



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:18 AM UTC

PDB ID : 4JCI / pdb_00004jci
Title : Crystal structure of csal_2705, a putative hydroxyproline epimerase from CHROMOHALOBACTER SALEXIGENS (TARGET EFI-506486), SPACE GROUP P212121, unliganded
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Deposited on : 2013-02-21
Resolution : 1.70 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)

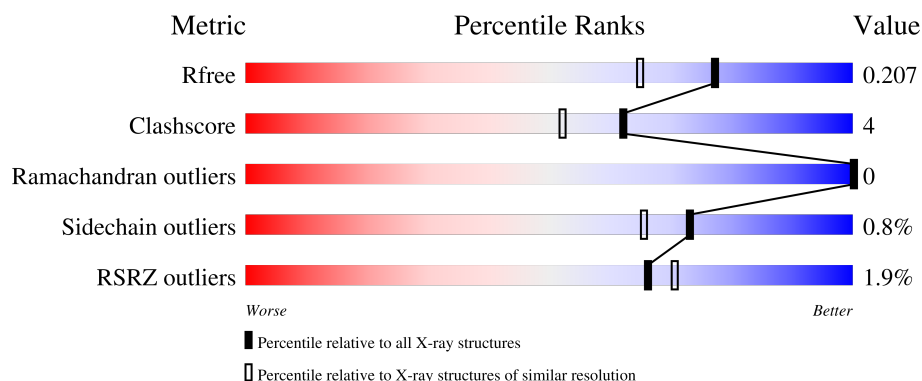
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

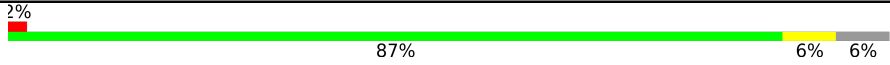
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	333	
1	B	333	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9875 atoms, of which 4597 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 Proline racemase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	0	4	0
			4724	1500	2319	434	455	16			
1	B	308	Total	C	H	N	O	S	0	2	0
			4639	1471	2278	427	447	16			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q1QU06
A	-20	HIS	-	expression tag	UNP Q1QU06
A	-19	HIS	-	expression tag	UNP Q1QU06
A	-18	HIS	-	expression tag	UNP Q1QU06
A	-17	HIS	-	expression tag	UNP Q1QU06
A	-16	HIS	-	expression tag	UNP Q1QU06
A	-15	HIS	-	expression tag	UNP Q1QU06
A	-14	SER	-	expression tag	UNP Q1QU06
A	-13	SER	-	expression tag	UNP Q1QU06
A	-12	GLY	-	expression tag	UNP Q1QU06
A	-11	VAL	-	expression tag	UNP Q1QU06
A	-10	ASP	-	expression tag	UNP Q1QU06
A	-9	LEU	-	expression tag	UNP Q1QU06
A	-8	GLY	-	expression tag	UNP Q1QU06
A	-7	THR	-	expression tag	UNP Q1QU06
A	-6	GLU	-	expression tag	UNP Q1QU06
A	-5	ASN	-	expression tag	UNP Q1QU06
A	-4	LEU	-	expression tag	UNP Q1QU06
A	-3	TYR	-	expression tag	UNP Q1QU06
A	-2	PHE	-	expression tag	UNP Q1QU06
A	-1	GLN	-	expression tag	UNP Q1QU06
A	0	SER	-	expression tag	UNP Q1QU06
B	-21	MET	-	expression tag	UNP Q1QU06
B	-20	HIS	-	expression tag	UNP Q1QU06
B	-19	HIS	-	expression tag	UNP Q1QU06

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	expression tag	UNP Q1QU06
B	-17	HIS	-	expression tag	UNP Q1QU06
B	-16	HIS	-	expression tag	UNP Q1QU06
B	-15	HIS	-	expression tag	UNP Q1QU06
B	-14	SER	-	expression tag	UNP Q1QU06
B	-13	SER	-	expression tag	UNP Q1QU06
B	-12	GLY	-	expression tag	UNP Q1QU06
B	-11	VAL	-	expression tag	UNP Q1QU06
B	-10	ASP	-	expression tag	UNP Q1QU06
B	-9	LEU	-	expression tag	UNP Q1QU06
B	-8	GLY	-	expression tag	UNP Q1QU06
B	-7	THR	-	expression tag	UNP Q1QU06
B	-6	GLU	-	expression tag	UNP Q1QU06
B	-5	ASN	-	expression tag	UNP Q1QU06
B	-4	LEU	-	expression tag	UNP Q1QU06
B	-3	TYR	-	expression tag	UNP Q1QU06
B	-2	PHE	-	expression tag	UNP Q1QU06
B	-1	GLN	-	expression tag	UNP Q1QU06
B	0	SER	-	expression tag	UNP Q1QU06

