



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:04 AM UTC

PDB ID : 3IG2 / pdb_00003ig2
Title : The Crystal Structure of a Putative Phenylalanyl-tRNA synthetase (PheRS) beta chain domain from Bacteroides fragilis to 2.1Å
Authors : Stein, A.J.; Sather, A.; Hendricks, R.; Keigher, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2009-07-27
Resolution : 2.09 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
Mogul : 2022.3.0, CSD as543be (2022)
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

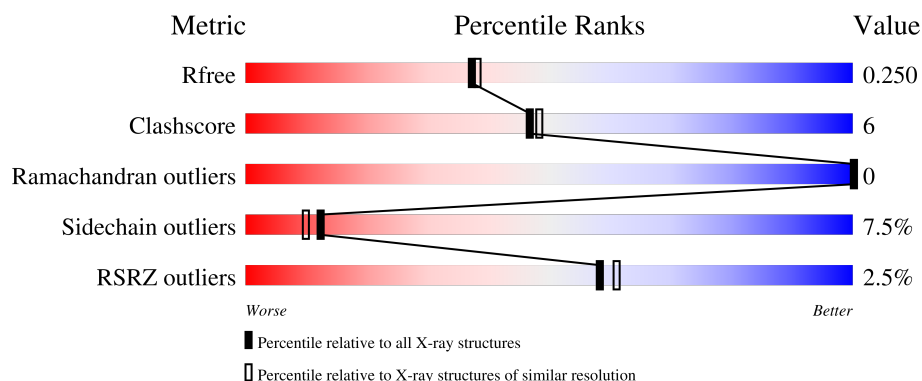
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	213	 72% 15% • 11%
1	B	213	 3% 80% 11% • 8%
1	C	213	 4% 75% 12% 12%
1	D	213	 2% 75% 15% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6285 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 Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	Se	0	2	0
			1502	965	245	283	3	6			
1	B	197	Total	C	N	O	S	Se	0	2	0
			1547	989	254	296	3	5			
1	C	187	Total	C	N	O	S	Se	0	3	0
			1475	944	240	284	3	4			
1	D	194	Total	C	N	O	S	Se	0	0	0
			1502	958	246	291	3	4			

There are 12 discrepancies between the modelled and reference sequences:

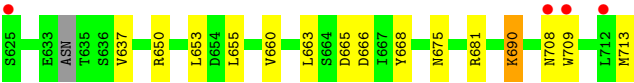
Chain	Residue	Modelled	Actual	Comment	Reference
A	501	SER	-	expression tag	UNP Q64T65
A	502	ASN	-	expression tag	UNP Q64T65
A	503	ALA	-	expression tag	UNP Q64T65
B	501	SER	-	expression tag	UNP Q64T65
B	502	ASN	-	expression tag	UNP Q64T65
B	503	ALA	-	expression tag	UNP Q64T65
C	501	SER	-	expression tag	UNP Q64T65
C	502	ASN	-	expression tag	UNP Q64T65
C	503	ALA	-	expression tag	UNP Q64T65
D	501	SER	-	expression tag	UNP Q64T65
D	502	ASN	-	expression tag	UNP Q64T65
D	503	ALA	-	expression tag	UNP Q64T65

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	73	Total 73	O 73	0	0
3	B	89	Total 89	O 89	0	0
3	C	64	Total 64	O 64	0	0
3	D	32	Total 32	O 32	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.50Å 60.34Å 78.81Å 99.04° 100.37° 105.08°	Depositor
Resolution (Å)	28.45 – 2.09 28.45 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.5 (28.45-2.09) 97.4 (28.45-2.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.51 (at 2.10Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0102	Depositor
R, R_{free}	0.195 , 0.236 0.216 , 0.250	Depositor DCC
R_{free} test set	2416 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6285	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.20% 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: MG

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	0.69	0/1533	0.83	0/2067
1	B	0.81	3/1576 (0.2%)	0.92	3/2125 (0.1%)
1	C	0.71	0/1507	0.84	0/2034
1	D	0.58	0/1526	0.82	0/2064
All	All	0.71	3/6142 (0.0%)	0.85	3/8290 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	640	LEU	C-O	6.50	1.31	1.24
1	B	638	TYR	C-N	5.59	1.41	1.33
1	B	638	TYR	N-CA	5.17	1.52	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	TYR	CA-C-O	-8.73	111.17	120.42
1	B	638	TYR	O-C-N	5.79	128.75	122.15
1	B	692	MSE	CG-SE-CE	-5.71	86.36	98.92

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	1502	0	1449	22	0
1	B	1547	0	1503	15	0
1	C	1475	0	1415	11	0
1	D	1502	0	1411	23	0
2	C	1	0	0	0	0
3	A	73	0	0	2	0
3	B	89	0	0	1	0
3	C	64	0	0	0	0
3	D	32	0	0	0	0
All	All	6285	0	5778	67	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 6.

