



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 08:20 PM UTC

PDB ID : 7OK9 / pdb_00007ok9
Title : Crystal structure of Penicillin-Binding Protein 1 (PBP1) from *Staphylococcus aureus* in complex with pentaglycine
Authors : Martinez Caballero, S.; Hermoso, J.A.
Deposited on : 2021-05-17
Resolution : 3.36 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 ⓘ 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

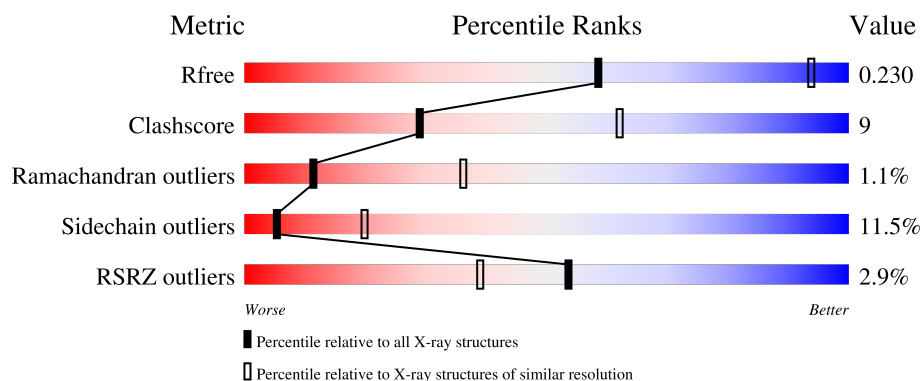
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.36 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	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	650	2% 59%18%20%
1	B	650	2% 60%16%19%
1	C	650	2% 59%17%20%
1	D	650	4% 57%16%24%
1	E	650	2% 60%17%19%

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Mol	Chain	Length	Quality of chain
1	F	650	
1	G	650	
1	H	650	
1	I	650	
1	J	650	
1	K	650	
1	L	650	
2	P	5	
2	Q	5	
2	R	5	
2	S	5	
2	T	5	
2	U	5	
2	V	5	
2	W	5	
2	X	5	
2	Y	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	D	802	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 47917 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 Penicillin-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4113	2613	707	777	16			
1	B	525	Total	C	N	O	S	0	0	0
			4138	2628	712	782	16			
1	C	522	Total	C	N	O	S	0	0	0
			4114	2614	708	776	16			
1	D	496	Total	C	N	O	S	0	0	0
			3913	2489	668	740	16			
1	E	524	Total	C	N	O	S	0	0	0
			4129	2623	711	779	16			
1	F	523	Total	C	N	O	S	0	0	0
			4122	2618	710	778	16			
1	G	520	Total	C	N	O	S	0	0	0
			4098	2604	705	773	16			
1	H	465	Total	C	N	O	S	0	0	0
			3661	2326	626	694	15			
1	I	519	Total	C	N	O	S	0	0	0
			4089	2598	703	772	16			
1	J	518	Total	C	N	O	S	0	0	0
			4080	2592	701	771	16			
1	K	462	Total	C	N	O	S	0	0	0
			3629	2306	619	690	14			
1	L	462	Total	C	N	O	S	0	0	0
			3646	2318	622	691	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	cloning artifact	UNP A0A0H2WVW5
B	64	MET	-	cloning artifact	UNP A0A0H2WVW5
C	64	MET	-	cloning artifact	UNP A0A0H2WVW5
D	64	MET	-	cloning artifact	UNP A0A0H2WVW5
E	64	MET	-	cloning artifact	UNP A0A0H2WVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
F	64	MET	-	cloning artifact	UNP A0A0H2WVW5
G	64	MET	-	cloning artifact	UNP A0A0H2WVW5
H	64	MET	-	cloning artifact	UNP A0A0H2WVW5
I	64	MET	-	cloning artifact	UNP A0A0H2WVW5
J	64	MET	-	cloning artifact	UNP A0A0H2WVW5
K	64	MET	-	cloning artifact	UNP A0A0H2WVW5
L	64	MET	-	cloning artifact	UNP A0A0H2WVW5

