



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:36 AM UTC

PDB ID : 4RYJ / pdb_00004ryj
Title : Crystal structure of apo dimer of BcTSPO
Authors : Guo, Y.; Liu, Q.; Hendrickson, W.A.; New York Consortium on Membrane Protein Structure (NYCOMPS)
Deposited on : 2014-12-15
Resolution : 4.10 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
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

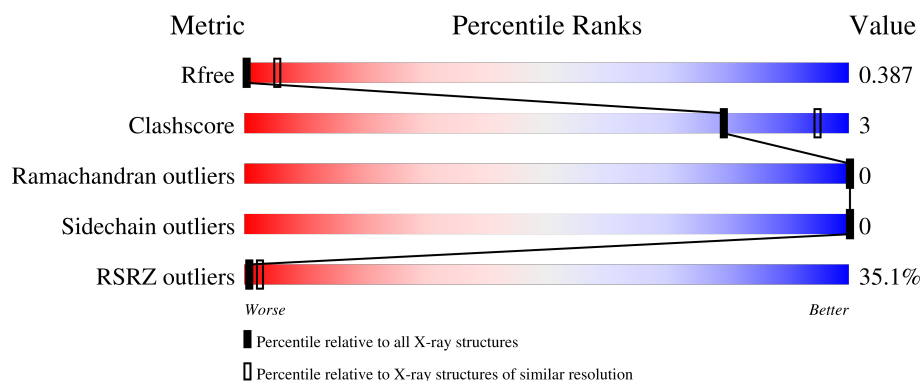
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	181	28% 76% 7% 17%
1	B	181	31% 75% 8% 17%

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 2444 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 Integral membrane protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1222	843	172	204	3			
1	B	151	Total	C	N	O	S	0	0	0
			1222	843	172	204	3			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP Q81BL7
A	-26	ASP	-	expression tag	UNP Q81BL7
A	-25	TYR	-	expression tag	UNP Q81BL7
A	-24	LYS	-	expression tag	UNP Q81BL7
A	-23	ASP	-	expression tag	UNP Q81BL7
A	-22	ASP	-	expression tag	UNP Q81BL7
A	-21	ASP	-	expression tag	UNP Q81BL7
A	-20	ASP	-	expression tag	UNP Q81BL7
A	-19	LYS	-	expression tag	UNP Q81BL7
A	-18	HIS	-	expression tag	UNP Q81BL7
A	-17	HIS	-	expression tag	UNP Q81BL7
A	-16	HIS	-	expression tag	UNP Q81BL7
A	-15	HIS	-	expression tag	UNP Q81BL7
A	-14	HIS	-	expression tag	UNP Q81BL7
A	-13	HIS	-	expression tag	UNP Q81BL7
A	-12	HIS	-	expression tag	UNP Q81BL7
A	-11	HIS	-	expression tag	UNP Q81BL7
A	-10	HIS	-	expression tag	UNP Q81BL7
A	-9	HIS	-	expression tag	UNP Q81BL7
A	-8	GLU	-	expression tag	UNP Q81BL7
A	-7	ASN	-	expression tag	UNP Q81BL7
A	-6	LEU	-	expression tag	UNP Q81BL7
A	-5	TYR	-	expression tag	UNP Q81BL7
A	-4	PHE	-	expression tag	UNP Q81BL7
A	-3	GLN	-	expression tag	UNP Q81BL7

