



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:16 AM UTC

PDB ID : 1ANF / pdb_00001anf
Title : MALTODEXTRIN BINDING PROTEIN WITH BOUND MALTOSE
Authors : Spurlino, J.C.; Quioco, F.A.
Deposited on : 1997-06-25
Resolution : 1.67 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

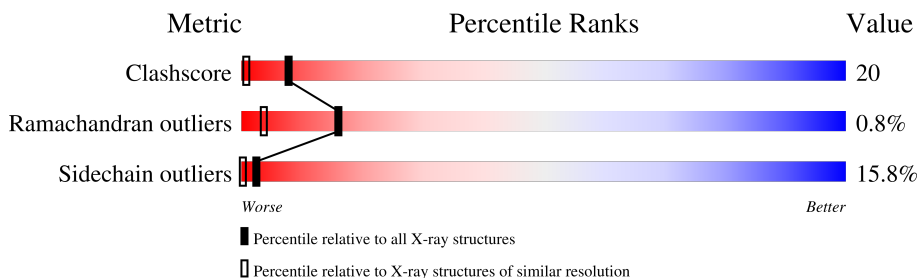
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)

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	2	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 2987 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
			2860	1843	468	543	6			

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
2	B	2	Total	C	O	0	0	0
			23	12	11			

- Molecule 3 is water.

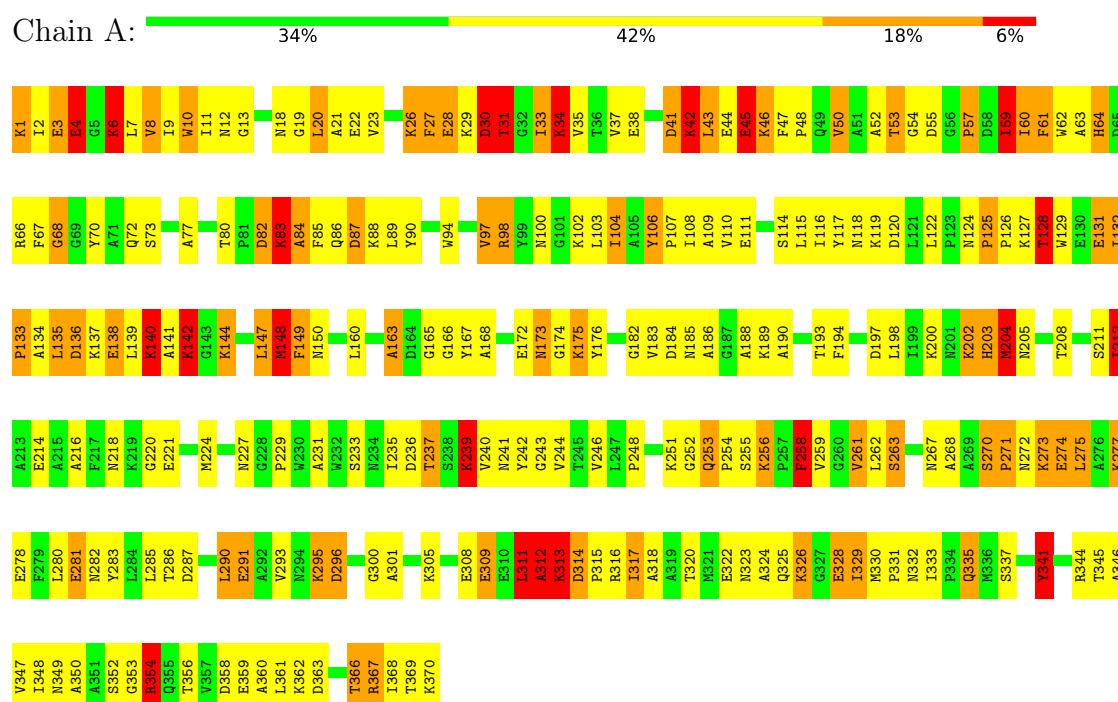
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	104	Total	O	0	0
			104	104		