All (67) 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:680:LYS:NZ	1:B:711:GLU:OE1	1.82	1.13
1:D:690:LYS:HE3	1:D:690:LYS:H	1.35	0.91
1:B:680:LYS:NZ	1:B:711:GLU:CD	2.31	0.88
1:B:680:LYS:HZ1	1:B:711:GLU:CD	1.89	0.81
1:B:533:ALA:H	1:B:559:ASN:HD21	1.27	0.80
1:C:533:ALA:H	1:C:559:ASN:HD21	1.27	0.79
1:D:576:ASN:HD22	1:D:578:ASN:H	1.31	0.78
1:D:543:PRO:HG2	1:D:546:ASN:OD1	1.86	0.75
1:D:709:TRP:NE1	1:D:713:MSE:CE	2.52	0.72
1:D:690:LYS:H	1:D:690:LYS:CE	2.02	0.70
1:D:576:ASN:ND2	1:D:578:ASN:H	1.89	0.70
1:A:511:ASN:HD21	1:D:511:ASN:ND2	1.91	0.68
1:D:665:ASP:HB3	1:D:668:TYR:H	1.59	0.68
1:B:680:LYS:HZ2	1:B:711:GLU:CD	2.01	0.67
1:A:584:LEU:HG	1:A:586:PHE:CZ	2.30	0.66
1:D:690:LYS:HE3	1:D:690:LYS:N	2.09	0.66
1:C:543:PRO:HB3	1:C:545:LYS:HE3	1.79	0.65
1:A:690:LYS:H	1:A:690:LYS:CD	2.10	0.64
1:C:532:ARG:CZ	1:C:557:ASP:OD1	2.48	0.61
1:C:587:PHE:HB2	1:C:617[A]:LEU:HD23	1.86	0.58
1:A:690:LYS:N	1:A:690:LYS:HD2	2.19	0.57
1:A:539:LEU:HD11	1:A:567:PHE:HZ	1.69	0.57
1:A:528:ASN:HD22	1:A:529:SER:N	2.04	0.54
1:D:576:ASN:HD22	1:D:578:ASN:N	2.04	0.54
1:B:559:ASN:HD22	1:B:559:ASN:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:42:HOH:O	1:D:528:ASN:HB3	2.08	0.53
1:A:647:ILE:O	1:A:651:LEU:HG	2.10	0.52
1:C:617[B]:LEU:HB2	1:C:705:ALA:HB3	1.92	0.51
1:C:587:PHE:CB	1:C:617[A]:LEU:HD23	2.41	0.50
1:B:569:GLY:HA3	1:B:618:TRP:CE2	2.47	0.50
1:C:569:GLY:HA3	1:C:618:TRP:CE2	2.47	0.50
1:A:506:SER:O	1:A:510:GLN:HG3	2.13	0.49
1:C:532:ARG:NH1	1:C:557:ASP:OD1	2.46	0.49
1:A:569:GLY:HA3	1:A:618:TRP:CE2	2.49	0.48
1:D:675:ASN:HD21	1:D:681:ARG:HE	1.62	0.48
1:B:511:ASN:O	1:B:515:GLU:HG3	2.13	0.48
1:D:709:TRP:CE2	1:D:713:MSE:CE	2.97	0.47
1:D:524:GLU:HB2	1:D:587:PHE:CZ	2.50	0.46
1:D:709:TRP:CE2	1:D:713:MSE:HE1	2.51	0.46
1:B:559:ASN:HD22	1:B:559:ASN:N	2.13	0.46
1:D:523:ASN:O	1:D:586:PHE:HA	2.15	0.46
1:A:690:LYS:CD	1:A:690:LYS:N	2.74	0.45
1:A:511:ASN:ND2	1:D:511:ASN:ND2	2.63	0.45
1:D:569:GLY:HA3	1:D:618:TRP:CE2	2.52	0.44
1:D:709:TRP:NE1	1:D:713:MSE:HE1	2.30	0.44
1:A:664:SER:HB2	1:A:669:SER:O	2.18	0.44
1:B:656:HIS:CE1	1:C:538:GLY:O	2.70	0.44
1:A:667:ILE:HD13	1:A:692:MSE:HE3	1.99	0.44
1:D:517:LEU:O	1:D:522:PHE:HB2	2.18	0.43
1:A:528:ASN:HD22	1:A:529:SER:H	1.66	0.43
1:A:626:ASN:C	1:A:626:ASN:HD22	2.25	0.43
1:B:650:ARG:HA	1:B:650:ARG:HD3	1.60	0.43
1:A:611:GLU:OE2	1:D:528:ASN:HB3	2.19	0.43
1:B:637:VAL:O	1:B:641:LYS:HB2	2.19	0.43
1:B:566:LEU:HD21	1:B:692:MSE:HE1	2.00	0.43
1:C:559:ASN:C	1:C:559:ASN:HD22	2.28	0.42
1:C:700:ASN:HB3	1:C:701:GLU:H	1.66	0.42
1:A:633:GLU:HB3	1:A:687:VAL:HG21	2.01	0.41
1:A:690:LYS:H	1:A:690:LYS:CE	2.32	0.41
1:A:532:ARG:NH1	3:A:124:HOH:O	2.53	0.41
1:D:650:ARG:HA	1:D:650:ARG:HD2	1.92	0.41
1:A:549:MSE:HE3	1:A:549:MSE:HB3	1.94	0.41
1:B:623:MSE:HG3	3:B:38:HOH:O	2.20	0.41
1:B:624:VAL:HG13	1:B:690:LYS:HE2	2.03	0.40
1:A:524:GLU:HB2	1:A:587:PHE:CZ	2.57	0.40
1:D:653:LEU:HD12	1:D:653:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:LYS:HD2	1:A:711:GLU:OE1	2.22	0.40