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

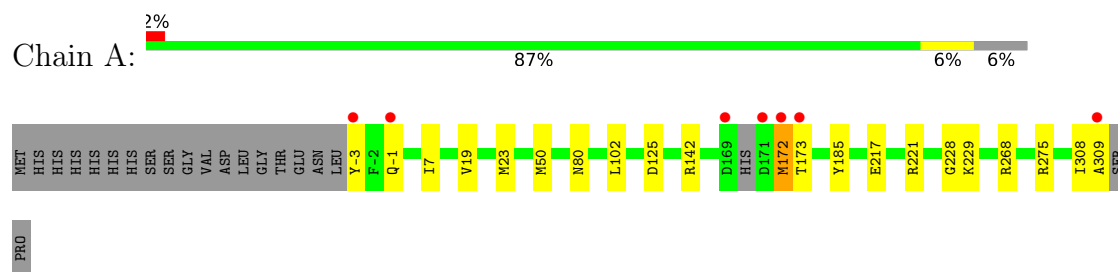
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	284	Total O 297 297	0	13
3	B	210	Total O 214 214	0	4

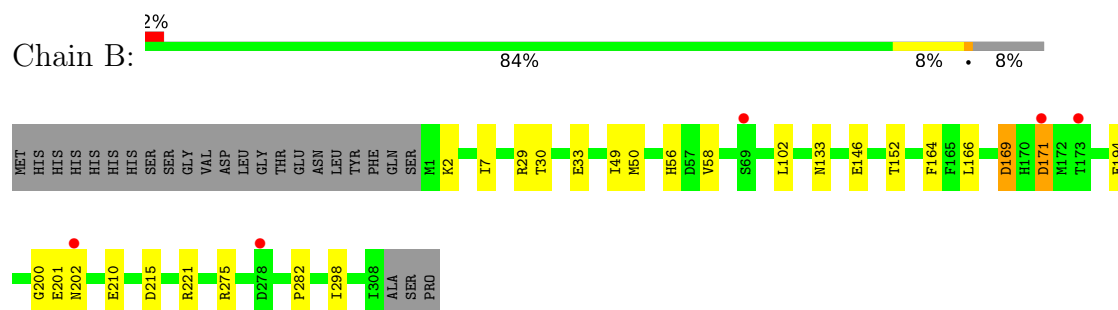
3 Residue-property plots [i](#)

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: Proline racemase



• Molecule 1: Proline racemase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.09Å 54.45Å 253.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.94 – 1.70 23.94 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.8 (23.94-1.70) 96.7 (23.94-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.169 , 0.205 0.175 , 0.207	Depositor DCC
R_{free} test set	3628 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9875	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: NA

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	0.68	0/2475	0.84	1/3358 (0.0%)
1	B	0.63	0/2422	0.83	1/3289 (0.0%)
All	All	0.66	0/4897	0.84	2/6647 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	172	MET	N-CA-C	-7.37	98.61	110.32
1	B	169	ASP	N-CA-C	7.05	117.82	107.88

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	173	THR	Peptide

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	2405	2319	2297	16	1
1	B	2361	2278	2262	22	0
2	A	1	0	0	0	0
3	A	297	0	0	2	0
3	B	214	0	0	3	0
All	All	5278	4597	4559	38	1

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 4.

