



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2017 – 04:55 PM EDT

PDB ID : 2QB0
Title : Structure of the 2TEL crystallization module fused to T4 lysozyme with an Ala-Gly-Pro linker.
Authors : Nauli, S.; Bowie, J.U.
Deposited on : unknown
Resolution : 2.56 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

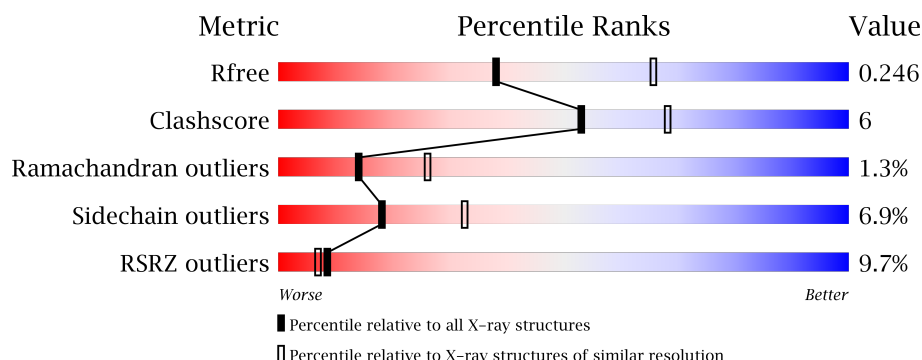
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	100719	3689 (2.60-2.52)
Clashscore	112137	4096 (2.60-2.52)
Ramachandran outliers	110173	4037 (2.60-2.52)
Sidechain outliers	110143	4037 (2.60-2.52)
RSRZ outliers	101464	3700 (2.60-2.52)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	77	<div> <div>5%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
1	C	77	<div> <div>6%</div> <div>74%</div> <div>22%</div> <div>..</div> </div>
2	B	241	<div> <div>10%</div> <div>87%</div> <div>10%</div> <div>.</div> </div>
2	D	241	<div> <div>12%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria.

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MN	B	257	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5372 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 E80-TELSAM domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	77	Total	C	N	O	S	0	1	0
			664	426	116	121	1			
1	C	77	Total	C	N	O	S	0	1	0
			669	432	117	119	1			

- Molecule 2 is a protein called TELSAM domain - Lysozyme chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1951	1239	351	354	7			
2	D	241	Total	C	N	O	S	0	0	0
			1936	1227	349	353	7			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	ALA	-	SEE REMARK 999	UNP P00720
B	93	GLY	-	SEE REMARK 999	UNP P00720
B	94	PRO	-	SEE REMARK 999	UNP P00720
B	147	THR	CYS	CONFLICT	UNP P00720
B	161	CYS	ASN	CONFLICT	UNP P00720
B	186	CYS	ALA	CONFLICT	UNP P00720
B	190	ALA	CYS	CONFLICT	UNP P00720
D	92	ALA	-	SEE REMARK 999	UNP P00720
D	93	GLY	-	SEE REMARK 999	UNP P00720
D	94	PRO	-	SEE REMARK 999	UNP P00720
D	147	THR	CYS	CONFLICT	UNP P00720
D	161	CYS	ASN	CONFLICT	UNP P00720
D	186	CYS	ALA	CONFLICT	UNP P00720
D	190	ALA	CYS	CONFLICT	UNP P00720

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mn 2	0	0
3	D	2	Total 2	Mn 2	0	0
3	C	1	Total 1	Mn 1	0	0

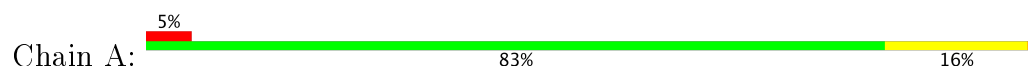
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	49	Total 49	O 49	0	0
4	C	27	Total 27	O 27	0	0
4	D	44	Total 44	O 44	0	0

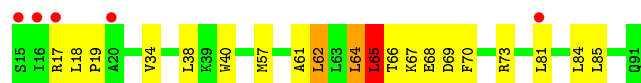
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

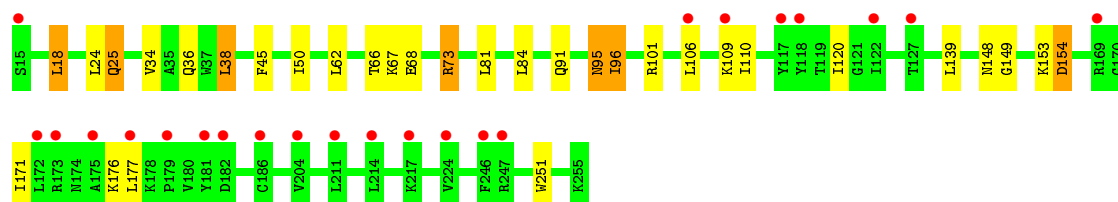
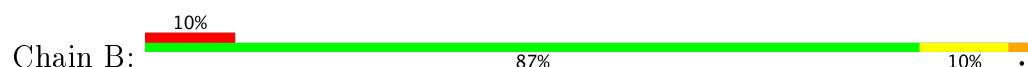
- Molecule 1: E80-TELSAM domain



