



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3MBP
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

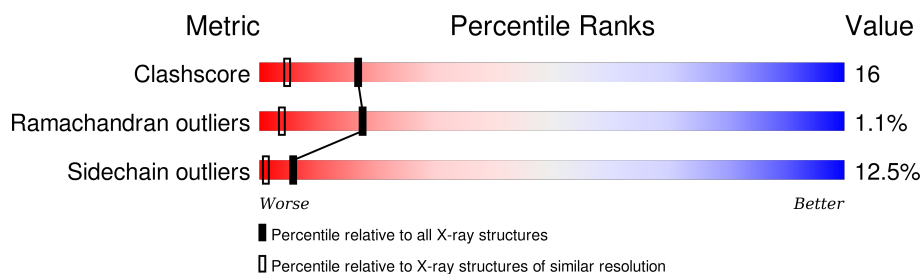
1 Overall quality at a glance

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	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	

2 Entry composition

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 a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is water.

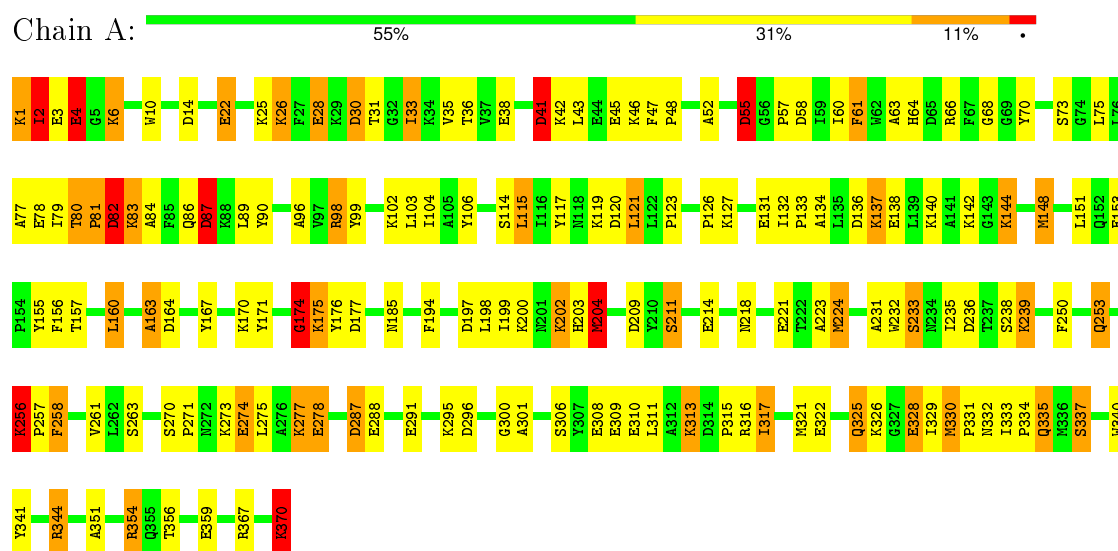
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: MALTODEXTRIN-BINDING PROTEIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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	1.58	10/2947 (0.3%)	2.36	135/3998 (3.4%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	370	LYS	C-OXT	31.43	1.83	1.23
1	A	238	SER	CB-OG	10.15	1.55	1.42
1	A	238	SER	CA-CB	7.62	1.64	1.52
1	A	4	GLU	C-N	7.28	1.46	1.33
1	A	117	TYR	CG-CD2	5.78	1.46	1.39
1	A	300	GLY	N-CA	5.66	1.54	1.46
1	A	131	GLU	CD-OE2	-5.65	1.19	1.25
1	A	340	TRP	CG-CD1	5.43	1.44	1.36
1	A	114	SER	CB-OG	-5.12	1.35	1.42
1	A	22	GLU	CA-CB	-5.04	1.42	1.53