- Molecule 2 is a protein called pentaglycine.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	5	Total	C	N	O	0	0	0
			21	10	5	6			
2	Q	5	Total	C	N	O	0	0	0
			21	10	5	6			
2	R	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	S	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	T	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	U	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	V	5	Total	C	N	O	0	0	1
			17	8	5	4			
2	W	4	Total	C	N	O	0	0	1
			13	6	4	3			
2	X	4	Total	C	N	O	0	0	1
			13	6	4	3			
2	Y	4	Total	C	N	O	0	0	1
			13	6	4	3			

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cd	0	0
			1	1		
3	B	1	Total	Cd	0	0
			1	1		
3	C	1	Total	Cd	0	0
			1	1		
3	D	1	Total	Cd	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Cd	0	0
			1	1		
3	F	1	Total	Cd	0	0
			1	1		
3	G	1	Total	Cd	0	0
			1	1		
3	H	1	Total	Cd	0	0
			1	1		
3	I	1	Total	Cd	0	0
			1	1		
3	J	1	Total	Cd	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

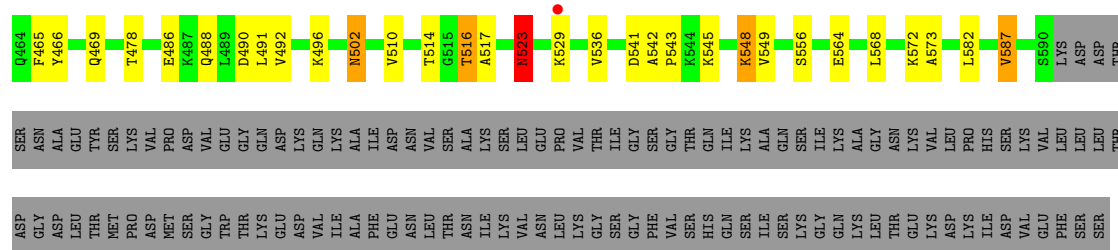
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		
4	F	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

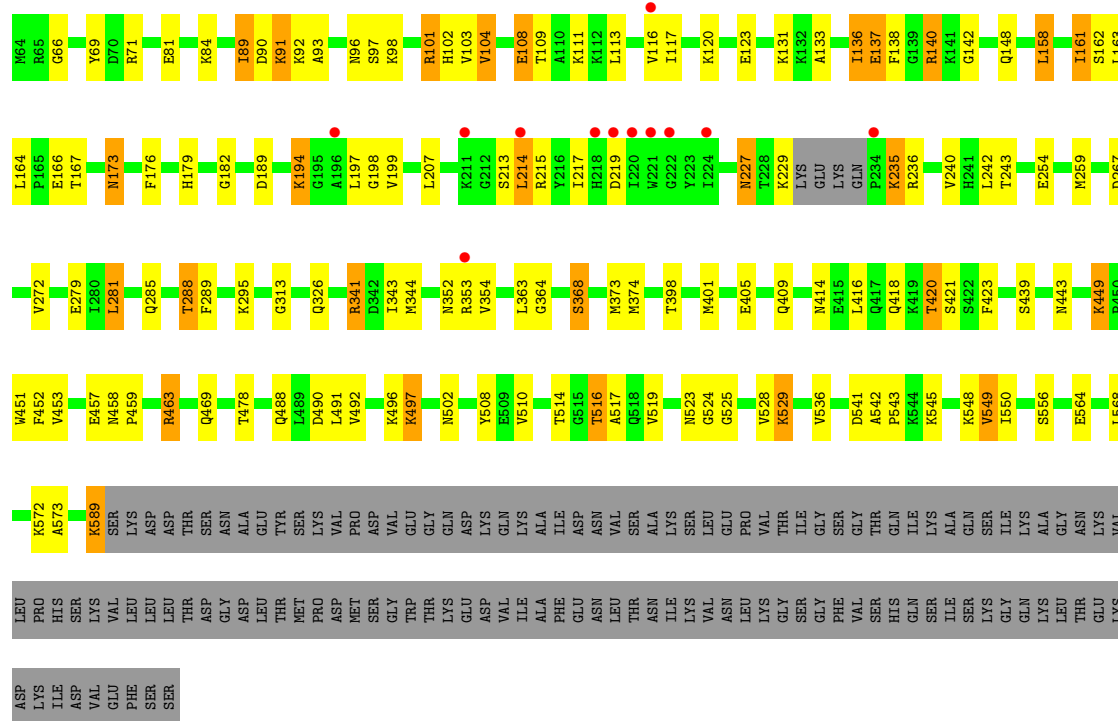
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	F	2	Total	O	0	0
			2	2		
5	H	1	Total	O	0	0
			1	1		
5	J	1	Total	O	0	0
			1	1		

