



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:16 AM UTC

PDB ID : 3MBP / pdb_00003mbp
Title : MALTODEXTRIN-BINDING PROTEIN WITH BOUND MALTOTRIOSE
Authors : Spurlino, J.C.; Quioco, F.A.
Deposited on : 1997-06-25
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

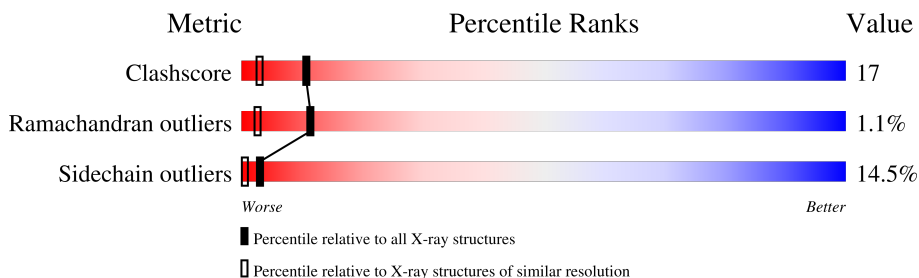
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)

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	370	
2	B	3	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3156 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 MALTODEXTRIN-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2878	1853	469	550	6			

- Molecule 2 is an oligosaccharide called alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	3	Total	C	O	0	0	0
			34	18	16			

- Molecule 3 is water.

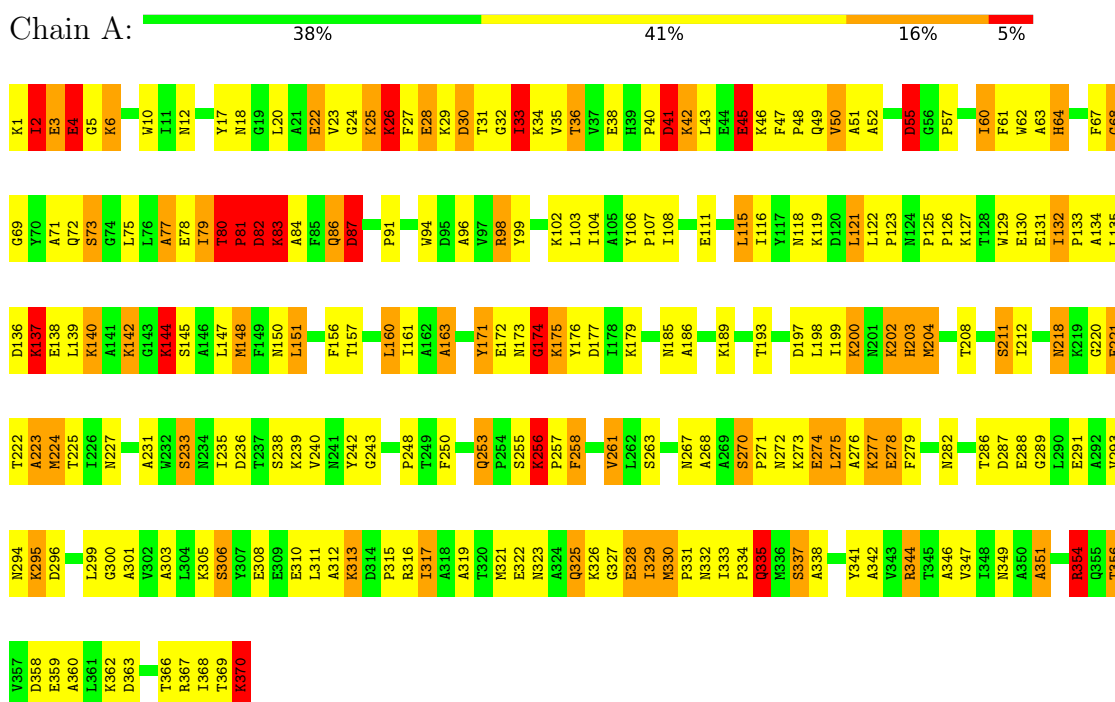
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		

3 Residue-property plots

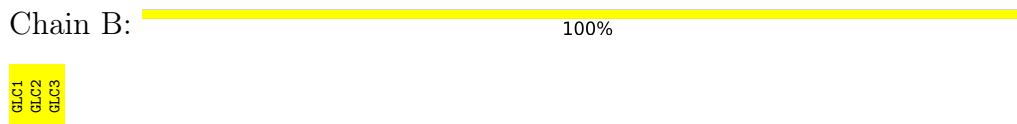
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose



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	106.07Å 68.43Å 57.94Å 90.00° 112.51° 90.00°	Depositor
Resolution (Å)	10.00 – 1.70	Depositor
% Data completeness (in resolution range)	75.0 (10.00-1.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3156	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: GLC

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	1.98	57/2947 (1.9%)	2.89	310/3998 (7.8%)