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	ARG	CD-NE-CZ	27.69	162.37	123.60
1	A	22	GLU	CA-CB-CG	24.80	167.95	113.40
1	A	354	ARG	NE-CZ-NH1	17.96	129.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ARG	NE-CZ-NH1	-16.88	111.86	120.30
1	A	177	ASP	CB-CG-OD1	14.15	131.04	118.30
1	A	30	ASP	CA-CB-CG	13.56	143.24	113.40
1	A	55	ASP	CB-CG-OD2	-12.86	106.72	118.30
1	A	55	ASP	CB-CG-OD1	12.37	129.43	118.30
1	A	367	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	A	98	ARG	NE-CZ-NH1	-12.27	114.17	120.30
1	A	344	ARG	NE-CZ-NH2	12.01	126.31	120.30
1	A	98	ARG	NE-CZ-NH2	11.21	125.90	120.30
1	A	354	ARG	NE-CZ-NH2	-11.20	114.70	120.30
1	A	236	ASP	CB-CG-OD1	11.11	128.30	118.30
1	A	167	TYR	CB-CG-CD2	-10.79	114.53	121.00
1	A	142	LYS	CA-CB-CG	10.57	136.66	113.40
1	A	41	ASP	CB-CG-OD1	-10.26	109.06	118.30
1	A	30	ASP	CB-CG-OD2	10.18	127.46	118.30
1	A	344	ARG	CD-NE-CZ	-10.14	109.40	123.60
1	A	287	ASP	CB-CG-OD1	10.12	127.41	118.30
1	A	164	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	A	328	GLU	CA-CB-CG	9.96	135.31	113.40
1	A	278	GLU	CA-CB-CG	9.65	134.62	113.40
1	A	204	MET	CA-CB-CG	9.64	129.69	113.30
1	A	209	ASP	CB-CG-OD2	9.29	126.66	118.30
1	A	58	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	316	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	291	GLU	CA-CB-CG	8.84	132.86	113.40
1	A	238	SER	CA-CB-OG	-8.78	87.49	111.20
1	A	204	MET	N-CA-CB	8.66	126.18	110.60
1	A	160	LEU	CA-CB-CG	8.24	134.26	115.30
1	A	22	GLU	CG-CD-OE1	-7.86	102.59	118.30
1	A	256	LYS	CA-CB-CG	7.86	130.68	113.40
1	A	194	PHE	CB-CG-CD1	-7.78	115.36	120.80
1	A	61	PHE	CB-CG-CD2	-7.77	115.36	120.80
1	A	155	TYR	CB-CG-CD1	-7.60	116.44	121.00
1	A	296	ASP	CB-CG-OD1	7.52	125.06	118.30
1	A	310	GLU	OE1-CD-OE2	-7.50	114.30	123.30
1	A	90	TYR	CB-CG-CD2	-7.41	116.55	121.00
1	A	370	LYS	N-CA-CB	7.37	123.87	110.60
1	A	164	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	155	TYR	CG-CD1-CE1	-7.31	115.45	121.30
1	A	148	MET	O-C-N	7.26	134.32	122.70
1	A	66	ARG	NE-CZ-NH1	-7.25	116.68	120.30
1	A	41	ASP	OD1-CG-OD2	7.21	137.00	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LYS	CA-CB-CG	7.01	128.81	113.40
1	A	175	LYS	CB-CA-C	-6.96	96.48	110.40
1	A	233	SER	CB-CA-C	6.76	122.94	110.10
1	A	209	ASP	CB-CG-OD1	-6.74	112.24	118.30
1	A	63	ALA	N-CA-CB	6.70	119.48	110.10
1	A	142	LYS	CB-CA-C	6.67	123.75	110.40
1	A	78	GLU	C-N-CA	-6.66	105.04	121.70
1	A	153	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	14	ASP	CB-CG-OD2	6.63	124.27	118.30
1	A	177	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	278	GLU	CG-CD-OE1	6.57	131.44	118.30
1	A	119	LYS	O-C-N	6.55	133.18	122.70
1	A	310	GLU	CB-CG-CD	6.55	131.88	114.20
1	A	70	TYR	CB-CG-CD2	-6.54	117.07	121.00
1	A	197	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	131	GLU	CG-CD-OE2	6.40	131.11	118.30
1	A	291	GLU	C-N-CA	6.40	137.70	121.70
1	A	102	LYS	CB-CA-C	-6.38	97.65	110.40
1	A	104	ILE	CA-CB-CG1	-6.38	98.89	111.00
1	A	177	ASP	O-C-N	-6.38	112.50	122.70
1	A	115	LEU	CB-CG-CD2	-6.28	100.32	111.00
