wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 07:09 PM GMT

PDB ID	:	1EA9
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

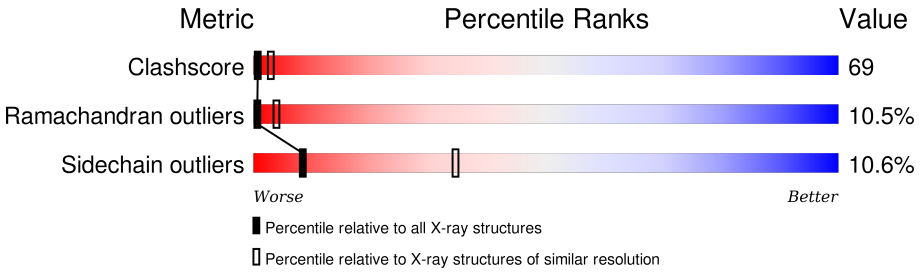
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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 <=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	C	583	20% 66% 13%
1	D	583	19% 64% 16%

2 Entry composition (i)

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
1	C	583	Total	C	N	O	S	0	0	0
			4791	3092	804	876	19			
1	D	583	Total	C	N	O	S	0	0	0
			4791	3092	804	876	19			

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

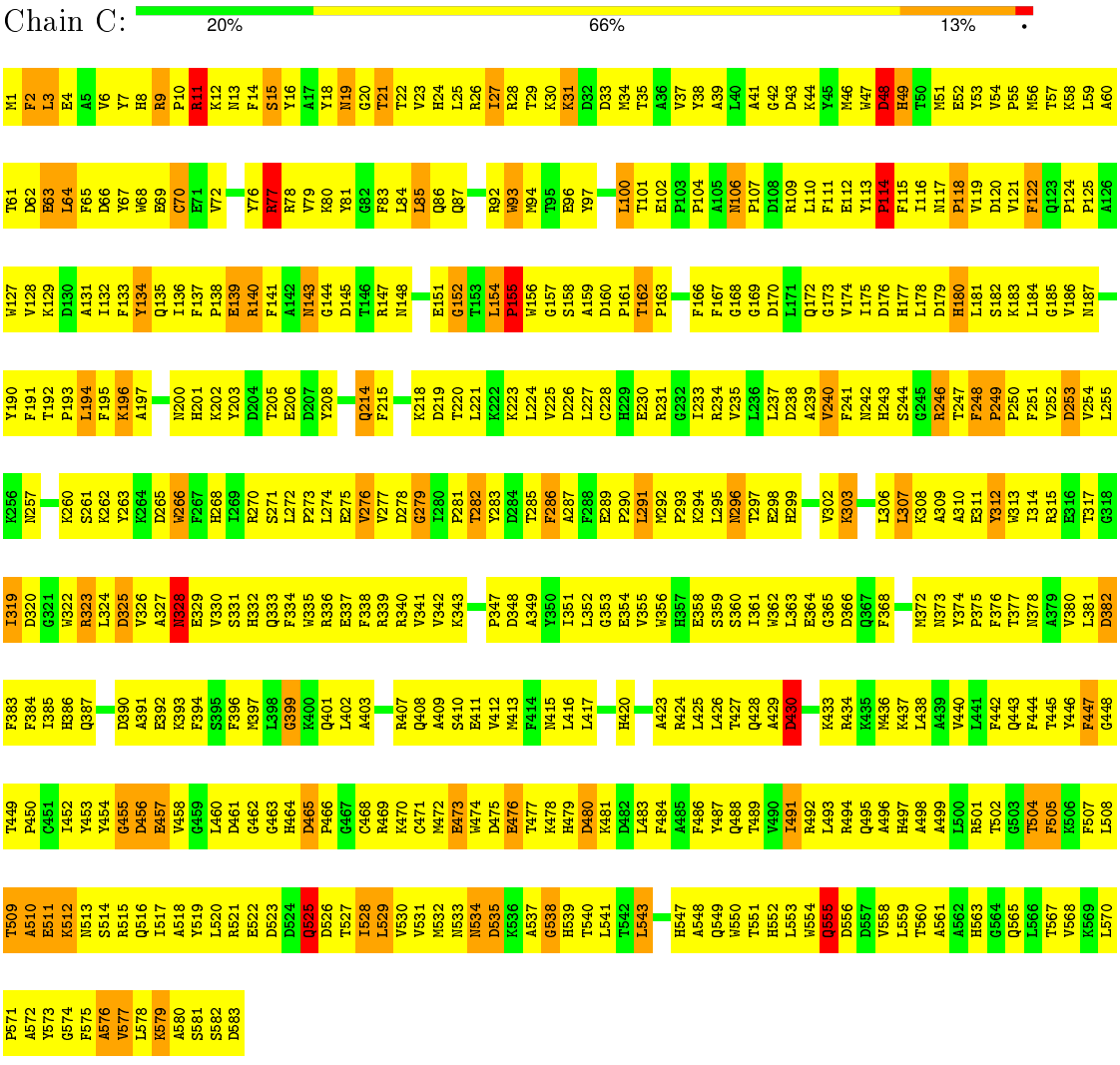
3 Residue-property plots (i)

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.

