



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 09:49 AM UTC

PDB ID : 7W76 / pdb_00007w76
Title : Crystal structure of the K. lactis Bre1 RBD in complex with Rad6, crystal form II
Authors : Shi, M.; Zhao, J.; Xiang, S.
Deposited on : 2021-12-03
Resolution : 3.05 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
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

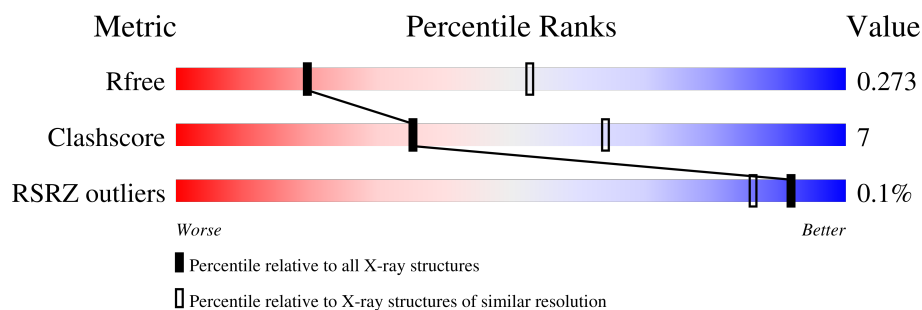
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	167	76% 19% 5%
1	B	167	66% 25% 10%
2	C	206	70% 6% 24%
2	D	206	75% 7% 18%
2	E	206	53% 18% 29%
2	F	206	66% 12% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7503 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 Ubiquitin-conjugating enzyme E2 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	Se	0	0	0
			1282	810	215	248	1	8			
1	B	151	Total	C	N	O	S	Se	0	0	0
			1207	763	201	234	1	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q6CUD9
A	-1	SER	-	expression tag	UNP Q6CUD9
A	0	HIS	-	expression tag	UNP Q6CUD9
B	-2	GLY	-	expression tag	UNP Q6CUD9
B	-1	SER	-	expression tag	UNP Q6CUD9
B	0	HIS	-	expression tag	UNP Q6CUD9

- Molecule 2 is a protein called E3 ubiquitin-protein ligase BRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	157	Total	C	N	O	S		0	0	0
			1247	773	213	256	5				
2	D	168	Total	C	N	O	S		0	0	0
			1325	818	229	273	5				
2	E	146	Total	C	N	O	S		0	0	0
			1160	722	197	236	5				
2	F	160	Total	C	N	O	S		0	0	0
			1265	782	219	259	5				

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



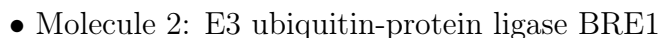
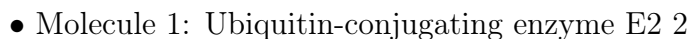
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



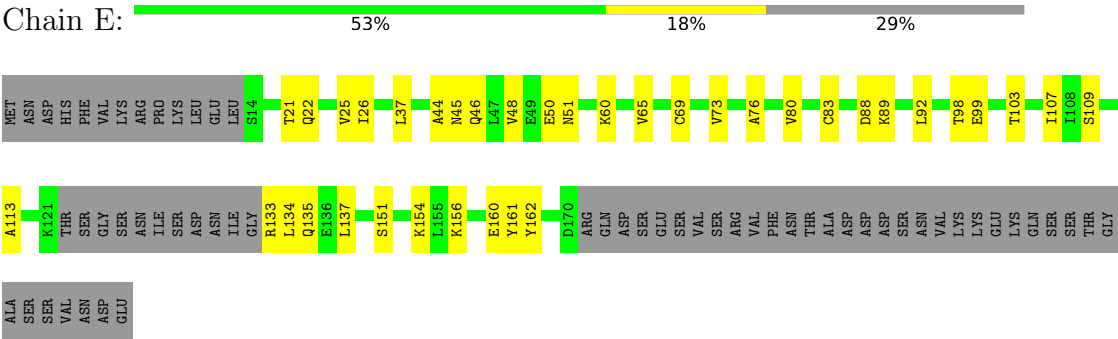
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 1: Ubiquitin-conjugating enzyme E2 2