- Molecule 1: Penicillin-binding protein 1

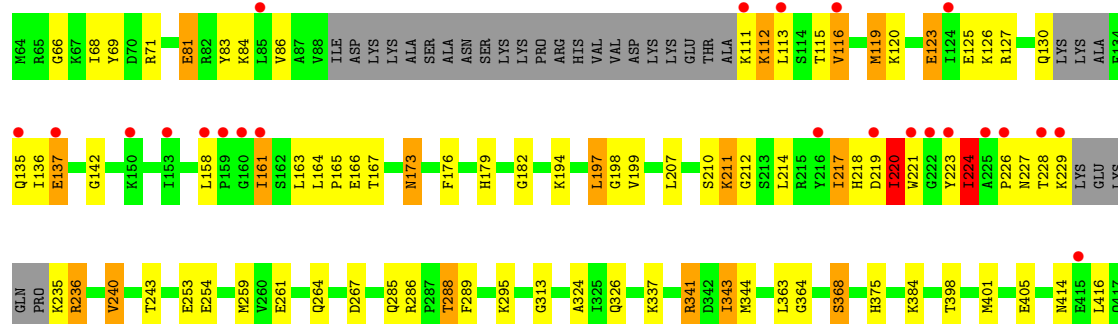




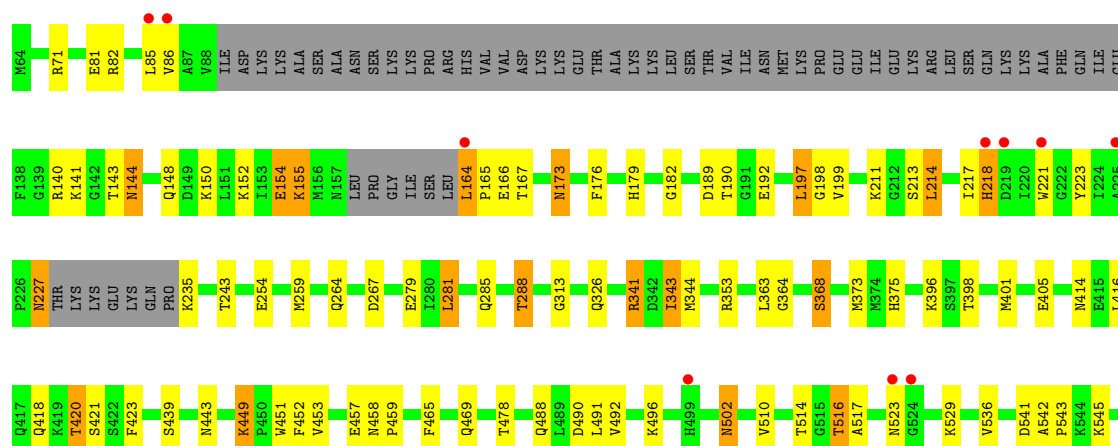
• Molecule 1: Penicillin-binding protein 1

