wwPDB X-ray Structure Validation Summary Report (i)

Jun 24, 2024 – 02:28 AM EDT

PDB ID	:	6QER
Title	:	Apo Form Of ComR From S. Thermophilus in space group C2
Authors	:	Thuillier, J.; Nessler, S.
Deposited on	:	2019-01-08
Resolution	:	2.46 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 (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 (1)) were used in the production of this report:

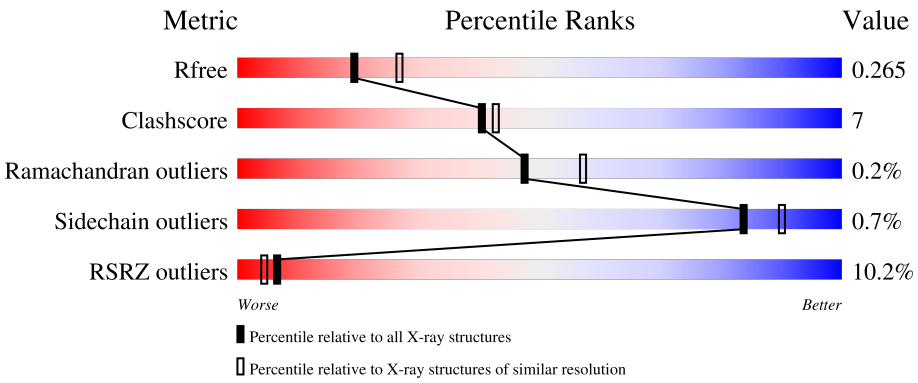
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.46 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	310	2% 79% 17% •
1	B	310	6% 76% 20% • •
1	C	310	% 83% 16% •
1	D	310	30% 71% 23% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10054 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 Transcriptional regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2492	1609	406	471	6	0	0	0
1	B	300	2492	1609	406	471	6	0	0	0
1	C	305	2531	1634	414	477	6	0	0	0
1	D	294	2450	1585	399	461	5	0	0	0

- Molecule 2 is water.

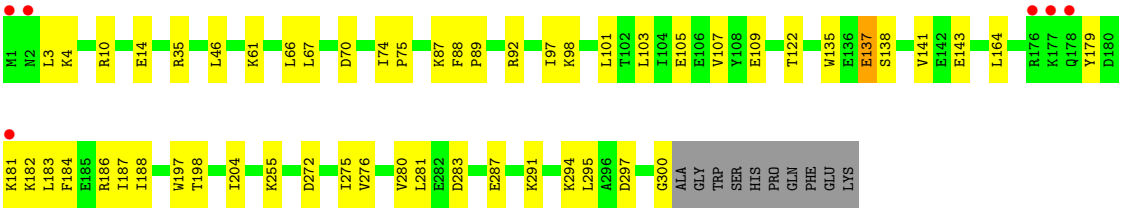
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	32	32	32	0	0
2	B	20	20	20	0	0
2	C	32	32	32	0	0
2	D	5	5	5	0	0

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.

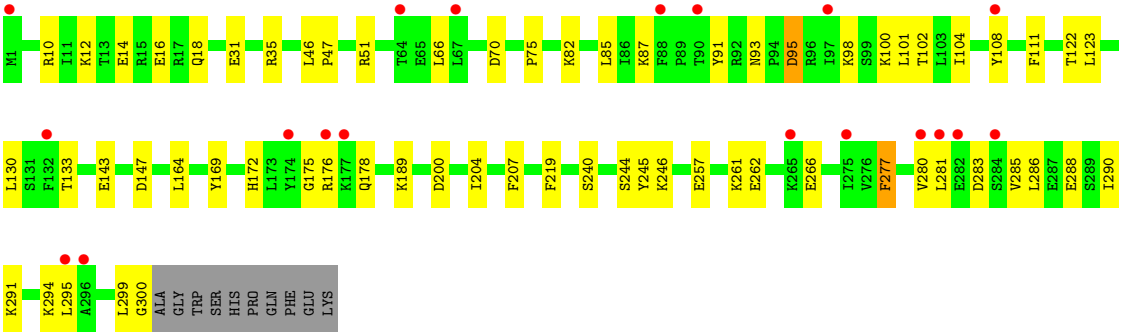
• Molecule 1: Transcriptional regulator

Chain A:



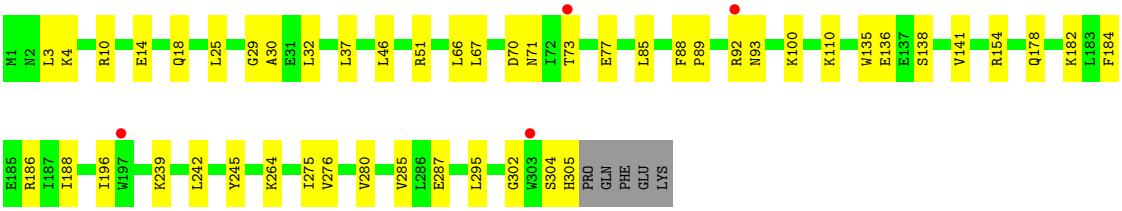
• Molecule 1: Transcriptional regulator

Chain B:



• Molecule 1: Transcriptional regulator

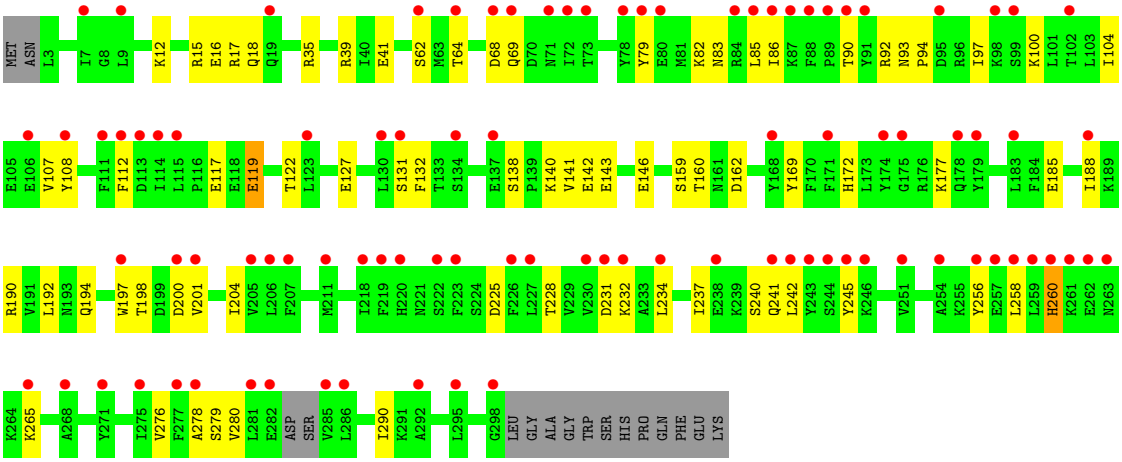
Chain C:



• Molecule 1: Transcriptional regulator

Chain D:

30%
71%
23%
5%


MET ASN L3 I7 G8 L9 K12 R15 E16 R17 Q18 Q19 R35 R39 I40 E41 S62 M63 T64 D68 Q69 D70 N71 I72 T73 Y78 Y79 E80 M81 K82 N83 R84 L85 I86 K87 F88 P89 T90 Y91 R92 N93 P94 D95 R96 I97 K98 S99 K100 L101 T102 L103 I104
E105 E106 V107 Y108 F111 F112 D113 I114 L115 P116 E117 E118 E119 T122 L123 E127 L130 S131 F132 T133 S134 E137 S138 P139 K140 V141 E142 E143 E146 S159 T160 N161 D162 Y168 Y169 F170 F171 H172 L173 Y174 G175 R176 K177 Q178 Y179 L183 F184 E185 I188 K189
R190 V191 L192 N193 Q194 W197 T198 D199 D200 V201 I204 V205 L206 F207 M211 I218 F219 H220 N221 S222 F223 S224 D225 F226 L227 T228 V229 V230 D231 K232 A233 L234 I237 E238 K239 S240 Q241 L242 Y243 S244 Y245 K246 V251 A254 K255 Y256 E257 L258 L259 H260 K261 E262 N263
K264 K265 A268 Y271 I275 V276 F277 A278 S279 V280 L281 E282 ASP SER V285 L286 I290 K291 A292 L295 G298 LEU GLY ALA GLY TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	271.79Å 73.72Å 78.31Å 90.00° 104.97° 90.00°	Depositor
Resolution (Å)	44.24 – 2.46 44.24 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.3 (44.24-2.46) 99.5 (44.24-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.231 , 0.264 0.237 , 0.265	Depositor DCC
R_{free} test set	2703 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10054	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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	0.66	0/2535	0.67	1/3411 (0.0%)
1	B	0.55	0/2535	0.61	0/3411
1	C	0.71	0/2577	0.65	0/3469
1	D	0.39	0/2492	0.56	1/3352 (0.0%)
All	All	0.59	0/10139	0.62	2/13643 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	LEU	CA-CB-CG	6.08	129.28	115.30
1	D	260	HIS	N-CA-C	-6.00	94.81	111.00

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	2492	0	2545	33	0
1	B	2492	0	2545	42	0
1	C	2531	0	2575	27	0
1	D	2450	0	2503	46	0
2	A	32	0	0	2	0
2	B	20	0	0	1	0
2	C	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	0	0
All	All	10054	0	10168	144	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 7.

The worst 5 of 144 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:B:257:GLU:HG2	1:B:266:GLU:HB2	1.51	0.90
1:D:79:TYR:O	1:D:83:ASN:ND2	2.17	0.78
1:A:272:ASP:OD1	1:A:294:LYS:NZ	2.16	0.78
1:B:108:TYR:CE1	1:B:123:LEU:HB3	2.18	0.78
1:B:178:GLN:N	1:B:178:GLN:OE1	2.22	0.71

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	298/310 (96%)	289 (97%)	9 (3%)	0	100	100
1	B	298/310 (96%)	289 (97%)	8 (3%)	1 (0%)	41	49
1	C	303/310 (98%)	295 (97%)	8 (3%)	0	100	100
1	D	290/310 (94%)	282 (97%)	7 (2%)	1 (0%)	41	49
All	All	1189/1240 (96%)	1155 (97%)	32 (3%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	PHE

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Mol	Chain	Res	Type
1	B	262	GLU

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	278/286 (97%)	277 (100%)	1 (0%)	91 94
1	B	278/286 (97%)	274 (99%)	4 (1%)	67 77
1	C	281/286 (98%)	280 (100%)	1 (0%)	91 94
1	D	273/286 (96%)	271 (99%)	2 (1%)	84 90
All	All	1110/1144 (97%)	1102 (99%)	8 (1%)	84 90

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	119	GLU
1	D	64	THR
1	B	277	PHE
1	B	133	THR
1	C	305	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	300/310 (96%)	0.16	6 (2%) 65 62	22, 34, 60, 88	0
1	B	300/310 (96%)	0.59	19 (6%) 20 16	25, 54, 117, 171	0
1	C	305/310 (98%)	0.09	4 (1%) 77 76	21, 32, 51, 68	0
1	D	294/310 (94%)	1.58	93 (31%) 0 0	37, 115, 178, 184	0
All	All	1199/1240 (96%)	0.60	122 (10%) 6 4	21, 44, 154, 184	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	TYR	9.4
1	D	258	LEU	8.4
1	D	111	PHE	6.2
1	D	278	ALA	5.9
1	D	223	PHE	5.8

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.