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	2

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	LYS	C-OXT	29.76	1.83	1.23
1	A	4	GLU	C-N	8.22	1.46	1.33
1	A	173	ASN	N-CA	7.04	1.55	1.46
1	A	193	THR	C-N	-7.02	1.24	1.33
1	A	129	TRP	N-CA	-6.89	1.37	1.46
1	A	289	GLY	CA-C	6.85	1.59	1.52
1	A	151	LEU	C-N	-6.84	1.23	1.33
1	A	356	THR	C-N	-6.79	1.25	1.33
1	A	238	SER	CB-OG	6.65	1.55	1.42
1	A	116	ILE	N-CA	6.63	1.54	1.46
1	A	330	MET	SD-CE	-6.53	1.63	1.79
1	A	22	GLU	CA-CB	-6.45	1.42	1.53
1	A	163	ALA	C-N	-6.44	1.24	1.33
1	A	258	PHE	C-O	6.44	1.31	1.23
1	A	233	SER	N-CA	6.39	1.54	1.46
1	A	300	GLY	N-CA	6.33	1.54	1.45
1	A	329	ILE	CA-CB	6.33	1.61	1.54
1	A	238	SER	CA-CB	6.22	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	HIS	CD2-NE2	-6.08	1.31	1.37
1	A	212	ILE	C-N	6.03	1.41	1.33
1	A	338	ALA	N-CA	-5.99	1.39	1.46
1	A	107	PRO	C-O	5.92	1.30	1.23
1	A	204	MET	SD-CE	5.82	1.94	1.79
1	A	175	LYS	N-CA	-5.81	1.38	1.46
1	A	63	ALA	CA-C	5.78	1.60	1.52
1	A	327	GLY	C-N	-5.71	1.24	1.33
1	A	137	LYS	C-O	5.70	1.30	1.24
1	A	83	LYS	C-N	-5.67	1.25	1.33
1	A	172	GLU	CA-C	-5.66	1.45	1.52
1	A	111	GLU	CA-C	-5.61	1.46	1.52
1	A	147	LEU	CA-CB	5.57	1.63	1.53
1	A	144	LYS	C-O	5.55	1.31	1.23
1	A	23	VAL	C-N	-5.54	1.27	1.34
1	A	137	LYS	N-CA	5.53	1.53	1.46
1	A	296	ASP	C-O	5.49	1.30	1.24
1	A	212	ILE	CA-CB	5.48	1.60	1.54
1	A	161	ILE	CA-CB	5.48	1.61	1.54
1	A	130	GLU	C-N	-5.47	1.25	1.33
1	A	193	THR	C-O	5.44	1.30	1.24
1	A	242	TYR	N-CA	5.42	1.52	1.45
1	A	108	ILE	CA-CB	5.41	1.62	1.55
1	A	366	THR	CA-CB	5.40	1.61	1.53
1	A	300	GLY	CA-C	5.39	1.59	1.51
1	A	248	PRO	C-O	5.37	1.30	1.23
1	A	132	ILE	CA-CB	5.36	1.61	1.54
1	A	161	ILE	C-O	5.35	1.30	1.24
1	A	3	GLU	N-CA	5.32	1.53	1.46
1	A	306	SER	N-CA	5.28	1.52	1.46
1	A	118	ASN	N-CA	5.27	1.52	1.46
1	A	323	ASN	C-O	-5.26	1.17	1.24
1	A	322	GLU	N-CA	-5.22	1.40	1.46
1	A	231	ALA	C-O	5.12	1.30	1.24
1	A	299	LEU	C-O	5.09	1.30	1.24
1	A	346	ALA	CA-C	-5.09	1.46	1.52
1	A	225	THR	C-N	-5.08	1.27	1.33
1	A	301	ALA	N-CA	5.07	1.52	1.46
1	A	156	PHE	CA-CB	5.01	1.61	1.53

