wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 26, 2014 – 10:08 PM GMT

PDB ID	:	1ANF
Title	:	MALTODEXTRIN BINDING PROTEIN WITH BOUND MALTOSE
Authors	:	Spurlino, J.C.; Quiocho, F.A.
Deposited on	:	1997-06-25
Resolution	:	1.67 Å(reported)

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		0.8%
Sidechain outliers		12.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
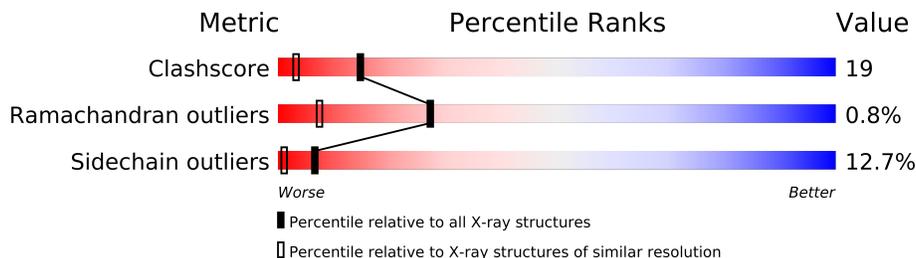
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4225 (1.70-1.66)
Ramachandran outliers	78287	4144 (1.70-1.66)
Sidechain outliers	78261	4143 (1.70-1.66)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 2987 atoms, of which 0 are hydrogen and 0 are deuterium.

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 2860	C 1843	N 468	O 543	S 6	0	0	0

- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 3 is water.

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

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

Chain A:
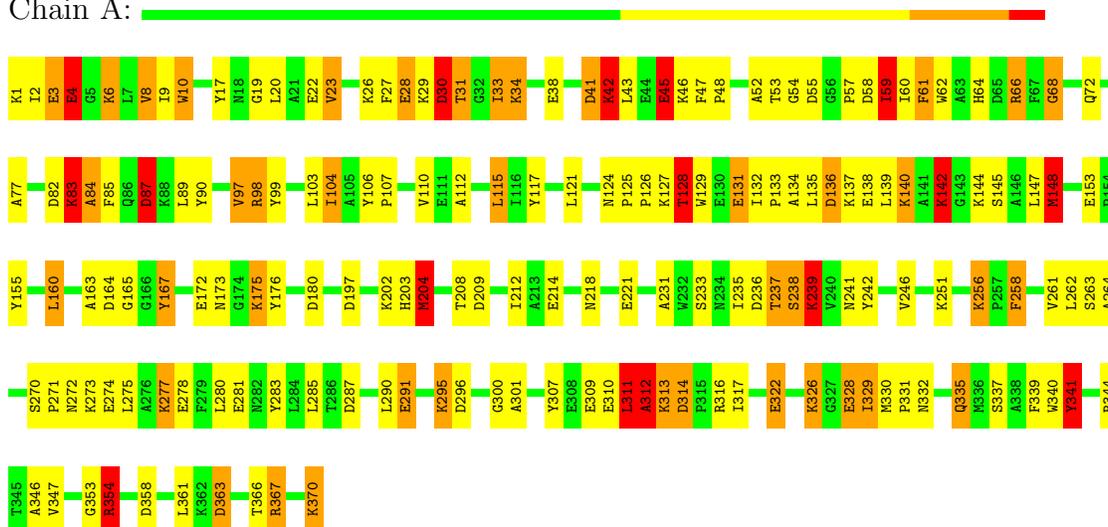
4 Data and refinement statistics ⓘ

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	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	1.47	9/2929 (0.3%)	2.43	146/3978 (3.7%)

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	238	SER	CB-OG	7.16	1.51	1.42
1	A	28	GLU	CD-OE2	-5.99	1.19	1.25
1	A	214	GLU	CD-OE1	-5.68	1.19	1.25
1	A	117	TYR	CG-CD2	5.55	1.46	1.39
1	A	138	GLU	C-O	5.46	1.33	1.23

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	354	ARG	NE-CZ-NH1	40.46	140.53	120.30
1	A	312	ALA	C-N-CA	19.76	171.09	121.70
1	A	341	TYR	CB-CG-CD2	-15.25	111.85	121.00
1	A	341	TYR	CB-CG-CD1	15.13	130.08	121.00
1	A	45	GLU	OE1-CD-OE2	14.94	141.22	123.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2860	0	2826	110	3
2	A	23	0	20	0	0
3	A	104	0	0	5	1
All	All	2987	0	2846	110	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

The worst 5 of 110 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:311:LEU:O	1:A:312:ALA:CB	1.98	0.99

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	Distance(Å)	Clash(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%)	27 7

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%)	255 (87%)	37 (13%)	6 1

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	LYS
1	A	173	ASN
1	A	341	TYR
1	A	142	LYS
1	A	148	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	335	GLN
1	A	203	HIS
1	A	49	GLN
1	A	218	ASN

5.3.3 RNA (i)

There are no RNA chains 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)

2 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	1.27	1 (8%)	17,17,17	2.46	5 (29%)
2	GLC	A	372	2	10,11,12	0.95	0	11,15,17	1.25	1 (9%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	371	GLC	O5-C1	-2.90	1.37	1.43

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	371	GLC	C1-O5-C5	6.68	125.37	113.40
2	A	371	GLC	O5-C1-C2	4.49	116.82	109.86
2	A	371	GLC	O1-C1-O5	-4.31	98.71	110.32
2	A	371	GLC	O6-C6-C5	-2.56	102.56	111.36
2	A	372	GLC	O5-C5-C4	-2.24	107.81	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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