3 Residue-property plots

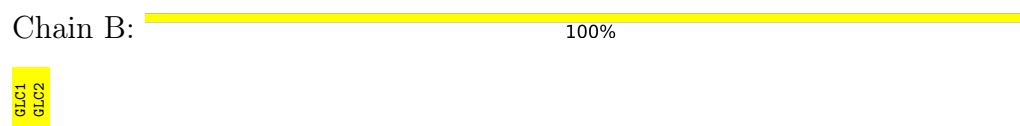
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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	105.88Å 68.44Å 57.94Å 90.00° 112.54° 90.00°	Depositor
Resolution (Å)	10.00 – 1.67	Depositor
% Data completeness (in resolution range)	80.0 (10.00-1.67)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2987	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: 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	1.88	50/2929 (1.7%)	2.90	304/3978 (7.6%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	GLU	C-O	8.21	1.33	1.24
1	A	149	PHE	N-CA	7.55	1.55	1.45
1	A	189	LYS	C-O	7.18	1.32	1.24
1	A	212	ILE	C-N	7.12	1.43	1.33
1	A	312	ALA	C-O	-6.81	1.16	1.23
1	A	55	ASP	N-CA	6.45	1.54	1.46
1	A	149	PHE	C-O	6.21	1.31	1.23
1	A	262	LEU	CA-C	6.11	1.60	1.52
1	A	31	THR	CA-CB	6.00	1.63	1.53
1	A	248	PRO	C-O	6.00	1.30	1.23
1	A	300	GLY	CA-C	5.90	1.60	1.51
1	A	147	LEU	CA-CB	5.88	1.64	1.53
1	A	296	ASP	C-O	5.81	1.31	1.24
1	A	30	ASP	N-CA	5.80	1.53	1.46
1	A	367	ARG	NE-CZ	5.78	1.39	1.33
1	A	312	ALA	C-N	-5.76	1.25	1.33
1	A	97	VAL	C-N	-5.74	1.25	1.33
1	A	111	GLU	N-CA	5.72	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	TYR	N-CA	5.71	1.53	1.45
1	A	261	VAL	CA-CB	5.71	1.60	1.53
1	A	368	ILE	CA-CB	5.70	1.61	1.54
1	A	125	PRO	CA-CB	-5.65	1.49	1.54
1	A	227	ASN	CA-C	5.65	1.59	1.52
1	A	80	THR	CA-CB	5.64	1.60	1.53
1	A	220	GLY	C-O	5.59	1.31	1.24
1	A	315	PRO	C-N	-5.58	1.26	1.33
1	A	194	PHE	C-N	-5.56	1.26	1.33
1	A	345	THR	C-O	5.56	1.30	1.24
1	A	313	LYS	N-CA	-5.49	1.39	1.46
1	A	224	MET	N-CA	5.45	1.52	1.45
1	A	188	ALA	C-O	5.45	1.30	1.24
1	A	341	TYR	N-CA	5.43	1.53	1.46
1	A	94	TRP	C-N	-5.42	1.26	1.34
1	A	366	THR	CA-CB	5.40	1.61	1.53
1	A	311	LEU	C-N	5.35	1.41	1.34
1	A	183	VAL	N-CA	5.35	1.53	1.46
1	A	286	THR	CB-OG1	5.34	1.52	1.43
1	A	252	GLY	C-O	5.33	1.31	1.24
1	A	108	ILE	CA-CB	5.32	1.60	1.55
1	A	254	PRO	C-O	5.29	1.30	1.23
1	A	3	GLU	C-O	5.27	1.30	1.24
1	A	63	ALA	C-O	5.26	1.30	1.23
1	A	268	ALA	N-CA	5.23	1.52	1.46
1	A	132	ILE	CA-CB	5.18	1.60	1.54
1	A	261	VAL	C-O	5.11	1.30	1.24
1	A	263	SER	C-N	5.11	1.40	1.33
1	A	350	ALA	C-O	5.10	1.30	1.24
1	A	61	PHE	CA-C	5.09	1.58	1.52
1	A	117	TYR	C-O	5.06	1.30	1.23
1	A	64	HIS	CD2-NE2	-5.06	1.32	1.37

