



wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 5T3R / pdb_00005t3r
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

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

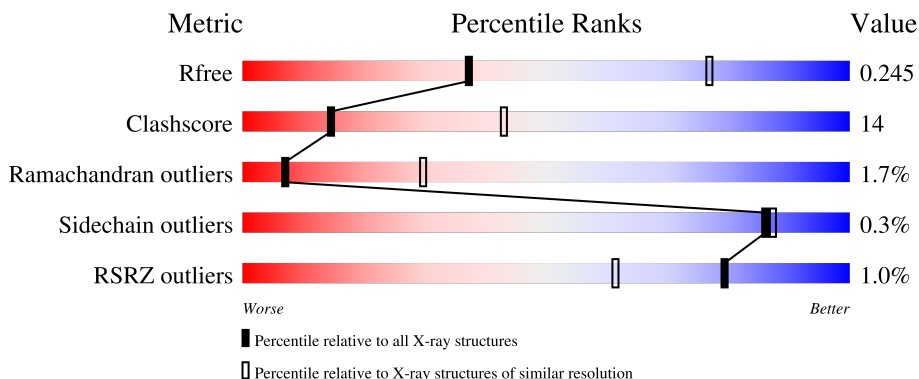
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 ≥ 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	% 72% 23% • •
2	D	1041	% 50% 26% • 23%

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 (CCD ID: 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 (CCD ID: NA) (formula: Na).

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

I964	P855	Y752	L669	M534	L443	D385
D971	T856	F758	P670	D537	R444	I356
R974	I865	G759	G672	G541	T446	L357
S978	Y869	L760	K674	S553	G448	G360
L982	K370	I768	R675	M561	N453	Q361
I985	D873	I775	R676	N562	P462	H362
K988	L874	E776	G679	A566	E465	F363
T991	T875	L778	N680	L571	M470	T364
G992	K878	E780	D681	S572	N471	R367
E993	V782	I781	H682	L573	G472	T368
D994	K787	V782	K684	D578	K473	V371
P998	G790	G792	E886	S581	S474	I377
S1001	N791	G793	Q690	R582	K479	I378
I1004	G796	V796	T691	F583	Q480	T380
P1005	V797	V797	I695	R588	E481	A381
V1006	T800	T800	L699	Y589	H482	L382
H1007	Q804	Q804	F700	A590	W483	D383
T1008	L808	L808	L704	N605	T484	I384
T1009	G811	G811	S707	K608	K485	P385
F1010	F813	F813	L708	L610	W486	V390
F1016	K814	K814	E709	T611	M487	S396
	S815	S815	Y712	L612	N489	W397
	E818	E818	K713	L613	A490	R408
	Q825	Q825	M722	L618	I491	M409
	A828	A828	V725	R619	Y494	R410
N834	R832	R832	G726	M627	E497	R411
E935	I833	I833	L728	Q628	K500	A412
Q936	R834	R834	L729	N632	H501	V413
R937	Y835	Y835	G731	L633	G503	L414
E944	R836	R836	G732	A634	D504	E415
F948	D837	D837	S733	R635	M509	K418
L949	I838	I838	R734	Y636	E510	R421
K950	D839	D839	Y735	T637	E514	Y422
L951	D845	D845	L736	Y639	D515	F428
I954	D848	D848	W737	Y643	D516	G429
G957	D848	D848	S738	T660	K623	D430
V963	Y853	Y853	G739	T661	F526	A431
	D854	D854	K742	N664	I528	Y432
			F748	G665	I529	V435
			N749	G666	T530	N434
			L750		P531	L435
			G751		D532	T436
					F441	P437
					N442	F438
						K439
						G440
						F441
						N442

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	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) 64.3 (75.89-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.82Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.259 (Not available) , 0.245	Depositor DCC
R_{free} test set	2708 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10860	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.45	0/4565	0.65	0/6194
2	D	0.50	0/6567	0.80	3/8904 (0.0%)
All	All	0.48	0/11132	0.74	3/15098 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	582	ARG	NE-CZ-NH2	-7.20	112.72	119.20
2	D	269	GLY	CA-C-N	5.97	133.65	121.48
2	D	269	GLY	C-N-CA	5.97	133.65	121.48

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	104	0
2	D	6402	0	6055	210	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	296	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 14.

The worst 5 of 296 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%)	24 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	804/1041 (77%)	691 (86%)	93 (12%)	20 (2%)	4	21
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%)	473 (100%)	2 (0%)	84	86
2	D	673/869 (77%)	671 (100%)	2 (0%)	86	87
All	All	1148/1364 (84%)	1144 (100%)	4 (0%)	86	87

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	TYR
1	A	204	LEU
2	D	368	THR
2	D	474	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	804	GLN
2	D	821	ASN

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Mol	Chain	Res	Type
2	D	953	ASN
2	D	906	ASN
2	D	470	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, 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	553/576 (96%)	-0.21	7 (1%) 75 56	39, 76, 118, 164	1 (0%)
2	D	806/1041 (77%)	-0.33	6 (0%) 84 68	34, 67, 125, 196	0
All	All	1359/1617 (84%)	-0.28	13 (0%) 79 61	34, 70, 122, 196	1 (0%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	738	SER	4.3
2	D	777	GLU	3.9
1	A	388	ASP	3.4
2	D	739	GLY	3.3
1	A	390	LEU	3.2

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	MG	D	1101	1/1	0.98	0.07	45,45,45,45	0
3	MG	A	601	1/1	0.99	0.08	53,53,53,53	0
4	NA	A	602	1/1	0.99	0.04	71,71,71,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.