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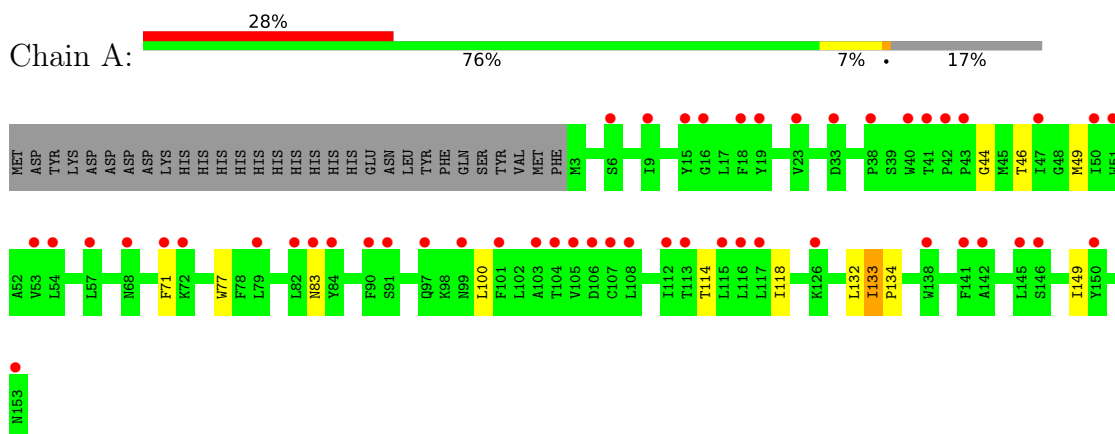
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q81BL7
A	-1	TYR	-	expression tag	UNP Q81BL7
A	0	VAL	-	expression tag	UNP Q81BL7
B	-27	MET	-	expression tag	UNP Q81BL7
B	-26	ASP	-	expression tag	UNP Q81BL7
B	-25	TYR	-	expression tag	UNP Q81BL7
B	-24	LYS	-	expression tag	UNP Q81BL7
B	-23	ASP	-	expression tag	UNP Q81BL7
B	-22	ASP	-	expression tag	UNP Q81BL7
B	-21	ASP	-	expression tag	UNP Q81BL7
B	-20	ASP	-	expression tag	UNP Q81BL7
B	-19	LYS	-	expression tag	UNP Q81BL7
B	-18	HIS	-	expression tag	UNP Q81BL7
B	-17	HIS	-	expression tag	UNP Q81BL7
B	-16	HIS	-	expression tag	UNP Q81BL7
B	-15	HIS	-	expression tag	UNP Q81BL7
B	-14	HIS	-	expression tag	UNP Q81BL7
B	-13	HIS	-	expression tag	UNP Q81BL7
B	-12	HIS	-	expression tag	UNP Q81BL7
B	-11	HIS	-	expression tag	UNP Q81BL7
B	-10	HIS	-	expression tag	UNP Q81BL7
B	-9	HIS	-	expression tag	UNP Q81BL7
B	-8	GLU	-	expression tag	UNP Q81BL7
B	-7	ASN	-	expression tag	UNP Q81BL7
B	-6	LEU	-	expression tag	UNP Q81BL7
B	-5	TYR	-	expression tag	UNP Q81BL7
B	-4	PHE	-	expression tag	UNP Q81BL7
B	-3	GLN	-	expression tag	UNP Q81BL7
B	-2	SER	-	expression tag	UNP Q81BL7
B	-1	TYR	-	expression tag	UNP Q81BL7
B	0	VAL	-	expression tag	UNP Q81BL7

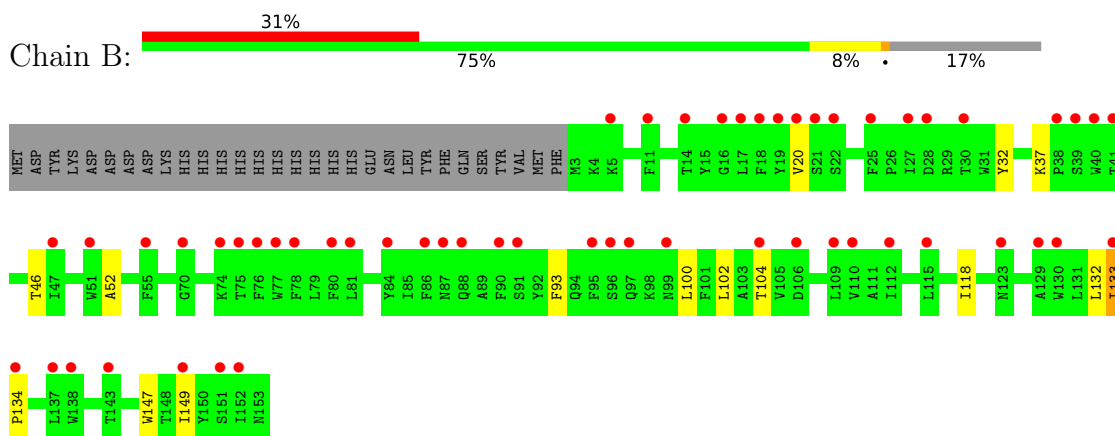
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Integral membrane protein



- Molecule 1: Integral membrane protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	33.98Å 104.93Å 53.86Å 90.00° 104.89° 90.00°	Depositor
Resolution (Å)	36.95 – 4.10 36.95 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (36.95-4.10) 99.3 (36.95-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.345 , 0.374 0.365 , 0.387	Depositor DCC
R_{free} test set	142 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.09 , 0.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	2444	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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](#)

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	0.41	0/1268	0.88	3/1741 (0.2%)
1	B	0.42	0/1268	0.92	3/1741 (0.2%)
All	All	0.41	0/2536	0.90	6/3482 (0.2%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	ILE	CB-CA-C	-6.91	107.02	114.35
1	A	46	THR	N-CA-C	-6.56	104.05	111.07
1	A	133	ILE	CB-CA-C	-6.30	107.67	114.35
1	B	46	THR	N-CA-C	-6.12	104.52	111.07
1	B	20	VAL	N-CA-C	5.97	116.15	110.42
1	A	44	GLY	N-CA-C	5.12	118.69	112.49

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	1222	0	1194	7	0
1	B	1222	0	1194	7	0
All	All	2444	0	2388	13	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 3.

