



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 08:12 PM UTC

PDB ID : 1EA9 / pdb_00001ea9
Title : Cyclomaltodextrinase
Authors : Cho, H.-S.; Kim, M.-S.; Oh, B.-H.
Deposited on : 2001-07-12
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
Xtrriage (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

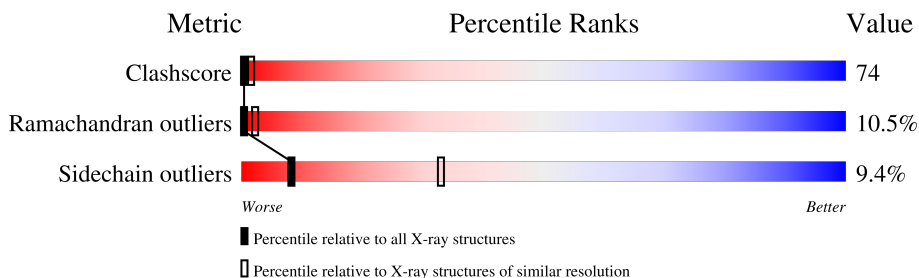
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

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	C	583	 18% 66% 14% •
1	D	583	 17% 64% 18% •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9582 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 CYCLOMALTODEXTRINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	583	4791	3092	804	876	19	0	0	0
1	D	583	4791	3092	804	876	19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

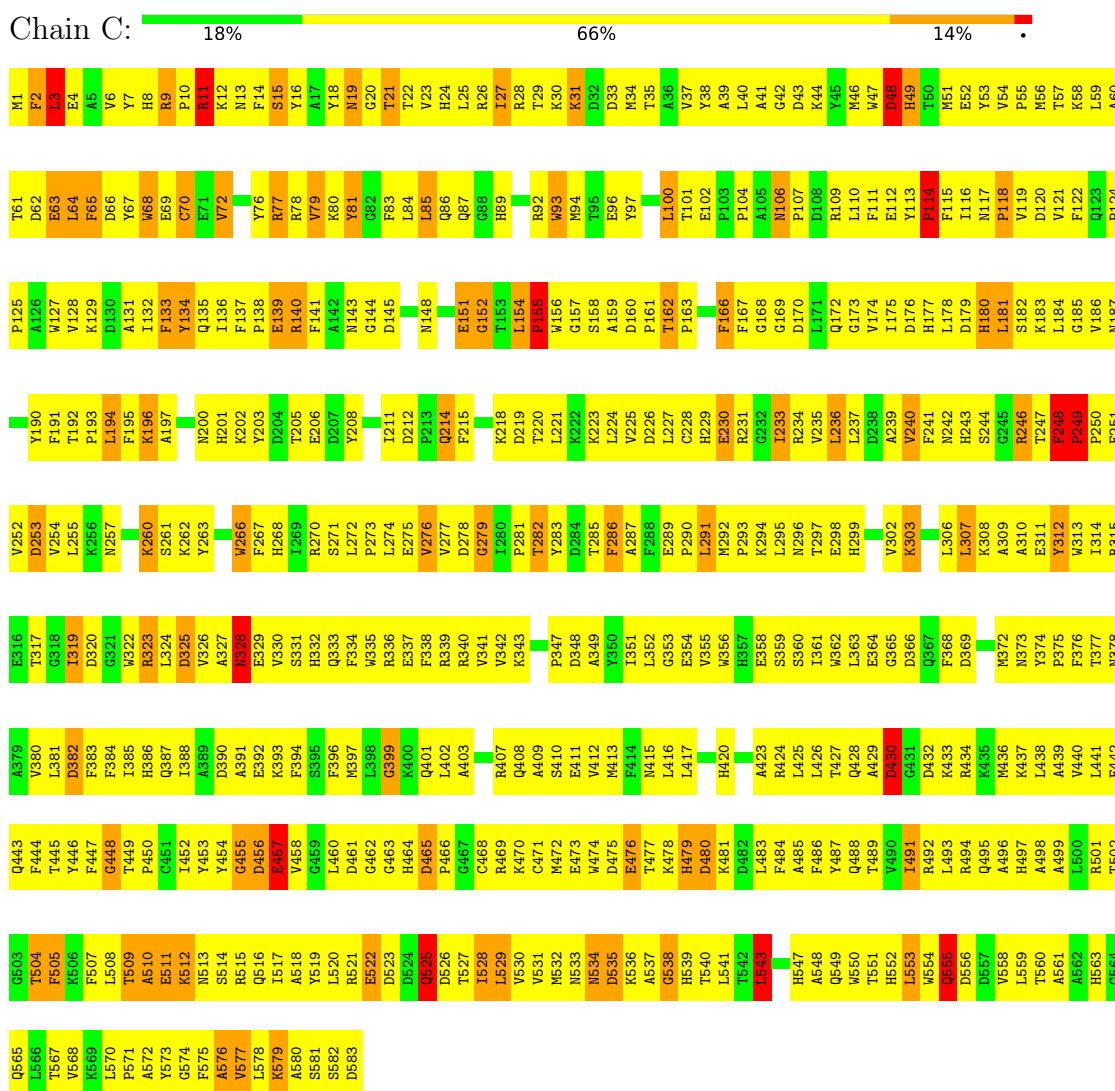
Chain	Residue	Modelled	Actual	Comment	Reference
C	14	PHE	TRP	conflict	UNP Q59226
C	105	ALA	ARG	conflict	UNP Q59226
D	14	PHE	TRP	conflict	UNP Q59226
D	105	ALA	ARG	conflict	UNP Q59226

