



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 03:22 PM UTC

PDB ID : 5L75 / pdb_00005L75
Title : A protein structure
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Deposited on : 2016-06-01
Resolution : 3.70 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

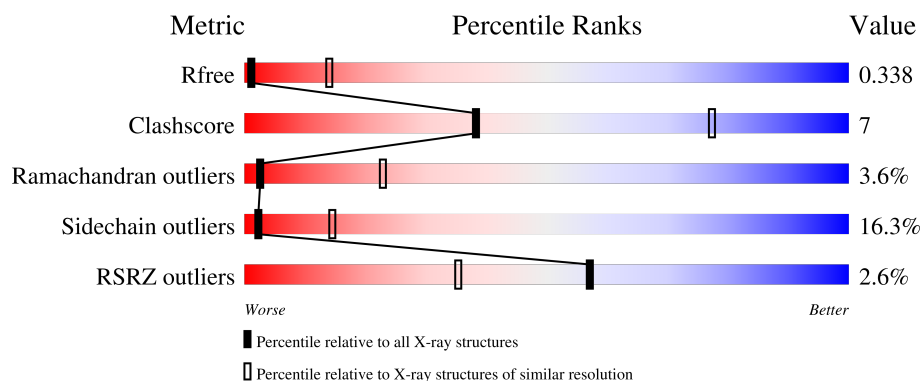
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

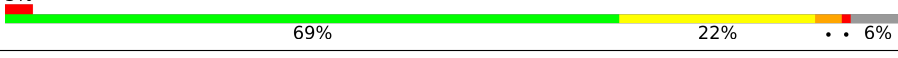
The reported resolution of this entry is 3.70 Å.

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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	241	
1	B	241	
2	F	365	
3	G	360	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8824 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 Lipopolysaccharide ABC transporter, ATP-binding protein LptB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1833	1149	335	345	4			
1	B	237	Total	C	N	O	S	0	0	0
			1850	1159	337	349	5			

- Molecule 2 is a protein called FIG000988: Predicted permease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	323	Total	C	N	O	S	0	0	0
			2503	1636	418	433	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	107	VAL	LEU	conflict	UNP W1B830
F	204	TYR	VAL	conflict	UNP W1B830

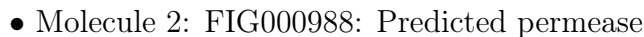
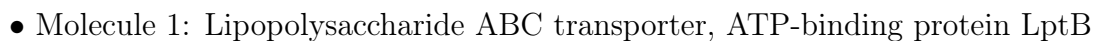
- Molecule 3 is a protein called FIG000906: Predicted Permease.

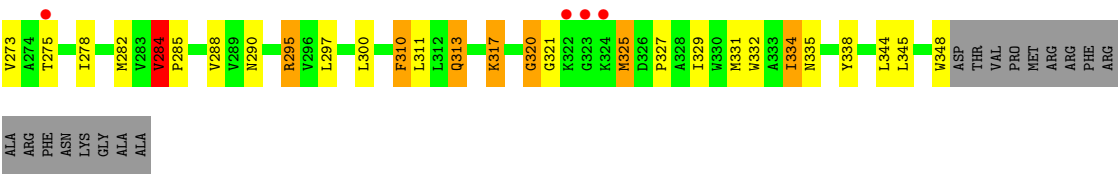
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	340	Total	C	N	O	S	0	0	0
			2636	1720	433	465	18			

- Molecule 4 is PLATINUM (II) ION (CCD ID: PT) (formula: Pt).

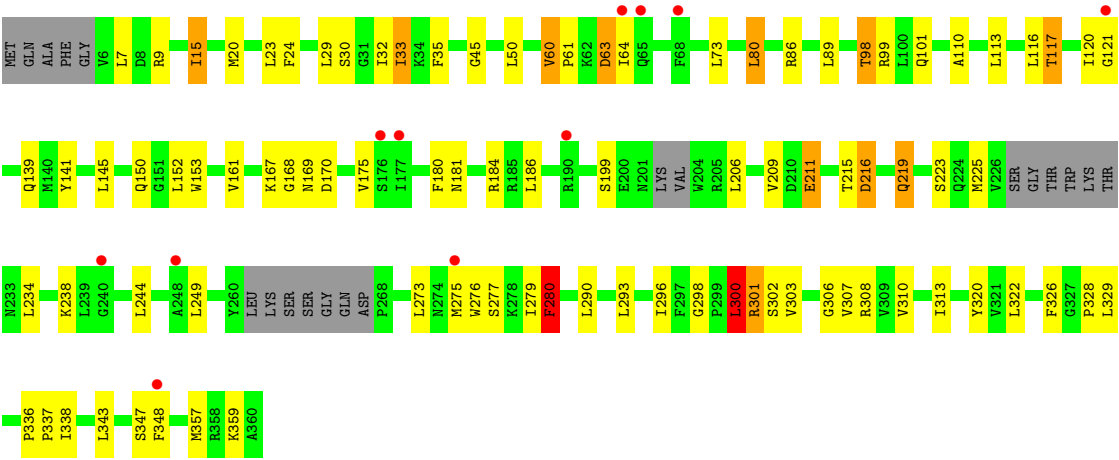
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Pt	0	0
			1	1		
4	G	1	Total	Pt	0	0
			1	1		