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	184/213 (86%)	182 (99%)	2 (1%)	0	100	100
1	B	193/213 (91%)	191 (99%)	2 (1%)	0	100	100
1	C	180/213 (84%)	178 (99%)	2 (1%)	0	100	100
1	D	184/213 (86%)	183 (100%)	1 (0%)	0	100	100
All	All	741/852 (87%)	734 (99%)	7 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	162/178 (91%)	150 (93%)	12 (7%)	13	10
1	B	166/178 (93%)	157 (95%)	9 (5%)	20	18
1	C	160/178 (90%)	145 (91%)	15 (9%)	8	6
1	D	157/178 (88%)	144 (92%)	13 (8%)	10	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	645/712 (91%)	596 (92%)	49 (8%)	12 9

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	511	ASN
1	A	512	LEU
1	A	550	LEU
1	A	563	GLN
1	A	584	LEU
1	A	626	ASN
1	A	634	ASN
1	A	635	THR
1	A	636	SER
1	A	650	ARG
1	A	653	LEU
1	A	690	LYS
1	B	512	LEU
1	B	526	LEU
1	B	559	ASN
1	B	606	LEU
1	B	627	SER
1	B	650	ARG
1	B	655	LEU
1	B	663	LEU
1	B	666	ASP
1	C	512	LEU
1	C	526	LEU
1	C	558	LEU
1	C	559	ASN
1	C	584	LEU
1	C	591	ASN
1	C	610	SER
1	C	627	SER
1	C	655	LEU
1	C	663	LEU
1	C	666	ASP
1	C	667	ILE
1	C	670[A]	THR
1	C	670[B]	THR
1	C	697	ASP
1	D	512	LEU

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Mol	Chain	Res	Type
1	D	540	GLU
1	D	544	SER
1	D	550	LEU
1	D	576	ASN
1	D	585	LYS
1	D	637	VAL
1	D	655	LEU
1	D	660	VAL
1	D	663	LEU
1	D	666	ASP
1	D	690	LYS
1	D	708	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	ASN
1	A	528	ASN
1	A	552	ASN
1	A	563	GLN
1	A	626	ASN
1	A	634	ASN
1	A	656	HIS
1	A	700	ASN
1	B	559	ASN
1	B	662	ASN
1	C	546	ASN
1	C	559	ASN
1	C	591	ASN
1	C	630	HIS
1	C	662	ASN
1	D	511	ASN
1	D	523	ASN
1	D	576	ASN
1	D	675	ASN

5.3.3 RNA ⓘ

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](#)

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 [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

6.1 Protein, DNA and RNA chains

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	185/213 (86%)	0.04	0	100	100	7, 15, 19, 20	1 (0%)
1	B	192/213 (90%)	0.16	6 (3%)	51	54	2, 14, 17, 20	2 (1%)
1	C	183/213 (85%)	0.23	8 (4%)	39	41	6, 13, 17, 18	3 (1%)
1	D	190/213 (89%)	0.18	5 (2%)	57	60	5, 16, 20, 23	0
All	All	750/852 (88%)	0.15	19 (2%)	58	61	2, 14, 19, 23	6 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	640	LEU	5.4
1	C	536	TYR	5.3
1	B	642	ALA	5.2
1	C	625	SER	5.1
1	D	709	TRP	4.8
1	B	643	TYR	4.4
1	B	644	VAL	4.0
1	B	638	TYR	3.7
1	C	635	THR	3.4
1	C	530	LEU	3.4
1	B	507	ASN	2.9
1	C	637	VAL	2.7
1	D	519	GLY	2.7
1	D	708	ASN	2.7
1	C	700	ASN	2.6
1	C	638	TYR	2.6
1	C	533	ALA	2.3
1	D	625	SER	2.2
1	D	712	LEU	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](#)

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($\text{\AA}^2$)	Q<0.9
2	MG	C	1	1/1	0.97	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.