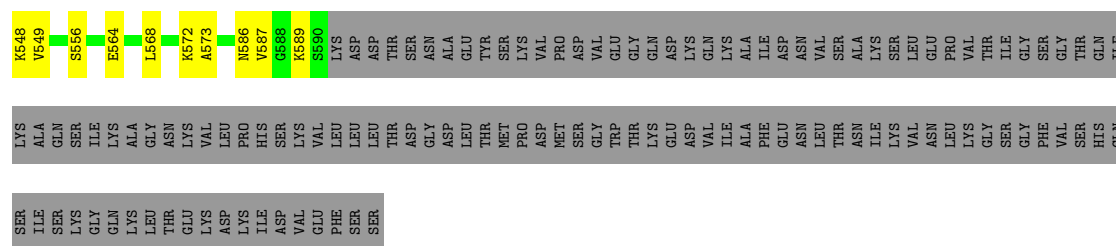


• Molecule 1: Penicillin-binding protein 1

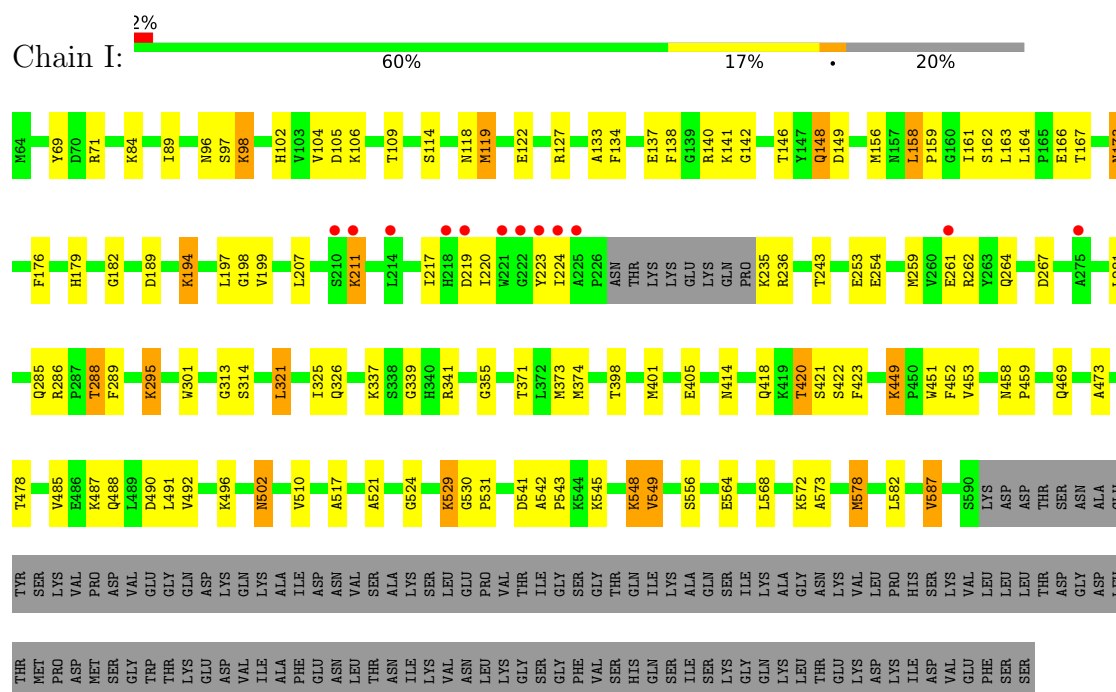