All (310) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ASP	CA-CB-CG	30.64	143.24	112.60
1	A	354	ARG	CD-NE-CZ	27.12	162.37	124.40
1	A	22	GLU	CA-CB-CG	26.93	167.95	114.10
1	A	291	GLU	CA-C-N	13.27	137.70	120.44
1	A	291	GLU	C-N-CA	13.27	137.70	120.44
1	A	35	VAL	CA-C-O	-12.50	107.27	120.39
1	A	326	LYS	CA-C-N	12.41	134.56	122.27
1	A	326	LYS	C-N-CA	12.41	134.56	122.27
1	A	238	SER	CA-CB-OG	-11.81	87.49	111.10
1	A	310	GLU	CB-CG-CD	11.34	131.88	112.60
1	A	142	LYS	CA-CB-CG	11.28	136.66	114.10
1	A	29	LYS	N-CA-C	-11.26	98.81	112.54
1	A	78	GLU	CA-C-N	-10.93	105.04	122.64
1	A	78	GLU	C-N-CA	-10.93	105.04	122.64
1	A	344	ARG	CD-NE-CZ	-10.71	109.40	124.40
1	A	163	ALA	CA-C-O	-10.70	109.45	120.90
1	A	328	GLU	CA-CB-CG	10.61	135.31	114.10
1	A	227	ASN	OD1-CG-ND2	-10.52	112.08	122.60
1	A	274	GLU	CB-CG-CD	10.44	130.35	112.60
1	A	278	GLU	CA-CB-CG	10.26	134.62	114.10
1	A	218	ASN	OD1-CG-ND2	-10.09	112.51	122.60
1	A	325	GLN	OE1-CD-NE2	9.99	132.59	122.60
1	A	311	LEU	CA-C-N	9.86	136.50	120.63
1	A	311	LEU	C-N-CA	9.86	136.50	120.63
1	A	344	ARG	NE-CZ-NH1	-9.64	111.86	121.50
1	A	50	VAL	CA-C-O	-9.43	110.29	120.47
1	A	291	GLU	CA-CB-CG	9.38	132.86	114.10
1	A	119	LYS	O-C-N	9.37	133.18	122.22
1	A	347	VAL	CA-C-O	-9.27	110.76	121.05
1	A	118	ASN	OD1-CG-ND2	9.26	131.85	122.60
1	A	325	GLN	CA-C-N	9.12	137.11	121.14
1	A	325	GLN	C-N-CA	9.12	137.11	121.14
1	A	84	ALA	N-CA-C	-9.07	100.33	111.40
1	A	38	GLU	CA-C-O	-9.01	110.92	121.46
1	A	84	ALA	CA-C-O	-8.99	110.93	120.55
1	A	148	MET	O-C-N	8.98	134.32	123.36
1	A	276	ALA	CA-C-O	8.88	130.14	120.82
1	A	177	ASP	O-C-N	-8.69	112.50	122.93
1	A	204	MET	N-CA-CB	8.70	126.18	111.66
1	A	185	ASN	CA-CB-CG	8.52	121.12	112.60
1	A	145	SER	CA-C-O	-8.43	111.59	121.46
1	A	253	GLN	CB-CG-CD	-8.43	98.26	112.60
1	A	211	SER	CA-CB-OG	-8.38	94.34	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	TYR	CA-C-O	-8.35	110.26	119.61
1	A	256	LYS	CA-CB-CG	8.29	130.68	114.10
1	A	29	LYS	CA-C-N	-8.14	109.71	122.49
1	A	29	LYS	C-N-CA	-8.14	109.71	122.49
1	A	33	ILE	CB-CA-C	8.08	120.93	110.91
1	A	121	LEU	N-CA-CB	-8.07	98.23	110.33
1	A	289	GLY	CA-C-O	-8.07	111.86	120.90
1	A	204	MET	O-C-N	8.06	132.43	123.25
1	A	67	PHE	N-CA-C	8.05	120.14	111.36
1	A	337	SER	CA-C-N	8.00	131.00	120.28
1	A	337	SER	C-N-CA	8.00	131.00	120.28
1	A	172	GLU	CB-CG-CD	7.98	126.17	112.60
1	A	321	MET	O-C-N	-7.98	113.66	122.12
1	A	272	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	A	323	ASN	CA-C-O	-7.95	111.99	120.42
1	A	49	GLN	OE1-CD-NE2	7.93	130.53	122.60
1	A	344	ARG	NE-CZ-NH2	7.90	126.31	119.20
1	A	370	LYS	N-CA-CB	7.87	123.87	110.50
1	A	204	MET	CA-CB-CG	7.80	129.69	114.10
1	A	354	ARG	NE-CZ-NH1	7.78	129.28	121.50
1	A	311	LEU	N-CA-C	7.75	119.81	111.36
1	A	331	PRO	O-C-N	-7.75	113.55	123.00
1	A	86	GLN	OE1-CD-NE2	7.73	130.33	122.60
1	A	142	LYS	CB-CA-C	7.71	123.75	110.72
1	A	25	LYS	CA-C-N	-7.63	110.44	122.73
1	A	25	LYS	C-N-CA	-7.63	110.44	122.73
1	A	325	GLN	CB-CG-CD	-7.61	99.67	112.60
1	A	60	ILE	CA-C-O	7.53	128.29	120.39
1	A	49	GLN	CB-CG-CD	-7.51	99.83	112.60
1	A	250	PHE	CA-C-O	-7.48	111.07	120.20
1	A	98	ARG	NE-CZ-NH2	7.45	125.90	119.20
1	A	27	PHE	N-CA-C	-7.44	101.33	112.04
1	A	176	TYR	CA-C-O	-7.43	112.14	120.54