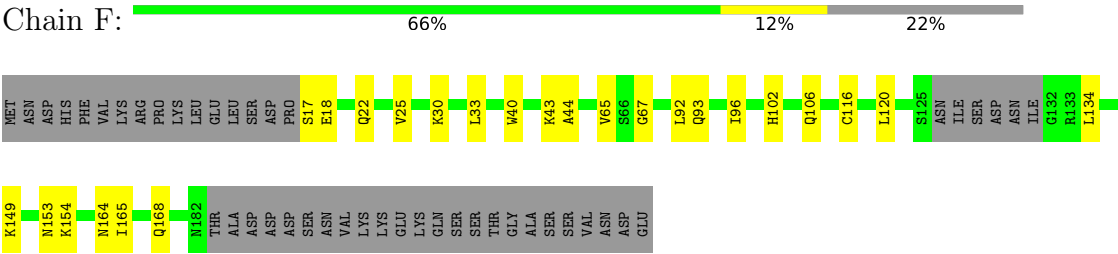


ALA
SER
SER
VAL
ASN
ASP
GLU

• Molecule 2: E3 ubiquitin-protein ligase BRE1



• Molecule 2: E3 ubiquitin-protein ligase BRE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.22Å 113.22Å 386.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.18 – 3.05 32.18 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.2 (32.18-3.05) 99.5 (32.18-3.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.237 , 0.286 (Not available) , 0.273	Depositor DCC
R_{free} test set	1486 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	85.8	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 99.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7503	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: SO4, GOL

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	0.15	0/1310	0.39	0/1770
1	B	0.17	0/1232	0.44	0/1660
2	C	0.14	0/1256	0.35	0/1692
2	D	0.13	0/1336	0.38	0/1801
2	E	0.13	0/1169	0.35	0/1575
2	F	0.13	0/1274	0.33	0/1714
All	All	0.14	0/7577	0.38	0/10212

There are no bond length outliers.

There are no bond angle outliers.

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	1282	0	1229	26	0
1	B	1207	0	1160	28	0
2	C	1247	0	1260	11	0
2	D	1325	0	1336	13	0
2	E	1160	0	1178	28	0
2	F	1265	0	1277	22	0
3	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	1	0
4	D	5	0	0	1	0
All	All	7503	0	7456	110	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 7.

The worst 5 of 110 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:8:ARG:HD3	1:B:64:PRO:HG3	1.58	0.85
1:B:57:LEU:HB3	1:B:70:VAL:HG13	1.62	0.80
2:E:137:LEU:HD12	2:F:134:LEU:HD22	1.65	0.79
2:E:48:VAL:HA	2:E:51:ASN:HB3	1.75	0.69
2:E:113:ALA:HB2	2:E:133:ARG:HG2	1.77	0.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

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](#)

3 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	$\# Z > 2$
3	GOL	B	1000	-	5,5,5	0.96	0	5,5,5	1.07	0
3	GOL	A	1000	-	5,5,5	0.97	0	5,5,5	1.09	0
4	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.12	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	1000	-	-	0/4/4/4	-
3	GOL	A	1000	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1000	GOL	1	0
4	D	301	SO4	1	0

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 [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	151/167 (90%)	-0.51	0 100 100	48, 78, 119, 170	0
1	B	143/167 (85%)	0.01	1 (0%) 84 66	98, 146, 196, 263	0
2	C	157/206 (76%)	-0.36	0 100 100	69, 108, 168, 210	0
2	D	168/206 (81%)	-0.38	0 100 100	70, 114, 169, 235	0
2	E	146/206 (70%)	-0.18	0 100 100	89, 137, 195, 220	0
2	F	160/206 (77%)	-0.35	0 100 100	69, 119, 198, 263	0
All	All	925/1158 (79%)	-0.30	1 (0%) 92 86	48, 114, 192, 263	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	4.2

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 [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
3	GOL	B	1000	6/6	0.55	0.14	119,128,133,134	0
3	GOL	A	1000	6/6	0.74	0.10	74,80,96,97	0
4	SO4	D	301	5/5	0.89	0.10	143,144,144,144	5

6.5 Other polymers [i](#)

There are no such residues in this entry.