



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:55 AM UTC

PDB ID : 8HML / pdb_00008hml
Title : Co-crystal structure of the C terminal DNA binding domain of Saccharopolyspora erythraea GlnR in complex with its conserved promoter DNA in 2.95 Angstrom resolution
Authors : Lin, W.; Xu, J.C.
Deposited on : 2022-12-04
Resolution : 2.95 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

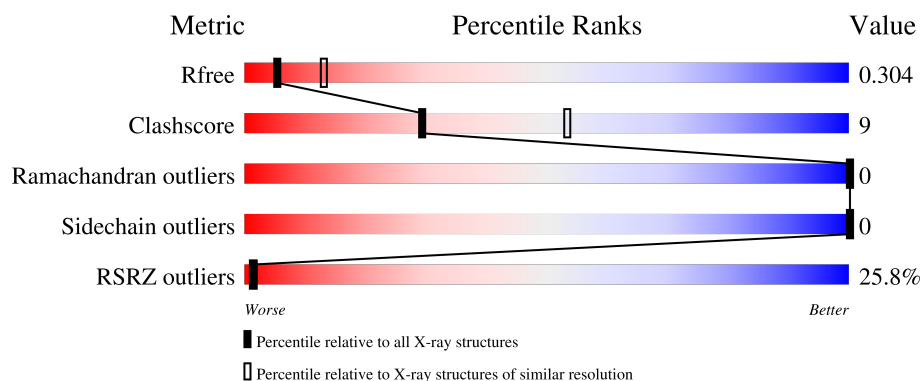
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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 $\leq 5\%$. 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	143	14% 55% 14% 31%
1	B	143	27% 54% 13% 34%
2	D	20	65% 35%
3	C	20	10% 70% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2351 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 DNA-binding response OmpR family regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			770	490	139	138	3			
1	B	95	Total	C	N	O	S	0	0	0
			754	482	136	135	1			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	MET	-	initiating methionine	UNP A4FQD5
A	114	HIS	-	expression tag	UNP A4FQD5
A	115	HIS	-	expression tag	UNP A4FQD5
A	116	HIS	-	expression tag	UNP A4FQD5
A	117	HIS	-	expression tag	UNP A4FQD5
A	118	HIS	-	expression tag	UNP A4FQD5
A	119	HIS	-	expression tag	UNP A4FQD5
A	120	MET	-	expression tag	UNP A4FQD5
A	121	ALA	-	expression tag	UNP A4FQD5
B	114	MET	-	initiating methionine	UNP A4FQD5
B	115	HIS	-	expression tag	UNP A4FQD5
B	116	HIS	-	expression tag	UNP A4FQD5
B	117	HIS	-	expression tag	UNP A4FQD5
B	118	HIS	-	expression tag	UNP A4FQD5
B	119	HIS	-	expression tag	UNP A4FQD5
B	120	HIS	-	expression tag	UNP A4FQD5
B	121	MET	-	expression tag	UNP A4FQD5
B	122	ALA	-	expression tag	UNP A4FQD5

- Molecule 2 is a DNA chain called DNA (5'-D(*AP*CP*GP*TP*AP*AP*CP*AP*TP*CP*GP*CP*GP*GP*TP*AP*AP*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	20	Total 406	C 194	N 79	O 114	P 19	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*GP*TP*TP*AP*CP*CP*GP*CP*GP*AP*TP*GP*TP*TP*AP*CP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	20	Total 406	C 195	N 71	O 121	P 19	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total 3	O 3	0	0
4	B	4	Total 4	O 4	0	0
4	D	4	Total 4	O 4	0	0
4	C	4	Total 4	O 4	0	0

- Molecule 1: DNA-binding response OmpR family regulator



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	46.28Å 46.28Å 366.86Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.84 – 2.95 39.84 – 2.95	Depositor EDS
% Data completeness (in resolution range)	86.5 (39.84-2.95) 86.5 (39.84-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.10 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.256 , 0.312 0.252 , 0.304	Depositor DCC
R_{free} test set	923 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.055 for -h,-k,l	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	2351	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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.

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	0.11	0/782	0.33	0/1052
1	B	0.16	0/768	0.43	0/1036
2	D	0.21	0/456	0.40	0/701
3	C	0.21	0/454	0.48	0/700
All	All	0.17	0/2460	0.41	0/3489

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 [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	770	0	778	17	0
1	B	754	0	752	14	0
2	D	406	0	225	9	0
3	C	406	0	225	4	0
4	A	3	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
All	All	2351	0	1980	37	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 9.

