87
1	A	193	ASP	CB-CG-OD2	9.17	139.48	118.40
1	A	188	PRO	CA-C-O	-9.16	110.43	123.07
1	A	329	LYS	O-C-N	-9.15	112.29	122.08
1	A	311	LYS	CA-CB-CG	9.15	132.40	114.10
1	A	135	ALA	N-CA-CB	9.06	123.43	110.12
1	A	125	GLN	CA-C-O	-9.05	110.12	121.88
1	A	265	THR	O-C-N	-9.03	112.55	122.12
1	A	307	ALA	CA-C-N	9.01	132.16	120.44
1	A	307	ALA	C-N-CA	9.01	132.16	120.44
1	A	270	LEU	CA-C-O	-8.98	110.71	121.66
1	A	240	THR	CA-C-O	-8.95	109.08	120.00
1	A	106	ILE	O-C-N	-8.94	113.53	123.10
1	A	351	ALA	O-C-N	-8.93	110.78	122.39
1	A	181	GLY	CA-C-O	-8.87	108.59	119.68
1	A	246	GLU	N-CA-CB	8.86	123.62	110.33
1	A	61	LEU	CA-C-O	-8.85	109.79	119.97
1	A	95	GLN	O-C-N	-8.81	112.11	122.15
1	A	133	ARG	CD-NE-CZ	8.75	136.65	124.40
1	A	52	GLU	N-CA-C	-8.67	102.28	113.12
1	A	68	ARG	NH1-CZ-NH2	8.66	130.55	119.30
1	A	161	LEU	N-CA-CB	-8.64	97.32	110.20
1	A	217	SER	N-CA-CB	-8.56	97.12	110.30
1	A	264	VAL	CA-C-O	-8.54	111.30	121.04
1	A	296	ALA	CA-C-O	-8.51	112.53	121.55
1	A	259	THR	CA-CB-CG2	8.49	124.93	110.50
1	A	243	PHE	O-C-N	-8.48	112.81	123.24
1	A	128	ASP	CA-C-N	8.45	135.99	120.87
1	A	128	ASP	C-N-CA	8.45	135.99	120.87
1	A	194	GLY	CA-C-O	-8.40	114.45	121.76
1	A	161	LEU	CA-C-O	8.39	129.55	120.24
1	A	120	GLY	O-C-N	-8.32	111.86	122.43
1	A	149	CYS	CA-C-O	-8.32	111.71	121.11
1	A	190	ILE	CA-C-O	-8.31	110.92	120.65
1	A	172	ARG	NE-CZ-NH2	8.31	126.67	119.20
1	A	249	ALA	O-C-N	-8.28	113.34	122.12
1	A	262	PRO	O-C-N	-8.27	110.77	122.35
1	A	45	SER	O-C-N	-8.25	112.79	122.20
1	A	15	LEU	O-C-N	-8.21	113.42	122.12
1	A	282	ASN	CA-C-O	-8.21	112.20	120.82
1	A	55	ARG	N-CA-C	-8.21	102.41	111.36
1	A	79	PHE	CA-C-N	8.21	134.24	121.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	PHE	C-N-CA	8.21	134.24	121.19
1	A	50	ASN	CA-CB-CG	-8.20	104.40	112.60
1	A	196	HIS	ND1-CE1-NE2	-8.20	100.20	108.40
1	A	247	GLU	CG-CD-OE1	-8.17	99.62	118.40
1	A	246	GLU	CA-C-N	-8.16	109.84	120.44
1	A	246	GLU	C-N-CA	-8.16	109.84	120.44
1	A	155	GLU	CA-C-N	-8.15	109.70	122.49
1	A	155	GLU	C-N-CA	-8.15	109.70	122.49
1	A	189	GLU	CA-C-N	-8.14	112.20	122.37
1	A	189	GLU	C-N-CA	-8.14	112.20	122.37
1	A	222	TYR	CA-C-O	8.14	129.63	120.84
1	A	261	PRO	CB-CA-C	8.12	120.83	110.92
1	A	231	ASN	CA-C-O	-8.10	112.73	121.56
1	A	105	GLY	CA-C-O	-8.09	112.47	121.77
1	A	219	HIS	ND1-CG-CD2	-8.07	98.03	106.10
1	A	21	ARG	NH1-CZ-NH2	8.07	129.79	119.30
1	A	247	GLU	CG-CD-OE2	8.06	136.95	118.40
1	A	321	LYS	O-C-N	-8.06	113.77	122.07
1	A	310	LEU	N-CA-C	-8.05	101.27	112.45
1	A	228	LEU	O-C-N	-8.03	113.54	123.01
1	A	118	THR	N-CA-CB	-8.02	96.77	111.37
1	A	330	ARG	CA-C-O	-8.02	111.04	120.10
1	A	178	GLN	CB-CG-CD	8.01	126.22	112.60
1	A	91	ARG	N-CA-CB	-8.00	98.47	110.32
1	A	61	LEU	N-CA-CB	8.00	122.68	110.28
1	A	160	ALA	CA-C-O	-7.99	111.25	120.20
1	A	207	LYS	CB-CG-CD	7.99	129.67	111.30
1	A	360	ASN	CA-C-O	7.98	131.07	121.17
1	A	269	PHE	O-C-N	-7.96	113.07	122.87
1	A	119	ASN	OD1-CG-ND2	-7.96	114.64	122.60
1	A	6	ALA	CB-CA-C	-7.95	97.60	110.79
1	A	272	GLY	O-C-N	-7.95	112.37	122.70
1	A	271	SER	CA-C-O	7.93	129.04	120.24
1	A	33	ASP	CA-CB-CG	7.92	120.52	112.60
1	A	271	SER	CA-CB-OG	7.92	126.94	111.10
1	A	3	GLN	CA-C-O	7.91	131.82	120.51
1	A	87	ALA	O-C-N	-7.91	113.00	122.65
1	A	193	ASP	O-C-N	-7.90	113.33	122.97
1	A	127	LEU	O-C-N	7.90	131.99	122.27
1	A	211	ALA	O-C-N	-7.89	113.64	122.08
1	A	83	LEU	N-CA-CB	7.87	121.69	110.12
1	A	258	ARG	CD-NE-CZ	-7.86	113.39	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	LYS	CA-C-N	7.84	131.59	120.53
1	A	207	LYS	C-N-CA	7.84	131.59	120.53
1	A	237	HIS	N-CA-CB	-7.81	98.63	110.12
1	A	267	ILE	CB-CA-C	7.81	122.47	110.83
1	A	119	ASN	CA-C-O	-7.81	111.98	122.44
1	A	360	ASN	CA-C-N	7.80	136.43	121.54
1	A	360	ASN	C-N-CA	7.80	136.43	121.54
1	A	107	LYS	CG-CD-CE	7.77	129.17	111.30
1	A	17	ASP	N-CA-C	-7.77	102.75	111.14
1	A	44	GLN	CG-CD-NE2	-7.73	104.81	116.40
