



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:58 am BST

PDB ID : 1QAZ
Title : CRYSTAL STRUCTURE OF ALGINATE LYASE A1-III FROM SPHINGOMONAS SPECIES A1 AT 1.78Å RESOLUTION
Authors : Yoon, H.-J.
Deposited on : 1999-04-08
Resolution : 1.78 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

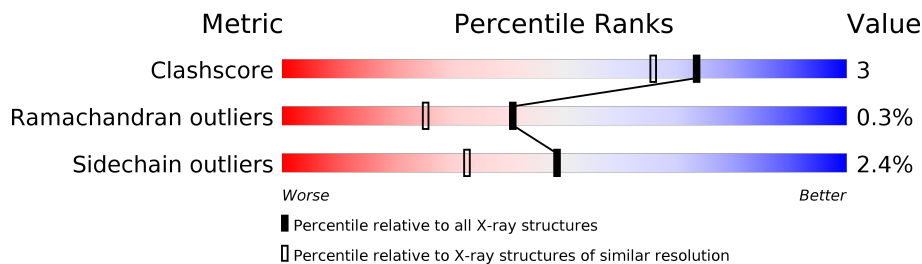
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	351	85% 13% .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 3101 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 PROTEIN (ALGINATE LYASE A1-III).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	351	2793	1767	489	524	13	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	ALA	conflict	UNP Q9KWU1
A	347	ALA	GLY	conflict	UNP Q9KWU1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	Total	O	S	0	0
			5	4	1		

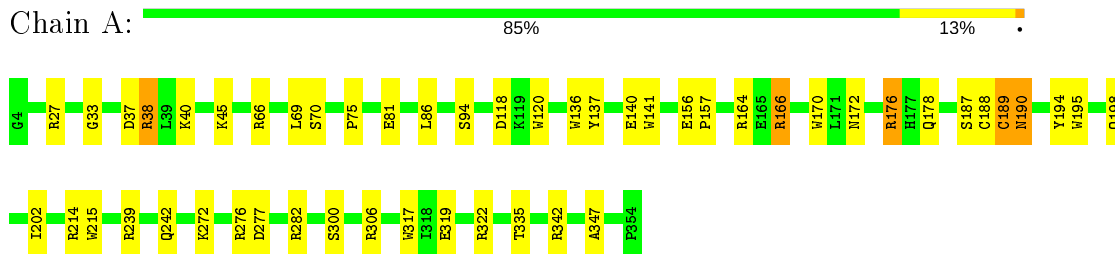
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	298	Total 298	O 298	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 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.

- Molecule 1: PROTEIN (ALGINATE LYASE A1-III)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	48.90Å 92.40Å 81.60Å 90.00° 104.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.78 42.21 – 1.29	Depositor EDS
% Data completeness (in resolution range)	89.9 (10.00-1.78) 8.7 (42.21-1.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.180 , 0.233 0.355 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 159.4	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.34	EDS
Total number of atoms	3101	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical 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.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.73	0/2866	1.40	38/3891 (1.0%)

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	1

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-18.34	111.13	120.30
1	A	38	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	A	215	TRP	CD1-CG-CD2	8.48	113.08	106.30
1	A	176	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	A	342	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	317	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	A	170	TRP	CD1-CG-CD2	7.79	112.53	106.30
1	A	136	TRP	CD1-CG-CD2	7.75	112.50	106.30
1	A	166	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	195	TRP	CD1-CG-CD2	7.52	112.31	106.30
1	A	170	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	A	141	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	A	239	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	120	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	141	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	120	TRP	CD1-CG-CD2	7.18	112.04	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	TRP	CE2-CD2-CG	-7.15	101.58	107.30
1	A	195	TRP	CE2-CD2-CG	-7.13	101.59	107.30
1	A	215	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	317	TRP	CE2-CD2-CG	-6.77	101.88	107.30
1	A	342	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	A	164	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	214	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	A	27	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	66	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	27	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	215	TRP	CG-CD1-NE1	-5.65	104.45	110.10
1	A	86	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	189	CYS	N-CA-C	5.55	126.00	111.00
1	A	214	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	282	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	120	TRP	CG-CD2-CE3	5.40	138.76	133.90
1	A	176	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	189	CYS	N-CA-CB	-5.21	101.21	110.60
1	A	166	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	276	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	317	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	A	170	TRP	CG-CD2-CE3	5.12	138.51	133.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	194	TYR	Sidechain

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	A	2793	0	2699	18	0
2	A	10	0	0	0	0
3	A	298	0	0	3	0
All	All	3101	0	2699	18	0

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 3.

All (18) 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:38:ARG:HD2	1:A:335:THR:O	1.96	0.65
1:A:242:GLN:HE22	1:A:306:ARG:HH12	1.48	0.62
1:A:137:TYR:O	1:A:140:GLU:HG2	2.05	0.56
1:A:188:CYS:SG	1:A:189:CYS:N	2.84	0.50
1:A:176:ARG:HD3	3:A:582:HOH:O	2.12	0.49
1:A:118:ASP:OD2	1:A:166:ARG:HD2	2.15	0.47
1:A:242:GLN:HE22	1:A:306:ARG:NH1	2.10	0.46
1:A:242:GLN:NE2	1:A:306:ARG:HH12	2.14	0.46
1:A:75:PRO:HD2	3:A:690:HOH:O	2.15	0.45
1:A:322:ARG:NH1	3:A:586:HOH:O	2.49	0.45
1:A:69:LEU:HD12	1:A:75:PRO:HB2	1.99	0.45
1:A:272:LYS:HG2	1:A:277:ASP:HB3	2.01	0.42
1:A:172:ASN:O	1:A:176:ARG:HG3	2.20	0.42
1:A:319:GLU:HB2	1:A:347:ALA:CB	2.50	0.42
1:A:198:GLN:O	1:A:202:ILE:HG22	2.20	0.41
1:A:187:SER:HA	1:A:190:ASN:ND2	2.36	0.40
1:A:37:ASP:HA	1:A:40:LYS:HE3	2.03	0.40
1:A:156:GLU:HA	1:A:157:PRO:HD2	2.00	0.40

There are no symmetry-related clashes.

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	A	349/351 (99%)	338 (97%)	10 (3%)	1 (0%)	41 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	33	GLY

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	A	293/293 (100%)	286 (98%)	7 (2%)	49 33

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	70	SER
1	A	81	GLU
1	A	94	SER
1	A	178	GLN
1	A	190	ASN
1	A	300	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	GLN
1	A	172	ASN
1	A	178	GLN
1	A	190	ASN
1	A	222	GLN
1	A	242	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	SO4	A	700	-	4,4,4	0.36	0	6,6,6	0.24	0
2	SO4	A	701	-	4,4,4	0.55	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.