



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 04:51 PM EST

PDB ID : 2P13
Title : Transporter associated domain CorC_HlyC from Nitrosomonas europaea
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Deposited on : 2007-03-01
Resolution : 1.65 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

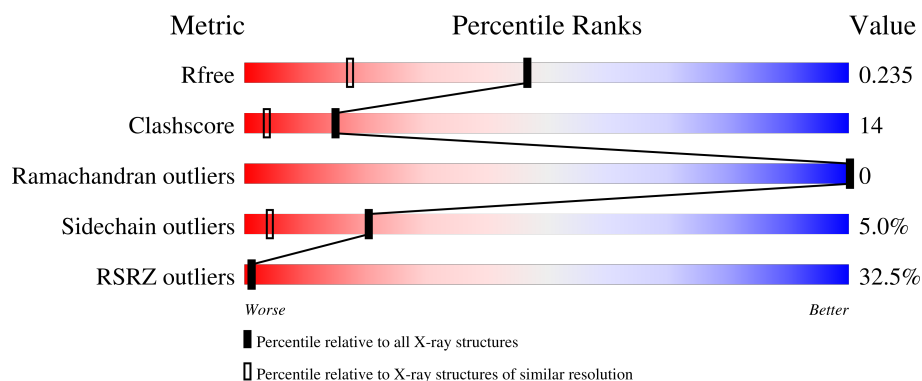
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	164625	2328 (1.66-1.66)
Clashscore	180529	2515 (1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (1.66-1.66)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	90	<div> <div>30%</div> <div>69%</div> <div>26%</div> <div>6%</div> </div>
1	B	90	<div> <div>30%</div> <div>70%</div> <div>16%</div> <div>7%</div> <div>8%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1655 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 CBS domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	Se	0	9	0
			754	483	131	139	1			
1	B	83	Total	C	N	O	Se	0	6	0
			718	458	130	129	1			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	427	SER	-	cloning artifact	UNP Q82SS8
A	428	ASN	-	cloning artifact	UNP Q82SS8
A	429	ALA	-	cloning artifact	UNP Q82SS8
A	445	MSE	MET	modified residue	UNP Q82SS8
B	427	SER	-	cloning artifact	UNP Q82SS8
B	428	ASN	-	cloning artifact	UNP Q82SS8
B	429	ALA	-	cloning artifact	UNP Q82SS8
B	445	MSE	MET	modified residue	UNP Q82SS8

- Molecule 2 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



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

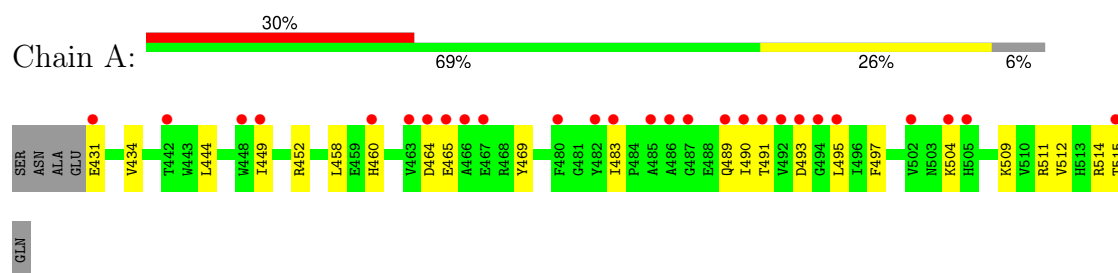
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	83	Total	O	0	0
			83	83		
3	B	96	Total	O	0	0
			96	96		

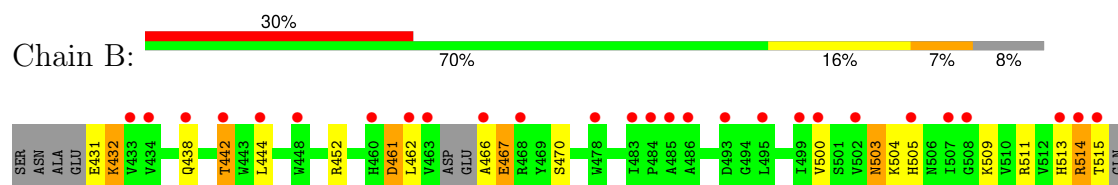
3 Residue-property plots [i](#)