1	A	348	ALA	O-C-N	-7.73	112.48	123.07
1	A	291	LEU	CA-C-N	7.72	132.92	121.72
1	A	291	LEU	C-N-CA	7.72	132.92	121.72
1	A	58	TYR	CA-C-N	7.72	130.62	120.28
1	A	58	TYR	C-N-CA	7.72	130.62	120.28
1	A	7	LEU	CA-C-O	-7.71	112.68	121.40
1	A	289	CYS	N-CA-CB	-7.70	95.95	109.73
1	A	68	ARG	CA-C-N	7.70	132.65	121.02
1	A	68	ARG	C-N-CA	7.70	132.65	121.02
1	A	246	GLU	N-CA-C	-7.68	102.83	112.90
1	A	111	GLY	CA-C-O	7.66	128.57	122.52
1	A	204	VAL	CA-C-O	-7.65	112.38	120.57
1	A	344	PRO	O-C-N	-7.65	112.32	122.64
1	A	70	ASN	O-C-N	-7.64	112.54	121.32
1	A	216	LEU	N-CA-CB	-7.64	97.58	110.49
1	A	43	LEU	CA-C-O	7.63	128.73	120.10
1	A	205	THR	N-CA-C	-7.63	103.04	111.36
1	A	306	GLN	O-C-N	-7.61	113.97	122.34
1	A	351	ALA	N-CA-C	7.61	121.66	112.38
1	A	68	ARG	NE-CZ-NH1	7.60	129.10	121.50
1	A	129	GLY	CA-C-N	7.58	131.20	120.28
1	A	129	GLY	C-N-CA	7.58	131.20	120.28
1	A	258	ARG	NH1-CZ-NH2	7.58	129.15	119.30
1	A	262	PRO	CA-C-N	7.56	133.34	120.72
1	A	262	PRO	C-N-CA	7.56	133.34	120.72
1	A	199	LYS	CA-CB-CG	-7.54	99.02	114.10
1	A	237	HIS	CA-CB-CG	-7.54	106.26	113.80
1	A	292	LEU	O-C-N	-7.48	113.82	123.02
1	A	268	THR	CB-CA-C	7.48	122.98	110.79
1	A	42	ARG	CG-CD-NE	7.47	128.44	112.00
1	A	133	ARG	NE-CZ-NH1	-7.47	114.03	121.50
1	A	240	THR	CA-CB-CG2	-7.47	97.80	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	ALA	CA-C-N	7.43	135.93	122.92
1	A	296	ALA	C-N-CA	7.43	135.93	122.92
1	A	347	GLN	N-CA-CB	-7.42	97.95	110.49
1	A	92	PRO	CA-C-N	7.40	128.87	120.06
1	A	92	PRO	C-N-CA	7.40	128.87	120.06
1	A	168	ASN	OD1-CG-ND2	7.38	129.98	122.60
1	A	53	GLU	CG-CD-OE1	7.38	135.37	118.40
1	A	115	LEU	CA-C-O	-7.35	112.72	120.58
1	A	219	HIS	CA-CB-CG	-7.34	106.46	113.80
1	A	215	ALA	O-C-N	-7.28	114.46	122.03
1	A	231	ASN	OD1-CG-ND2	-7.28	115.32	122.60
1	A	232	MET	O-C-N	-7.28	114.55	122.85
1	A	337	ALA	O-C-N	-7.27	114.58	122.07
1	A	109	ASP	CA-CB-CG	7.26	119.86	112.60
1	A	64	THR	CA-CB-CG2	7.26	122.84	110.50
1	A	25	PRO	N-CA-CB	7.25	109.72	103.19
1	A	3	GLN	CG-CD-NE2	-7.25	105.53	116.40
1	A	262	PRO	CA-C-O	-7.25	108.86	118.86
1	A	123	THR	CA-C-N	-7.23	109.93	122.37
1	A	123	THR	C-N-CA	-7.23	109.93	122.37
1	A	289	CYS	CA-C-O	7.23	126.55	119.75
1	A	152	LYS	CA-C-O	-7.21	111.94	120.60
1	A	268	THR	OG1-CB-CG2	-7.21	94.89	109.30
1	A	89	ASP	CA-C-O	7.19	128.40	119.05
1	A	325	GLU	N-CA-C	-7.15	103.42	111.07
1	A	139	LYS	CA-C-O	-7.13	113.27	120.90
1	A	245	HIS	ND1-CG-CD2	-7.13	98.97	106.10
1	A	27	LYS	O-C-N	-7.12	114.96	122.94
1	A	88	ASP	CA-C-N	7.12	135.28	121.18
1	A	88	ASP	C-N-CA	7.12	135.28	121.18
1	A	221	ILE	CA-C-O	-7.12	111.97	121.02
1	A	36	THR	CA-CB-OG1	-7.12	98.92	109.60
1	A	124	THR	CA-CB-CG2	7.12	122.60	110.50
1	A	263	ALA	CA-C-O	-7.09	110.66	119.38
1	A	241	GLN	CA-C-O	7.07	128.93	121.15
1	A	166	ASN	O-C-N	-7.06	114.10	122.15
1	A	330	ARG	NH1-CZ-NH2	7.05	128.47	119.30
1	A	115	LEU	O-C-N	-7.05	114.47	122.93
1	A	279	ALA	N-CA-C	7.02	119.54	111.11
1	A	107	LYS	O-C-N	-7.02	115.02	123.16
1	A	83	LEU	CA-C-O	-7.01	113.11	120.55
1	A	73	ILE	CA-C-O	-7.01	111.58	120.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	GLU	N-CA-CB	-6.96	99.75	109.91
1	A	10	GLU	CA-C-N	-6.95	109.74	120.31
1	A	10	GLU	C-N-CA	-6.95	109.74	120.31
1	A	120	GLY	CA-C-N	6.93	130.55	120.71
1	A	120	GLY	C-N-CA	6.93	130.55	120.71
1	A	288	LYS	N-CA-C	-6.93	104.98	113.50
1	A	89	ASP	CA-CB-CG	6.92	119.52	112.60
1	A	175	SER	N-CA-CB	-6.89	99.96	110.16
1	A	162	ALA	CA-C-O	-6.87	113.55	120.90
1	A	1	PRO	O-C-N	-6.86	112.02	123.00
1	A	72	CYS	N-CA-C	6.86	121.39	112.89
1	A	283	LEU	CA-C-O	-6.85	113.23	120.63
1	A	67	ASP	CB-CG-OD1	6.85	134.15	118.40
1	A	114	PRO	CA-C-O	-6.83	113.29	121.48
1	A	293	LYS	CB-CG-CD	6.81	126.96	111.30
1	A	348	ALA	CB-CA-C	-6.80	100.61	110.06
1	A	90	GLY	CA-C-O	6.78	127.41	119.13
1	A	260	VAL	CA-C-N	-6.78	113.39	120.38
1	A	260	VAL	C-N-CA	-6.78	113.39	120.38