1	A	151	LEU	CA-C-N	7.42	134.13	121.14
1	A	151	LEU	C-N-CA	7.42	134.13	121.14
1	A	122	LEU	CA-C-N	7.41	127.28	119.05
1	A	122	LEU	C-N-CA	7.41	127.28	119.05
1	A	83	LYS	O-C-N	-7.39	113.77	122.20
1	A	367	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	A	267	ASN	CA-CB-CG	7.36	119.96	112.60
1	A	6	LYS	CA-CB-CG	7.36	128.81	114.10
1	A	98	ARG	NE-CZ-NH1	-7.33	114.17	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	SER	CB-CA-C	7.32	122.94	110.79
1	A	360	ALA	CA-C-O	-7.25	112.73	120.42
1	A	142	LYS	O-C-N	-7.24	113.64	122.25
1	A	303	ALA	CA-C-O	-7.21	111.29	119.79
1	A	51	ALA	O-C-N	7.17	130.61	122.22
1	A	358	ASP	CA-C-O	-7.16	113.31	120.82
1	A	30	ASP	CB-CA-C	7.15	122.60	111.02
1	A	18	ASN	CA-C-N	7.14	127.91	119.98
1	A	18	ASN	C-N-CA	7.14	127.91	119.98
1	A	38	GLU	O-C-N	7.07	132.58	123.11
1	A	12	ASN	CA-CB-CG	-7.06	105.54	112.60
1	A	30	ASP	CA-C-O	-7.06	111.41	119.95
1	A	102	LYS	CB-CA-C	-7.04	97.65	109.48
1	A	275	LEU	O-C-N	7.04	130.18	122.15
1	A	294	ASN	CA-C-N	7.01	129.67	120.28
1	A	294	ASN	C-N-CA	7.01	129.67	120.28
1	A	315	PRO	O-C-N	7.01	131.26	122.22
1	A	115	LEU	O-C-N	-6.98	115.11	123.13
1	A	176	TYR	O-C-N	6.97	131.17	123.22
1	A	300	GLY	O-C-N	6.94	131.73	122.70
1	A	22	GLU	CG-CD-OE1	-6.87	102.59	118.40
1	A	87	ASP	O-C-N	6.86	131.93	122.46
1	A	208	THR	CA-CB-OG1	-6.85	99.33	109.60
1	A	278	GLU	CB-CG-CD	6.83	124.21	112.60
1	A	62	TRP	O-C-N	-6.83	116.46	123.29
1	A	312	ALA	CA-C-N	6.83	132.29	120.68
1	A	312	ALA	C-N-CA	6.83	132.29	120.68
1	A	67	PHE	CA-C-O	-6.82	113.19	120.42
1	A	349	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	A	2	ILE	CB-CA-C	6.78	121.87	110.95
1	A	104	ILE	CA-CB-CG1	-6.77	98.89	110.40
1	A	45	GLU	CA-C-O	6.75	127.03	119.41
1	A	94	TRP	N-CA-C	-6.70	104.58	112.89
1	A	51	ALA	CA-C-N	6.64	129.18	120.28
1	A	51	ALA	C-N-CA	6.64	129.18	120.28
1	A	125	PRO	O-C-N	-6.64	113.62	121.46
1	A	27	PHE	CA-C-N	6.63	130.40	120.31
1	A	27	PHE	C-N-CA	6.63	130.40	120.31
1	A	49	GLN	N-CA-CB	6.63	119.59	109.98
1	A	222	THR	CA-CB-OG1	-6.63	99.66	109.60
1	A	80	THR	O-C-N	6.61	126.56	121.27
1	A	366	THR	CA-CB-OG1	-6.60	99.70	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	LEU	N-CA-C	6.57	119.99	108.75
1	A	25	LYS	N-CA-C	-6.57	104.20	111.36
1	A	31	THR	N-CA-CB	6.56	121.58	110.49
1	A	308	GLU	CA-C-O	6.53	127.47	120.10
1	A	257	PRO	O-C-N	6.51	131.07	123.06
1	A	301	ALA	O-C-N	-6.51	115.01	123.02
1	A	175	LYS	CB-CA-C	-6.50	96.48	109.35
1	A	277	LYS	CA-CB-CG	6.49	127.08	114.10
1	A	69	GLY	O-C-N	-6.45	116.00	122.19
1	A	218	ASN	O-C-N	6.45	130.21	122.27
1	A	142	LYS	N-CA-CB	-6.44	100.74	110.73
1	A	63	ALA	N-CA-CB	6.42	119.48	110.04
1	A	175	LYS	CA-CB-CG	6.42	126.94	114.10
1	A	276	ALA	O-C-N	-6.42	115.46	122.07
1	A	282	ASN	CB-CG-ND2	-6.42	106.77	116.40
1	A	250	PHE	O-C-N	6.34	131.40	123.28
1	A	174	GLY	O-C-N	6.33	130.93	122.70
1	A	24	GLY	O-C-N	6.32	129.61	122.34
1	A	139	LEU	CA-C-O	-6.32	113.72	120.42
1	A	99	TYR	O-C-N	6.32	131.46	123.12
1	A	255	SER	N-CA-C	-6.30	101.10	110.23
1	A	197	ASP	CA-C-O	-6.29	113.88	120.55
1	A	367	ARG	CA-C-N	6.28	129.34	120.42
1	A	367	ARG	C-N-CA	6.28	129.34	120.42
1	A	306	SER	CA-C-O	-6.27	114.24	120.82
1	A	91	PRO	CB-CA-C	6.23	122.90	112.62
1	A	68	GLY	N-CA-C	-6.17	105.33	112.73
1	A	125	PRO	CB-CA-C	6.16	118.43	110.92
