



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 5T4Y / pdb_00005t4y
Title : Crystal structure of BT1762-1763
Authors : van den Berg, B.
Deposited on : 2016-08-30
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

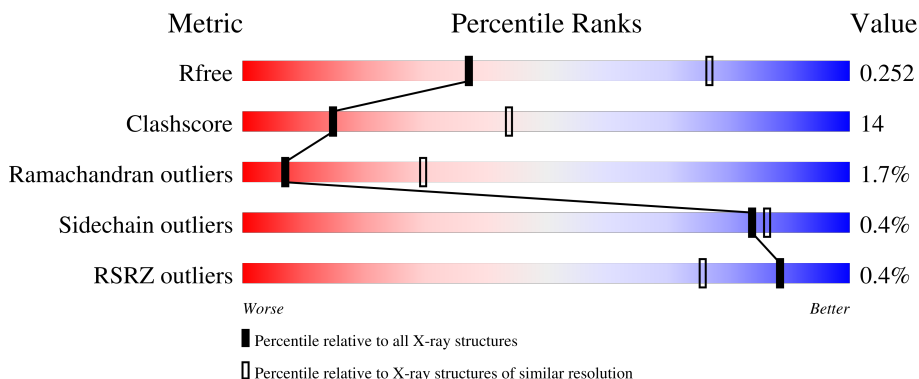
1 Overall quality at a glance ⓘ

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	76% 20% ••
1	B	576	% 75% 21% •
2	C	1041	49% 27% • 22%
2	D	1041	49% 27% • 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21727 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	552	Total	C	N	O	S	0	2	0
			4450	2818	737	874	21			
1	B	553	Total	C	N	O	S	0	2	0
			4460	2824	740	875	21			

There are 12 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
B	553	HIS	-	expression tag	UNP Q8A6W4
B	554	HIS	-	expression tag	UNP Q8A6W4
B	555	HIS	-	expression tag	UNP Q8A6W4
B	556	HIS	-	expression tag	UNP Q8A6W4
B	557	HIS	-	expression tag	UNP Q8A6W4
B	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			
2	C	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			

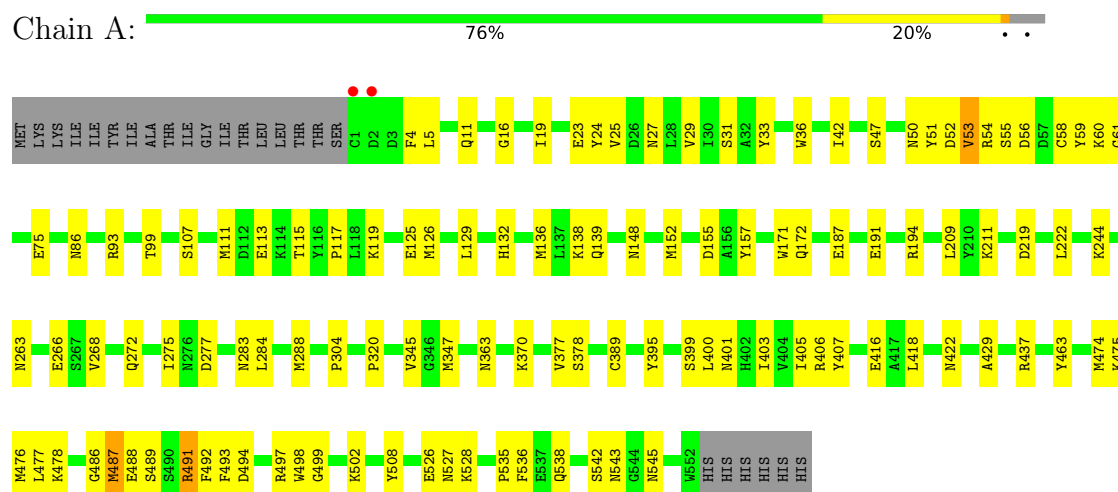
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0