All (304) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ALA	CA-C-N	25.95	171.09	121.54
1	A	312	ALA	C-N-CA	25.95	171.09	121.54
1	A	30	ASP	CA-CB-CG	22.44	135.04	112.60
1	A	354	ARG	NE-CZ-NH1	19.03	140.53	121.50
1	A	311	LEU	CA-C-N	-18.90	94.87	121.33
1	A	311	LEU	C-N-CA	-18.90	94.87	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ALA	O-C-N	15.21	139.14	123.62
1	A	124	ASN	CA-CB-CG	15.05	127.65	112.60
1	A	137	LYS	CA-CB-CG	13.35	140.80	114.10
1	A	136	ASP	O-C-N	11.14	133.93	122.12
1	A	236	ASP	O-C-N	11.14	133.93	122.12
1	A	4	GLU	CA-C-N	11.06	143.08	121.41
1	A	4	GLU	C-N-CA	11.06	143.08	121.41
1	A	341	TYR	CA-CB-CG	11.03	133.76	113.90
1	A	59	ILE	CA-CB-CG2	10.95	129.12	110.50
1	A	55	ASP	CA-CB-CG	10.73	123.33	112.60
1	A	354	ARG	NH1-CZ-NH2	-10.62	105.50	119.30
1	A	134	ALA	CA-C-O	10.51	131.86	120.82
1	A	358	ASP	CA-CB-CG	10.39	122.99	112.60
1	A	35	VAL	CA-C-O	-10.01	109.86	120.57
1	A	347	VAL	O-C-N	9.74	131.86	121.83
1	A	239	LYS	CB-CG-CD	9.28	132.65	111.30
1	A	272	ASN	CB-CG-ND2	9.26	130.29	116.40
1	A	316	ARG	CD-NE-CZ	9.25	137.35	124.40
1	A	84	ALA	N-CA-CB	9.13	123.65	110.13
1	A	278	GLU	CB-CG-CD	8.87	127.68	112.60
1	A	86	GLN	CA-C-N	8.86	133.03	120.28
1	A	86	GLN	C-N-CA	8.86	133.03	120.28
1	A	233	SER	CA-CB-OG	-8.68	93.73	111.10
1	A	274	GLU	CB-CG-CD	8.66	127.32	112.60
1	A	335	GLN	CG-CD-NE2	8.65	129.38	116.40
1	A	42	LYS	CB-CA-C	-8.48	99.41	111.80
1	A	50	VAL	CA-C-O	-8.48	111.32	120.47
1	A	33	ILE	N-CA-CB	8.40	120.58	111.00
1	A	141	ALA	CA-C-O	8.29	129.57	119.38
1	A	227	ASN	OD1-CG-ND2	-8.25	114.35	122.60
1	A	203	HIS	CA-CB-CG	-8.13	105.67	113.80
1	A	68	GLY	O-C-N	-8.08	114.43	122.19
1	A	278	GLU	CA-CB-CG	8.08	130.26	114.10
1	A	239	LYS	CG-CD-CE	8.07	129.87	111.30
1	A	104	ILE	O-C-N	8.06	130.88	122.09
1	A	270	SER	CA-C-N	8.05	127.77	119.64
1	A	270	SER	C-N-CA	8.05	127.77	119.64
1	A	328	GLU	CA-CB-CG	8.04	130.17	114.10
1	A	331	PRO	O-C-N	-8.02	113.21	122.91
1	A	84	ALA	N-CA-C	-8.01	101.63	111.40
1	A	272	ASN	CA-C-O	-7.87	109.26	119.80
1	A	27	PHE	N-CA-C	-7.83	100.76	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	251	LYS	CG-CD-CE	7.75	129.13	111.30
1	A	18	ASN	OD1-CG-ND2	-7.74	114.86	122.60
1	A	291	GLU	CA-C-O	-7.74	111.07	119.97
1	A	45	GLU	OE1-CD-OE2	7.63	141.22	122.90
1	A	45	GLU	N-CA-CB	-7.55	98.87	110.42
1	A	84	ALA	O-C-N	7.53	131.28	122.17
1	A	185	ASN	CA-CB-CG	7.53	120.13	112.60
1	A	282	ASN	CA-C-O	-7.53	110.92	118.97
1	A	33	ILE	CA-C-O	-7.51	111.86	120.65
1	A	84	ALA	CA-C-O	-7.47	112.56	120.55
1	A	67	PHE	CA-C-O	-7.42	112.55	120.42
1	A	38	GLU	O-C-N	7.39	133.01	123.11
1	A	109	ALA	CA-C-N	7.39	133.16	123.11
1	A	109	ALA	C-N-CA	7.39	133.16	123.11
1	A	29	LYS	N-CA-C	-7.37	103.75	112.89
1	A	349	ASN	CA-CB-CG	7.34	119.94	112.60
1	A	97	VAL	O-C-N	7.33	131.73	122.57
1	A	354	ARG	N-CA-CB	7.32	121.62	110.28
1	A	26	LYS	N-CA-C	-7.30	104.25	113.02
1	A	346	ALA	O-C-N	-7.30	114.50	122.09
1	A	142	LYS	CA-CB-CG	7.25	128.61	114.10
1	A	173	ASN	CA-CB-CG	7.24	119.84	112.60
1	A	278	GLU	CA-C-N	7.15	130.19	120.54
1	A	278	GLU	C-N-CA	7.15	130.19	120.54
1	A	128	THR	N-CA-CB	-7.14	98.35	111.13
1	A	106	TYR	O-C-N	7.13	129.27	121.36
1	A	353	GLY	O-C-N	7.12	131.02	122.34
1	A	30	ASP	CB-CA-C	7.03	122.74	110.64
1	A	262	LEU	O-C-N	7.01	131.65	122.95