1	A	359	SER	CB-CA-C	-6.78	101.46	109.80
1	A	241	GLN	N-CA-C	6.78	119.80	110.24
1	A	284	ASN	CA-C-O	-6.78	113.23	120.42
1	A	328	VAL	CA-C-O	-6.77	112.32	120.78
1	A	258	ARG	NE-CZ-NH2	-6.76	113.11	119.20
1	A	83	LEU	CD1-CG-CD2	-6.76	95.93	110.80
1	A	59	ARG	NH1-CZ-NH2	-6.76	110.52	119.30
1	A	108	VAL	O-C-N	6.75	131.01	122.57
1	A	183	VAL	CA-C-O	6.75	125.01	119.47
1	A	166	ASN	OD1-CG-ND2	6.74	129.34	122.60
1	A	282	ASN	CA-CB-CG	-6.73	105.87	112.60
1	A	220	HIS	CA-C-O	-6.73	112.49	120.57
1	A	135	ALA	O-C-N	6.73	129.25	122.12
1	A	346	GLY	N-CA-C	-6.72	97.25	113.18
1	A	147	TRP	CA-C-N	-6.71	112.65	122.65
1	A	147	TRP	C-N-CA	-6.71	112.65	122.65
1	A	104	VAL	CA-C-N	-6.70	116.51	122.47
1	A	104	VAL	C-N-CA	-6.70	116.51	122.47
1	A	83	LEU	CB-CA-C	-6.70	99.67	110.79
1	A	199	LYS	O-C-N	-6.70	114.38	122.22
1	A	55	ARG	O-C-N	-6.70	114.52	122.15
1	A	221	ILE	CA-C-N	6.69	132.15	122.85
1	A	221	ILE	C-N-CA	6.69	132.15	122.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	HIS	CA-C-N	6.69	134.32	121.54
1	A	361	HIS	C-N-CA	6.69	134.32	121.54
1	A	260	VAL	CA-C-O	6.68	123.53	119.19
1	A	16	SER	N-CA-CB	-6.67	100.03	110.30
1	A	207	LYS	CD-CE-NZ	6.67	133.23	111.90
1	A	116	ALA	CB-CA-C	-6.66	98.66	109.72
1	A	139	LYS	CG-CD-CE	6.66	126.62	111.30
1	A	342	TYR	CA-C-O	6.65	128.05	120.54
1	A	159	SER	CA-CB-OG	-6.64	97.81	111.10
1	A	294	PRO	CA-C-N	6.63	134.37	121.63
1	A	294	PRO	C-N-CA	6.63	134.37	121.63
1	A	319	ASN	O-C-N	-6.63	114.38	122.34
1	A	255	ALA	O-C-N	-6.61	115.11	122.12
1	A	60	GLN	CG-CD-NE2	6.61	126.31	116.40
1	A	156	HIS	CA-CB-CG	-6.60	107.20	113.80
1	A	208	VAL	O-C-N	-6.59	115.43	121.89
1	A	267	ILE	CA-CB-CG2	6.59	121.70	110.50
1	A	145	ALA	CA-C-O	-6.59	113.91	121.68
1	A	68	ARG	CB-CG-CD	-6.57	96.18	111.30
1	A	218	ASP	CA-C-N	6.57	135.08	121.94
1	A	218	ASP	C-N-CA	6.57	135.08	121.94
1	A	101	GLY	CA-C-O	-6.57	109.14	120.57
1	A	278	GLU	N-CA-CB	6.57	119.72	109.94
1	A	100	LYS	N-CA-C	-6.56	103.33	112.25
1	A	16	SER	CB-CA-C	6.56	123.76	110.38
1	A	168	ASN	N-CA-CB	-6.55	100.21	110.30
1	A	132	GLU	CB-CG-CD	-6.54	101.48	112.60
1	A	63	LEU	N-CA-C	6.53	121.10	113.20
1	A	45	SER	CB-CA-C	6.52	123.11	110.46
1	A	245	HIS	N-CA-C	-6.50	105.51	113.50
1	A	14	GLU	N-CA-CB	6.49	119.65	110.12
1	A	95	GLN	CB-CA-C	6.48	121.87	110.85
1	A	27	LYS	CA-CB-CG	6.48	127.06	114.10
1	A	54	ASN	OD1-CG-ND2	6.48	129.08	122.60
1	A	122	THR	CA-CB-OG1	-6.48	99.89	109.60
1	A	199	LYS	CB-CG-CD	6.47	126.18	111.30
1	A	189	GLU	N-CA-C	6.47	119.15	109.25
1	A	221	ILE	N-CA-C	6.45	118.67	108.87
1	A	119	ASN	CA-CB-CG	-6.45	106.16	112.60
1	A	293	LYS	CA-CB-CG	-6.45	101.21	114.10
1	A	191	LEU	CA-C-O	6.42	127.95	120.69
1	A	3	GLN	CB-CG-CD	6.42	123.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	GLN	CG-CD-OE1	-6.40	108.00	120.80
1	A	305	LEU	N-CA-C	-6.40	104.72	113.30
1	A	133	ARG	CA-C-O	-6.39	113.77	120.55
1	A	282	ASN	OD1-CG-ND2	-6.39	116.21	122.60
1	A	277	GLU	N-CA-CB	-6.39	100.42	109.94
1	A	355	SER	O-C-N	-6.38	115.48	123.01
1	A	235	PRO	N-CA-CB	6.35	109.92	103.25
1	A	226	THR	CA-C-O	-6.35	114.13	121.49
1	A	125	GLN	CA-C-N	6.33	133.82	121.41
1	A	125	GLN	C-N-CA	6.33	133.82	121.41
1	A	177	CYS	O-C-N	-6.33	115.55	122.07
1	A	127	LEU	CA-C-N	-6.32	111.67	121.02
1	A	127	LEU	C-N-CA	-6.32	111.67	121.02
1	A	10	GLU	O-C-N	6.32	128.82	122.12
1	A	203	TYR	N-CA-C	-6.31	104.09	110.97
1	A	351	ALA	N-CA-CB	-6.31	99.59	110.32
1	A	55	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	A	106	ILE	N-CA-CB	-6.31	101.09	111.44
1	A	67	ASP	CB-CG-OD2	-6.27	103.97	118.40
1	A	261	PRO	O-C-N	-6.27	114.06	121.46
1	A	238	ALA	CA-C-O	-6.26	109.58	119.23
1	A	32	ALA	CA-C-N	6.25	132.36	122.60
1	A	32	ALA	C-N-CA	6.25	132.36	122.60
1	A	81	GLU	CA-C-N	6.25	131.15	120.72
1	A	81	GLU	C-N-CA	6.25	131.15	120.72
1	A	86	LYS	CA-C-O	6.22	127.31	120.71
1	A	325	GLU	CA-CB-CG	-6.22	101.66	114.10
1	A	98	LYS	CA-C-O	6.21	127.55	120.90