1	A	120	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	211	SER	CA-CB-OG	-6.24	94.34	111.20
1	A	277	LYS	CA-CB-CG	6.22	127.08	113.40
1	A	38	GLU	O-C-N	6.17	132.58	122.70
1	A	325	GLN	C-N-CA	6.16	137.11	121.70
1	A	175	LYS	CA-CB-CG	6.16	126.94	113.40
1	A	89	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	170	LYS	CD-CE-NZ	6.13	125.80	111.70
1	A	35	VAL	CA-C-O	-6.11	107.27	120.10
1	A	30	ASP	CB-CA-C	6.10	122.60	110.40
1	A	121	LEU	N-CA-CB	-6.09	98.23	110.40
1	A	296	ASP	OD1-CG-OD2	-6.08	111.74	123.30
1	A	204	MET	O-C-N	6.08	132.43	122.70
1	A	84	ALA	N-CA-CB	6.00	118.51	110.10
1	A	106	TYR	CG-CD1-CE1	-6.00	116.50	121.30
1	A	274	GLU	CB-CG-CD	5.98	130.35	114.20
1	A	31	THR	N-CA-CB	5.94	121.58	110.30
1	A	311	LEU	C-N-CA	5.92	136.50	121.70
1	A	258	PHE	CB-CG-CD1	-5.91	116.66	120.80
1	A	321	MET	CG-SD-CE	-5.91	90.74	100.20
1	A	326	LYS	C-N-CA	5.84	134.56	122.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	LYS	N-CA-CB	5.80	121.05	110.60
1	A	87	ASP	O-C-N	5.77	131.93	122.70
1	A	330	MET	CG-SD-CE	5.76	109.41	100.20
1	A	22	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	A	331	PRO	O-C-N	-5.72	113.55	122.70
1	A	308	GLU	OE1-CD-OE2	5.69	130.13	123.30
1	A	321	MET	O-C-N	-5.65	113.66	122.70
1	A	174	GLY	N-CA-C	-5.64	99.00	113.10
1	A	300	GLY	O-C-N	5.64	131.73	122.70
1	A	142	LYS	O-C-N	-5.63	113.64	123.20
1	A	232	TRP	CH2-CZ2-CE2	-5.62	111.78	117.40
1	A	83	LYS	O-C-N	-5.58	113.77	122.70
1	A	142	LYS	N-CA-CB	-5.48	100.74	110.60
1	A	99	TYR	O-C-N	5.47	131.46	122.70
1	A	322	GLU	OE1-CD-OE2	5.47	129.86	123.30
1	A	90	TYR	CD1-CE1-CZ	-5.45	114.89	119.80
1	A	291	GLU	CG-CD-OE2	-5.44	107.41	118.30
1	A	296	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	250	PHE	O-C-N	5.43	131.40	122.70
1	A	214	GLU	CG-CD-OE2	-5.42	107.45	118.30
1	A	167	TYR	CZ-CE2-CD2	-5.42	114.93	119.80
1	A	315	PRO	O-C-N	5.35	131.26	122.70
1	A	317	ILE	CA-CB-CG1	-5.32	100.90	111.00
1	A	176	TYR	O-C-N	5.29	131.17	122.70
1	A	316	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	156	PHE	CB-CG-CD1	5.28	124.49	120.80
1	A	231	ALA	N-CA-CB	-5.24	102.76	110.10
1	A	224	MET	CG-SD-CE	-5.24	91.82	100.20
1	A	257	PRO	O-C-N	5.23	131.07	122.70
1	A	367	ARG	CG-CD-NE	-5.19	100.89	111.80
1	A	309	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	A	30	ASP	OD1-CG-OD2	-5.18	113.46	123.30
1	A	204	MET	CB-CA-C	-5.15	100.10	110.40
1	A	174	GLY	O-C-N	5.14	130.93	122.70
1	A	2	ILE	CB-CA-C	5.13	121.87	111.60
1	A	194	PHE	CD1-CE1-CZ	-5.13	113.94	120.10
1	A	253	GLN	CB-CG-CD	-5.13	98.26	111.60
1	A	28	GLU	CA-CB-CG	5.10	124.61	113.40
1	A	326	LYS	CD-CE-NZ	-5.09	99.98	111.70
1	A	185	ASN	CB-CA-C	5.09	120.58	110.40
1	A	163	ALA	CA-C-O	-5.07	109.45	120.10
1	A	337	SER	CA-C-N	5.07	128.35	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASP	OD1-CG-OD2	-5.07	113.67	123.30
1	A	296	ASP	CB-CA-C	5.05	120.50	110.40
1	A	148	MET	CG-SD-CE	-5.05	92.12	100.20
1	A	291	GLU	CG-CD-OE1	5.03	128.37	118.30
1	A	301	ALA	CA-C-N	5.03	128.26	117.20
1	A	123	PRO	N-CD-CG	-5.01	95.68	103.20