1	A	8	VAL	CB-CA-C	6.96	120.94	110.63
1	A	242	TYR	CA-C-N	-6.93	116.30	122.47
1	A	242	TYR	C-N-CA	-6.93	116.30	122.47
1	A	28	GLU	N-CA-C	6.92	119.85	111.82
1	A	64	HIS	CA-CB-CG	-6.91	106.89	113.80
1	A	291	GLU	OE1-CD-OE2	6.88	139.41	122.90
1	A	125	PRO	CB-CA-C	6.87	117.62	111.17
1	A	208	THR	O-C-N	6.84	131.27	123.06
1	A	353	GLY	CA-C-O	-6.82	110.71	119.58
1	A	33	ILE	O-C-N	6.82	131.26	122.94
1	A	120	ASP	CA-C-O	-6.82	111.75	119.79
1	A	55	ASP	CB-CA-C	6.81	123.98	110.42
1	A	133	PRO	O-C-N	6.79	129.84	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	A	293	VAL	CA-C-O	-6.78	113.53	121.05
1	A	94	TRP	CA-C-N	6.77	130.59	120.31
1	A	94	TRP	C-N-CA	6.77	130.59	120.31
1	A	361	LEU	O-C-N	6.77	131.40	122.33
1	A	366	THR	CA-CB-OG1	-6.75	99.47	109.60
1	A	312	ALA	N-CA-C	6.73	118.65	107.20
1	A	354	ARG	NE-CZ-NH2	-6.70	113.17	119.20
1	A	128	THR	OG1-CB-CG2	6.67	122.65	109.30
1	A	290	LEU	O-C-N	6.64	129.16	122.12
1	A	341	TYR	CB-CA-C	6.64	122.13	110.85
1	A	367	ARG	NE-CZ-NH2	6.60	125.14	119.20
1	A	204	MET	N-CA-CB	-6.54	100.74	111.66
1	A	140	LYS	CA-C-N	6.54	131.63	120.72
1	A	140	LYS	C-N-CA	6.54	131.63	120.72
1	A	122	LEU	N-CA-CB	-6.53	102.94	111.23
1	A	86	GLN	CB-CG-CD	6.52	123.68	112.60
1	A	285	LEU	O-C-N	-6.52	113.92	122.59
1	A	253	GLN	CB-CG-CD	-6.48	101.59	112.60
1	A	186	ALA	CA-C-O	-6.42	113.75	120.55
1	A	301	ALA	CA-C-O	-6.42	113.05	120.49
1	A	27	PHE	CA-C-O	6.41	128.33	120.31
1	A	305	LYS	CA-C-N	6.41	128.77	120.44
1	A	305	LYS	C-N-CA	6.41	128.77	120.44
1	A	33	ILE	CB-CA-C	-6.39	103.22	110.96
1	A	277	LYS	CB-CG-CD	6.37	125.95	111.30
1	A	165	GLY	CA-C-O	-6.35	109.53	120.57
1	A	70	TYR	CA-C-N	6.34	128.69	120.44
1	A	70	TYR	C-N-CA	6.34	128.69	120.44
1	A	274	GLU	CA-C-O	-6.33	113.71	120.42
1	A	53	THR	CA-CB-OG1	-6.33	100.11	109.60
1	A	29	LYS	CA-CB-CG	6.32	126.74	114.10
1	A	7	LEU	O-C-N	-6.31	115.92	123.31
1	A	111	GLU	O-C-N	-6.29	115.86	123.29
1	A	103	LEU	CB-CA-C	6.28	120.09	109.80
1	A	100	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	333	ILE	CA-C-N	6.27	126.18	119.28
1	A	333	ILE	C-N-CA	6.27	126.18	119.28
1	A	37	VAL	CA-C-O	-6.23	113.80	120.59
1	A	100	ASN	CB-CG-ND2	6.22	125.73	116.40
1	A	185	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	A	38	GLU	CA-C-O	-6.21	114.20	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	THR	O-C-N	6.20	128.46	122.07
1	A	193	THR	CA-CB-OG1	-6.20	100.31	109.60
1	A	3	GLU	CB-CA-C	6.19	122.73	110.42
1	A	341	TYR	CB-CG-CD1	6.19	130.08	120.80
1	A	21	ALA	CA-C-O	-6.17	114.01	120.55
1	A	273	LYS	N-CA-C	6.16	118.00	111.28
1	A	88	LYS	CG-CD-CE	6.15	125.44	111.30
1	A	10	TRP	CB-CG-CD2	-6.15	118.19	126.80
1	A	18	ASN	N-CA-C	-6.13	104.15	111.69
1	A	214	GLU	CA-C-O	-6.12	114.39	120.82
1	A	41	ASP	CA-C-O	-6.12	114.89	121.56
1	A	354	ARG	CA-CB-CG	6.12	126.34	114.10
1	A	200	LYS	CB-CA-C	-6.10	100.62	110.74
1	A	175	LYS	CA-C-O	6.06	127.94	121.45
1	A	204	MET	CA-C-O	-6.05	114.79	121.33
1	A	323	ASN	O-C-N	6.05	129.04	122.15
1	A	229	PRO	CA-C-N	6.04	128.99	120.28
1	A	229	PRO	C-N-CA	6.04	128.99	120.28
1	A	282	ASN	CB-CG-ND2	-6.04	107.34	116.40
1	A	13	GLY	O-C-N	6.03	129.17	122.54
1	A	11	ILE	CA-C-N	6.02	129.85	120.75
1	A	11	ILE	C-N-CA	6.02	129.85	120.75
1	A	64	HIS	ND1-CE1-NE2	-6.02	102.38	108.40