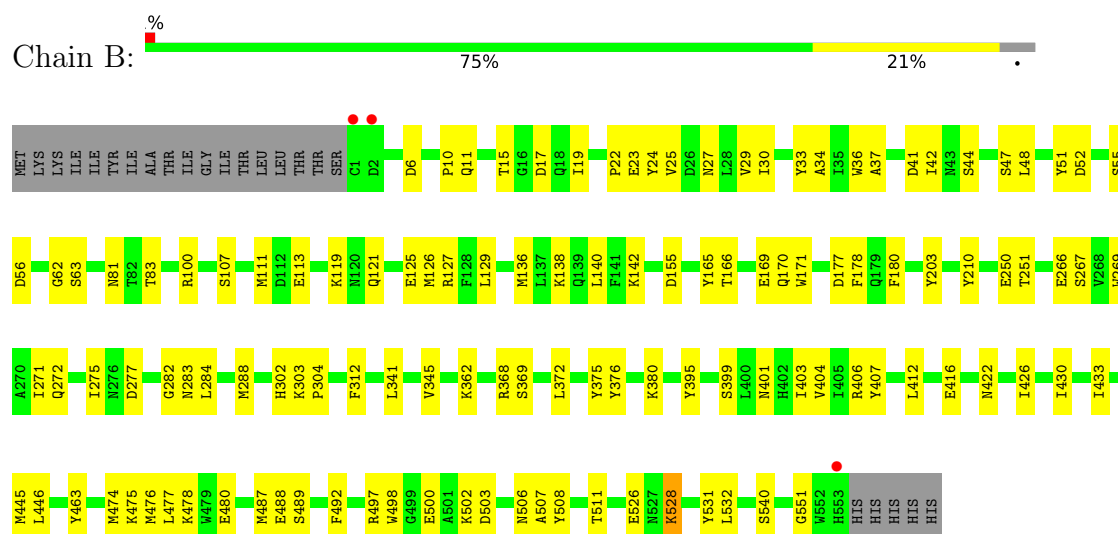
3 Residue-property plots

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: SusD homolog



• Molecule 1: SusD homolog



• Molecule 2: SusC homolog





LEU	K318	G403	G503	E604	G706	A823	P925
TYR	G319	D406	D504	M605	S707	T824	A926
ILE	S320	R407	V505	K608	L708	Q825	L927
ASP	S321	R408	I507	W612	E709	E826	T928
GLY	V231	N409	G508	L616	Y712	A827	N933
VAL	L232	P410	M509	L617	I718	A828	K934
PRO	N233	R411	E510	L618	L719	R832	E935
THR	T234	E415	D516	L624	T720	R833	Q936
LYS	E235	Y422	S520	Q628	G731	D837	R937
ALA	Q236	W425	D525	N632	G732	E838	V943
GLY	Y237	R426	I528	L633	R734	D845	G944
MET	G238	M427	T530	T637	W735	E846	K950
HIS	R239	D338	Y533	L638	I736	R847	L951
GLU	Q243	D338	M534	A640	G739	D848	Q955
LEU	A244	D338	W535	P641	K742	R850	L956
ASN	Y245	D429	G541	N642	F748	T852	G965
GLY	Y246	D430	Y546	D647	G751	P857	K966
ASN	N247	A431	G547	S648	Y752	T865	M970
ASP	N247	Y432	A548	L658	L764	F872	D971
ILE	P252	N434	G549	P641	I768	D873	R972
GLU	N255	L435	G549	N642	I768	L874	L973
SER	Q258	T436	Y562	T656	L776	T875	R974
ILE	Y259	I353	Y563	A657	E777	T884	N981
GLN	G258	D354	S564	L658	K787	D885	L982
VAL	Y259	D354	Y565	I660	F788	T886	K986
LYS	N262	I356	G568	L669	N791	L887	S987
ASP	W263	L357	Y569	P670	G792	S888	K988
ALA	N266	G360	N562	P670	V797	D889	N989
SER	N266	Q361	Y563	L669	Y801	T890	F990
ALA	V272	Q362	S564	P670	I797	K892	G992
SER	L273	F363	Y565	L669	Y801	S894	E993
ILE	Y274	T364	R568	L669	Q804	D895	E996
TYR	Y274	T364	Y569	P670	V805	N901	K997
GLY	K280	R367	T574	P670	G806	Y902	P998
SER	Y281	E370	L575	F673	G807	G903	P1003
ARG	L282	V371	R576	K674	I808	F904	V1006
ALA	V290	P374	R577	K675	A809	L905	V1007
ASN	A291	G375	D578	N676	D810	N906	I1008
GLY	D292	G376	T469	N677	T812	G908	T1009
VAL	T293	I377	M470	Q677	F813	T909	L1012
ILE	T293	I378	N471	I678	K814	R910	L1013
ILE	W295	E379	G472	G679	D817	L911	I1014
THR	F296	T380	K487	L679	E818	L912	G1015
THR	D297	E298	N489	W685	E822	R913	F1016
LYS	E298	D383	A590	T691		L914	
GLN	R301	V390	Y588	T691		L915	
LYS	V304	S396	Y589	T691		L916	
G210	I305	W397	A590	T691		L917	
G211	S313	P400	G499	T691		L918	
I212	G315	V401	K500	T691		L919	
A218			H501	T691		L920	
S219			G603	T691		L921	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.83Å 152.09Å 253.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.35 – 3.10 130.35 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (130.35-3.10) 98.9 (130.35-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.270 (Not available) , 0.252	Depositor DCC
R_{free} test set	4422 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21727	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 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	0.38	0/4562	0.61	1/6190 (0.0%)
1	B	0.42	0/4573	0.68	0/6205
2	C	0.52	0/6571	0.78	5/8909 (0.1%)
2	D	0.48	0/6571	0.78	4/8909 (0.0%)
All	All	0.46	0/22277	0.73	10/30213 (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	4