1	A	18	ILE	N-CA-C	-6.21	104.45	110.72
1	A	158	PRO	CA-N-CD	-6.21	102.81	111.50
1	A	169	VAL	CA-C-O	-6.20	113.56	120.25
1	A	292	LEU	CA-C-N	6.20	132.22	123.30
1	A	292	LEU	C-N-CA	6.20	132.22	123.30
1	A	121	GLU	CB-CG-CD	-6.19	102.08	112.60
1	A	231	ASN	N-CA-C	-6.19	101.78	110.50
1	A	27	LYS	CA-C-O	6.19	129.02	121.72
1	A	133	ARG	O-C-N	-6.18	115.56	122.12
1	A	138	LYS	CA-C-O	-6.18	113.38	120.24
1	A	225	GLY	O-C-N	-6.17	114.68	122.70
1	A	167	ALA	CA-C-N	-6.17	110.19	120.68
1	A	167	ALA	C-N-CA	-6.17	110.19	120.68
1	A	274	GLN	CG-CD-NE2	6.14	125.61	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	92	PRO	CB-CA-C	-6.11	102.98	110.98
1	A	32	ALA	CB-CA-C	6.10	120.95	111.13
1	A	84	TYR	N-CA-CB	-6.10	101.27	110.91
1	A	113	VAL	CG1-CB-CG2	-6.10	97.39	110.80
1	A	219	HIS	ND1-CE1-NE2	-6.08	102.32	108.40
1	A	155	GLU	N-CA-CB	6.05	119.11	110.16
1	A	362	ALA	N-CA-CB	6.05	120.71	110.49
1	A	200	ARG	CD-NE-CZ	-6.04	115.94	124.40
1	A	173	TYR	CA-C-N	6.03	128.28	120.44
1	A	173	TYR	C-N-CA	6.03	128.28	120.44
1	A	217	SER	O-C-N	-6.03	114.25	122.33
1	A	213	TYR	CA-CB-CG	-6.03	103.05	113.90
1	A	302	GLY	CA-C-N	6.02	128.66	120.54
1	A	302	GLY	C-N-CA	6.02	128.66	120.54
1	A	313	TRP	CA-C-N	6.02	131.24	120.77
1	A	313	TRP	C-N-CA	6.02	131.24	120.77
1	A	44	GLN	CA-CB-CG	6.01	126.12	114.10
1	A	153	ILE	CA-CB-CG2	-6.01	100.28	110.50
1	A	83	LEU	CA-C-N	-6.00	113.59	122.83
1	A	83	LEU	C-N-CA	-6.00	113.59	122.83
1	A	168	ASN	CB-CG-OD1	-5.99	108.81	120.80
1	A	254	THR	CA-C-N	-5.97	112.20	120.38
1	A	254	THR	C-N-CA	-5.97	112.20	120.38
1	A	213	TYR	CA-C-N	-5.96	112.30	120.28
1	A	213	TYR	C-N-CA	-5.96	112.30	120.28
1	A	256	LEU	O-C-N	-5.95	114.46	122.43
1	A	326	GLU	O-C-N	5.94	128.21	122.03
1	A	261	PRO	CA-C-O	5.93	129.16	120.56
1	A	17	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	152	LYS	CA-C-N	-5.93	115.31	122.90
1	A	152	LYS	C-N-CA	-5.93	115.31	122.90
1	A	32	ALA	O-C-N	-5.93	114.61	122.20
1	A	175	SER	CA-C-N	5.92	128.14	120.56
1	A	175	SER	C-N-CA	5.92	128.14	120.56
1	A	189	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	208	VAL	CG1-CB-CG2	-5.91	97.80	110.80
1	A	8	THR	O-C-N	-5.90	115.38	120.99
1	A	81	GLU	CG-CD-OE2	5.89	131.95	118.40
1	A	115	LEU	CD1-CG-CD2	5.89	123.76	110.80
1	A	261	PRO	N-CA-C	5.89	117.88	110.70
1	A	220	HIS	CA-C-N	-5.89	113.08	122.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	220	HIS	C-N-CA	-5.89	113.08	122.50
1	A	19	ALA	CA-C-N	5.88	128.16	120.28
1	A	19	ALA	C-N-CA	5.88	128.16	120.28
1	A	46	ILE	CB-CG1-CD1	5.87	126.12	113.80
1	A	297	LEU	CD1-CG-CD2	-5.86	97.90	110.80
1	A	221	ILE	O-C-N	-5.86	116.03	122.83
1	A	291	LEU	O-C-N	-5.86	116.09	123.12
1	A	148	ARG	NE-CZ-NH1	5.84	127.34	121.50
1	A	93	PHE	CA-CB-CG	5.84	119.64	113.80
1	A	166	ASN	CA-C-N	5.83	128.02	120.44
1	A	166	ASN	C-N-CA	5.83	128.02	120.44
1	A	124	THR	CB-CA-C	5.83	121.21	109.38
1	A	207	LYS	CG-CD-CE	5.82	124.69	111.30
1	A	252	THR	CA-C-O	-5.82	114.67	121.07
1	A	170	LEU	O-C-N	-5.82	115.95	122.12
1	A	259	THR	CA-CB-OG1	-5.82	100.88	109.60
1	A	357	PHE	CB-CA-C	5.81	119.33	109.80
1	A	223	LEU	CA-CB-CG	5.80	136.62	116.30
1	A	81	GLU	OE1-CD-OE2	-5.80	108.98	122.90
1	A	257	ARG	NE-CZ-NH2	5.79	124.42	119.20
1	A	168	ASN	CA-C-O	5.79	126.62	119.79
1	A	248	ILE	N-CA-C	-5.79	104.71	110.62
1	A	27	LYS	N-CA-C	5.79	119.09	110.52
1	A	82	THR	N-CA-C	-5.79	105.48	112.54
1	A	333	ALA	CB-CA-C	5.79	120.39	110.79
1	A	201	CYS	O-C-N	5.77	128.24	122.12
1	A	313	TRP	CE3-CZ3-CH2	-5.75	113.62	121.10
1	A	92	PRO	O-C-N	-5.74	116.00	123.06
1	A	54	ASN	CB-CG-OD1	-5.73	109.34	120.80
1	A	224	GLU	CG-CD-OE2	5.72	131.56	118.40
1	A	48	THR	N-CA-CB	-5.72	100.65	111.00
1	A	20	HIS	O-C-N	-5.72	116.06	122.12
1	A	274	GLN	CA-C-O	5.71	127.61	121.55
1	A	303	ARG	CB-CA-C	-5.70	101.69	110.81
1	A	53	GLU	CG-CD-OE2	-5.69	105.32	118.40
1	A	268	THR	CA-CB-OG1	-5.68	101.08	109.60