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 ⓘ

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	2857	95	5
2	A	34	0	30	0	0
3	A	244	0	0	10	5
All	All	3156	0	2887	95	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 16.

All (95) 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	1.20	1.15
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HG	3:A:508:HOH:O	1.70	0.91
1:A:356:THR:OG1	1:A:359:GLU:HG3	1.74	0.87
1:A:26:LYS:O	1:A:26:LYS:HE3	1.74	0.87
1:A:26:LYS:C	1:A:26:LYS:HE3	1.96	0.85
1:A:33:ILE:HD13	1:A:275:LEU:HD13	1.57	0.85
1:A:313:LYS:HE3	1:A:313:LYS:HA	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:C	2.01	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:CE	1:A:313:LYS:HA	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: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: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:26:LYS:HE3	1:A:26:LYS:CA	2.10	0.56
1:A:313:LYS:CE	1:A:313:LYS:CA	2.83	0.55
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:HB2	1:A:273:LYS:HE3	1.91	0.53
1:A:126:PRO:HD2	1:A:224:MET:HE3	1.90	0.52
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:148:MET:HE3	3:A:640:HOH:O	2.10	0.51
1:A:132:ILE:N	1:A:133:PRO:CD	2.73	0.51
1:A:329:ILE:CG2	1:A:329:ILE:O	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:80:THR:HG22	1:A:80:THR:O	2.12	0.50
1:A:171:TYR:HH	1:A:174:GLY:HA2	1.75	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:115:LEU:CD2	1:A:224:MET:HE1	2.15	0.48
1:A:121:LEU:HD23	1:A:223:ALA:HA	1.95	0.48
1:A:82:ASP:OD1	1:A:82:ASP:C	2.52	0.48
1:A:83:LYS:HG3	1:A:83:LYS:O	2.12	0.47
1:A:270:SER:HA	1:A:271:PRO:HD3	1.71	0.47
1:A:115:LEU:CD2	1:A:224:MET:CE	2.79	0.47
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:288:GLU:CD	1:A:288:GLU:H	2.20	0.45
1:A:42:LYS:HB3	1:A:45:GLU:HG3	1.98	0.45
1:A:3:GLU:O	1:A:4:GLU:C	2.55	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:HD3	1:A:370:LYS:HA	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:132:ILE:N	1:A:133:PRO:HD3	2.34	0.42
1:A:140:LYS:HA	1:A:140:LYS:HD3	1.78	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:204:MET:HE3	1:A:204:MET:HB3	1.75	0.42
1:A:332:ASN:OD1	1:A:332:ASN:C	2.58	0.41
1:A:10:TRP:CG	1:A:57:PRO:HG3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:O	1:A:87:ASP:HB2	2.21	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:HG3	1:A:98:ARG:HH11	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%)	17 4

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%)	260 (88%)	37 (12%)	6 1

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
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	55	ASP
1	A	80	THR
1	A	82	ASP
1	A	87	ASP
1	A	127	LYS
1	A	137	LYS
1	A	138	GLU
1	A	144	LYS
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	239	LYS
1	A	253	GLN
1	A	256	LYS
1	A	258	PHE
1	A	274	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	370	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	86	GLN
1	A	203	HIS
1	A	218	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 carbohydrates 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	A	371	2	12,12,12	0.90	0	17,17,17	1.47	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	A	372	2	11,11,12	0.80	0	14,15,17	1.56	4 (28%)
2	GLC	A	373	2	11,11,12	1.58	2 (18%)	14,15,17	1.62	3 (21%)

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	A	371	2	-	0/2/22/22	0/1/1/1
2	GLC	A	372	2	-	0/2/19/22	0/1/1/1
2	GLC	A	373	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	A	373	GLC	O5-C1	-3.95	1.37	1.43
2	A	373	GLC	O4-C4	-2.47	1.37	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	372	GLC	C1-C2-C3	-2.88	106.13	109.54
2	A	371	GLC	O4-C4-C3	-2.76	104.12	110.34
2	A	372	GLC	O4-C4-C3	-2.75	104.14	110.34
2	A	373	GLC	O3-C3-C4	-2.42	104.88	110.34
2	A	371	GLC	O1-C1-O5	-2.26	104.05	110.25
2	A	372	GLC	C2-C3-C4	-2.19	107.31	111.04
2	A	373	GLC	C2-C3-C4	-2.00	107.64	111.04
2	A	372	GLC	C1-O5-C5	2.58	115.53	112.25
2	A	371	GLC	C1-O5-C5	2.89	118.83	113.47
2	A	373	GLC	C1-O5-C5	4.50	117.95	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.