



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 3, 2017 – 07:40 PM EST

PDB ID : 5OCQ
Title : Crystal structure of the complex of the kappa-carrageenase from *Pseudoalteromonas carrageenovora* with an oligotetrasaccharide of kappa-carrageenan
Authors : Czjzek, M.; Leroux, C.; Bernard, T.; Matard-Mann, M.; Jeudy, A.; Michel, G.
Deposited on : unknown
Resolution : 1.70 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 ⓘ symbol.

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

MolProbity : **FAILED**
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

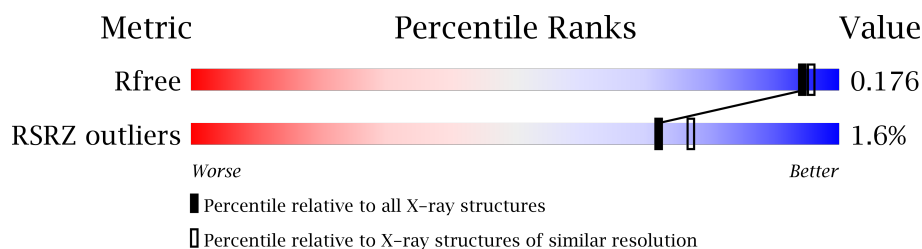
1 Overall quality at a glance

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))
R_{free}	100719	3453 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	A	405	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5272 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.

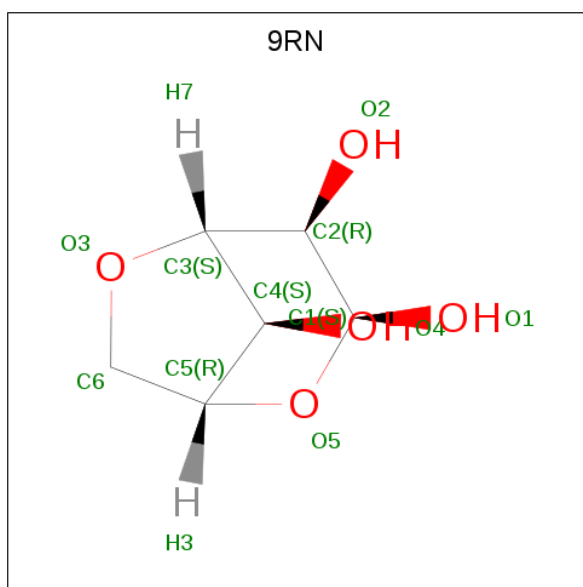
- Molecule 1 is a protein called Kappa-carrageenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	10	0
			2250	1427	395	421	7			
1	B	279	Total	C	N	O	S	0	7	0
			2309	1462	407	433	7			

There are 20 discrepancies between the modelled and reference sequences:

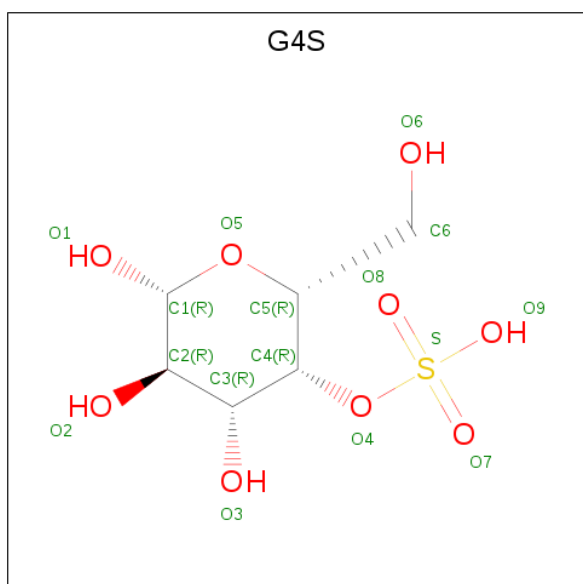
Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP P43478
A	168	ASP	GLU	engineered mutation	UNP P43478
A	302	LEU	-	expression tag	UNP P43478
A	303	GLU	-	expression tag	UNP P43478
A	304	HIS	-	expression tag	UNP P43478
A	305	HIS	-	expression tag	UNP P43478
A	306	HIS	-	expression tag	UNP P43478
A	307	HIS	-	expression tag	UNP P43478
A	308	HIS	-	expression tag	UNP P43478
A	309	HIS	-	expression tag	UNP P43478
B	25	MET	-	initiating methionine	UNP P43478
B	168	ASP	GLU	engineered mutation	UNP P43478
B	302	LEU	-	expression tag	UNP P43478
B	303	GLU	-	expression tag	UNP P43478
B	304	HIS	-	expression tag	UNP P43478
B	305	HIS	-	expression tag	UNP P43478
B	306	HIS	-	expression tag	UNP P43478
B	307	HIS	-	expression tag	UNP P43478
B	308	HIS	-	expression tag	UNP P43478
B	309	HIS	-	expression tag	UNP P43478