1	A	285	LEU	CA-C-O	6.01	129.10	120.51
1	A	291	GLU	CA-C-N	6.00	128.32	120.28
1	A	291	GLU	C-N-CA	6.00	128.32	120.28
1	A	308	GLU	CA-C-O	6.00	126.88	120.10
1	A	114	SER	CA-C-O	-5.99	114.43	121.44
1	A	341	TYR	CB-CG-CD2	-5.97	111.85	120.80
1	A	131	GLU	CG-CD-OE1	5.97	132.12	118.40
1	A	168	ALA	CA-C-N	5.96	131.39	122.99
1	A	168	ALA	C-N-CA	5.96	131.39	122.99
1	A	271	PRO	CA-C-O	5.95	126.77	118.86
1	A	291	GLU	CG-CD-OE2	-5.95	104.72	118.40
1	A	360	ALA	O-C-N	5.94	128.42	122.12
1	A	315	PRO	CA-C-N	5.92	128.14	120.44
1	A	315	PRO	C-N-CA	5.92	128.14	120.44
1	A	117	TYR	O-C-N	5.92	130.85	123.15
1	A	61	PHE	O-C-N	5.92	130.27	123.29
1	A	13	GLY	CA-C-O	-5.91	112.67	119.65
1	A	110	VAL	O-C-N	5.91	130.62	122.88
1	A	256	LYS	CA-CB-CG	5.89	125.89	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLY	CA-C-N	-5.89	112.21	121.87
1	A	174	GLY	C-N-CA	-5.89	112.21	121.87
1	A	50	VAL	O-C-N	5.89	128.45	121.80
1	A	90	TYR	CA-C-O	5.89	125.28	119.75
1	A	35	VAL	CA-C-N	5.88	131.29	123.05
1	A	35	VAL	C-N-CA	5.88	131.29	123.05
1	A	94	TRP	O-C-N	-5.84	115.09	122.27
1	A	43	LEU	O-C-N	5.83	129.45	122.27
1	A	314	ASP	CA-C-O	-5.83	113.72	119.49
1	A	86	GLN	CG-CD-NE2	-5.80	107.70	116.40
1	A	312	ALA	CA-C-O	-5.80	114.23	120.09
1	A	325	GLN	O-C-N	-5.79	115.44	122.22
1	A	243	GLY	N-CA-C	-5.79	101.50	111.57
1	A	316	ARG	NE-CZ-NH1	5.78	127.28	121.50
1	A	118	ASN	CA-C-O	-5.77	114.41	120.58
1	A	82	ASP	O-C-N	5.77	129.40	122.94
1	A	135	LEU	CA-C-N	5.77	128.01	120.28
1	A	135	LEU	C-N-CA	5.77	128.01	120.28
1	A	275	LEU	CA-C-O	5.75	126.86	120.82
1	A	53	THR	CA-CB-CG2	5.75	120.28	110.50
1	A	366	THR	OG1-CB-CG2	5.74	120.78	109.30
1	A	46	LYS	CA-C-O	-5.74	114.34	120.42
1	A	262	LEU	N-CA-CB	5.74	118.47	109.69
1	A	44	GLU	CA-C-O	5.73	126.43	119.38
1	A	22	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	67	PHE	CA-C-N	5.72	126.33	119.98
1	A	67	PHE	C-N-CA	5.72	126.33	119.98
1	A	324	ALA	CA-C-O	5.72	126.61	120.55
1	A	135	LEU	CB-CA-C	5.72	120.28	110.79
1	A	1	LYS	CA-C-N	5.70	132.22	121.97
1	A	1	LYS	C-N-CA	5.70	132.22	121.97
1	A	144	LYS	CB-CG-CD	5.69	124.39	111.30
1	A	97	VAL	CA-C-O	-5.67	113.70	120.78
1	A	184	ASP	N-CA-CB	-5.65	101.88	111.20
1	A	367	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	A	129	TRP	CE2-CD2-CE3	5.63	124.43	118.80
1	A	312	ALA	CB-CA-C	5.56	118.33	111.43
1	A	369	THR	CA-C-O	-5.55	112.56	119.28
1	A	104	ILE	CB-CA-C	-5.54	104.89	111.65
1	A	197	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	311	LEU	O-C-N	-5.53	114.92	122.33
1	A	20	LEU	CA-C-O	-5.52	115.02	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	356	THR	N-CA-C	-5.52	103.10	110.55
1	A	60	ILE	CA-C-O	5.52	126.18	120.39
1	A	205	ASN	CA-C-N	5.51	129.42	120.60
1	A	205	ASN	C-N-CA	5.51	129.42	120.60
1	A	305	LYS	N-CA-C	5.50	117.99	111.33
1	A	208	THR	CA-CB-OG1	-5.50	101.35	109.60
1	A	147	LEU	N-CA-CB	-5.50	101.18	111.13
1	A	244	VAL	CA-C-O	-5.49	114.72	120.27
1	A	205	ASN	OD1-CG-ND2	5.49	128.09	122.60
1	A	281	GLU	N-CA-C	5.48	118.18	111.82
1	A	356	THR	N-CA-CB	5.48	118.78	110.45
1	A	262	LEU	CA-C-O	-5.48	114.68	120.92
1	A	176	TYR	O-C-N	5.47	129.44	123.04
1	A	34	LYS	CA-C-O	5.46	127.20	120.92
1	A	142	LYS	N-CA-CB	-5.45	102.20	110.92
1	A	255	SER	N-CA-C	-5.45	102.33	110.23