3 Residue-property plots

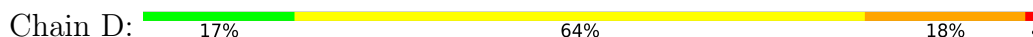
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 1: CYCLOMALTODEXTRINASE



H563	H564	G564	G565	L566	T567	Y568	K569	L570	P571	A572	G573	G574	F575	A576	V577	L578	K579	A580	S581	S582	D583																																						
I500	R501	T502	G503	T504	F505	L506	L507	T508	F509	A510	E511	E512	G513	T514	S514	R515	O516	A517	A518	Y519	L520	E522																																					
Q525	R526	T527	L528	L529	V530	M532	M533	M534	D535	K536	A537	G538	R539	T540	L541	T542	L543	P544	V545	R546	Q549	W550	T551	H552	L553	W554	O555	D556	D557	V558	L559	T560	A561	A562																									
R434	K435	M436	K437	L438	A439	V440	L441	F442	Q443	F444	T445	L446	F447	G448	G449	P450	C451	L452	Y453	Y454	D455	D456	F457	C458	C459	L460	G461	R469	K470	C471	M472	M473	W474	D475	E476	T477	K478	H479	D480	K481	D482	L483	F484	A485	F486	Y487	Q488	T489	W490	T491	R492	L493	L494	Q495	A498	D499	K433		
N373	Y374	P375	F376	T377	N378	A379	V380	L381	D382	F383	F384	L385	H386	Q387	I388	A389	D390	A391	E392	K393	F394	S395	F396	M397	L398	G399	K400	Q401	G404	Y405	P406	R407	Q408	A409	S410	E411	Y412	M413	N414	N415	D416	L417	D418	S419	H420	D421	T422	A423	R424	L425	L426	T427	Q428	A429	D430	G431	D432	K433	
Y312	W313	I314	R315	E316	T317	G318	I319	D320	G321	W322	F323	L324	D325	V326	A327	N328	E329	V330	S331	H332	Q333	F334	W335	R336	E337	F338	R339	R340	V341	V342	K343	N346	P347	Q348	D349	Y350	I351	L352	G353	E354	V355	H356	E358	S359	S360	I361	K362	L363	E364	G365	G366	Q367	L368	D369	A370	V371	M372		
V252	D253	V254	L255	K256	N257	G258	E259	K260	S261	K262	H263	Y264	D265	W266	F267	H268	I269	R270	S271	L272	P273	L274	E275	V276	V277	D278	G279	K280	I281	V282	Y283	D284	K285	T286	F287	A288	F289	P290	L291	M292	P293	K294	L295	T297	E298	H299	S300	D301	V302	K303	E304	Y305	G306	L307	L308	K308	A309	A310	E311
F191	T192	P193	L194	K195	R196	A197	T198	T199	N200	H201	K202	Y203	D204	T205	E206	H207	Y208	F209	Q210	I211	D212	P213	Q214	G216	D217	K218	L219	T220	L221	K222	K223	L224	V225	D226	L227	C228	H229	E230	T233	R234	V235	L236	L237	D238	A239	H240	F241	N242	H243	G244	G245	L246	T247	F248	P249	V250	F251		
M1	F2	L3	V6	Y7	H8	R9	P10	R11	K12	M13	F14	S15	Y16	R17	Y18	M19	G20	T21	T22	V23	H24	L25	L27	R28	K29	R30	K31	D32	D33	M34	V37	Y38	A39	L40	A41	G42	D43	Y45	M46	W47	D48	H49	T50	M51	F52	Y53	V54	P55	M56	T57	K58	L59	A60	Q123	P124				
E63	L64	F65	D66	Y67	W68	E69	C70	E71	V72	T73	P74	F75	Y76	R77	A78	W79	K80	Y81	G82	F83	L84	L85	Q86	H89	E90	K91	R92	W93	M94	T95	E96	Y97	D98	F99	L100	T101	E102	P103	P104	A105	M106	P107	D108	R109	L110	F111	E112	Y113	P114	F115	L116	N117	P118	V121	F122	Q123	P124		
P125	A126	M127	K129	D130	A131	I132	F133	Y134	Q135	T136	F137	P138	E139	R140	F141	Y142	K143	M148	D149	G152	L153	L154	P155	W156	A159	D160	P161	T162	P163	S164	C165	F166	F167	G168	E169	D170	L171	A172	Q173	G174	V174	I175	D176	H177	L178	D179	H180	K183	L184	G185	V186	M187	A188	V189	Q190	Y190			