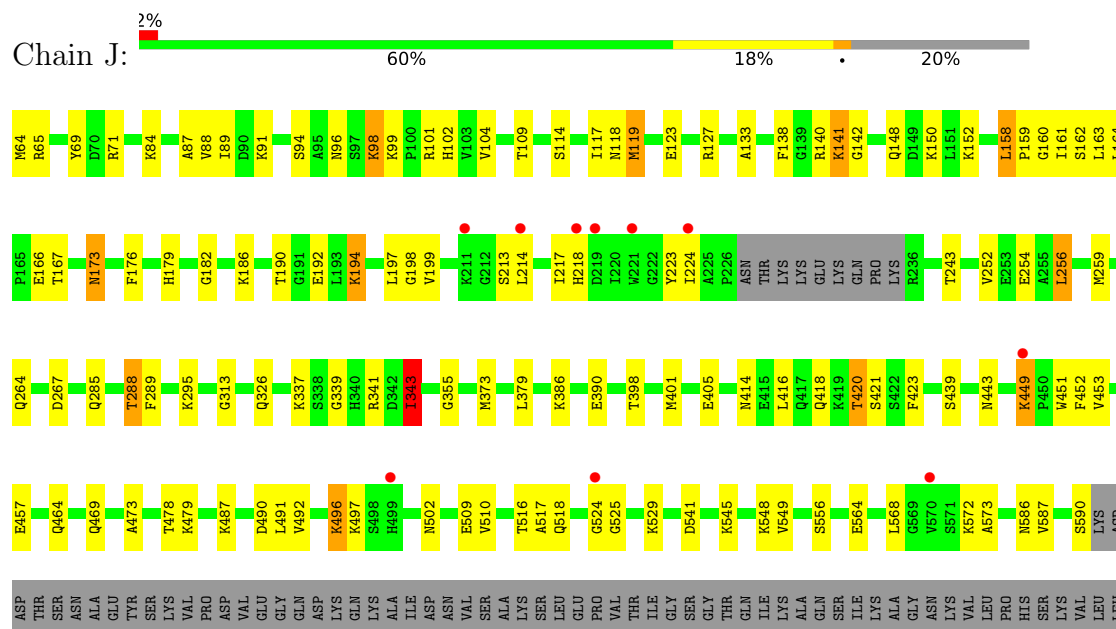


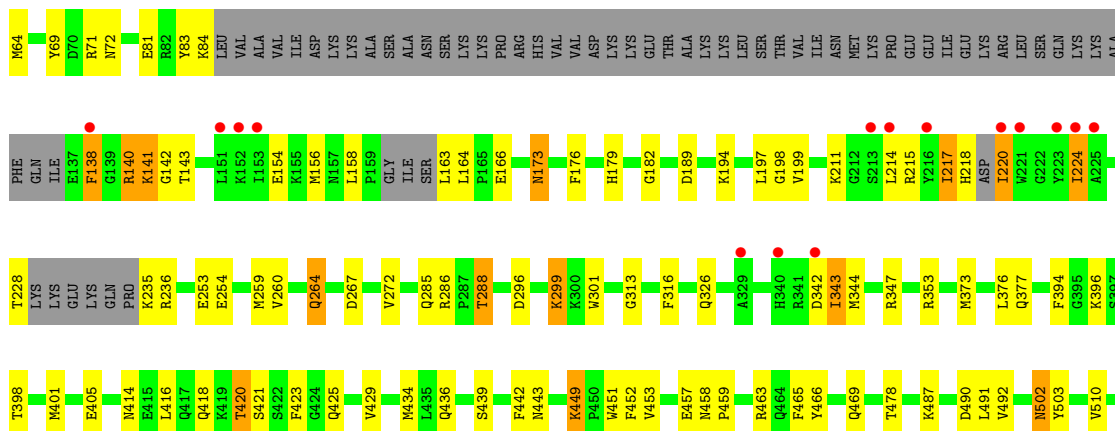


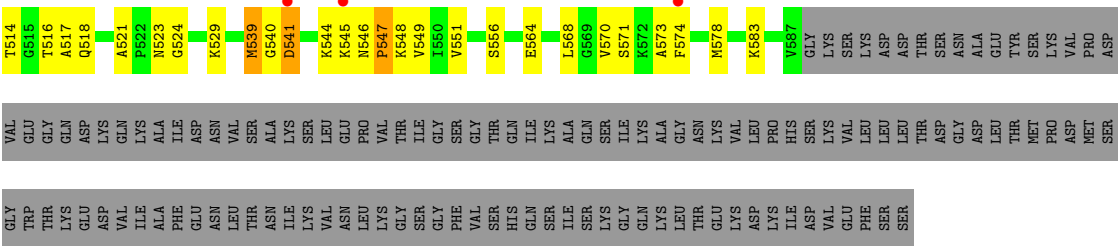
• Molecule 1: Penicillin-binding protein 1