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. 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: CBS domain



- Molecule 1: CBS domain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	49.40Å 49.40Å 127.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.80 – 1.65 42.78 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.80-1.65) 99.4 (42.78-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.243 0.195 , 0.235	Depositor DCC
R_{free} test set	2243 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1655	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.05% 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

5.1 Standard geometry

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

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	0.79	0/766	0.80	0/1032
1	B	0.75	0/732	0.85	0/987
All	All	0.77	0/1498	0.83	0/2019

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

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	754	0	752	19	0
1	B	718	0	699	22	0
2	A	4	0	3	0	0
3	A	83	0	0	4	0
3	B	96	0	0	3	0
All	All	1655	0	1454	40	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 14.

All (40) 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:444[A]:LEU:HD21	1:A:509[A]:LYS:HE3	1.01	1.00
1:A:444[A]:LEU:HD21	1:A:509[A]:LYS:CE	1.96	0.94
1:A:444[A]:LEU:CD2	1:A:509[A]:LYS:HE3	1.96	0.94
1:B:442:THR:HG21	3:B:126:HOH:O	1.77	0.83
1:B:503:ASN:HD22	1:B:505[A]:HIS:H	1.28	0.81
1:A:483:ILE:O	1:B:505[B]:HIS:HD2	1.68	0.75
1:B:503:ASN:HD22	1:B:505[B]:HIS:H	1.35	0.72
1:B:442:THR:HB	1:B:513[A]:HIS:HB3	1.75	0.66
1:B:442:THR:HG22	1:B:513[B]:HIS:CD2	2.31	0.66
1:B:503:ASN:ND2	1:B:505[A]:HIS:H	1.95	0.64
1:A:464:ASP:HB2	1:A:469:TYR:CZ	2.34	0.62
1:A:434:VAL:HB	1:A:449[B]:ILE:HG22	1.80	0.62
1:A:511[A]:ARG:NH1	3:A:48:HOH:O	2.31	0.62
1:B:503:ASN:ND2	1:B:505[B]:HIS:H	2.00	0.59
1:B:438:GLN:HE22	1:B:511[B]:ARG:NH2	2.00	0.59
1:B:452:ARG:HH11	1:B:452:ARG:HG3	1.70	0.56
1:B:467:GLU:O	1:B:470:SER:HB2	2.06	0.56
1:A:460:HIS:NE2	1:A:493:ASP:OD2	2.39	0.52
1:A:465:GLU:HG2	3:A:137:HOH:O	2.10	0.51
1:B:444[B]:LEU:CD2	1:B:511[B]:ARG:HG2	2.43	0.49
1:B:500:VAL:HG21	1:B:511[B]:ARG:HG3	1.95	0.48
1:B:461[A]:ASP:OD2	1:B:461[A]:ASP:N	2.37	0.48
1:A:489:GLN:HA	1:A:497:PHE:O	2.14	0.48
1:A:504[B]:LYS:N	1:A:504[B]:LYS:HD3	2.29	0.48
1:A:504[B]:LYS:HB2	1:A:504[B]:LYS:HE2	1.59	0.45
1:B:504:LYS:HE2	3:B:97:HOH:O	2.17	0.45
1:B:511[A]:ARG:NH2	3:B:126:HOH:O	2.50	0.45
1:B:514:ARG:HB3	1:B:515:THR:HG23	2.00	0.44
1:A:434:VAL:HB	1:A:449[B]:ILE:CG2	2.46	0.44
1:B:462:LEU:O	1:B:466:ALA:N	2.50	0.44
1:B:444[B]:LEU:HD21	1:B:511[B]:ARG:HH11	1.82	0.43
1:A:431:GLU:N	3:A:18:HOH:O	2.51	0.43
1:A:491:THR:HA	1:A:495:LEU:O	2.18	0.43
1:B:431:GLU:HG3	1:B:432:LYS:H	1.84	0.43
1:A:458[B]:LEU:HD21	1:A:512:VAL:HG11	2.02	0.42
1:A:504[B]:LYS:HD3	1:A:504[B]:LYS:H	1.83	0.41
1:B:444[A]:LEU:HD11	1:B:509:LYS:HB3	2.03	0.41
1:B:452:ARG:HG3	1:B:452:ARG:NH1	2.35	0.41
1:A:452:ARG:NH2	3:A:56:HOH:O	2.54	0.40
1:A:514:ARG:O	1:A:515:THR:HB	2.22	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	92/90 (102%)	91 (99%)	1 (1%)	0	100	100
1	B	85/90 (94%)	81 (95%)	4 (5%)	0	100	100
All	All	177/180 (98%)	172 (97%)	5 (3%)	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	80/74 (108%)	79 (99%)	1 (1%)	65	47
1	B	75/74 (101%)	68 (91%)	7 (9%)	7	1
All	All	155/148 (105%)	147 (95%)	8 (5%)	20	4