1	A	273	LYS	CB-CA-C	-5.45	101.75	110.79
1	A	211	SER	CA-CB-OG	-5.44	100.21	111.10
1	A	293	VAL	CA-C-N	5.44	128.12	120.28
1	A	293	VAL	C-N-CA	5.44	128.12	120.28
1	A	21	ALA	CA-C-N	5.43	128.10	120.28
1	A	21	ALA	C-N-CA	5.43	128.10	120.28
1	A	194	PHE	CA-C-O	-5.41	115.14	120.82
1	A	346	ALA	CA-C-O	5.40	126.68	120.90
1	A	28	GLU	CA-C-O	5.38	126.16	119.97
1	A	147	LEU	N-CA-C	5.38	117.95	108.75
1	A	326	LYS	CA-CB-CG	-5.38	103.34	114.10
1	A	59	ILE	CA-C-O	5.37	126.69	120.67
1	A	237	THR	O-C-N	5.37	128.50	122.22
1	A	344	ARG	O-C-N	5.33	127.56	122.07
1	A	316	ARG	NH1-CZ-NH2	-5.32	112.38	119.30
1	A	348	ILE	CB-CG1-CD1	-5.32	102.63	113.80
1	A	28	GLU	CG-CD-OE1	-5.31	106.18	118.40
1	A	103	LEU	CA-C-O	-5.30	114.55	120.54
1	A	166	GLY	N-CA-C	-5.29	106.50	112.33
1	A	172	GLU	CG-CD-OE2	-5.29	106.24	118.40
1	A	148	MET	CG-SD-CE	-5.29	89.27	100.90
1	A	190	ALA	CA-C-N	5.28	125.81	119.94
1	A	190	ALA	C-N-CA	5.28	125.81	119.94
1	A	118	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	A	80	THR	CA-CB-OG1	-5.26	101.71	109.60
1	A	119	LYS	O-C-N	5.25	129.22	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ASN	O-C-N	5.24	129.45	122.95
1	A	114	SER	O-C-N	5.23	129.95	123.15
1	A	231	ALA	N-CA-CB	-5.23	101.62	110.41
1	A	314	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	281	GLU	CB-CG-CD	-5.21	103.74	112.60
1	A	68	GLY	CA-C-O	5.21	126.11	120.75
1	A	142	LYS	CA-C-N	5.20	132.57	121.18
1	A	142	LYS	C-N-CA	5.20	132.57	121.18
1	A	28	GLU	CG-CD-OE2	5.20	130.36	118.40
1	A	124	ASN	CB-CG-ND2	-5.17	108.65	116.40
1	A	258	PHE	N-CA-C	-5.17	101.55	109.76
1	A	277	LYS	O-C-N	-5.16	116.65	122.12
1	A	102	LYS	CB-CA-C	-5.15	100.70	109.51
1	A	175	LYS	CB-CA-C	5.15	122.78	111.09
1	A	3	GLU	O-C-N	-5.14	115.76	122.59
1	A	22	GLU	CA-C-O	5.14	125.90	120.10
1	A	59	ILE	CB-CA-C	5.13	118.41	110.50
1	A	259	VAL	O-C-N	-5.13	117.49	122.93
1	A	57	PRO	O-C-N	-5.13	116.89	123.14
1	A	198	LEU	O-C-N	5.13	127.55	122.12
1	A	242	TYR	N-CA-C	5.12	118.10	109.95
1	A	12	ASN	CA-C-O	5.10	126.96	121.55
1	A	135	LEU	N-CA-CB	-5.09	102.63	110.12
1	A	287	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	352	SER	CA-C-N	5.09	130.87	120.80
1	A	352	SER	C-N-CA	5.09	130.87	120.80
1	A	116	ILE	CA-C-N	-5.08	114.61	122.59
1	A	116	ILE	C-N-CA	-5.08	114.61	122.59
1	A	300	GLY	N-CA-C	-5.07	101.16	113.18
1	A	53	THR	N-CA-CB	5.05	118.24	110.46
1	A	163	ALA	N-CA-C	5.05	117.17	111.11
1	A	316	ARG	O-C-N	5.05	127.27	122.07
1	A	324	ALA	CA-C-N	5.04	127.54	120.28
1	A	324	ALA	C-N-CA	5.04	127.54	120.28
1	A	6	LYS	CA-C-N	5.04	130.50	122.74
1	A	6	LYS	C-N-CA	5.04	130.50	122.74
1	A	98	ARG	CA-CB-CG	5.04	124.17	114.10
1	A	239	LYS	CD-CE-NZ	5.03	127.98	111.90
1	A	182	GLY	O-C-N	5.02	129.23	122.70
1	A	73	SER	CA-C-N	5.01	131.29	121.06
1	A	73	SER	C-N-CA	5.01	131.29	121.06
1	A	359	GLU	CB-CA-C	-5.01	103.01	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	ALA	CA-C-O	5.01	125.86	120.55
1	A	251	LYS	N-CA-C	-5.01	105.83	112.24
1	A	344	ARG	NE-CZ-NH2	5.01	123.70	119.20
1	A	270	SER	CB-CA-C	-5.00	101.81	108.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ALA	Peptide
1	A	354	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	2860	0	2827	114	3
2	B	23	0	20	0	0
3	A	104	0	0	5	1
All	All	2987	0	2847	114	4