1	A	225	THR	O-C-N	-6.15	115.21	122.96
1	A	177	ASP	CA-CB-CG	-6.15	106.45	112.60
1	A	317	ILE	CA-C-O	6.12	127.34	120.85
1	A	368	ILE	O-C-N	6.12	128.13	121.83
1	A	72	GLN	CA-C-N	6.10	134.13	121.94
1	A	72	GLN	C-N-CA	6.10	134.13	121.94
1	A	253	GLN	O-C-N	6.09	128.58	121.39
1	A	42	LYS	CB-CA-C	-6.08	102.92	111.80
1	A	256	LYS	CB-CA-C	-6.04	101.42	110.97
1	A	329	ILE	N-CA-CB	6.04	117.73	110.31
1	A	351	ALA	CA-C-O	6.00	126.87	119.97
1	A	306	SER	O-C-N	6.00	128.25	122.07
1	A	363	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	174	GLY	N-CA-C	-5.99	99.00	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	49	GLN	CA-C-O	-5.97	114.75	120.90
1	A	63	ALA	N-CA-C	-5.95	102.26	110.35
1	A	41	ASP	CA-CB-CG	-5.95	106.65	112.60
1	A	369	THR	CA-C-N	5.94	132.39	121.70
1	A	369	THR	C-N-CA	5.94	132.39	121.70
1	A	78	GLU	O-C-N	5.92	130.21	122.93
1	A	41	ASP	OD1-CG-OD2	5.88	137.00	122.90
1	A	317	ILE	CB-CA-C	5.88	120.33	112.22
1	A	137	LYS	N-CA-CB	5.87	118.75	110.12
1	A	356	THR	CA-C-N	5.86	128.16	120.60
1	A	356	THR	C-N-CA	5.86	128.16	120.60
1	A	80	THR	CA-C-N	5.85	127.16	119.84
1	A	80	THR	C-N-CA	5.85	127.16	119.84
1	A	197	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	189	LYS	CA-C-O	-5.83	114.24	120.42
1	A	295	LYS	CB-CA-C	-5.82	101.12	110.79
1	A	6	LYS	N-CA-CB	5.82	121.05	111.62
1	A	22	GLU	N-CA-CB	5.80	119.24	110.30
1	A	119	LYS	CA-C-O	-5.78	113.56	120.10
1	A	31	THR	CA-CB-OG1	-5.78	100.93	109.60
1	A	270	SER	CA-CB-OG	5.77	122.65	111.10
1	A	163	ALA	O-C-N	5.77	128.09	122.09
1	A	172	GLU	CA-C-N	-5.77	109.34	121.80
1	A	172	GLU	C-N-CA	-5.77	109.34	121.80
1	A	179	LYS	N-CA-C	-5.76	106.29	113.38
1	A	258	PHE	CA-C-O	-5.76	114.18	120.81
1	A	221	GLU	CA-C-O	-5.76	112.33	119.18
1	A	211	SER	N-CA-C	5.75	117.22	111.07
1	A	335	GLN	CG-CD-NE2	5.75	125.02	116.40
1	A	221	GLU	CB-CG-CD	-5.74	102.84	112.60
1	A	203	HIS	CA-CB-CG	-5.74	108.06	113.80
1	A	274	GLU	CA-C-N	5.74	128.44	120.29
1	A	274	GLU	C-N-CA	5.74	128.44	120.29
1	A	366	THR	O-C-N	5.73	127.98	122.07
1	A	278	GLU	CA-C-N	5.72	128.74	120.79
1	A	278	GLU	C-N-CA	5.72	128.74	120.79
1	A	349	ASN	CA-CB-CG	5.70	118.30	112.60
1	A	257	PRO	CA-C-O	-5.69	114.72	121.67
1	A	261	VAL	CA-C-O	-5.69	114.00	120.66
1	A	186	ALA	CA-C-N	5.68	132.54	121.41
1	A	186	ALA	C-N-CA	5.68	132.54	121.41
1	A	278	GLU	CG-CD-OE1	5.67	131.44	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	ALA	N-CA-CB	5.66	118.51	110.13
1	A	236	ASP	O-C-N	5.65	128.11	122.12
1	A	135	LEU	CA-C-O	-5.65	114.44	120.42
1	A	131	GLU	CB-CG-CD	5.64	122.18	112.60
1	A	84	ALA	O-C-N	5.62	128.97	122.17
1	A	268	ALA	CA-C-N	5.62	133.18	121.94
1	A	268	ALA	C-N-CA	5.62	133.18	121.94
1	A	337	SER	O-C-N	-5.62	115.74	122.15
1	A	49	GLN	O-C-N	5.62	128.09	122.03
1	A	81	PRO	O-C-N	5.61	130.21	122.64
1	A	329	ILE	CB-CG1-CD1	5.60	125.55	113.80
1	A	64	HIS	ND1-CE1-NE2	-5.59	102.81	108.40
1	A	347	VAL	O-C-N	5.59	127.72	121.90
1	A	317	ILE	CA-CB-CG1	-5.59	100.90	110.40
1	A	193	THR	CA-C-N	5.58	127.76	120.28
1	A	193	THR	C-N-CA	5.58	127.76	120.28
1	A	34	LYS	CA-C-O	5.56	127.87	121.47
1	A	323	ASN	O-C-N	5.56	128.49	122.15
1	A	71	ALA	CA-C-O	-5.54	115.00	120.82
1	A	32	GLY	CA-C-O	5.53	124.90	119.04
1	A	131	GLU	CG-CD-OE2	5.53	131.11	118.40
1	A	312	ALA	N-CA-C	5.51	119.51	112.34