1	A	306	GLN	CB-CG-CD	-5.68	102.94	112.60
1	A	295	TRP	CA-CB-CG	5.68	124.39	113.60
1	A	345	SER	CA-CB-OG	-5.68	99.75	111.10
1	A	215	ALA	CB-CA-C	5.67	119.69	110.96
1	A	94	PRO	O-C-N	-5.66	115.43	122.23
1	A	221	ILE	CA-CB-CG1	-5.66	100.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	180	ASN	CA-C-O	5.66	126.27	119.59
1	A	41	LYS	CA-CB-CG	5.65	125.41	114.10
1	A	241	GLN	OE1-CD-NE2	5.65	128.25	122.60
1	A	91	ARG	NE-CZ-NH1	-5.64	115.86	121.50
1	A	162	ALA	N-CA-CB	5.64	118.34	109.94
1	A	219	HIS	CG-ND1-CE1	5.63	118.88	109.30
1	A	257	ARG	CA-C-O	5.63	126.29	119.31
1	A	317	LYS	CB-CG-CD	5.63	124.25	111.30
1	A	44	GLN	N-CA-CB	-5.63	101.85	110.12
1	A	292	LEU	CB-CA-C	5.63	119.52	110.29
1	A	148	ARG	N-CA-C	5.62	118.98	109.76
1	A	33	ASP	OD1-CG-OD2	-5.61	109.44	122.90
1	A	318	GLU	CA-CB-CG	5.59	125.28	114.10
1	A	173	TYR	CA-C-O	5.58	126.47	120.55
1	A	58	TYR	CA-CB-CG	-5.58	103.86	113.90
1	A	158	PRO	N-CD-CG	5.58	110.49	103.80
1	A	155	GLU	CA-C-O	-5.57	114.52	120.42
1	A	223	LEU	CA-C-O	5.55	126.30	120.42
1	A	270	LEU	N-CA-CB	5.55	119.21	110.56
1	A	57	PHE	N-CA-C	-5.54	105.15	111.14
1	A	164	MET	CA-C-N	5.54	127.65	120.44
1	A	164	MET	C-N-CA	5.54	127.65	120.44
1	A	193	ASP	OD1-CG-OD2	-5.54	109.60	122.90
1	A	313	TRP	CZ3-CH2-CZ2	5.53	128.69	121.50
1	A	98	LYS	O-C-N	-5.53	116.34	122.09
1	A	35	SER	O-C-N	5.52	129.76	122.36
1	A	238	ALA	CA-C-N	5.52	129.31	121.42
1	A	238	ALA	C-N-CA	5.52	129.31	121.42
1	A	324	GLN	CG-CD-OE1	5.52	131.83	120.80
1	A	359	SER	CA-C-O	-5.51	115.70	120.88
1	A	120	GLY	N-CA-C	5.50	122.90	115.32
1	A	322	ALA	CA-C-O	-5.49	113.89	120.10
1	A	49	GLU	CA-C-O	5.49	127.31	121.16
1	A	347	GLN	CB-CA-C	5.47	121.31	110.42
1	A	73	ILE	CB-CA-C	5.46	117.93	111.32
1	A	143	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	15	LEU	N-CA-C	5.43	117.20	111.28
1	A	118	THR	CA-C-N	-5.43	114.17	122.21
1	A	118	THR	C-N-CA	-5.43	114.17	122.21
1	A	304	ALA	O-C-N	-5.41	115.23	122.43
1	A	39	ILE	CA-C-O	5.41	126.31	120.47
1	A	284	ASN	CB-CA-C	-5.40	101.66	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	ALA	N-CA-CB	-5.39	102.20	110.12
1	A	198	LEU	O-C-N	-5.39	116.27	122.09
1	A	230	PRO	CB-CA-C	-5.39	102.67	111.56
1	A	5	PRO	O-C-N	-5.38	115.37	122.64
1	A	317	LYS	O-C-N	-5.38	116.42	122.12
1	A	243	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	260	VAL	O-C-N	-5.37	116.73	121.61
1	A	19	ALA	N-CA-C	5.36	117.12	111.28
1	A	128	ASP	CB-CG-OD2	5.35	130.71	118.40
1	A	344	PRO	CA-C-N	5.35	131.75	121.54
1	A	344	PRO	C-N-CA	5.35	131.75	121.54
1	A	95	GLN	N-CA-C	-5.34	105.53	111.36
1	A	23	VAL	O-C-N	-5.33	115.91	122.57
1	A	343	THR	CA-C-N	-5.33	113.18	119.84
1	A	343	THR	C-N-CA	-5.33	113.18	119.84
1	A	297	LEU	CA-C-O	5.32	131.04	121.62
1	A	198	LEU	CA-C-O	5.32	126.18	120.70
1	A	267	ILE	N-CA-C	-5.32	100.72	108.17
1	A	251	ALA	N-CA-CB	5.32	117.90	109.82
1	A	21	ARG	CG-CD-NE	-5.31	100.31	112.00
1	A	274	GLN	CA-C-N	5.31	131.05	121.06
1	A	274	GLN	C-N-CA	5.31	131.05	121.06
1	A	181	GLY	N-CA-C	-5.31	105.74	114.76
1	A	357	PHE	CA-CB-CG	-5.30	108.50	113.80
1	A	120	GLY	CA-C-O	5.30	125.00	119.06
1	A	222	TYR	CA-C-N	5.30	127.81	120.29
1	A	222	TYR	C-N-CA	5.30	127.81	120.29
1	A	267	ILE	CA-CB-CG1	-5.28	101.43	110.40
1	A	8	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	174	ALA	N-CA-C	-5.25	105.45	111.07
1	A	80	HIS	CA-CB-CG	-5.24	108.56	113.80
1	A	284	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	108	VAL	CA-CB-CG2	-5.24	101.50	110.40
1	A	343	THR	N-CA-CB	5.23	120.75	110.61
1	A	141	GLY	N-CA-C	5.22	123.26	115.64
1	A	108	VAL	CB-CA-C	-5.21	102.75	111.29
1	A	133	ARG	CG-CD-NE	-5.21	100.55	112.00
1	A	252	THR	N-CA-C	5.21	117.37	111.02
1	A	14	GLU	CG-CD-OE2	5.20	130.37	118.40
1	A	319	ASN	OD1-CG-ND2	-5.20	117.40	122.60
1	A	54	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	60	GLN	CA-C-O	-5.19	115.05	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	CYS	O-C-N	-5.17	115.55	122.43