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 20.

All (114) 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:239:LYS:O	1:A:239:LYS:HE3	1.39	1.19
1:A:311:LEU:O	1:A:312:ALA:HB2	1.34	1.14
1:A:31:THR:HG23	1:A:33:ILE:H	1.09	1.07
1:A:239:LYS:O	1:A:239:LYS:CE	2.07	1.02
1:A:31:THR:CG2	1:A:33:ILE:H	1.75	0.99
1:A:311:LEU:O	1:A:312:ALA:CB	1.98	0.99
1:A:312:ALA:HB3	1:A:317:ILE:CG2	1.92	0.98
1:A:239:LYS:O	1:A:239:LYS:CD	2.14	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:MET:HE2	3:A:499:HOH:O	1.67	0.93
1:A:312:ALA:CB	1:A:317:ILE:CG2	2.45	0.93
1:A:204:MET:CE	3:A:499:HOH:O	2.19	0.91
1:A:1:LYS:HA	1:A:54:GLY:O	1.72	0.90
1:A:312:ALA:CB	1:A:317:ILE:HB	2.04	0.88
1:A:309:GLU:O	1:A:313:LYS:HE3	1.74	0.88
1:A:31:THR:HG23	1:A:33:ILE:N	1.91	0.85
1:A:312:ALA:HB3	1:A:317:ILE:HG21	1.61	0.82
1:A:295:LYS:HD3	1:A:295:LYS:C	2.06	0.80
1:A:239:LYS:O	1:A:239:LYS:CG	2.27	0.79
1:A:33:ILE:HG12	1:A:275:LEU:HD13	1.63	0.79
1:A:6:LYS:HA	1:A:33:ILE:HG23	1.65	0.79
1:A:312:ALA:HB3	1:A:317:ILE:HG22	1.66	0.77
1:A:31:THR:HG23	1:A:33:ILE:HD12	1.67	0.76
1:A:64:HIS:HD2	1:A:261:VAL:H	1.34	0.76
1:A:28:GLU:HA	1:A:31:THR:HG22	1.68	0.75
1:A:312:ALA:HA	1:A:314:ASP:H	1.51	0.74
1:A:312:ALA:CB	1:A:317:ILE:HG21	2.15	0.74
1:A:136:ASP:OD2	1:A:203:HIS:HD2	1.69	0.73
1:A:341:TYR:CD1	1:A:367:ARG:NH2	2.57	0.73
1:A:312:ALA:CB	1:A:317:ILE:CB	2.66	0.73
1:A:27:PHE:O	1:A:31:THR:HB	1.89	0.72
1:A:341:TYR:HD1	1:A:367:ARG:NH2	1.88	0.71
1:A:312:ALA:HB1	1:A:317:ILE:HB	1.72	0.71
1:A:64:HIS:HE1	1:A:330:MET:O	1.73	0.70
1:A:68:GLY:HA3	1:A:332:ASN:O	1.92	0.69
1:A:43:LEU:CD1	1:A:60:ILE:HD11	2.24	0.67
1:A:312:ALA:HB2	1:A:317:ILE:HB	1.77	0.67
1:A:83:LYS:O	1:A:87:ASP:HB2	1.96	0.66
1:A:59:ILE:HD12	1:A:280:LEU:HD11	1.75	0.66
1:A:237:THR:HG22	1:A:237:THR:O	1.96	0.64
1:A:59:ILE:CD1	1:A:280:LEU:HD21	2.28	0.64
1:A:43:LEU:HD13	1:A:60:ILE:HD11	1.79	0.63
1:A:48:PRO:O	1:A:52:ALA:HB2	1.99	0.62
1:A:149:PHE:CE1	1:A:204:MET:HE1	2.36	0.61
1:A:309:GLU:O	1:A:313:LYS:CE	2.47	0.60
1:A:45:GLU:O	1:A:48:PRO:HD2	2.01	0.60
1:A:136:ASP:O	1:A:140:LYS:HB2	2.02	0.59
1:A:128:THR:HG21	3:A:412:HOH:O	2.03	0.59
1:A:64:HIS:CD2	1:A:261:VAL:H	2.19	0.58
1:A:1:LYS:CA	1:A:54:GLY:O	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:THR:HG22	1:A:131:GLU:H	1.69	0.57
1:A:295:LYS:HD3	1:A:296:ASP:N	2.19	0.56
1:A:3:GLU:O	1:A:4:GLU:CB	2.51	0.56
1:A:30:ASP:OD1	1:A:283:TYR:OH	2.24	0.56
1:A:329:ILE:HG23	1:A:329:ILE:O	2.06	0.55
1:A:136:ASP:OD2	1:A:203:HIS:CD2	2.56	0.54
1:A:140:LYS:HD2	1:A:144:LYS:O	2.07	0.54
1:A:19:GLY:O	1:A:23:VAL:HG23	2.08	0.53
1:A:202:LYS:HA	1:A:202:LYS:HE2	1.91	0.53
1:A:34:LYS:O	1:A:34:LYS:HG2	2.09	0.53
1:A:132:ILE:N	1:A:133:PRO:CD	2.71	0.53
1:A:335:GLN:NE2	1:A:335:GLN:H	2.08	0.52
1:A:136:ASP:OD2	1:A:140:LYS:NZ	2.35	0.51
1:A:82:ASP:O	1:A:85:PHE:N	2.43	0.51
1:A:9:ILE:HG21	1:A:20:LEU:HD21	1.92	0.51
1:A:363:ASP:O	1:A:367:ARG:HG3	2.11	0.51
1:A:167:TYR:HE2	3:A:504:HOH:O	1.94	0.50
1:A:322:GLU:O	1:A:326:LYS:HG3	2.10	0.50
1:A:85:PHE:CD1	1:A:85:PHE:C	2.89	0.49
1:A:239:LYS:NZ	1:A:241:ASN:HB2	2.27	0.49
1:A:312:ALA:HB2	1:A:317:ILE:CB	2.39	0.49
1:A:64:HIS:CE1	1:A:330:MET:O	2.62	0.49
1:A:204:MET:HE3	3:A:499:HOH:O	1.97	0.48
1:A:61:PHE:HA	1:A:263:SER:O	2.13	0.48
1:A:277:LYS:O	1:A:281:GLU:HG3	2.13	0.48
1:A:212:ILE:N	1:A:212:ILE:HD13	2.27	0.48
1:A:136:ASP:HB3	1:A:203:HIS:CD2	2.48	0.48
1:A:147:LEU:O	1:A:148:MET:HG2	2.13	0.48
1:A:237:THR:O	1:A:237:THR:CG2	2.60	0.47
1:A:82:ASP:C	1:A:84:ALA:N	2.73	0.46
1:A:62:TRP:CD1	1:A:66:ARG:HG3	2.50	0.46
1:A:136:ASP:CG	1:A:203:HIS:HD2	2.24	0.46
1:A:144:LYS:HE2	1:A:221:GLU:HA	1.98	0.46
1:A:270:SER:HA	1:A:271:PRO:HD3	1.74	0.45
1:A:366:THR:O	1:A:370:LYS:HG3	2.15	0.45
1:A:41:ASP:O	1:A:42:LYS:HB2	2.16	0.45
1:A:312:ALA:CB	1:A:317:ILE:HG22	2.32	0.45
1:A:239:LYS:HZ1	1:A:241:ASN:HB2	1.80	0.44
1:A:6:LYS:HD2	1:A:8:VAL:HG23	1.99	0.44
1:A:97:VAL:O	1:A:104:ILE:HG12	2.17	0.44
1:A:139:LEU:HA	1:A:142:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:PRO:HA	1:A:126:PRO:HD3	1.82	0.43
1:A:132:ILE:N	1:A:133:PRO:HD3	2.33	0.43
1:A:59:ILE:HD11	1:A:280:LEU:HD21	2.00	0.43
1:A:148:MET:HE3	1:A:216:ALA:CB	2.48	0.43
1:A:31:THR:HG23	1:A:33:ILE:CD1	2.42	0.43
1:A:6:LYS:HA	1:A:33:ILE:CG2	2.41	0.42
1:A:362:LYS:C	1:A:362:LYS:HE2	2.44	0.42
1:A:31:THR:CG2	1:A:33:ILE:N	2.60	0.42
1:A:106:TYR:HA	1:A:107:PRO:HD3	1.86	0.42
1:A:31:THR:CG2	1:A:33:ILE:HD12	2.43	0.41
1:A:312:ALA:HB2	1:A:317:ILE:CG2	2.45	0.41
1:A:59:ILE:HD13	1:A:59:ILE:HG21	1.70	0.41
1:A:42:LYS:N	1:A:42:LYS:HD2	2.35	0.41
1:A:128:THR:CG2	1:A:131:GLU:H	2.31	0.41
1:A:10:TRP:CD1	1:A:57:PRO:HB3	2.55	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.73	0.41
1:A:77:ALA:HB2	1:A:273:LYS:HE2	2.01	0.41
1:A:163:ALA:HA	1:A:256:LYS:HD3	2.02	0.41
1:A:31:THR:CG2	1:A:33:ILE:CD1	2.99	0.41
1:A:47:PHE:HB3	1:A:48:PRO:HD3	2.03	0.41
1:A:72:GLN:O	1:A:72:GLN:HG2	2.20	0.41
1:A:149:PHE:CD1	1:A:204:MET:HE1	2.56	0.40
1:A:218:ASN:HD21	1:A:235:ILE:HG12	1.87	0.40
1:A:258:PHE:CG	1:A:330:MET:HG2	2.57	0.40