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	470	ASN	N-CA-C	-8.99	100.15	114.09
2	C	565	TYR	CA-CB-CG	5.42	123.65	113.90
2	C	992	GLY	CA-C-N	5.34	131.75	121.54
2	C	992	GLY	C-N-CA	5.34	131.75	121.54
1	A	53	VAL	N-CA-C	-5.26	106.40	112.98

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	317	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	D	353	ILE	Peptide
2	D	470	ASN	Peptide
2	D	584	GLY	Peptide

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	4450	0	4219	90	0
1	B	4460	0	4227	89	0
2	C	6406	0	6058	217	0
2	D	6406	0	6058	231	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	21727	0	20562	585	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 585 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)
2:D:427:MET:HE3	2:C:427:MET:SD	1.39	1.58
2:D:427:MET:CE	2:C:427:MET:SD	2.35	1.12
1:B:275:ILE:HG22	1:B:284:LEU:HD11	1.47	0.95
2:D:365:LEU:HD13	2:D:427:MET:SD	2.12	0.90
2:C:986:LYS:H	2:C:986:LYS:HD2	1.38	0.87

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	552/576 (96%)	500 (91%)	48 (9%)	4 (1%)	18	49
1	B	553/576 (96%)	514 (93%)	36 (6%)	3 (0%)	24	57
2	C	805/1041 (77%)	716 (89%)	68 (8%)	21 (3%)	4	21
2	D	805/1041 (77%)	714 (89%)	72 (9%)	19 (2%)	4	22
All	All	2715/3234 (84%)	2444 (90%)	224 (8%)	47 (2%)	7	30

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	608	LYS
2	D	826	GLU
2	D	993	GLU
2	C	732	GLY
2	C	971	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%)	475 (100%)	0	100	100
1	B	476/495 (96%)	474 (100%)	2 (0%)	84	86
2	C	673/869 (77%)	668 (99%)	5 (1%)	76	82
2	D	673/869 (77%)	670 (100%)	3 (0%)	84	86
All	All	2297/2728 (84%)	2287 (100%)	10 (0%)	84	86

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	504	ASP
2	C	564	SER
2	C	709	GLU
1	B	203	TYR
1	B	251	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	GLN
2	C	934	ASN
2	C	330	ASN
2	C	882	GLN
2	C	262	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 5 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	552/576 (95%)	-0.38	2 (0%)	88 76	44, 83, 111, 146	2 (0%)
1	B	553/576 (96%)	-0.56	3 (0%)	87 73	37, 65, 94, 124	2 (0%)
2	C	807/1041 (77%)	-0.37	2 (0%)	91 83	37, 64, 104, 150	0
2	D	807/1041 (77%)	-0.30	5 (0%)	85 70	35, 71, 111, 146	0
All	All	2719/3234 (84%)	-0.39	12 (0%)	88 76	35, 70, 108, 150	4 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	HIS	4.4
1	A	1	CYS	3.5
1	B	1	CYS	3.0
1	B	2	ASP	2.7
2	D	427	MET	2.5

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	B	602	1/1	0.92	0.12	113,113,113,113	0
3	MG	A	602	1/1	0.97	0.05	84,84,84,84	0
3	MG	C	1101	1/1	0.98	0.11	47,47,47,47	0
3	MG	A	601	1/1	0.99	0.03	28,28,28,28	0
3	MG	B	601	1/1	1.00	0.05	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.