1	A	259	THR	CA-C-O	-5.17	112.03	118.54
1	A	83	LEU	CB-CG-CD1	5.17	126.20	110.70
1	A	325	GLU	CA-C-O	5.17	126.25	120.82
1	A	180	ASN	O-C-N	-5.16	116.11	122.25
1	A	267	ILE	O-C-N	-5.16	117.77	123.18
1	A	66	ASP	O-C-N	-5.15	114.99	121.74
1	A	196	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	210	ALA	N-CA-CB	-5.14	102.55	110.01
1	A	20	HIS	N-CA-C	5.13	116.88	111.28
1	A	136	GLN	CG-CD-NE2	5.13	124.10	116.40
1	A	231	ASN	CB-CG-ND2	5.13	124.10	116.40
1	A	306	GLN	N-CA-C	5.13	120.93	114.31
1	A	155	GLU	O-C-N	5.13	128.00	122.15
1	A	19	ALA	O-C-N	-5.13	116.69	122.12
1	A	237	HIS	CB-CA-C	5.12	119.29	110.79
1	A	256	LEU	N-CA-CB	-5.12	101.89	110.39
1	A	273	GLY	CA-C-O	-5.12	111.66	120.57
1	A	121	GLU	N-CA-CB	-5.08	102.16	109.83
1	A	121	GLU	CA-C-O	5.08	126.78	121.19
1	A	180	ASN	CB-CA-C	5.06	119.27	110.72
1	A	75	GLY	CA-C-N	-5.05	115.81	122.98
1	A	75	GLY	C-N-CA	-5.05	115.81	122.98
1	A	132	GLU	CA-C-O	-5.05	115.51	121.07
1	A	356	LEU	CA-C-O	5.05	127.30	121.34
1	A	330	ARG	CA-CB-CG	-5.05	104.01	114.10
1	A	179	GLN	O-C-N	-5.04	115.07	122.43
1	A	250	MET	O-C-N	5.04	127.53	122.09
1	A	104	VAL	CB-CA-C	-5.03	104.68	110.91
1	A	129	GLY	O-C-N	-5.03	116.98	122.41
1	A	71	PRO	CA-C-N	5.02	129.93	121.14
1	A	71	PRO	C-N-CA	5.02	129.93	121.14
1	A	91	ARG	CA-CB-CG	5.00	124.10	114.10

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	LYS	Mainchain
1	A	103	VAL	Mainchain
1	A	105	GLY	Mainchain
1	A	108	VAL	Mainchain

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Mol	Chain	Res	Type	Group
1	A	119	ASN	Mainchain
1	A	121	GLU	Mainchain
1	A	122	THR	Mainchain
1	A	124	THR	Mainchain
1	A	129	GLY	Mainchain
1	A	138	LYS	Mainchain
1	A	139	LYS	Mainchain
1	A	140	ASP	Mainchain
1	A	15	LEU	Mainchain
1	A	156	HIS	Mainchain
1	A	157	THR	Mainchain
1	A	164	MET	Mainchain
1	A	181	GLY	Mainchain
1	A	190	ILE	Mainchain
1	A	195	ASP	Mainchain
1	A	204	VAL	Mainchain
1	A	207	LYS	Mainchain
1	A	212	VAL	Mainchain
1	A	217	SER	Mainchain
1	A	221	ILE	Mainchain
1	A	23	VAL	Mainchain
1	A	235	PRO	Mainchain
1	A	240	THR	Mainchain
1	A	242	LYS	Mainchain
1	A	256	LEU	Mainchain
1	A	259	THR	Mainchain
1	A	260	VAL	Mainchain
1	A	262	PRO	Mainchain
1	A	264	VAL	Mainchain
1	A	266	GLY	Mainchain
1	A	272	GLY	Mainchain
1	A	279	ALA	Mainchain
1	A	281	ILE	Mainchain
1	A	282	ASN	Mainchain
1	A	287	ASN	Mainchain
1	A	290	PRO	Mainchain
1	A	292	LEU	Mainchain
1	A	301	TYR	Mainchain
1	A	307	ALA	Mainchain
1	A	314	GLY	Mainchain
1	A	330	ARG	Mainchain
1	A	331	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	A	338	CYS	Mainchain
1	A	348	ALA	Mainchain
1	A	350	ALA	Peptide
1	A	360	ASN	Mainchain
1	A	4	TYR	Mainchain
1	A	5	PRO	Mainchain
1	A	50	ASN	Mainchain
1	A	68	ARG	Mainchain
1	A	78	LEU	Peptide
1	A	8	THR	Mainchain
1	A	83	LEU	Mainchain
1	A	84	TYR	Mainchain
1	A	99	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2763	0	2783	119	0
2	A	20	0	9	9	0
All	All	2783	0	2792	121	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 22.

All (121) 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)
2:A:364:2FP:C5	2:A:364:2FP:O5	1.68	1.42
1:A:178:GLN:HE22	1:A:222:TYR:H	0.97	0.96
1:A:311:LYS:HE2	1:A:351:ALA:HB2	1.58	0.84
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.58	0.83
1:A:94:PRO:O	1:A:98:LYS:HD3	1.83	0.78
1:A:124:THR:HG21	1:A:148:ARG:O	1.83	0.76
1:A:244:SER:OG	1:A:247:GLU:HG3	1.85	0.76
1:A:250:MET:HE3	1:A:250:MET:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:VAL:O	1:A:188:PRO:HD3	1.90	0.71
1:A:118:THR:HG23	1:A:121:GLU:H	1.54	0.70
1:A:292:LEU:C	1:A:292:LEU:HD12	2.19	0.67
1:A:221:ILE:HD12	1:A:221:ILE:C	2.20	0.65
1:A:86:LYS:HA	1:A:92:PRO:HA	1.79	0.65
1:A:292:LEU:HD12	1:A:293:LYS:N	2.12	0.63
1:A:317:LYS:HG2	1:A:318:GLU:OE1	1.99	0.63
1:A:107:LYS:NZ	2:A:364:2FP:O61	2.32	0.62