All (4) 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:84:ALA:CA	1:A:341:TYR:OH[4_547]	1.59	0.61
3:A:502:HOH:O	3:A:504:HOH:O[2_657]	2.00	0.20
1:A:84:ALA:CB	1:A:341:TYR:OH[4_547]	2.04	0.16
1:A:84:ALA:N	1:A:341:TYR:OH[4_547]	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	368/370 (100%)	349 (95%)	16 (4%)	3 (1%)	16	4

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	83	LYS
1	A	2	ILE

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	292/297 (98%)	246 (84%)	46 (16%)	2	0

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	26	LYS
1	A	30	ASP
1	A	31	THR
1	A	34	LYS
1	A	42	LYS
1	A	45	GLU
1	A	46	LYS
1	A	50	VAL
1	A	53	THR
1	A	59	ILE
1	A	83	LYS
1	A	87	ASP
1	A	89	LEU

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Mol	Chain	Res	Type
1	A	98	ARG
1	A	115	LEU
1	A	127	LYS
1	A	128	THR
1	A	135	LEU
1	A	138	GLU
1	A	140	LYS
1	A	142	LYS
1	A	148	MET
1	A	160	LEU
1	A	173	ASN
1	A	175	LYS
1	A	202	LYS
1	A	204	MET
1	A	212	ILE
1	A	239	LYS
1	A	240	VAL
1	A	246	VAL
1	A	253	GLN
1	A	258	PHE
1	A	274	GLU
1	A	291	GLU
1	A	295	LYS
1	A	309	GLU
1	A	311	LEU
1	A	313	LYS
1	A	317	ILE
1	A	328	GLU
1	A	329	ILE
1	A	337	SER
1	A	341	TYR
1	A	354	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	49	GLN
1	A	64	HIS
1	A	173	ASN
1	A	201	ASN
1	A	203	HIS

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Mol	Chain	Res	Type
1	A	205	ASN
1	A	218	ASN
1	A	272	ASN
1	A	325	GLN
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 ⓘ

2 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	1.19	1 (8%)	17,17,17	2.25	5 (29%)
2	GLC	B	2	2	11,11,12	1.52	1 (9%)	15,15,17	1.45	1 (6%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	GLC	O5-C1	-3.91	1.37	1.43
2	B	1	GLC	O5-C1	-2.28	1.37	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	GLC	C1-O5-C5	6.06	125.37	113.65
2	B	2	GLC	C1-O5-C5	4.22	117.84	112.19
2	B	1	GLC	O1-C1-O5	-3.94	98.71	110.41
2	B	1	GLC	O5-C1-C2	3.71	116.82	110.30
2	B	1	GLC	O6-C6-C5	-2.58	102.56	111.33
2	B	1	GLC	O4-C4-C5	-2.18	103.94	109.32

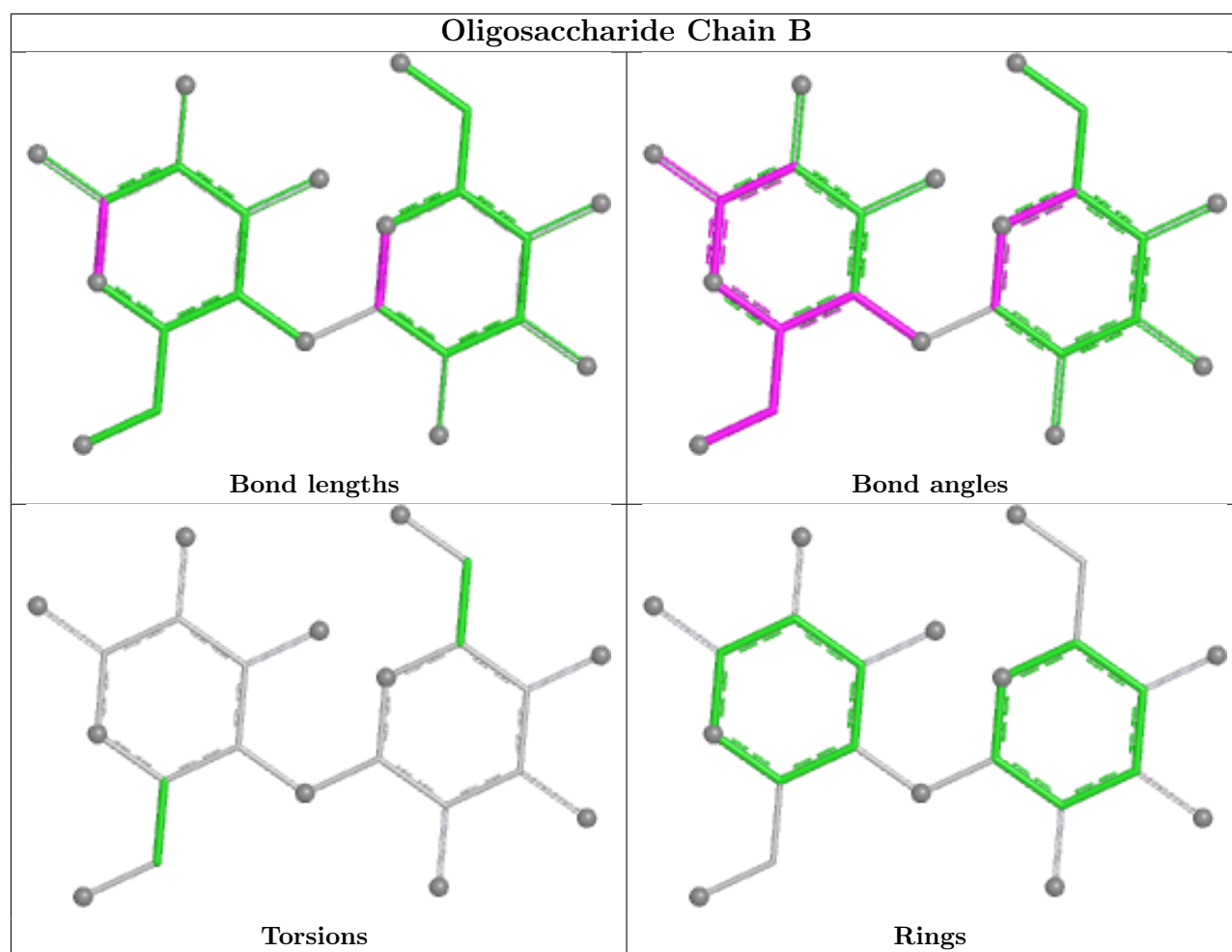
There are no chirality outliers.

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 [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.