Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 11:26 PM EDT

PDB ID	:	1HE9
Title	:	Crystal structure of the GAP domain of the Pseudomonas aeruginosa ExoS toxin
Authors	:	Wurtele, M.; Renault, L.; Barbieri, J.T.; Wittinghofer, A.; Wolf, E.
Deposited on	:	2000-11-21
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

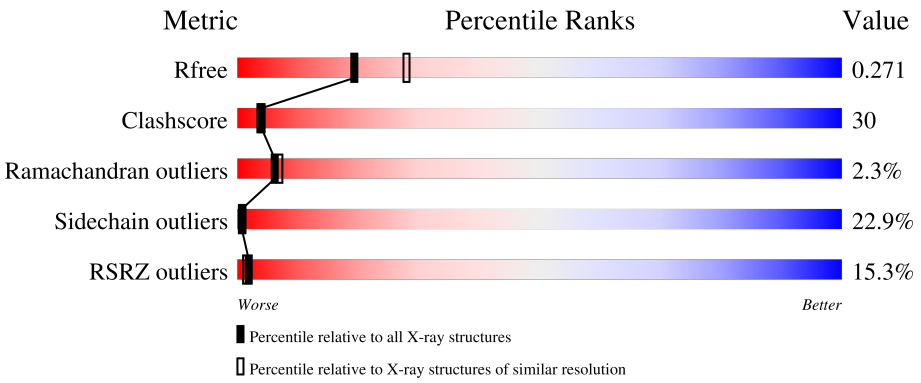
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

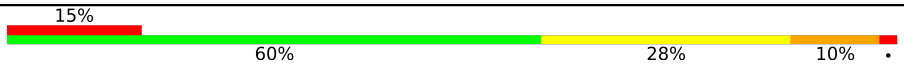
The reported resolution of this entry is 2.40 Å.

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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.

Mol	Chain	Length	Quality of chain
1	A	134	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 1065 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 EXOENZYME S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	134	1000	611	186	200	3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	235	TYR	LYS	cloning artifact	UNP Q51451
A	104	MSE	MET	modified residue	UNP Q51451
A	112	MSE	MET	modified residue	UNP Q51451
A	214	MSE	MET	modified residue	UNP Q51451

- Molecule 2 is water.

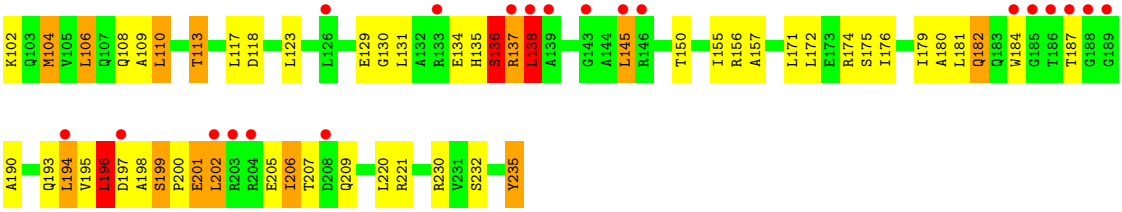
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	65	65	65	0	0

3 Residue-property plots (i)

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 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.

- Molecule 1: EXOENZYME S

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	42.90Å 55.65Å 107.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 16.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.40) 99.2 (16.82-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	7.20 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.265 0.259 , 0.271	Depositor DCC
R_{free} test set	518 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	42.0	Xtriage
Anisotropy	0.845	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	1065	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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)

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	0.88	0/1004	1.07	4/1347 (0.3%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	A	118	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	138	LEU	CA-CB-CG	5.97	129.03	115.30
1	A	196	LEU	CA-CB-CG	5.92	128.92	115.30

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	A	1000	0	1023	61	0
2	A	65	0	0	8	0
All	All	1065	0	1023	61	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 30.