4 Data and refinement statistics

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

Property	Value	Source
Space group	F 2 3	Depositor
Cell constants a, b, c, α , β , γ	334.61Å 334.61Å 334.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.20	Depositor
% Data completeness (in resolution range)	83.4 (10.00-3.20)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.214 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	C	0.38	0/4940	0.94	24/6714 (0.4%)
1	D	0.37	0/4940	0.93	29/6714 (0.4%)
All	All	0.37	0/9880	0.94	53/13428 (0.4%)

There are no bond length outliers.

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	79	VAL	N-CA-C	7.80	118.96	108.27
1	D	376	PHE	N-CA-C	-7.75	102.38	112.68
1	D	393	LYS	N-CA-C	-7.25	103.38	111.28
1	C	323	ARG	N-CA-C	-6.67	98.81	109.76
1	C	151	GLU	N-CA-C	6.58	119.02	110.53

There are no chirality outliers.

There are no planarity outliers.

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	C	4791	0	4588	679	1
1	D	4791	0	4588	715	0
All	All	9582	0	9176	1392	1

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 74.

The worst 5 of 1392 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:C:128:VAL:HG21	1:C:412:VAL:HG13	1.27	1.10
1:D:326:VAL:H	1:D:354:GLU:HB3	1.22	1.03
1:C:132:ILE:H	1:C:187:ASN:HB2	1.22	1.03
1:C:19:ASN:HD21	1:C:22:THR:N	1.56	1.02
1:C:19:ASN:ND2	1:C:22:THR:H	1.58	1.00

All (1) 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:C:12:LYS:NZ	1:C:12:LYS:NZ[4_566]	1.77	0.43

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	C	581/583 (100%)	384 (66%)	138 (24%)	59 (10%)	0 2
1	D	581/583 (100%)	360 (62%)	158 (27%)	63 (11%)	0 2
All	All	1162/1166 (100%)	744 (64%)	296 (26%)	122 (10%)	0 2

5 of 122 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	15	SER
1	C	31	LYS
1	C	49	HIS
1	C	70	CYS
1	C	114	PRO

5.3.2 Protein sidechains [i](#)

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	C	508/508 (100%)	464 (91%)	44 (9%)	9	36
1	D	508/508 (100%)	456 (90%)	52 (10%)	7	29
All	All	1016/1016 (100%)	920 (91%)	96 (9%)	8	33

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	156	TRP
1	D	328	ASN
1	D	184	LEU
1	D	237	LEU
1	D	373	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	187	ASN
1	D	378	ASN
1	D	296	ASN
1	D	332	HIS
1	D	387	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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.