- Molecule 2 is 3,6-anhydro-D-galactose (three-letter code: 9RN) (formula: C₆H₁₀O₅).



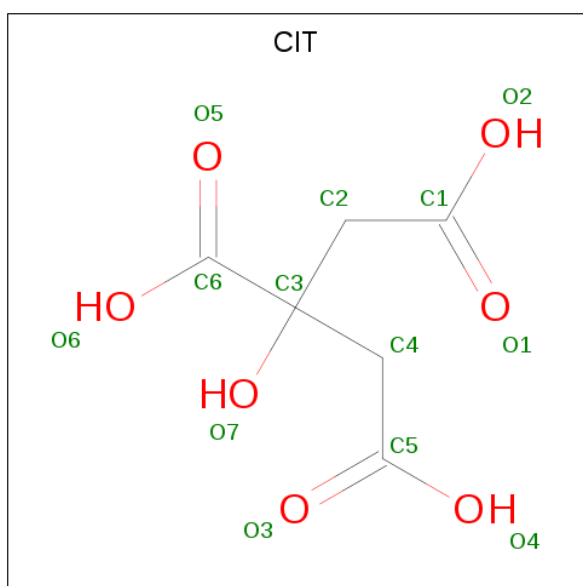
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	6	5		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			11	6	5		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is 4-O-sulfo-beta-D-galactopyranose (three-letter code: G4S) (formula: $C_6H_{12}O_9S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			15	6	8	1		
3	A	1	Total	C	O	S	0	0
			15	6	8	1		
3	B	1	Total	C	O	S	0	0
			15	6	8	1		
3	B	1	Total	C	O	S	0	0
			15	6	8	1		

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	261	Total	O	0	0
			261	261		
5	B	324	Total	O	0	0
			324	324		

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3 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.61Å 67.36Å 158.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.65 – 1.70 34.62 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.65-1.70) 99.4 (34.62-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.136 , 0.166 0.149 , 0.176	Depositor DCC
R_{free} test set	3733 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	9.5	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5272	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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4.3.3 RNA [i](#)

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

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4.5 Carbohydrates [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.6 Ligand geometry [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.7 Other polymers [i](#)

validation-pack failed to run properly - this section is therefore empty.

4.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	271/285 (95%)	-0.30	6 (2%) 62 68	4, 12, 28, 53	6 (2%)
1	B	279/285 (97%)	-0.44	3 (1%) 80 84	3, 9, 22, 46	3 (1%)
All	All	550/570 (96%)	-0.37	9 (1%) 72 77	3, 10, 26, 53	9 (1%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	GLY	3.3
1	A	27	SER	3.1
1	A	189	ASN	3.1
1	B	189	ASN	2.8
1	A	191	LYS	2.6

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

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

5.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CIT	A	405	13/13	0.93	0.17	12.84	11,37,60,61	0
4	CIT	B	405	13/13	0.92	0.20	1.47	12,28,39,40	0
3	G4S	A	402	15/16	0.95	0.10	0.73	11,14,22,23	0
2	9RN	B	403	10/11	0.98	0.07	-0.37	6,6,7,8	0
2	9RN	A	403	10/11	0.97	0.06	-0.55	10,11,12,12	0
3	G4S	A	404	15/16	0.98	0.06	-0.58	10,11,12,15	0
3	G4S	B	402	15/16	0.98	0.06	-1.17	7,10,18,20	0
3	G4S	B	404	15/16	0.99	0.05	-1.63	6,7,9,9	0
2	9RN	A	401	11/11	0.89	0.12	-	20,28,34,43	0
2	9RN	B	401	11/11	0.94	0.10	-	12,22,24,33	0

5.5 Other polymers [i](#)

There are no such residues in this entry.