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	490	ILE
1	B	432	LYS
1	B	442	THR
1	B	461[A]	ASP
1	B	461[B]	ASP
1	B	467	GLU
1	B	503	ASN
1	B	514	ARG

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	456	ASN
1	A	489	GLN
1	B	438	GLN
1	B	503	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](#)

1 ligand is 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	ACY	A	201	-	3,3,3	0.75	0	3,3,3	1.03	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.2883, which does not match the depositor's R factor of 0.199. Please interpret the results in this section carefully.

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	84/90 (93%)	1.67	27 (32%) 1 1	14, 36, 54, 64	9 (10%)
1	B	82/90 (91%)	1.65	27 (32%) 1 1	18, 37, 48, 59	6 (7%)
All	All	166/180 (92%)	1.66	54 (32%) 1 1	14, 37, 53, 64	15 (9%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505[A]	HIS	4.9
1	B	466	ALA	4.9
1	A	466	ALA	4.2
1	B	513[A]	HIS	3.6
1	B	433	VAL	3.5
1	A	504[A]	LYS	3.4
1	A	515	THR	3.3
1	A	490	ILE	3.2
1	A	460	HIS	3.2
1	B	463	VAL	3.0
1	A	494	GLY	3.0
1	B	515	THR	2.9
1	B	483	ILE	2.8
1	B	434	VAL	2.7
1	B	468	ARG	2.7
1	A	464	ASP	2.6
1	B	500	VAL	2.6
1	A	465	GLU	2.6
1	A	505	HIS	2.6
1	B	493	ASP	2.5
1	A	449[A]	ILE	2.5
1	A	492	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	438	GLN	2.5
1	B	508	GLY	2.4
1	A	491	THR	2.4
1	A	489	GLN	2.4
1	A	483	ILE	2.4
1	B	485	ALA	2.4
1	A	495	LEU	2.3
1	A	493	ASP	2.3
1	B	460[A]	HIS	2.3
1	A	463	VAL	2.3
1	B	499	ILE	2.2
1	A	486	ALA	2.2
1	A	482	TYR	2.2
1	A	448	TRP	2.2
1	B	448	TRP	2.2
1	A	480	PHE	2.2
1	A	485	ALA	2.2
1	A	442	THR	2.2
1	B	486	ALA	2.2
1	B	502	VAL	2.2
1	A	487	GLY	2.2
1	B	444[A]	LEU	2.1
1	B	514	ARG	2.1
1	B	442	THR	2.1
1	A	502	VAL	2.1
1	A	431	GLU	2.1
1	B	462	LEU	2.1
1	B	495	LEU	2.1
1	B	478	TRP	2.0
1	A	467[A]	GLU	2.0
1	B	507	ILE	2.0
1	B	484	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands

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. 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	B-factors(Å ²)	Q<0.9
2	ACY	A	201	4/4	0.75	0.18	63,64,64,64	0

6.5 Other polymers

There are no such residues in this entry.