1:A:267:ILE:HD11	1:A:269:PHE:CZ	2.35	0.61
1:A:267:ILE:HG12	1:A:297:LEU:HD23	1.81	0.61
1:A:216:LEU:HG	1:A:221:ILE:HG12	1.82	0.61
1:A:123:THR:HG21	1:A:165:GLU:OE2	2.00	0.61
1:A:35:SER:N	2:A:364:2FP:O61	2.34	0.61
1:A:78:LEU:O	1:A:106:ILE:HA	2.01	0.60
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.36	0.60
1:A:146:LYS:NZ	2:A:364:2FP:H4	2.18	0.59
2:A:364:2FP:C5	2:A:364:2FP:HO5	2.11	0.58
1:A:92:PRO:HB2	1:A:94:PRO:HD2	1.86	0.58
1:A:195:ASP:OD1	1:A:195:ASP:C	2.45	0.57
1:A:193:ASP:OD2	1:A:360:ASN:HB2	2.04	0.57
1:A:118:THR:CG2	1:A:121:GLU:HB2	2.36	0.56
1:A:146:LYS:HZ1	2:A:364:2FP:H4	1.71	0.56
1:A:277:GLU:HG2	1:A:330:ARG:NH2	2.20	0.55
1:A:324:GLN:O	1:A:325:GLU:C	2.49	0.55
1:A:106:ILE:HD12	1:A:107:LYS:N	2.22	0.55
1:A:319:ASN:O	1:A:320:LEU:C	2.50	0.53
1:A:8:THR:O	1:A:9:PRO:C	2.51	0.53
1:A:284:ASN:ND2	1:A:288:LYS:HE2	2.22	0.53
1:A:358:VAL:HG12	1:A:359:SER:N	2.24	0.53
1:A:65:ALA:O	1:A:100:LYS:NZ	2.35	0.52
1:A:12:LYS:HG2	1:A:222:TYR:CE1	2.45	0.51
1:A:303:ARG:NH2	1:A:356:LEU:HD22	2.25	0.51
1:A:134:CYS:HB3	1:A:182:ILE:HD12	1.93	0.51
1:A:221:ILE:CD1	1:A:226:THR:HG21	2.41	0.51
1:A:178:GLN:HE22	1:A:222:TYR:N	1.83	0.51
1:A:115:LEU:O	1:A:118:THR:HB	2.11	0.51
1:A:44:GLN:O	1:A:45:SER:C	2.50	0.50
1:A:241:GLN:HB3	1:A:243:PHE:CE2	2.47	0.50
1:A:8:THR:O	1:A:11:GLN:N	2.45	0.50
1:A:283:LEU:CD2	1:A:299:PHE:HB3	2.42	0.50
1:A:60:GLN:OE1	1:A:87:ALA:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:TYR:OH	1:A:306:GLN:NE2	2.34	0.49
1:A:98:LYS:HD2	1:A:104:VAL:HG23	1.94	0.49
1:A:254:THR:O	1:A:255:ALA:C	2.50	0.49
1:A:221:ILE:HD11	1:A:226:THR:HG21	1.96	0.48
1:A:267:ILE:O	1:A:267:ILE:HG13	2.09	0.48
1:A:21:ARG:O	1:A:22:ILE:C	2.53	0.48
1:A:172:ARG:HH11	1:A:172:ARG:HD2	1.31	0.48
1:A:12:LYS:HG2	1:A:222:TYR:CZ	2.49	0.48
1:A:359:SER:OG	1:A:361:HIS:HB2	2.13	0.48
1:A:24:ALA:O	1:A:25:PRO:C	2.56	0.48
1:A:330:ARG:HD3	1:A:330:ARG:HA	1.46	0.48
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.49	0.47
1:A:321:LYS:O	1:A:322:ALA:C	2.54	0.47
1:A:66:ASP:OD1	1:A:68:ARG:HD3	2.15	0.47
1:A:303:ARG:CZ	1:A:356:LEU:HD22	2.45	0.47
1:A:244:SER:OG	1:A:247:GLU:CG	2.61	0.46
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.50	0.46
1:A:211:ALA:O	1:A:212:VAL:C	2.57	0.46
1:A:221:ILE:HD12	1:A:222:TYR:N	2.30	0.46
1:A:311:LYS:HE2	1:A:351:ALA:CB	2.37	0.46
1:A:271:SER:N	2:A:364:2FP:O11	2.46	0.46
1:A:217:SER:O	1:A:218:ASP:C	2.58	0.46
1:A:66:ASP:OD2	1:A:68:ARG:NH1	2.48	0.45
1:A:344:PRO:O	1:A:345:SER:C	2.59	0.45
1:A:283:LEU:HD22	1:A:299:PHE:HB3	1.98	0.45
1:A:276:GLU:HB2	1:A:352:ALA:HA	1.98	0.45
1:A:115:LEU:HD22	1:A:122:THR:O	2.16	0.45
1:A:267:ILE:HD11	1:A:269:PHE:CE2	2.52	0.45
1:A:187:GLU:HG3	1:A:229:LYS:O	2.17	0.45
1:A:267:ILE:HD11	1:A:269:PHE:CE1	2.51	0.45
1:A:70:ASN:ND2	1:A:100:LYS:HB3	2.31	0.44
1:A:105:GLY:HA2	1:A:144:PHE:O	2.18	0.44
1:A:59:ARG:HG2	1:A:82:THR:HG21	1.99	0.44
1:A:120:GLY:O	1:A:152:LYS:HE2	2.18	0.44
1:A:34:GLU:HA	2:A:364:2FP:O61	2.18	0.44
1:A:118:THR:HG23	1:A:121:GLU:N	2.29	0.44
1:A:21:ARG:HH11	1:A:21:ARG:HD2	1.38	0.43
1:A:274:GLN:HB3	1:A:278:GLU:HB3	2.00	0.43
1:A:53:GLU:O	1:A:54:ASN:C	2.59	0.43
1:A:8:THR:HG23	1:A:11:GLN:OE1	2.18	0.43
1:A:12:LYS:HG2	1:A:222:TYR:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD22	1:A:186:VAL:HG13	2.01	0.43
1:A:306:GLN:O	1:A:307:ALA:C	2.61	0.43
1:A:118:THR:HG21	1:A:121:GLU:HB2	2.01	0.42
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.89	0.42
1:A:224:GLU:HG3	1:A:263:ALA:O	2.19	0.42
1:A:193:ASP:OD1	1:A:193:ASP:N	2.29	0.42
1:A:276:GLU:OE1	1:A:352:ALA:HA	2.19	0.42
1:A:277:GLU:HG2	1:A:330:ARG:HH22	1.81	0.42
1:A:359:SER:C	1:A:361:HIS:H	2.25	0.42
1:A:349:GLY:O	1:A:350:ALA:CB	2.67	0.42
1:A:298:THR:OG1	1:A:299:PHE:N	2.47	0.42
1:A:13:LYS:O	1:A:13:LYS:HD2	2.19	0.42
1:A:212:VAL:O	1:A:216:LEU:HB2	2.20	0.42
1:A:191:LEU:HD13	1:A:360:ASN:HB3	2.02	0.41