All (13) 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:A:118:ILE:HG12	1:A:132:LEU:HB2	1.85	0.59
1:B:32:TYR:O	1:B:37:LYS:NZ	2.38	0.54
1:B:100:LEU:HD13	1:B:149:ILE:HG22	1.94	0.49
1:A:100:LEU:HD13	1:A:149:ILE:HG22	1.95	0.49
1:A:83:ASN:ND2	1:A:114:THR:OG1	2.47	0.47
1:A:133:ILE:HB	1:A:134:PRO:HD3	1.96	0.47
1:A:49:MET:HA	1:B:52:ALA:HB2	1.97	0.46
1:B:118:ILE:HG12	1:B:132:LEU:HB2	1.97	0.45
1:A:118:ILE:HD13	1:A:133:ILE:HD13	1.98	0.45
1:A:71:PHE:HA	1:A:77:TRP:NE1	2.33	0.44
1:B:93:PHE:CD1	1:B:102:LEU:HB3	2.55	0.42
1:B:133:ILE:HB	1:B:134:PRO:HD3	2.02	0.41
1:B:104:THR:HG21	1:B:147:TRP:HB2	2.04	0.40

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	149/181 (82%)	147 (99%)	2 (1%)	0	100	100
1	B	149/181 (82%)	147 (99%)	2 (1%)	0	100	100
All	All	298/362 (82%)	294 (99%)	4 (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	129/166 (78%)	129 (100%)	0	100	100
1	B	129/166 (78%)	129 (100%)	0	100	100
All	All	258/332 (78%)	258 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	151/181 (83%)	1.89	50 (33%)  	99, 124, 153, 176	0
1	B	151/181 (83%)	2.41	56 (37%)  	103, 121, 141, 160	0
All	All	302/362 (83%)	2.15	106 (35%)  	99, 122, 147, 176	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	88	GLN	17.2
1	B	87	ASN	13.8
1	A	42	PRO	13.3
1	B	17	LEU	13.0
1	B	18	PHE	12.0
1	B	75	THR	11.0
1	B	16	GLY	11.0
1	B	74	LYS	10.6
1	B	84	TYR	9.9
1	A	19	TYR	8.8
1	A	41	THR	8.4
1	A	40	TRP	7.5
1	B	22	SER	7.5
1	A	145	LEU	7.2
1	B	134	PRO	6.9
1	B	138	TRP	6.8
1	B	86	PHE	6.7
1	A	71	PHE	6.7
1	B	91	SER	6.5
1	A	107	CYS	6.3
1	A	72	LYS	6.2
1	B	80	PHE	6.2
1	B	106	ASP	6.2
1	A	91	SER	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	152	ILE	6.0
1	B	19	TYR	5.9
1	A	106	ASP	5.8
1	B	21	SER	5.7
1	B	77	TRP	5.7
1	B	78	PHE	4.9
1	A	141	PHE	4.8
1	B	137	LEU	4.7
1	A	103	ALA	4.6
1	A	23	VAL	4.6
1	B	51	TRP	4.6
1	A	16	GLY	4.3
1	B	90	PHE	4.3
1	A	68	ASN	4.2
1	A	142	ALA	4.1
1	A	43	PRO	4.1
1	A	47	ILE	4.0
1	B	96	SER	3.9
1	B	112	ILE	3.8
1	B	39	SER	3.7
1	B	130	TRP	3.7
1	B	151	SER	3.7
1	A	84	TYR	3.6
1	B	97	GLN	3.6
1	A	53	VAL	3.5
1	A	112	ILE	3.5
1	B	25	PHE	3.4
1	B	38	PRO	3.3
1	B	81	LEU	3.3
1	A	108	LEU	3.3
1	B	27	ILE	3.3
1	B	41	THR	3.3
1	B	40	TRP	3.1
1	A	6	SER	3.1
1	A	138	TRP	3.1
1	A	79	LEU	3.0
1	B	129	ALA	3.0
1	A	150	TYR	2.9
1	A	90	PHE	2.9
1	A	105	VAL	2.8
1	A	146	SER	2.7
1	A	115	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	15	TYR	2.6
1	A	54	LEU	2.6
1	B	20	VAL	2.6
1	B	95	PHE	2.6
1	B	70	GLY	2.6
1	B	104	THR	2.6
1	B	76	PHE	2.5
1	B	133	ILE	2.5
1	B	109	LEU	2.5
1	A	116	LEU	2.5
1	A	97	GLN	2.4
1	A	50	ILE	2.4
1	B	30	THR	2.4
1	A	57	LEU	2.4
1	B	14	THR	2.4
1	A	101	PHE	2.4
1	A	99	ASN	2.4
1	B	149	ILE	2.4
1	A	82	LEU	2.3
1	B	110	VAL	2.3
1	A	113	THR	2.3
1	A	18	PHE	2.3
1	A	153	ASN	2.3
1	B	123	ASN	2.3
1	A	38	PRO	2.3
1	B	47	ILE	2.2
1	B	115	LEU	2.2
1	B	11	PHE	2.2
1	A	9	ILE	2.2
1	A	83	ASN	2.2
1	A	126	LYS	2.2
1	B	5	LYS	2.1
1	A	33	ASP	2.1
1	B	143	THR	2.1
1	A	117	LEU	2.1
1	B	55	PHE	2.1
1	A	51	TRP	2.1
1	B	28	ASP	2.1
1	A	104	THR	2.1
1	B	99	ASN	2.0

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.