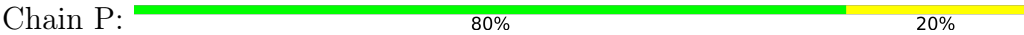
• Molecule 1: Penicillin-binding protein 1







• Molecule 2: pentaglycine



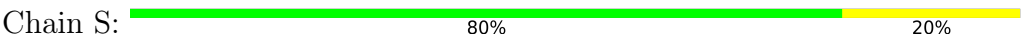
• Molecule 2: pentaglycine



• Molecule 2: pentaglycine



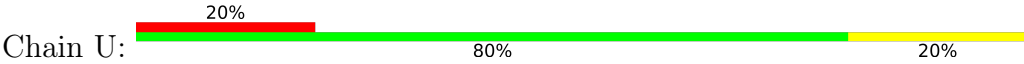
• Molecule 2: pentaglycine



• Molecule 2: pentaglycine



• Molecule 2: pentaglycine

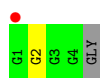




- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



- Molecule 2: pentaglycine



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	313.99Å 198.19Å 220.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.32 – 3.36 49.32 – 3.36	Depositor EDS
% Data completeness (in resolution range)	44.1 (49.32-3.36) 44.1 (49.32-3.36)	Depositor EDS
R_{merge}	0.67	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.230 , 0.267 (Not available) , 0.230	Depositor DCC
R_{free} test set	4313 reflections (2.20%)	wwPDB-VP
Wilson B-factor (Å ²)	69.4	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 115.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	47917	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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](#)

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

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	1.03	3/4203 (0.1%)	1.23	4/5652 (0.1%)
1	B	1.03	6/4228 (0.1%)	1.22	4/5685 (0.1%)
1	C	1.04	4/4204 (0.1%)	1.22	8/5654 (0.1%)
1	D	1.03	7/3998 (0.2%)	1.22	6/5378 (0.1%)
1	E	1.03	5/4219 (0.1%)	1.21	2/5673 (0.0%)
1	F	1.04	5/4211 (0.1%)	1.21	4/5662 (0.1%)
1	G	1.02	5/4188 (0.1%)	1.21	2/5633 (0.0%)
1	H	1.06	8/3743 (0.2%)	1.21	7/5037 (0.1%)
1	I	1.02	5/4178 (0.1%)	1.20	7/5619 (0.1%)
1	J	1.04	8/4169 (0.2%)	1.22	3/5608 (0.1%)
1	K	1.03	5/3708 (0.1%)	1.18	6/4989 (0.1%)
1	L	1.02	4/3728 (0.1%)	1.18	3/5017 (0.1%)
2	P	1.21	0/20	1.81	0/22
2	Q	1.42	0/20	2.13	0/22
2	R	1.44	0/16	0.98	0/19
2	S	1.81	0/16	1.62	1/19 (5.3%)
2	T	2.25	1/16 (6.2%)	1.22	0/19
2	U	1.27	0/16	1.22	0/19
2	V	1.34	0/16	1.68	1/19 (5.3%)
2	W	1.23	0/12	2.63	2/14 (14.3%)
2	X	1.34	0/12	1.36	0/14
2	Y	1.47	0/12	0.73	0/14
All	All	1.03	66/48933 (0.1%)	1.21	60/65788 (0.1%)

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	ALA	C-O	7.23	1.32	1.24
1	H	85	LEU	C-O	-6.94	1.15	1.24
1	B	69	TYR	C-O	6.27	1.31	1.23
1	J	586	ASN	C-O	6.25	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	69	TYR	C-O	6.12	1.31	1.23

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	523	ASN	CA-C-O	-11.09	112.79	119.55
1	C	354	VAL	N-CA-C	-10.54	103.36	111.90
1	J	587	VAL	CA-C-O	-9.92	110.09	120.71
1	H	587	VAL	CA-C-O	-9.89	110.13	120.71
1	K	409	GLN	CB-CG-CD	-7.28	100.23	112.60