1	A	73	SER	CA-C-N	5.51	130.74	120.87
1	A	73	SER	C-N-CA	5.51	130.74	120.87
1	A	41	ASP	O-C-N	5.50	129.36	122.86
1	A	40	PRO	CA-C-O	5.50	128.83	121.95
1	A	223	ALA	CA-C-O	-5.50	113.64	119.97
1	A	174	GLY	CA-C-N	5.50	131.63	122.73
1	A	174	GLY	C-N-CA	5.50	131.63	122.73
1	A	177	ASP	CB-CG-OD1	5.49	131.04	118.40
1	A	223	ALA	O-C-N	5.49	129.02	122.27
1	A	35	VAL	O-C-N	5.48	129.18	123.26
1	A	349	ASN	CA-C-O	-5.47	115.08	120.82
1	A	26	LYS	CB-CA-C	5.46	119.94	110.94
1	A	286	THR	CA-C-N	5.44	127.57	120.28
1	A	286	THR	C-N-CA	5.44	127.57	120.28
1	A	286	THR	CA-C-O	-5.44	115.27	121.58
1	A	150	ASN	OD1-CG-ND2	-5.41	117.19	122.60
1	A	218	ASN	CA-C-O	-5.41	113.75	119.97
1	A	319	ALA	O-C-N	5.41	128.92	122.27
1	A	17	TYR	CA-C-O	-5.40	113.76	119.97
1	A	171	TYR	CA-CB-CG	-5.40	104.19	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	282	ASN	CA-C-O	-5.40	113.00	119.15
1	A	55	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	142	LYS	CA-C-O	5.37	125.92	119.59
1	A	31	THR	CA-C-N	5.36	131.15	122.09
1	A	31	THR	C-N-CA	5.36	131.15	122.09
1	A	123	PRO	O-C-N	5.35	128.65	122.23
1	A	18	ASN	CA-C-O	-5.34	114.76	120.42
1	A	200	LYS	CA-CB-CG	-5.34	103.43	114.10
1	A	123	PRO	CA-C-N	-5.33	112.57	122.06
1	A	123	PRO	C-N-CA	-5.33	112.57	122.06
1	A	185	ASN	CB-CA-C	5.33	120.58	110.51
1	A	208	THR	CA-C-O	-5.31	115.17	120.96
1	A	316	ARG	CA-C-O	-5.30	114.80	120.42
1	A	200	LYS	N-CA-C	-5.29	105.62	111.71
1	A	342	ALA	O-C-N	-5.28	116.52	122.12
1	A	77	ALA	CA-C-O	-5.28	115.03	121.05
1	A	224	MET	CA-C-O	5.27	127.02	121.33
1	A	319	ALA	CA-C-N	5.26	127.28	120.44
1	A	319	ALA	C-N-CA	5.26	127.28	120.44
1	A	325	GLN	CA-C-O	-5.26	114.97	120.55
1	A	36	THR	CB-CA-C	5.26	119.33	109.71
1	A	28	GLU	CA-CB-CG	5.26	124.61	114.10
1	A	129	TRP	CA-C-O	5.23	125.96	120.42
1	A	220	GLY	CA-C-O	5.20	126.20	119.44
1	A	119	LYS	CB-CA-C	-5.18	101.04	110.63
1	A	305	LYS	O-C-N	5.18	127.61	122.12
1	A	148	MET	CA-C-O	-5.17	113.92	120.28
1	A	267	ASN	OD1-CG-ND2	-5.16	117.44	122.60
1	A	293	VAL	N-CA-CB	5.15	117.16	110.57
1	A	86	GLN	CG-CD-NE2	-5.15	108.68	116.40
1	A	310	GLU	CA-CB-CG	5.14	124.38	114.10
1	A	369	THR	CA-C-O	-5.14	113.06	119.28
1	A	160	LEU	CA-CB-CG	5.13	134.26	116.30
1	A	20	LEU	CA-C-N	5.13	127.67	120.28
1	A	20	LEU	C-N-CA	5.13	127.67	120.28
1	A	107	PRO	N-CA-CB	5.12	108.10	103.34
1	A	308	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	279	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	270	SER	CA-C-O	5.10	124.47	120.19
1	A	368	ILE	CA-C-O	-5.09	115.45	120.85
1	A	240	VAL	N-CA-C	-5.08	103.04	109.80
1	A	225	THR	CA-CB-OG1	-5.08	101.98	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CB-CG-OD2	-5.08	106.72	118.40
1	A	289	GLY	O-C-N	5.07	127.06	122.19
1	A	296	ASP	CB-CA-C	5.07	120.50	110.42
1	A	325	GLN	CB-CA-C	-5.06	102.38	110.79
1	A	106	TYR	O-C-N	5.05	129.88	121.59
1	A	367	ARG	CG-CD-NE	-5.05	100.89	112.00
1	A	243	GLY	N-CA-C	-5.04	103.42	111.18
1	A	335	GLN	OE1-CD-NE2	-5.04	117.56	122.60
1	A	367	ARG	O-C-N	-5.03	116.78	122.12
1	A	242	TYR	N-CA-CB	-5.02	103.22	110.70
1	A	255	SER	CA-CB-OG	-5.02	101.06	111.10
1	A	346	ALA	O-C-N	-5.02	116.87	122.09
1	A	123	PRO	N-CD-CG	-5.01	95.68	103.20
1	A	268	ALA	O-C-N	5.01	128.08	122.22
1	A	116	ILE	CB-CA-C	5.01	118.29	110.83