All (38) 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:194:GLU:OE1	3:B:502:HOH:O	1.87	0.93
1:A:142:ARG:NH2	3:A:610:HOH:O	2.02	0.93
1:B:201:GLU:O	1:B:202:ASN:OD1	1.98	0.81
1:A:19:VAL:HG11	1:A:23:MET:HG3	1.66	0.77
1:A:19:VAL:HG11	1:A:23:MET:CG	2.16	0.74
1:B:7:ILE:CD1	1:B:102:LEU:HD11	2.20	0.71
1:B:49:ILE:HG22	1:B:50:MET:CE	2.21	0.70
1:A:228:GLY:O	1:A:229:LYS:HG2	1.92	0.69
1:B:275:ARG:NH2	3:B:596:HOH:O	2.28	0.65
1:B:30:THR:HG23	1:B:33:GLU:H	1.62	0.64
1:B:49:ILE:HG22	1:B:50:MET:HE2	1.78	0.63
1:A:50:MET:HE2	1:A:80:ASN:HA	1.84	0.60
1:B:146:GLU:OE2	1:B:152:THR:OG1	2.16	0.59
1:A:-3:TYR:HD2	1:A:-1:GLN:NE2	2.01	0.58
1:A:308:ILE:O	1:A:309:ALA:C	2.47	0.56
1:B:166:LEU:HD12	1:B:166:LEU:N	2.23	0.54
1:B:133:ASN:HB3	1:B:282:PRO:HG2	1.89	0.54
1:B:7:ILE:HD11	1:B:102:LEU:HD11	1.93	0.49
1:B:49:ILE:HG22	1:B:50:MET:HE3	1.94	0.49
1:A:217:GLU:CB	1:A:268:ARG:HH12	2.27	0.47
1:A:19:VAL:CG1	1:A:23:MET:HG3	2.41	0.46
1:A:221:ARG:NE	3:A:697:HOH:O	2.49	0.45
1:A:-3:TYR:CD2	1:A:-1:GLN:NE2	2.83	0.45
1:A:19:VAL:CG1	1:A:23:MET:CG	2.92	0.43
1:B:58:VAL:HG22	1:B:58:VAL:O	2.17	0.43
1:B:201:GLU:C	1:B:202:ASN:OD1	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:LYS:HB2	1:B:298:ILE:HB	2.01	0.43
1:A:217:GLU:HB3	1:A:268:ARG:HH12	1.84	0.42
1:B:58:VAL:HG23	3:B:438:HOH:O	2.19	0.41
1:B:30:THR:CG2	1:B:33:GLU:H	2.32	0.41
1:B:171:ASP:OD2	1:B:171:ASP:N	2.54	0.41
1:B:164:PHE:CD2	1:B:210:GLU:HG3	2.56	0.41
1:A:172:MET:HG3	1:A:185:TYR:CD2	2.56	0.41
1:B:200:GLY:C	1:B:201:GLU:O	2.63	0.41
1:B:164:PHE:HD2	1:B:210:GLU:HG3	1.86	0.41
1:A:217:GLU:HB2	1:A:268:ARG:NH1	2.36	0.40
1:B:215:ASP:OD2	1:B:221:ARG:NH2	2.52	0.40
1:A:7:ILE:CD1	1:A:102:LEU:HD11	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASP:OD1	1:A:275[A]:ARG:HH22[3_645]	1.54	0.06

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	312/333 (94%)	309 (99%)	3 (1%)	0	100	100
1	B	308/333 (92%)	300 (97%)	8 (3%)	0	100	100
All	All	620/666 (93%)	609 (98%)	11 (2%)	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	251/267 (94%)	251 (100%)	0	100	100
1	B	246/267 (92%)	242 (98%)	4 (2%)	55	41
All	All	497/534 (93%)	493 (99%)	4 (1%)	73	65

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	29	ARG
1	B	56	HIS
1	B	169	ASP
1	B	171	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	191	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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 [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	312/333 (93%)	-0.42	7 (2%) 62 66	9, 20, 44, 87	2 (0%)
1	B	308/333 (92%)	-0.18	5 (1%) 70 75	12, 27, 52, 83	1 (0%)
All	All	620/666 (93%)	-0.30	12 (1%) 66 71	9, 23, 49, 87	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	-3	TYR	5.8
1	A	-1	GLN	3.5
1	A	173	THR	3.5
1	B	173	THR	3.5
1	A	309	ALA	2.9
1	B	202	ASN	2.9
1	A	171	ASP	2.7
1	A	169	ASP	2.7
1	B	278	ASP	2.6
1	A	172	MET	2.5
1	B	69	SER	2.3
1	B	171	ASP	2.2

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

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	NA	A	401	1/1	0.93	0.08	42,42,42,42	0

6.5 Other polymers

There are no such residues in this entry.