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	4113	0	4100	102	0
1	B	4138	0	4128	83	0
1	C	4114	0	4104	68	0
1	D	3913	0	3877	74	0
1	E	4129	0	4122	70	0
1	F	4122	0	4114	74	0
1	G	4098	0	4084	82	0
1	H	3661	0	3597	54	0
1	I	4089	0	4075	62	0
1	J	4080	0	4062	62	0
1	K	3629	0	3570	53	0
1	L	3646	0	3579	77	0
2	P	21	0	17	1	0
2	Q	21	0	17	0	0
2	R	17	0	14	0	0
2	S	17	0	14	0	0
2	T	17	0	14	0	0
2	U	17	0	14	0	0
2	V	17	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	W	13	0	11	0	0
2	X	13	0	11	1	0
2	Y	13	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	D	1	0	0	2	0
4	F	1	0	0	0	0
4	H	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	F	2	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
All	All	47917	0	47549	830	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.

The worst 5 of 830 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:D:66:GLY:HA2	1:D:236:ARG:NH2	1.40	1.36
1:A:539:MET:HE1	1:A:550:ILE:CG2	1.62	1.26
1:D:84:LYS:CE	1:D:137:GLU:HG2	1.71	1.17
1:F:439:SER:HB2	1:F:448:LEU:CD1	1.80	1.11
1:L:429:VAL:HG21	1:L:434:MET:HE3	1.28	1.11

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	518/650 (80%)	468 (90%)	43 (8%)	7 (1%)	9	30
1	B	521/650 (80%)	473 (91%)	40 (8%)	8 (2%)	8	29
1	C	518/650 (80%)	467 (90%)	46 (9%)	5 (1%)	12	38
1	D	488/650 (75%)	438 (90%)	40 (8%)	10 (2%)	6	24
1	E	520/650 (80%)	473 (91%)	39 (8%)	8 (2%)	8	29
1	F	519/650 (80%)	479 (92%)	36 (7%)	4 (1%)	16	44
1	G	516/650 (79%)	472 (92%)	40 (8%)	4 (1%)	16	44
1	H	457/650 (70%)	416 (91%)	38 (8%)	3 (1%)	18	46
1	I	515/650 (79%)	472 (92%)	40 (8%)	3 (1%)	21	49
1	J	514/650 (79%)	465 (90%)	43 (8%)	6 (1%)	10	33
1	K	452/650 (70%)	409 (90%)	39 (9%)	4 (1%)	14	41
1	L	452/650 (70%)	414 (92%)	37 (8%)	1 (0%)	43	70
2	P	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	Q	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	R	3/5 (60%)	1 (33%)	2 (67%)	0	100	100
2	S	3/5 (60%)	2 (67%)	1 (33%)	0	100	100
2	T	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
2	U	3/5 (60%)	2 (67%)	0	1 (33%)	0	0
2	V	3/5 (60%)	3 (100%)	0	0	100	100
2	W	2/5 (40%)	2 (100%)	0	0	100	100
2	X	2/5 (40%)	2 (100%)	0	0	100	100
2	Y	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	6017/7850 (77%)	5465 (91%)	487 (8%)	65 (1%)	11	36

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	HIS
1	B	211	LYS
1	B	218	HIS
1	D	211	LYS
1	E	98	LYS

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	439/552 (80%)	388 (88%)	51 (12%)	5	20
1	B	442/552 (80%)	390 (88%)	52 (12%)	5	19
1	C	439/552 (80%)	378 (86%)	61 (14%)	3	14
1	D	417/552 (76%)	370 (89%)	47 (11%)	5	20
1	E	441/552 (80%)	393 (89%)	48 (11%)	6	22
1	F	440/552 (80%)	390 (89%)	50 (11%)	5	20
1	G	437/552 (79%)	390 (89%)	47 (11%)	6	22
1	H	387/552 (70%)	347 (90%)	40 (10%)	7	25
1	I	436/552 (79%)	388 (89%)	48 (11%)	6	22
1	J	435/552 (79%)	385 (88%)	50 (12%)	5	20
1	K	384/552 (70%)	339 (88%)	45 (12%)	5	19
1	L	386/552 (70%)	338 (88%)	48 (12%)	4	18
All	All	5083/6624 (77%)	4496 (88%)	587 (12%)	5	20