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	ARG	Sidechain
1	A	4	GLU	Mainchain

5.2 Too-close contacts [i](#)

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	2878	0	2859	97	5
2	B	34	0	30	0	0
3	A	244	0	0	10	5
All	All	3156	0	2889	97	5

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 17.

All (97) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:224:MET:HE1	1.38	1.05
1:A:115:LEU:HD21	1:A:224:MET:CE	1.91	1.01
1:A:2:ILE:CD1	1:A:55:ASP:HA	1.94	0.96
1:A:43:LEU:CD1	1:A:60:ILE:HD11	1.95	0.96
1:A:171:TYR:CZ	1:A:174:GLY:HA2	2.02	0.94
1:A:171:TYR:OH	1:A:174:GLY:HA2	1.68	0.94
1:A:198:LEU:HG	3:A:508:HOH:O	1.70	0.91
1:A:26:LYS:C	1:A:26:LYS:HE3	1.96	0.90
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.74	0.87
1:A:26:LYS:HE3	1:A:26:LYS:O	1.74	0.87
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.57	0.85
1:A:2:ILE:HD11	1:A:55:ASP:C	2.01	0.84
1:A:313:LYS:HA	1:A:313:LYS:HE3	1.60	0.83
1:A:64:HIS:HD2	1:A:261:VAL:H	1.26	0.80
1:A:2:ILE:HD11	1:A:55:ASP:HA	1.62	0.79
1:A:2:ILE:HD12	1:A:55:ASP:HA	1.65	0.77
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.68	0.77
1:A:43:LEU:HD13	1:A:60:ILE:HD11	1.66	0.76
1:A:2:ILE:HD11	1:A:55:ASP:CA	2.16	0.76
1:A:157:THR:HG23	3:A:522:HOH:O	1.89	0.72
1:A:43:LEU:HD13	1:A:60:ILE:CD1	2.23	0.69
1:A:33:ILE:CD1	1:A:275:LEU:HD13	2.22	0.69
1:A:64:HIS:HE1	1:A:330:MET:O	1.75	0.68
1:A:2:ILE:CD1	1:A:55:ASP:CA	2.72	0.67
1:A:313:LYS:HA	1:A:313:LYS:CE	2.24	0.66
1:A:81:PRO:O	1:A:82:ASP:HB3	1.95	0.66
1:A:96:ALA:HB2	1:A:329:ILE:HD11	1.80	0.64
1:A:329:ILE:HG23	1:A:329:ILE:O	1.96	0.64
1:A:26:LYS:O	1:A:26:LYS:CE	2.45	0.63
1:A:48:PRO:O	1:A:52:ALA:HB2	1.99	0.63
1:A:41:ASP:O	1:A:46:LYS:HE2	1.99	0.63
1:A:171:TYR:CE1	1:A:174:GLY:HA2	2.35	0.61
1:A:115:LEU:HD21	1:A:224:MET:HE2	1.80	0.61
1:A:295:LYS:HE3	3:A:572:HOH:O	1.99	0.61
1:A:64:HIS:CD2	1:A:261:VAL:H	2.15	0.61
1:A:287:ASP:OD1	1:A:306:SER:OG	2.16	0.61
1:A:68:GLY:HA3	1:A:332:ASN:O	2.01	0.60
1:A:171:TYR:OH	1:A:174:GLY:CA	2.48	0.59
1:A:148:MET:HE3	3:A:640:HOH:O	2.01	0.59
1:A:45:GLU:OE2	1:A:341:TYR:OH	2.22	0.58
1:A:198:LEU:CG	3:A:508:HOH:O	2.38	0.57
1:A:313:LYS:CE	1:A:313:LYS:CA	2.83	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:HG2	1:A:271:PRO:HB2	1.88	0.55
1:A:10:TRP:CD2	1:A:57:PRO:HG3	2.42	0.55
1:A:28:GLU:HB2	1:A:33:ILE:O	2.06	0.54
1:A:126:PRO:HD2	1:A:224:MET:CE	2.37	0.54
1:A:136:ASP:OD2	1:A:203:HIS:CD2	2.57	0.54
1:A:144:LYS:HE2	1:A:221:GLU:HA	1.89	0.53
1:A:126:PRO:HD2	1:A:224:MET:HE1	1.89	0.53
1:A:77:ALA:HB2	1:A:273:LYS:HE3	1.91	0.53
1:A:82:ASP:OD1	1:A:82:ASP:C	2.52	0.52
1:A:115:LEU:CG	1:A:224:MET:HE2	2.40	0.51
1:A:317:ILE:HD11	3:A:428:HOH:O	2.10	0.51
1:A:96:ALA:HB2	1:A:329:ILE:CD1	2.40	0.51
1:A:132:ILE:N	1:A:133:PRO:CD	2.73	0.51
1:A:329:ILE:O	1:A:329:ILE:CG2	2.58	0.51
1:A:335:GLN:NE2	1:A:335:GLN:H	2.09	0.51
1:A:140:LYS:HA	1:A:144:LYS:O	2.11	0.50
1:A:288:GLU:CD	1:A:288:GLU:H	2.20	0.50
1:A:80:THR:HG22	1:A:80:THR:O	2.12	0.50
1:A:3:GLU:O	1:A:4:GLU:C	2.55	0.49
1:A:73:SER:HB3	3:A:470:HOH:O	2.12	0.48
1:A:163:ALA:O	1:A:256:LYS:NZ	2.46	0.48
1:A:121:LEU:HD23	1:A:223:ALA:HA	1.95	0.48
1:A:115:LEU:CD2	1:A:224:MET:HE2	2.43	0.48
1:A:83:LYS:O	1:A:83:LYS:HG3	2.12	0.47
1:A:270:SER:HA	1:A:271:PRO:HD3	1.71	0.47
1:A:332:ASN:OD1	1:A:332:ASN:C	2.58	0.46
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.81	0.45
1:A:337:SER:HB3	3:A:475:HOH:O	2.15	0.45
1:A:42:LYS:HB3	1:A:45:GLU:HG3	1.98	0.45
1:A:98:ARG:CG	1:A:98:ARG:HH11	2.29	0.45
1:A:48:PRO:HA	1:A:75:LEU:HD13	1.99	0.45
1:A:136:ASP:OD2	1:A:140:LYS:NZ	2.47	0.44
1:A:96:ALA:CB	1:A:329:ILE:HD11	2.45	0.44
1:A:200:LYS:O	1:A:202:LYS:HE3	2.18	0.44
1:A:81:PRO:HG2	1:A:86:GLN:NE2	2.32	0.44
1:A:239:LYS:HA	3:A:563:HOH:O	2.18	0.44
1:A:370:LYS:HA	1:A:370:LYS:HD3	1.45	0.44
1:A:43:LEU:HD12	1:A:60:ILE:HD11	1.92	0.44
1:A:198:LEU:CD2	3:A:508:HOH:O	2.65	0.43
1:A:43:LEU:HD12	1:A:43:LEU:C	2.44	0.43
1:A:132:ILE:N	1:A:133:PRO:HD3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:HA	1:A:140:LYS:HD3	1.78	0.42
1:A:5:GLY:C	1:A:33:ILE:HD12	2.44	0.42
1:A:47:PHE:N	1:A:48:PRO:HD2	2.34	0.42
1:A:61:PHE:HA	1:A:263:SER:O	2.20	0.42
1:A:26:LYS:HE3	1:A:26:LYS:CA	2.10	0.42
1:A:10:TRP:CG	1:A:57:PRO:HG3	2.56	0.41
1:A:83:LYS:O	1:A:87:ASP:HB2	2.21	0.41
1:A:115:LEU:HD11	1:A:224:MET:HE2	2.03	0.41
1:A:136:ASP:HB3	1:A:203:HIS:CD2	2.55	0.41
1:A:333:ILE:HA	1:A:334:PRO:HD3	1.88	0.41
1:A:134:ALA:HA	1:A:137:LYS:HG2	2.01	0.41
1:A:98:ARG:HH11	1:A:98:ARG:HG3	1.86	0.41
1:A:199:ILE:HD13	1:A:351:ALA:HB1	2.03	0.40
1:A:79:ILE:HD11	1:A:103:LEU:HB3	2.04	0.40

All (5) 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:1:LYS:NZ	3:A:515:HOH:O[4_556]	1.12	1.08
1:A:1:LYS:CE	3:A:515:HOH:O[4_556]	1.57	0.63
1:A:1:LYS:CD	3:A:515:HOH:O[4_556]	1.93	0.27
1:A:46:LYS:NZ	3:A:602:HOH:O[4_556]	2.11	0.09
1:A:354:ARG:CD	3:A:563:HOH:O[4_556]	2.14	0.06

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	368/370 (100%)	353 (96%)	11 (3%)	4 (1%)	11 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ASP
1	A	4	GLU
1	A	81	PRO
1	A	174	GLY

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	297/297 (100%)	254 (86%)	43 (14%)	3 0