- Molecule 1: Lipopolysaccharide ABC transporter, ATP-binding protein LptB





• Molecule 3: FIG000906: Predicted Permease



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.26Å 210.52Å 258.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.70 29.96 – 3.70	Depositor EDS
% Data completeness (in resolution range)	65.3 (29.96-3.70) 65.2 (29.96-3.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 3.75Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.284 , 0.322 0.306 , 0.338	Depositor DCC
R_{free} test set	1041 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	124.0	Xtriage
Anisotropy	1.734	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 54.1	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	0.90	EDS
Total number of atoms	8824	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: PT

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	0.78	0/1858	1.37	3/2512 (0.1%)
1	B	0.80	0/1875	1.34	4/2534 (0.2%)
2	F	0.81	1/2550 (0.0%)	1.40	5/3459 (0.1%)
3	G	0.82	0/2691	1.43	22/3639 (0.6%)
All	All	0.80	1/8974 (0.0%)	1.39	34/12144 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	284	VAL	CA-CB	5.42	1.56	1.54

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	284	VAL	N-CA-CB	11.00	117.89	110.52
3	G	280	PHE	CA-CB-CG	7.88	121.68	113.80
2	F	222	PHE	CA-CB-CG	6.79	120.59	113.80
3	G	348	PHE	CA-CB-CG	6.73	120.53	113.80
3	G	110	ALA	CA-C-N	6.57	125.59	120.33

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	1833	0	1871	28	0
1	B	1850	0	1889	20	0
2	F	2503	0	2595	50	3
3	G	2636	0	2715	30	0
4	A	1	0	0	0	0
4	G	1	0	0	0	0
All	All	8824	0	9070	123	3

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 7.

The worst 5 of 123 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)
2:F:257:THR:HG23	2:F:258:HIS:H	1.31	0.96
2:F:253:THR:HG22	2:F:256:LYS:NZ	1.89	0.87
1:A:89:ILE:HA	1:A:150:ARG:HH21	1.42	0.83
2:F:275:THR:HA	2:F:278:ILE:HG22	1.61	0.83
2:F:253:THR:HG22	2:F:256:LYS:HZ1	1.49	0.77

All (3) 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)
2:F:94:SER:CB	2:F:258:HIS:NE2[8_554]	1.39	0.81
2:F:94:SER:OG	2:F:258:HIS:NE2[8_554]	1.77	0.43
2:F:94:SER:OG	2:F:258:HIS:CD2[8_554]	1.93	0.27

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	233/241 (97%)	203 (87%)	23 (10%)	7 (3%)	3	26
1	B	235/241 (98%)	194 (83%)	37 (16%)	4 (2%)	7	34
2	F	313/365 (86%)	253 (81%)	41 (13%)	19 (6%)	1	14
3	G	332/360 (92%)	271 (82%)	51 (15%)	10 (3%)	3	26
All	All	1113/1207 (92%)	921 (83%)	152 (14%)	40 (4%)	2	23

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	ALA
2	F	144	LEU
2	F	146	GLN
2	F	260	ASP
3	G	63	ASP

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	196/202 (97%)	159 (81%)	37 (19%)	1	10
1	B	198/202 (98%)	175 (88%)	23 (12%)	5	24
2	F	266/301 (88%)	209 (79%)	57 (21%)	1	7
3	G	283/300 (94%)	246 (87%)	37 (13%)	4	20
All	All	943/1005 (94%)	789 (84%)	154 (16%)	2	14

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	344	LEU
3	G	249	LEU
3	G	15	ILE
3	G	117	THR
3	G	313	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	231	GLN
3	G	38	GLN
3	G	255	HIS
2	F	313	GLN
3	G	65	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 2 ligands modelled in this entry, 2 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	179:ALA	C	180:PHE	N	3.86

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	235/241 (97%)	-0.31	7 (2%) 52 32	51, 93, 131, 162	0
1	B	237/241 (98%)	-0.60	0 100 100	79, 126, 164, 195	0
2	F	323/365 (88%)	-0.21	11 (3%) 48 30	30, 113, 186, 252	0
3	G	340/360 (94%)	-0.15	11 (3%) 50 31	47, 96, 180, 254	0
All	All	1135/1207 (94%)	-0.29	29 (2%) 57 35	30, 107, 176, 254	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	90	ALA	5.8
2	F	86	THR	5.7
3	G	65	GLN	5.2
2	F	87	VAL	5.2
3	G	240	GLY	5.1

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
4	PT	A	301	1/1	0.77	0.10	160,160,160,160	1
4	PT	G	401	1/1	0.88	0.28	236,236,236,236	1

6.5 Other polymers [i](#)

There are no such residues in this entry.