



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 29, 2026 – 05:25 PM UTC

PDB ID : 4XKT / pdb_00004xkt
Title : E coli BFR variant Y149F
Authors : Bradley, J.M.; Hemmings, A.M.; Le Brun, N.E.
Deposited on : 2015-01-12
Resolution : 1.82 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	:	FAILED
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

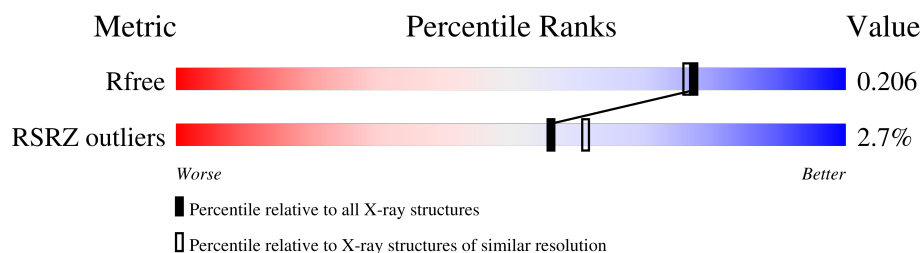
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19321 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	15	1
			1393	879	231	276	7			
1	B	158	Total	C	N	O	S	0	16	1
			1396	883	234	272	7			
1	C	158	Total	C	N	O	S	0	14	1
			1376	872	229	268	7			
1	D	158	Total	C	N	O	S	0	12	1
			1365	864	231	263	7			
1	E	158	Total	C	N	O	S	0	13	1
			1374	870	229	268	7			
1	F	158	Total	C	N	O	S	0	15	1
			1390	877	236	270	7			
1	G	158	Total	C	N	O	S	0	16	1
			1392	881	233	271	7			
1	H	158	Total	C	N	O	S	0	13	1
			1379	868	233	271	7			
1	I	158	Total	C	N	O	S	0	14	1
			1375	869	232	267	7			
1	J	158	Total	C	N	O	S	0	8	1
			1337	845	225	260	7			
1	K	158	Total	C	N	O	S	0	10	1
			1350	852	227	264	7			
1	L	158	Total	C	N	O	S	0	11	1
			1360	860	228	265	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	PHE	TYR	engineered mutation	UNP E2QFJ1
B	149	PHE	TYR	engineered mutation	UNP E2QFJ1
C	149	PHE	TYR	engineered mutation	UNP E2QFJ1
D	149	PHE	TYR	engineered mutation	UNP E2QFJ1
E	149	PHE	TYR	engineered mutation	UNP E2QFJ1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	149	PHE	TYR	engineered mutation	UNP E2QFJ1
G	149	PHE	TYR	engineered mutation	UNP E2QFJ1
H	149	PHE	TYR	engineered mutation	UNP E2QFJ1
I	149	PHE	TYR	engineered mutation	UNP E2QFJ1
J	149	PHE	TYR	engineered mutation	UNP E2QFJ1
K	149	PHE	TYR	engineered mutation	UNP E2QFJ1
L	149	PHE	TYR	engineered mutation	UNP E2QFJ1

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	233	Total	O	0	0
			233	233		
3	B	234	Total	O	0	0
			234	234		
3	C	246	Total	O	0	0
			246	246		
3	D	231	Total	O	0	0
			231	231		
3	E	228	Total	O	0	0
			228	228		
3	F	232	Total	O	0	0
			232	232		
3	G	236	Total	O	0	0
			236	236		
3	H	220	Total	O	0	0
			220	220		
3	I	219	Total	O	0	0
			219	219		
3	J	229	Total	O	0	0
			229	229		
3	K	230	Total	O	0	0
			230	230		
3	L	231	Total	O	0	0
			231	231		

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.47Å 208.47Å 142.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.75 – 1.82 31.75 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.75-1.82) 99.8 (31.75-1.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.167 , 0.206 0.170 , 0.206	Depositor DCC
R_{free} test set	13933 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19321	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.41 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4915e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 Ligand geometry [i](#)