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	6	LYS
1	A	22	GLU
1	A	25	LYS
1	A	26	LYS
1	A	30	ASP
1	A	33	ILE
1	A	36	THR
1	A	41	ASP
1	A	45	GLU
1	A	50	VAL
1	A	55	ASP
1	A	79	ILE
1	A	80	THR
1	A	82	ASP
1	A	83	LYS
1	A	87	ASP
1	A	127	LYS
1	A	137	LYS
1	A	138	GLU
1	A	140	LYS
1	A	142	LYS
1	A	144	LYS

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Mol	Chain	Res	Type
1	A	151	LEU
1	A	160	LEU
1	A	175	LYS
1	A	202	LYS
1	A	204	MET
1	A	211	SER
1	A	233	SER
1	A	253	GLN
1	A	256	LYS
1	A	258	PHE
1	A	274	GLU
1	A	277	LYS
1	A	278	GLU
1	A	313	LYS
1	A	325	GLN
1	A	328	GLU
1	A	335	GLN
1	A	354	ARG
1	A	362	LYS
1	A	370	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	86	GLN
1	A	124	ASN
1	A	203	HIS
1	A	218	ASN
1	A	282	ASN
1	A	335	GLN

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

3 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GLC	B	1	2	12,12,12	0.83	0	17,17,17	1.40	3 (17%)
2	GLC	B	2	2	11,11,12	0.79	0	15,15,17	1.43	4 (26%)
2	GLC	B	3	2	11,11,12	1.57	2 (18%)	15,15,17	1.54	2 (13%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLC	B	2	2	-	0/2/19/22	0/1/1/1
2	GLC	B	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	GLC	O5-C1	-3.92	1.37	1.43
2	B	3	GLC	O4-C4	-2.39	1.37	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLC	C1-O5-C5	4.30	117.95	112.19
2	B	1	GLC	C1-O5-C5	2.67	118.83	113.65
2	B	1	GLC	O4-C4-C3	-2.65	104.12	110.38
2	B	2	GLC	O4-C4-C3	-2.65	104.14	110.38
2	B	2	GLC	C1-O5-C5	2.49	115.53	112.19
2	B	2	GLC	C1-C2-C3	-2.41	106.13	109.64
2	B	3	GLC	O3-C3-C4	-2.33	104.88	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	O1-C1-O5	-2.14	104.05	110.41
2	B	2	GLC	C2-C3-C4	-2.02	107.31	110.86

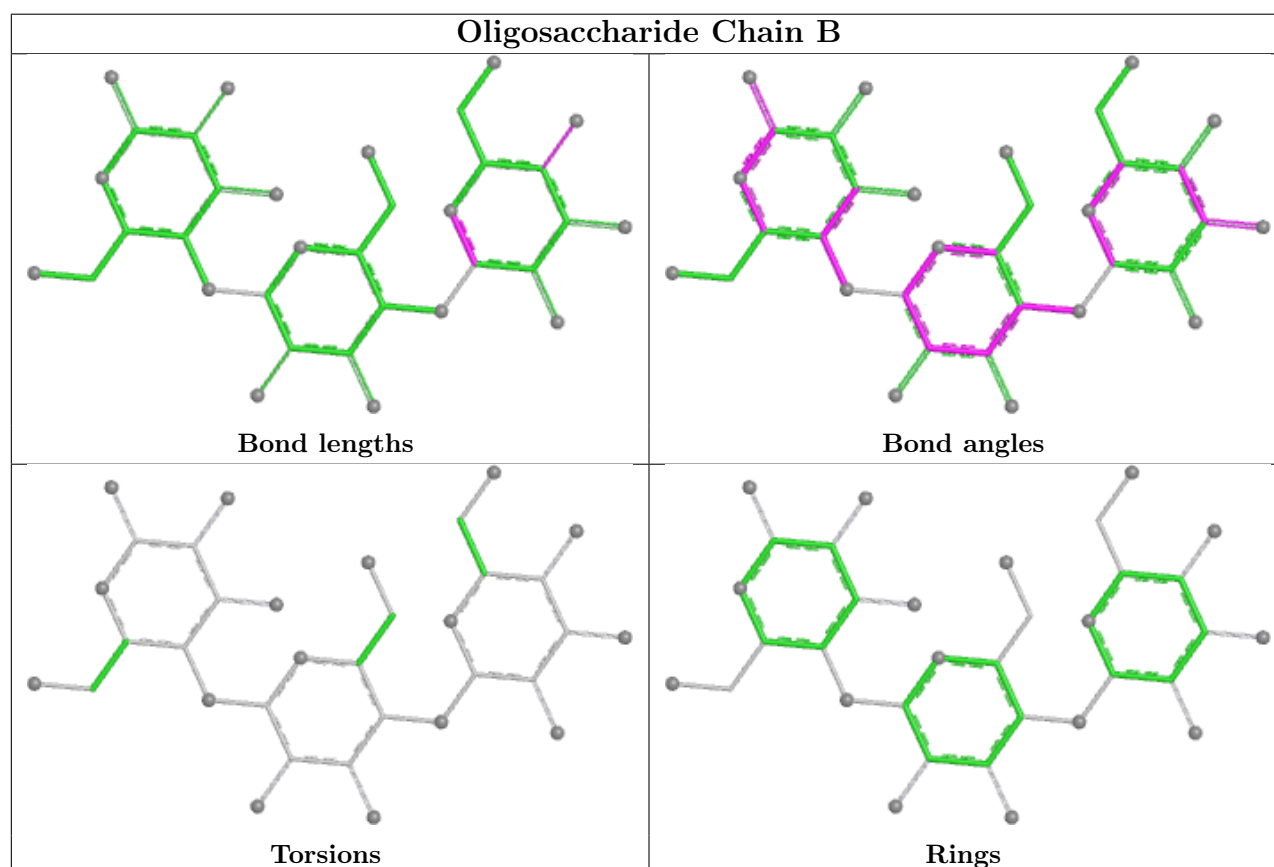
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

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.