



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 12:17 am GMT

PDB ID : 5T3R  
Title : Crystal structure of BT1762-1763  
Authors : van den Berg, B.  
Deposited on : 2016-08-26  
Resolution : 3.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

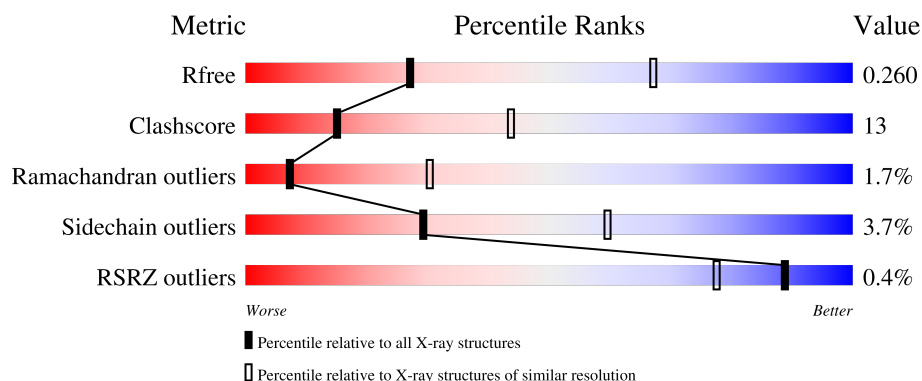
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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  $\geq 3$ , 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	576	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
2	D	1041	<div> <div>50%</div> <div>25%</div> <div>•</div> <div>23%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10860 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	1	0
			4455	2821	740	873	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	HIS	-	expression tag	UNP Q8A6W4
A	554	HIS	-	expression tag	UNP Q8A6W4
A	555	HIS	-	expression tag	UNP Q8A6W4
A	556	HIS	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	806	Total	C	N	O	S	0	0	0
			6402	4055	1088	1240	19			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

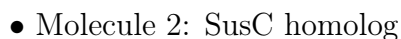
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

**i**

- Molecule 1: SusD homolog



R341	F441	M534	I664	L750	Y853	V963
L352	N442	G541	L669	G751	D854	1964
D355	L443	P670	P670	Y752	P855	R969
I356	R444	S553	S671	R753	T856	N970
L357	S445	M561	G672	F758	I865	D971
G360	T446	M562	F673	G759	Y869	R974
Q361	F447	Y565	K674	L760	K870	S978
H362	G448	N676	N677	I768	D873	L982
F363	N453	A566	1678	I775	L874	I985
T364	K454	L571	G679	L776	T875	K988
R367	Y463	S572	M680	E777	W878	T981
V371	E465	L573	D681	L778	I886	Q992
I377	E465	D578	N682	P779	K891	E993
I378	N470	S581	1683	E780	K892	D994
E379	M471	R582	K684	T781	S894	P998
T380	G472	F583	W685	W782	W897	I1004
A381	K479	R588	E686	K787	L905	P1005
D382	Q480	Y589	Q690	G790	N906	V1006
I384	E481	A590	T691	N791	K907	N1007
P385	H482	L597	1695	G792	G908	I1008
V390	W483	R600	L699	W793	T909	T1009
S396	L484	N605	L704	T800	K910	F1010
W397	K485	K608	L707	Q804	L912	F1016
R408	W486	E609	E708	I808	N913	
N409	M487	L610	E709	1812	N921	
P410	A490	T611	Y712	F813	S922	
R411	L491	W612	K713	K814	D923	
A412	Y494	D614	Y722	S815	A926	
V413	K500	L618	W725	E818	L927	
L414	H501	R619	G726	Q825	T928	
E415	R502	N627	V727	A828	D931	
K418	D504	Q628	L728	E829	N934	
R421	E510	N632	G730	I832	E935	
Y422	E514	L633	G731	R833	Q936	
F428	D515	A634	G732	R834	R937	
G429	D516	R635	S733	Y835	E944	
D430	K623	Y636	R734	D836	F948	
A431	F526	T637	W735	I837	L949	
Y432	V433	Y639	I736	D839	K950	
F437	N434	I528	N737	D845	L951	
V438	L435	I529	S738	D848	T954	
T436	T436	T530	K742	D848	G957	
P437	T530	P531	F748	D848		
K439	D532	T661	N749	D848		
G440	Y533					

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.77Å 117.33Å 119.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.89 – 3.10 75.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.89-3.10) 99.9 (75.89-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.197 , 0.259 0.197 , 0.260	Depositor DCC
$R_{free}$ test set	2072 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 47.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NA, MG

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	0.47	0/4565	0.66	1/6194 (0.0%)
2	D	0.55	0/6567	0.78	4/8904 (0.0%)
All	All	0.52	0/11132	0.73	5/15098 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	582	ARG	NE-CZ-NH2	-15.16	112.72	120.30
1	A	275	ILE	CG1-CB-CG2	-7.07	95.84	111.40
2	D	282	LEU	CA-CB-CG	6.43	130.09	115.30
2	D	778	LEU	CA-CB-CG	6.11	129.34	115.30
2	D	905	LEU	CA-CB-CG	5.71	128.42	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	582	ARG	Sidechain

## 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	4455	0	4222	98	0
2	D	6402	0	6055	205	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
All	All	10860	0	10277	285	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 13.

The worst 5 of 285 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:178:PHE:CZ	1:A:203:TYR:CD2	2.11	1.39
1:A:178:PHE:CZ	1:A:203:TYR:CE2	2.30	1.19
1:A:178:PHE:CE1	1:A:203:TYR:HD2	1.63	1.15
1:A:178:PHE:CE1	1:A:203:TYR:CD2	2.43	1.03
1:A:178:PHE:HZ	1:A:203:TYR:CE2	1.78	0.90

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	552/576 (96%)	505 (92%)	44 (8%)	3 (0%)	25 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	804/1041 (77%)	691 (86%)	93 (12%)	20 (2%)	4	22
All	All	1356/1617 (84%)	1196 (88%)	137 (10%)	23 (2%)	7	30

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	501	HIS
2	D	610	LEU
2	D	612	TRP
2	D	759	GLY
2	D	845	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	475/495 (96%)	462 (97%)	13 (3%)	40	67
2	D	673/869 (77%)	644 (96%)	29 (4%)	25	55
All	All	1148/1364 (84%)	1106 (96%)	42 (4%)	29	59

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	664	ASN
2	D	873	ASP
2	D	671	SER
2	D	753	ARG
2	D	937	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	906	ASN
2	D	804	GLN

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Mol	Chain	Res	Type
2	D	243	GLN
2	D	236	GLN
2	D	247	ASN

### 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](#)

Of 3 ligands modelled in this entry, 3 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	553/576 (96%)	-0.33	3 (0%)	87 75	39, 76, 118, 164	1 (0%)
2	D	806/1041 (77%)	-0.41	2 (0%)	92 85	34, 67, 125, 196	0
All	All	1359/1617 (84%)	-0.38	5 (0%)	89 77	34, 70, 122, 196	1 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	388	ASP	3.8
2	D	777	GLU	3.1
1	A	140	LEU	2.7
2	D	738	SER	2.1
1	A	387	CYS	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 monosaccharides 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, 95<sup>th</sup> 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	MG	A	601	1/1	0.94	0.10	53,53,53,53	0
4	NA	A	602	1/1	0.97	0.07	71,71,71,71	0
3	MG	D	1101	1/1	0.99	0.05	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.