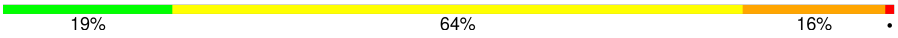
- Molecule 1: CYCLOMALTODEXTRINASE

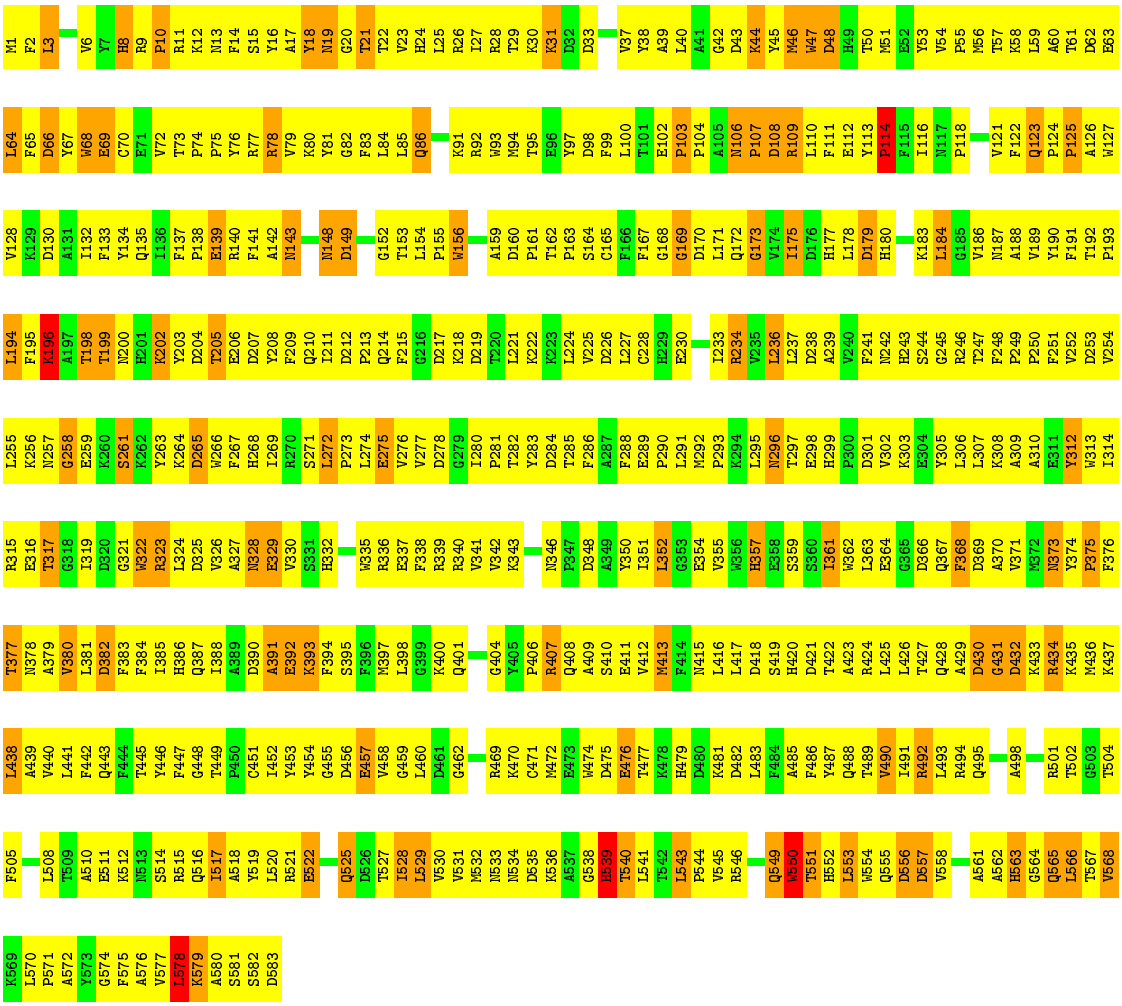
Chain C:



- Molecule 1: CYCLOMALTODEXTRINASE

Chain D:




M1 F2 L3 V6 Y7 H8 R9 P10 R11 K12 N13 F14 S15 Y16 A17 Y18 N19 G20 T21 T22 V23 H24 L25 R26 I27 R28 T29 K30 K31 D32 D33 V37 Y38 A39 L40 A41 G42 D43 K44 Y45 M46 W47 D48 H49 T50 M51 E52 Y53 V54 P55 M56 T57 K58 L59 A60 T61 D62 E63
L64 F65 D66 Y67 W68 E69 C70 E71 V72 T73 P74 P75 Y76 R77 R78 V79 K80 Y81 G82 F83 L84 L85 Q86 K91 R92 W93 M94 T95 E96 Y97 D98 F99 L100 T101 E102 P103 P104 A105 N106 P107 D108 R109 L110 F111 E112 Y113 P114 F115 I116 N117 P118 V121 F122 Q123 P124 P125 A126 W127
V128 K129 D130 A131 I132 F133 Y134 Q135 I136 F137 P138 E139 R140 F141 A142 N143 N148 D149 G152 T153 L154 P155 W156 A159 D160 P161 T162 P163 S164 C165 F166 F167 G168 G169 D170 L171 Q172 G173 V174 I175 D176 H177 L178 D179 H180 K183 L184 G185 V186 N187 A188 V189 Y190 F191 T192 P193
L194 F195 K196 A197 T198 T199 N200 H201 K202 Y203 D204 T205 E206 D207 Y208 F209 Q210 I211 D212 P213 Q214 F215 G216 D217 K218 D219 T220 L221 K222 K223 L224 V225 D226 L227 C228 H229 E230 I233 R234 V235 L236 I237 D238 A239 Y240 F241 N242 H243 S244 G245 R246 T247 F248 P249 P250 F251 V252 D253 V254
L255 K256 N257 G258 E259 K260 S261 K262 Y263 K264 D265 W266 F267 H268 I269 R270 S271 L272 P273 L274 E275 V276 V277 D278 G279 I280 P281 T282 Y283 D284 T285 F286 A287 F288 E289 P290 L291 M292 P293 K294 L295 N296 T297 E298 H299 P300 D301 V302 K303 E304 Y305 L306 L307 K308 A309 A310 E311 Y312 W313 I314
R315 E316 T317 G318 I319 D320 G321 W322 R323 I324 D325 V326 A327 N328 E329 V330 S331 H332 W335 R336 E337 F338 R339 R340 V341 V342 K343 N346 P347 D348 A349 Y350 I351 I352 G353 E354 V355 W356 H357 E358 S359 S360 I361 W362 L363 E364 G365 D366 Q367 F368 D369 A370 V371 N372 N373 Y374 P375 F376
T377 N378 A379 V380 L381 D382 F383 F384 I385 H386 Q387 I388 A389 D390 A391 E392 K393 F394 S395 F396 M397 L398 G399 K400 Q401 G404 Y405 P406 R407 Q408 A409 S410 E411 V412 M413 F414 N415 L416 L417 D418 S419 H420 D421 T422 A423 R424 L425 L426 T427 Q428 A429 D430 G431 D432 K433 R434 K435 M436 K437
L438 A439 V440 L441 F442 Q443 F444 T445 Y446 F447 G448 T449 P450 C451 I452 Y453 Y454 G455 D456 E457 V458 G459 L460 D461 G462 R469 K470 C471 M472 E473 W474 D475 E476 T477 K478 H479 D480 K481 D482 L483 F484 A485 F486 Y487 Q488 T489 V490 I491 R492 L493 R494 Q495 A498 R501 T502 G503 T504
F505 L508 T509 A510 E511 K512 N513 S514 R515 Q516 I517 A518 Y519 L520 R521 E522 Q525 D526 T527 I528 L529 V530 V531 N532 N533 N534 D535 K536 A537 G538 H539 T540 L541 T542 L543 P544 V545 R546 Q549 N550 T551 H552 L553 W554 Q555 D556 D557 V558 A561 A562 H563 G564 Q565 L566 T567 V568
R569 L570 P571 A572 Y573 G574 F575 A576 V577 L578 K579 A580 S581 S582 D583

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	9582	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.33	0/4940	0.59	0/6714
1	D	0.34	0/4940	0.59	0/6714
All	All	0.33	0/9880	0.59	0/13428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	C	4791	0	4588	638	1
1	D	4791	0	4588	656	0
All	All	9582	0	9176	1292	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 69.

The worst 5 of 1292 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	1 4
1	D	581/583 (100%)	360 (62%)	158 (27%)	63 (11%)	0 3
All	All	1162/1166 (100%)	744 (64%)	296 (26%)	122 (10%)	1 4

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%)	458 (90%)	50 (10%)	10 38
1	D	508/508 (100%)	450 (89%)	58 (11%)	7 31
All	All	1016/1016 (100%)	908 (89%)	108 (11%)	8 34

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	573	TYR
1	D	98	ASP
1	D	528	ILE
1	D	3	LEU
1	D	64	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	495	GLN
1	D	19	ASN
1	D	495	GLN
1	C	534	ASN
1	D	106	ASN

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 carbohydrates in this entry.

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

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.