13 ligands are 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	SO4	C	201	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	E	201	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	H	201	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	H	202	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	K	201	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	C	203	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	L	201	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	G	201	-	4,4,4	0.20	0	6,6,6	0.09	0
2	SO4	J	201	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	D	201	-	4,4,4	0.26	0	6,6,6	0.09	0
2	SO4	B	201	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	C	202	-	4,4,4	0.22	0	6,6,6	0.08	0
2	SO4	F	201	-	4,4,4	0.21	0	6,6,6	0.09	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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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	158/158 (100%)	-0.53	5 (3%)	50	57	3, 9, 19, 77	15 (9%)
1	B	158/158 (100%)	-0.59	4 (2%)	58	64	4, 9, 21, 78	16 (10%)
1	C	158/158 (100%)	-0.60	4 (2%)	58	64	4, 9, 20, 77	14 (8%)
1	D	158/158 (100%)	-0.54	4 (2%)	58	64	4, 9, 22, 86	12 (7%)
1	E	158/158 (100%)	-0.57	6 (3%)	44	50	4, 9, 22, 83	13 (8%)
1	F	158/158 (100%)	-0.62	3 (1%)	66	72	3, 9, 19, 81	15 (9%)
1	G	158/158 (100%)	-0.59	5 (3%)	50	57	4, 8, 20, 79	16 (10%)
1	H	158/158 (100%)	-0.58	5 (3%)	50	57	4, 9, 20, 82	13 (8%)
1	I	158/158 (100%)	-0.64	3 (1%)	66	72	4, 9, 21, 76	14 (8%)
1	J	158/158 (100%)	-0.58	5 (3%)	50	57	4, 9, 22, 80	8 (5%)
1	K	158/158 (100%)	-0.57	4 (2%)	58	64	4, 9, 19, 80	10 (6%)
1	L	158/158 (100%)	-0.61	4 (2%)	58	64	4, 9, 21, 80	11 (6%)
All	All	1896/1896 (100%)	-0.59	52 (2%)	56	61	3, 9, 21, 86	157 (8%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	158	GLY	7.3
1	A	158	GLY	7.0
1	D	158	GLY	6.2
1	F	158	GLY	6.0
1	E	158	GLY	5.9
1	B	158	GLY	5.2
1	D	157	GLU	4.5
1	C	155	ARG	4.3
1	G	155	ARG	4.3
1	L	155	ARG	4.2
1	A	157	GLU	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	156[A]	GLU	3.9
1	G	157	GLU	3.9
1	J	158	GLY	3.8
1	B	39	ARG	3.7
1	G	158	GLY	3.6
1	B	155	ARG	3.5
1	E	99	LYS	3.4
1	F	155	ARG	3.4
1	A	39	ARG	3.3
1	C	157	GLU	3.3
1	L	157	GLU	3.3
1	H	155	ARG	3.3
1	I	155	ARG	3.3
1	C	158	GLY	3.1
1	G	156	GLU	3.1
1	G	39	ARG	3.0
1	J	157	GLU	3.0
1	H	39[A]	ARG	2.9
1	E	142	GLN	2.9
1	J	39	ARG	2.9
1	B	157	GLU	2.9
1	J	155	ARG	2.9
1	K	156	GLU	2.8
1	H	156	GLU	2.8
1	K	155	ARG	2.8
1	L	156	GLU	2.8
1	D	156	GLU	2.7
1	E	156	GLU	2.7
1	K	157	GLU	2.7
1	J	156	GLU	2.6
1	F	157	GLU	2.5
1	E	155	ARG	2.5
1	C	156	GLU	2.5
1	K	158	GLY	2.4
1	L	158	GLY	2.4
1	A	155	ARG	2.3
1	D	155	ARG	2.3
1	I	157	GLU	2.3
1	I	156[A]	GLU	2.1
1	E	157	GLU	2.1
1	H	154	ILE	2.0

5.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.4 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	SO4	J	201	5/5	0.77	0.34	38,44,48,51	0
2	SO4	C	202	5/5	0.81	0.23	72,76,77,81	0
2	SO4	D	201	5/5	0.92	0.12	40,45,48,54	0
2	SO4	C	203	5/5	0.92	0.15	45,46,47,51	0
2	SO4	F	201	5/5	0.93	0.10	46,52,53,58	0
2	SO4	H	202	5/5	0.94	0.10	44,47,52,52	0
2	SO4	K	201	5/5	0.94	0.18	39,40,45,50	0
2	SO4	L	201	5/5	0.94	0.15	41,43,46,48	0
2	SO4	G	201	5/5	0.96	0.08	44,49,56,61	0
2	SO4	C	201	5/5	0.99	0.03	10,11,11,12	0
2	SO4	E	201	5/5	0.99	0.04	11,12,14,16	0
2	SO4	B	201	5/5	1.00	0.02	8,10,12,13	0
2	SO4	H	201	5/5	1.00	0.02	10,10,11,12	0

5.5 Other polymers [i](#)

There are no such residues in this entry.