All (37) 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:166:VAL:HA	1:A:216:LYS:HB3	1.69	0.74
1:B:194:ARG:NH2	2:D:3:DG:O6	2.31	0.63
2:D:2:DC:H2''	2:D:3:DG:C8	2.35	0.61
1:B:154:GLU:HB3	1:B:176:VAL:HG13	1.85	0.58
3:C:1:DG:H2'	3:C:2:DT:C6	2.41	0.56
2:D:4:DT:H2''	2:D:5:DA:C8	2.41	0.55
1:B:141:LEU:HD13	1:B:203:TYR:CD2	2.42	0.54
1:A:158:TYR:CE1	1:A:175:GLU:HG2	2.43	0.53
1:B:151:LYS:HZ3	1:B:177:TRP:CD1	2.27	0.52
1:A:186:ARG:NH2	3:C:3:DG:N7	2.58	0.52
3:C:14:DG:H2''	3:C:15:DT:O5'	2.08	0.52
2:D:1:DA:H2''	2:D:2:DC:H5''	1.92	0.52
1:A:190:VAL:HG21	2:D:15:DT:H71	1.93	0.51
1:A:186:ARG:O	1:A:190:VAL:HG23	2.12	0.49
2:D:4:DT:H2''	2:D:5:DA:H8	1.79	0.48
1:A:166:VAL:HB	1:A:216:LYS:HD3	1.96	0.48
1:B:136:THR:OG1	1:B:138:THR:OG1	2.26	0.47
1:A:173:LEU:O	1:A:177:TRP:HB2	2.14	0.47
1:B:127:VAL:HA	1:B:130:LEU:O	2.14	0.47
1:A:203:TYR:HD1	1:A:206:MET:HE3	1.80	0.46
1:B:136:THR:HG1	1:B:138:THR:HG1	1.55	0.46
1:A:193:ARG:C	1:A:193:ARG:HD3	2.42	0.45
1:A:149:THR:CG2	1:A:152:GLU:H	2.29	0.45
1:B:196:ARG:NH2	1:B:209:THR:OG1	2.34	0.44
1:B:132:ILE:O	1:B:132:ILE:HG13	2.17	0.44
1:A:192:VAL:O	1:A:196:ARG:HG3	2.18	0.44
1:B:173:LEU:O	1:B:177:TRP:HB2	2.18	0.43
1:A:193:ARG:NE	3:C:5:DT:OP2	2.40	0.43
1:B:187:THR:OG1	2:D:3:DG:OP2	2.29	0.43
1:A:203:TYR:CD1	1:A:206:MET:HE3	2.54	0.42
1:A:146:LEU:HB3	1:A:148:LEU:HD21	2.01	0.42
1:A:159:LEU:HD21	1:A:172:LEU:HD21	2.01	0.42
1:B:189:ASP:OD1	1:B:189:ASP:N	2.52	0.42
1:A:137:TYR:HB2	1:B:166:VAL:HG11	2.01	0.42
1:A:149:THR:OG1	2:D:12:DC:H3'	2.20	0.41
2:D:3:DG:H2''	2:D:4:DT:H72	2.03	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	94/143 (66%)	87 (93%)	7 (7%)	0	100	100
1	B	93/143 (65%)	85 (91%)	8 (9%)	0	100	100
All	All	187/286 (65%)	172 (92%)	15 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	78/117 (67%)	78 (100%)	0	100	100
1	B	76/117 (65%)	76 (100%)	0	100	100
All	All	154/234 (66%)	154 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	212	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 oligosaccharides 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	98/143 (68%)	1.52	20 (20%) 3 2	9, 19, 43, 53	0
1	B	95/143 (66%)	1.96	38 (40%) 1 0	6, 26, 65, 77	0
2	D	20/20 (100%)	0.63	0 100 100	11, 15, 24, 24	0
3	C	20/20 (100%)	0.95	2 (10%) 12 11	8, 19, 27, 27	0
All	All	233/326 (71%)	1.58	60 (25%) 1 1	6, 20, 57, 77	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	143	GLY	6.0
1	B	185	THR	6.0
1	B	150	TYR	5.9
1	B	182	PHE	5.8
1	A	179	TYR	5.6
1	A	221	SER	5.5
1	B	145	ALA	5.1
1	A	185	THR	5.0
1	B	144	ARG	4.8
1	B	135	SER	4.4
1	B	179	TYR	4.3
1	B	181	PHE	4.1
1	B	147	GLU	4.1
1	B	142	LYS	4.0
1	B	128	GLY	3.9
1	B	178	GLY	3.8
1	A	204	ASP	3.8
1	B	221	SER	3.7
1	B	141	LEU	3.7
1	A	183	GLY	3.6
1	B	183	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	136	THR	3.5
1	B	154	GLU	3.5
1	B	220	PRO	3.4
1	B	184	GLY	3.3
1	A	134	GLU	3.2
1	B	127	VAL	3.2
1	A	136	THR	3.2
1	A	213	VAL	3.1
1	B	171	GLN	3.1
1	B	140	ARG	3.1
1	B	146	LEU	3.1
1	B	180	ASP	3.0
1	B	133	GLU	3.0
1	B	137	TYR	3.0
1	A	120	MET	2.9
3	C	1	DG	2.7
1	A	218	VAL	2.7
1	A	161	GLN	2.6
1	A	184	GLY	2.6
1	A	135	SER	2.5
1	A	138	THR	2.4
3	C	6	DA	2.4
1	A	205	SER	2.3
1	B	174	GLN	2.3
1	A	140	ARG	2.3
1	B	210	VAL	2.3
1	A	137	TYR	2.3
1	B	129	ASP	2.3
1	A	187	THR	2.2
1	B	148	LEU	2.2
1	B	195	LEU	2.2
1	B	202	GLU	2.2
1	B	201	PRO	2.2
1	B	132	ILE	2.2
1	B	187	THR	2.2
1	A	139	ALA	2.1
1	B	203	TYR	2.1
1	B	161	GLN	2.1
1	A	165	ARG	2.1

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 oligosaccharides 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.