All (61) 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:179:ILE:HD12	1:A:194:LEU:HD12	1.42	1.00
1:A:135:HIS:HB3	1:A:195:VAL:HG11	1.53	0.89
1:A:134:GLU:HG3	1:A:138:LEU:HG	1.57	0.87
1:A:110:LEU:O	1:A:113:THR:HB	1.75	0.85
1:A:135:HIS:CB	1:A:195:VAL:HG11	2.08	0.83
1:A:184:TRP:CH2	1:A:206:ILE:HD13	2.13	0.83
1:A:205:GLU:HG2	1:A:209:GLN:NE2	1.93	0.82
1:A:156:ARG:CD	2:A:2024:HOH:O	2.27	0.81
1:A:102:LYS:O	1:A:106:LEU:HD22	1.82	0.79
1:A:102:LYS:O	1:A:102:LYS:HG2	1.82	0.77
1:A:202:LEU:O	1:A:206:ILE:HG23	1.88	0.73
1:A:205:GLU:HG2	1:A:209:GLN:HE22	1.52	0.73
1:A:156:ARG:HD3	2:A:2024:HOH:O	1.88	0.72
1:A:199:SER:O	1:A:201:GLU:N	2.23	0.70
1:A:135:HIS:ND1	1:A:136:SER:N	2.41	0.69
1:A:194:LEU:O	1:A:198:ALA:HB2	1.95	0.66
1:A:194:LEU:HD21	1:A:202:LEU:CD1	2.26	0.65
1:A:190:ALA:O	1:A:194:LEU:HB2	1.97	0.64
1:A:136:SER:OG	1:A:137:ARG:N	2.32	0.61
1:A:194:LEU:HD21	1:A:202:LEU:HD13	1.82	0.61
1:A:179:ILE:HD12	1:A:194:LEU:CD1	2.25	0.61
1:A:184:TRP:CZ3	1:A:206:ILE:HD13	2.35	0.60
1:A:129:GLU:HB2	2:A:2017:HOH:O	2.02	0.59
1:A:175:SER:HB3	2:A:2039:HOH:O	2.01	0.59
1:A:102:LYS:O	1:A:102:LYS:CG	2.52	0.58
1:A:179:ILE:CD1	1:A:194:LEU:HD12	2.26	0.58
1:A:104:MSE:H	1:A:104:MSE:SE	2.38	0.57
1:A:106:LEU:HG	1:A:157:ALA:HB1	1.87	0.57
1:A:109:ALA:O	1:A:110:LEU:C	2.43	0.56
1:A:199:SER:C	1:A:201:GLU:H	2.10	0.55
1:A:235:TYR:CD1	1:A:235:TYR:N	2.74	0.55
1:A:194:LEU:O	1:A:198:ALA:N	2.40	0.54
1:A:135:HIS:O	1:A:138:LEU:HD12	2.08	0.54
1:A:156:ARG:HD2	2:A:2024:HOH:O	2.02	0.53
1:A:134:GLU:O	1:A:135:HIS:C	2.46	0.53
1:A:137:ARG:C	1:A:137:ARG:HD2	2.30	0.52
1:A:135:HIS:HB2	1:A:195:VAL:HG11	1.92	0.51
1:A:176:ILE:HB	1:A:184:TRP:NE1	2.25	0.51
1:A:156:ARG:NH1	2:A:2024:HOH:O	2.30	0.50
1:A:135:HIS:CG	1:A:136:SER:H	2.30	0.49
1:A:135:HIS:CG	1:A:136:SER:N	2.81	0.48
1:A:187:THR:HG23	1:A:187:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:HD22	1:A:182:GLN:HB2	1.96	0.47
1:A:123:LEU:HD11	1:A:145:LEU:HD13	1.96	0.47
1:A:130:GLY:O	1:A:134:GLU:HG2	2.15	0.46
1:A:176:ILE:HG22	1:A:206:ILE:HB	1.98	0.45
1:A:205:GLU:CG	1:A:209:GLN:HE22	2.25	0.45
1:A:131:LEU:CD2	1:A:206:ILE:HG12	2.45	0.45
1:A:194:LEU:O	1:A:198:ALA:CB	2.61	0.45
1:A:201:GLU:HG3	1:A:202:LEU:H	1.82	0.45
1:A:230:ARG:HD3	2:A:2062:HOH:O	2.17	0.44
1:A:184:TRP:CZ3	1:A:206:ILE:CD1	3.01	0.43
1:A:196:LEU:HD23	2:A:2046:HOH:O	2.17	0.43
1:A:199:SER:C	1:A:201:GLU:N	2.68	0.43
1:A:129:GLU:CD	1:A:129:GLU:H	2.21	0.43
1:A:180:ALA:O	1:A:181:LEU:C	2.57	0.43
1:A:232:SER:HA	1:A:235:TYR:CD1	2.54	0.43
1:A:102:LYS:HG2	1:A:106:LEU:HD22	2.01	0.42
1:A:205:GLU:CG	1:A:209:GLN:NE2	2.74	0.42
1:A:194:LEU:CD2	1:A:202:LEU:HD13	2.49	0.41
1:A:113:THR:HG23	1:A:155:ILE:HD11	2.03	0.41

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	132/134 (98%)	118 (89%)	11 (8%)	3 (2%)	6 7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	SER
1	A	137	ARG

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Mol	Chain	Res	Type
1	A	200	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	A	105/102 (103%)	81 (77%)	24 (23%)	1 1

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	MSE
1	A	106	LEU
1	A	108	GLN
1	A	110	LEU
1	A	113	THR
1	A	117	LEU
1	A	136	SER
1	A	138	LEU
1	A	145	LEU
1	A	150	THR
1	A	171	LEU
1	A	182	GLN
1	A	193	GLN
1	A	194	LEU
1	A	196	LEU
1	A	197	ASP
1	A	199	SER
1	A	201	GLU
1	A	202	LEU
1	A	206	ILE
1	A	207	THR
1	A	220	LEU
1	A	221	ARG
1	A	235	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	A	108	GLN
1	A	193	GLN
1	A	222	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 monosaccharides 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 (i)

6.1 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	131/134 (97%)	0.95	20 (15%) 2 1	29, 51, 112, 119	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	THR	9.0
1	A	187	THR	8.1
1	A	185	GLY	7.8
1	A	139	ALA	6.4
1	A	188	GLY	4.8
1	A	189	GLY	4.1
1	A	184	TRP	3.4
1	A	146	ARG	3.3
1	A	145	LEU	3.3
1	A	203	ARG	3.3
1	A	143	GLY	2.9
1	A	138	LEU	2.8
1	A	202	LEU	2.7
1	A	133	ARG	2.4
1	A	197	ASP	2.4
1	A	204	ARG	2.3
1	A	208	ASP	2.2
1	A	137	ARG	2.2
1	A	194	LEU	2.0
1	A	126	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.