1:A:147:TRP:HB3	1:A:173:TYR:CE2	2.55	0.41
1:A:70:ASN:HD21	1:A:100:LYS:HB3	1.86	0.41
1:A:271:SER:HB3	2:A:364:2FP:O11	2.21	0.41
1:A:46:ILE:HB	1:A:314:GLY:HA2	2.02	0.41
1:A:27:LYS:HD3	1:A:71:PRO:O	2.21	0.41
1:A:39:ILE:HG21	1:A:55:ARG:HD2	2.01	0.41
1:A:70:ASN:ND2	1:A:100:LYS:HE3	2.36	0.41
1:A:344:PRO:O	1:A:347:GLN:HB2	2.20	0.41
1:A:68:ARG:CZ	1:A:328:VAL:HG11	2.51	0.40
1:A:151:LEU:HD12	1:A:151:LEU:N	2.36	0.40
1:A:183:VAL:HA	1:A:184:PRO:HD3	1.83	0.40
1:A:310:LEU:O	1:A:311:LYS:C	2.61	0.40
1:A:3:GLN:H	1:A:3:GLN:HG3	1.15	0.40
1:A:95:GLN:O	1:A:96:VAL:C	2.62	0.40
1:A:161:LEU:O	1:A:162:ALA:C	2.64	0.40
1:A:202:GLN:HB2	1:A:233:VAL:HG11	2.03	0.40
1:A:303:ARG:CZ	1:A:356:LEU:HB3	2.52	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	352/363 (97%)	315 (90%)	29 (8%)	8 (2%)	5	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	SER
1	A	350	ALA
1	A	361	HIS
1	A	362	ALA
1	A	347	GLN
1	A	344	PRO
1	A	349	GLY
1	A	230	PRO

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	291/291 (100%)	238 (82%)	53 (18%)	2	6

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	13	LYS
1	A	16	SER
1	A	27	LYS
1	A	30	LEU
1	A	41	LYS
1	A	44	GLN
1	A	59	ARG
1	A	61	LEU
1	A	69	VAL
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	83	LEU
1	A	91	ARG
1	A	98	LYS
1	A	100	LYS
1	A	106	ILE
1	A	107	LYS
1	A	109	ASP
1	A	115	LEU
1	A	118	THR
1	A	123	THR
1	A	124	THR
1	A	139	LYS
1	A	146	LYS
1	A	152	LYS
1	A	164	MET
1	A	165	GLU
1	A	169	VAL
1	A	185	ILE
1	A	193	ASP
1	A	207	LYS
1	A	214	LYS
1	A	216	LEU
1	A	221	ILE
1	A	240	THR
1	A	241	GLN
1	A	247	GLU
1	A	267	ILE
1	A	270	LEU
1	A	271	SER
1	A	280	SER
1	A	287	ASN
1	A	292	LEU
1	A	293	LYS
1	A	295	TRP
1	A	303	ARG
1	A	308	SER
1	A	316	LYS
1	A	317	LYS
1	A	318	GLU
1	A	326	GLU
1	A	329	LYS
1	A	355	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	119	ASN
1	A	178	GLN
1	A	245	HIS
1	A	287	ASN
1	A	306	GLN
1	A	339	GLN
1	A	347	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2FP	A	364	-	19,19,19	7.35	16 (84%)	21,28,28	4.56	11 (52%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FP	A	364	-	-	15/24/24/24	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	364	2FP	O2-C2	20.46	1.55	1.21
2	A	364	2FP	O5-C5	11.97	1.68	1.43
2	A	364	2FP	O1-C1	-10.08	1.33	1.43
2	A	364	2FP	O3-C3	8.67	1.59	1.42
2	A	364	2FP	C6-C5	7.79	1.62	1.51
2	A	364	2FP	P6-O63	6.71	1.71	1.50
2	A	364	2FP	P1-O11	6.30	1.70	1.50
2	A	364	2FP	P6-O62	5.14	1.73	1.54
2	A	364	2FP	C1-C2	-4.96	1.43	1.51
2	A	364	2FP	C5-C4	4.90	1.62	1.53
2	A	364	2FP	P1-O12	4.16	1.70	1.54
2	A	364	2FP	P1-O13	3.39	1.67	1.54
2	A	364	2FP	P6-O6	3.18	1.70	1.60
2	A	364	2FP	P1-O1	3.17	1.70	1.60
2	A	364	2FP	O4-C4	2.91	1.50	1.43
2	A	364	2FP	P6-O61	2.16	1.62	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	364	2FP	C5-C4-C3	12.33	132.28	112.05
2	A	364	2FP	O61-P6-O6	10.34	133.62	106.67
2	A	364	2FP	O4-C4-C5	-8.46	89.70	108.93
2	A	364	2FP	O4-C4-C3	-5.56	99.31	109.29
2	A	364	2FP	O5-C5-C6	4.12	119.07	109.99
2	A	364	2FP	O13-P1-O1	3.41	115.55	106.67
2	A	364	2FP	O3-C3-C4	3.14	117.19	110.38
2	A	364	2FP	O1-P1-O11	2.73	113.82	106.44
2	A	364	2FP	O61-P6-O63	-2.70	100.31	110.83
2	A	364	2FP	O13-P1-O11	-2.39	101.54	110.83
2	A	364	2FP	O62-P6-O61	-2.19	99.58	107.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

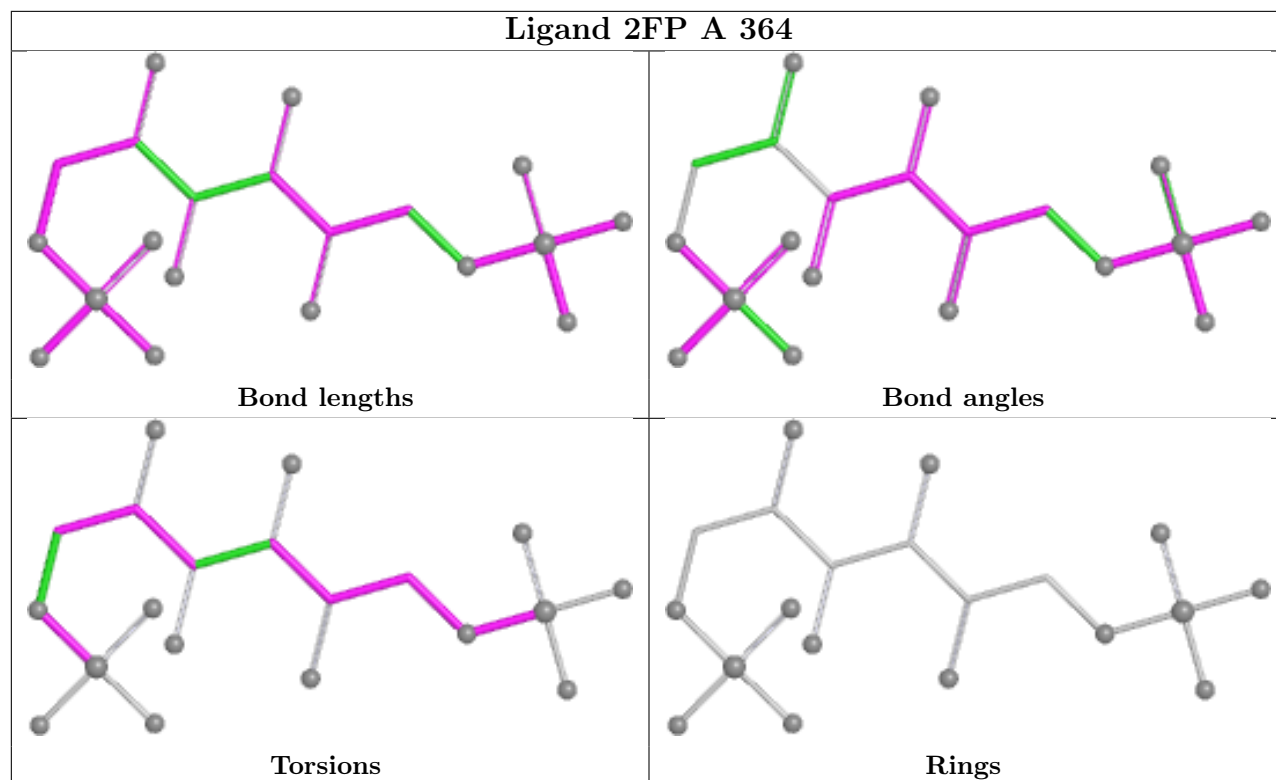
Mol	Chain	Res	Type	Atoms
2	A	364	2FP	C6-O6-P6-O61
2	A	364	2FP	O5-C5-C6-O6
2	A	364	2FP	C4-C5-C6-O6
2	A	364	2FP	O4-C4-C5-C6
2	A	364	2FP	C3-C4-C5-C6
2	A	364	2FP	O4-C4-C5-O5
2	A	364	2FP	O2-C2-C3-O3
2	A	364	2FP	C1-O1-P1-O11
2	A	364	2FP	C1-O1-P1-O12
2	A	364	2FP	C1-O1-P1-O13
2	A	364	2FP	C3-C4-C5-O5
2	A	364	2FP	C5-C6-O6-P6
2	A	364	2FP	C6-O6-P6-O62
2	A	364	2FP	C6-O6-P6-O63
2	A	364	2FP	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	364	2FP	9	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.