5 of 587 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	173	ASN
1	L	490	ASP
1	J	453	VAL
1	J	167	THR
1	K	358	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	559	GLN
1	L	580	ASN
1	K	144	ASN
1	K	580	ASN
1	D	494	ASN

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 13 ligands modelled in this entry, 13 are 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 ⓘ

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	522/650 (80%)	-0.07	5 (0%) 79 66	38, 80, 156, 226	0
1	B	525/650 (80%)	-0.17	9 (1%) 69 53	39, 84, 139, 184	1 (0%)
1	C	522/650 (80%)	0.06	12 (2%) 61 45	50, 93, 183, 243	0
1	D	496/650 (76%)	0.11	23 (4%) 37 27	44, 89, 212, 320	0
1	E	524/650 (80%)	0.03	13 (2%) 58 43	45, 97, 141, 192	1 (0%)
1	F	523/650 (80%)	0.08	23 (4%) 39 28	56, 101, 172, 236	1 (0%)
1	G	520/650 (80%)	-0.03	6 (1%) 76 63	43, 87, 134, 195	0
1	H	465/650 (71%)	-0.08	10 (2%) 62 46	46, 85, 148, 206	0
1	I	519/650 (79%)	-0.10	12 (2%) 61 45	48, 96, 137, 173	0
1	J	518/650 (79%)	0.08	10 (1%) 66 49	46, 102, 197, 236	0
1	K	462/650 (71%)	0.41	28 (6%) 27 20	65, 119, 175, 229	0
1	L	462/650 (71%)	0.30	18 (3%) 43 30	69, 131, 181, 236	0
2	P	5/5 (100%)	0.42	0 100 100	103, 103, 120, 131	0
2	Q	5/5 (100%)	0.37	1 (20%) 3 4	90, 107, 144, 158	0
2	R	5/5 (100%)	1.08	1 (20%) 3 4	96, 100, 134, 135	0
2	S	5/5 (100%)	0.60	0 100 100	84, 86, 122, 128	0
2	T	5/5 (100%)	1.24	1 (20%) 3 4	96, 98, 129, 132	0
2	U	5/5 (100%)	0.91	1 (20%) 3 4	103, 106, 129, 133	0
2	V	5/5 (100%)	0.57	0 100 100	90, 106, 134, 135	0
2	W	4/5 (80%)	0.72	1 (25%) 2 3	84, 87, 108, 122	0
2	X	4/5 (80%)	0.29	0 100 100	97, 111, 115, 116	0
2	Y	4/5 (80%)	0.49	0 100 100	80, 93, 97, 105	0
All	All	6105/7850 (77%)	0.05	174 (2%) 53 39	38, 97, 169, 320	3 (0%)

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	221	TRP	7.9
1	L	221	TRP	7.6
1	C	221	TRP	6.4
1	D	153	ILE	5.8
1	I	219	ASP	5.5

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(Å ²)	Q<0.9
3	CD	F	801	1/1	0.78	0.11	184,184,184,184	0
3	CD	A	801	1/1	0.83	0.09	139,139,139,139	0
3	CD	E	801	1/1	0.85	0.09	181,181,181,181	0
3	CD	B	801	1/1	0.85	0.11	243,243,243,243	0
3	CD	C	801	1/1	0.87	0.08	72,72,72,72	0
3	CD	G	801	1/1	0.87	0.08	150,150,150,150	0
3	CD	I	801	1/1	0.90	0.12	171,171,171,171	0
3	CD	D	801	1/1	0.91	0.06	120,120,120,120	0
4	CL	D	802	1/1	0.91	0.06	77,77,77,77	0
4	CL	F	802	1/1	0.92	0.05	80,80,80,80	0
3	CD	J	801	1/1	0.95	0.05	104,104,104,104	0
3	CD	H	801	1/1	0.97	0.04	76,76,76,76	0
4	CL	H	802	1/1	0.97	0.04	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.