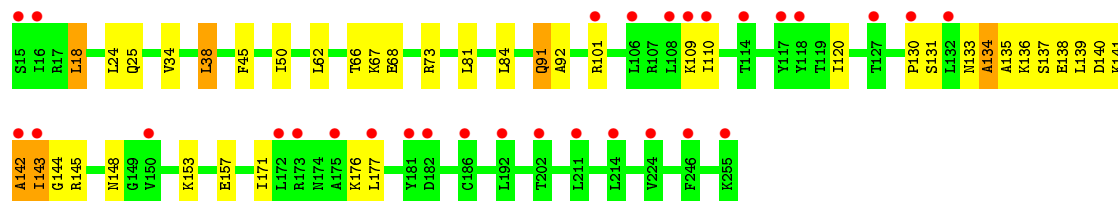
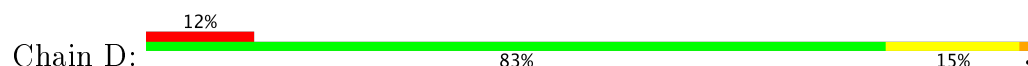
- Molecule 1: E80-TELSAM domain



- Molecule 2: TELSAM domain - Lysozyme chimera



- Molecule 2: TELSAM domain - Lysozyme chimera



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	122.62Å 122.62Å 53.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.56 61.31 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.56) 99.7 (61.31-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.55Å)	Xtriage
Refinement program	REFMAC refmac _5.2.0019	Depositor
R, R_{free}	0.211 , 0.252 0.208 , 0.246	Depositor DCC
R_{free} test set	1469 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.039 for h,-h-k,-l 0.038 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5372	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1080e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.31	0/682	0.74	2/922 (0.2%)
1	C	0.32	0/689	0.96	7/933 (0.8%)
2	B	0.30	0/1991	0.72	6/2690 (0.2%)
2	D	0.31	0/1975	0.67	2/2670 (0.1%)
All	All	0.31	0/5337	0.74	17/7215 (0.2%)

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	B	1	0

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	LEU	C-N-CA	11.19	149.68	121.70
2	B	73	ARG	NE-CZ-NH1	-10.00	115.30	120.30
1	C	73	ARG	NE-CZ-NH1	-9.60	115.50	120.30
2	B	73	ARG	NE-CZ-NH2	9.41	125.01	120.30
1	C	73	ARG	NE-CZ-NH2	8.98	124.79	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	96	ILE	CA

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	664	0	648	7	0
1	C	669	0	651	14	0
2	B	1951	0	1968	19	0
2	D	1936	0	1924	27	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	27	0	0	1	0
4	B	49	0	0	8	0
4	C	27	0	0	7	0
4	D	44	0	0	3	0
All	All	5372	0	5191	65	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 6.

The worst 5 of 65 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:66:THR:HB	4:A:99:HOH:O	1.45	1.16
1:C:66:THR:HB	4:C:217:HOH:O	1.48	1.14
2:D:144:GLY:HA2	2:D:145:ARG:HG3	1.40	1.02
2:D:91:GLN:C	2:D:92:ALA:N	2.14	1.00
2:D:138:GLU:HB3	2:D:139:LEU:HD23	1.42	0.97

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	76/77 (99%)	75 (99%)	1 (1%)	0	100	100
1	C	76/77 (99%)	74 (97%)	1 (1%)	1 (1%)	14	26
2	B	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	22	41
2	D	237/241 (98%)	220 (93%)	12 (5%)	5 (2%)	8	14
All	All	628/636 (99%)	600 (96%)	20 (3%)	8 (1%)	14	26

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	ILE
2	B	154	ASP
1	C	65	LEU
2	D	131	SER
2	D	142	ALA

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	72/71 (101%)	67 (93%)	5 (7%)	18	33
1	C	72/71 (101%)	64 (89%)	8 (11%)	7	11
2	B	207/207 (100%)	194 (94%)	13 (6%)	21	38
2	D	202/207 (98%)	189 (94%)	13 (6%)	20	37
All	All	553/556 (100%)	514 (93%)	39 (7%)	18	31

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	176	LYS
1	C	40[B]	TRP
2	D	109	LYS

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Mol	Chain	Res	Type
1	C	34	VAL
1	C	38	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	91	GLN
2	D	133	ASN
2	D	215	GLN
1	C	91	GLN
2	D	148	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	91:GLN	C	92:ALA	N	2.14

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	77/77 (100%)	0.90	4 (5%) 28 25	38, 46, 83, 152	0
1	C	77/77 (100%)	0.92	5 (6%) 20 17	38, 47, 83, 152	0
2	B	241/241 (100%)	0.79	23 (9%) 9 7	34, 56, 79, 146	0
2	D	241/241 (100%)	0.87	30 (12%) 4 3	34, 56, 90, 146	0
All	All	636/636 (100%)	0.85	62 (9%) 8 7	34, 55, 87, 152	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	181	TYR	6.5
2	D	142	ALA	5.7
2	B	181	TYR	5.6
2	D	211	LEU	4.6
2	B	211	LEU	4.4

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MN	B	257	1/1	0.98	0.30	6.20	48,48,48,48	0
3	MN	C	207	1/1	0.96	0.12	-2.30	92,92,92,92	0
3	MN	D	257	1/1	0.79	0.17	-	103,103,103,103	0
3	MN	B	256	1/1	0.80	0.33	-	104,104,104,104	0
3	MN	D	256	1/1	0.82	0.31	-	108,108,108,108	0

6.5 Other polymers [i](#)

There are no such residues in this entry.