



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:49 PM UTC

PDB ID : 1SKY / pdb_00001sky
Title : CRYSTAL STRUCTURE OF THE NUCLEOTIDE FREE ALPHA3BETA3
SUB-COMPLEX OF F1-ATPASE FROM THE THERMOPHILIC BACIL-
LUS PS3
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Deposited on : 1997-02-26
Resolution : 3.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

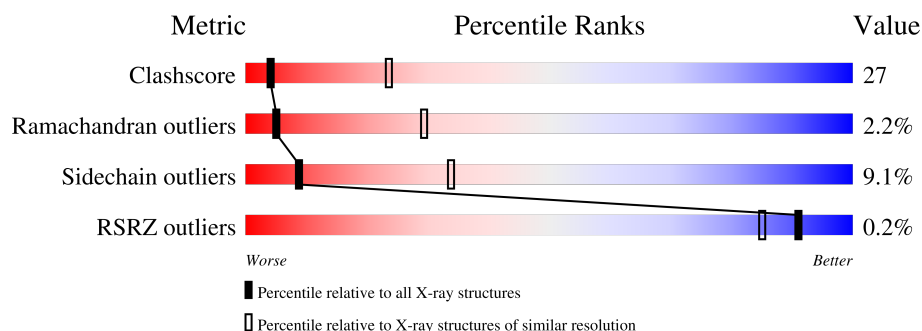
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

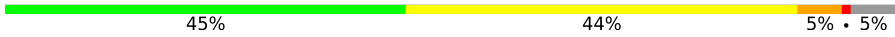
The reported resolution of this entry is 3.20 Å.

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))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	B	502	
2	E	473	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7299 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 F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	479	Total	C	N	O	S	0	0	0
			3660	2312	640	697	11			

- Molecule 2 is a protein called F1-ATPASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	470	Total	C	N	O	S	0	0	0
			3629	2289	630	696	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

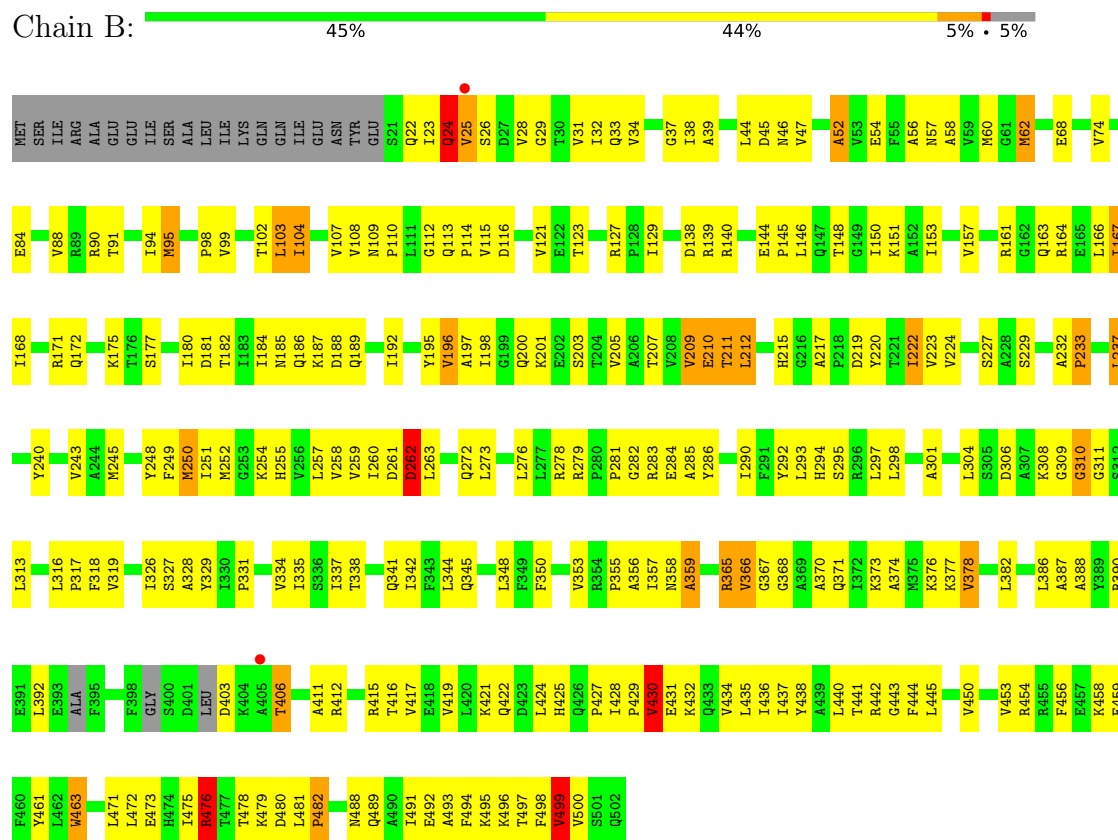


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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: F1-ATPASE



• Molecule 2: F1-ATPASE



S411	Q412	N413	F414	H415	F420	Q423	P424	G425	S426	Y427	V428	P429	V430	K431	E432	T433	V434	R435	G436	F437	K438	E439	I440	G443	L448	P449	E450	D451	R452	F453	R454	L455	V456	I459	E460	E461	V462	V463	A466	G470	VAL	GLU	VAL						
T329	N330	L331	E332	R333	K334	P342	A343	V344	V348	S349	T350	S351	R352	A353	L354	A355	P356	E357	I358	V359	E362	H363	Y364	Q365	V366	A367	R368	Q372	E375	R376	Y377	L380	Q381	D382	I383	I384	M389	L392	S393	D394	E395	D396	K397	L398	V399	V400	H401	R402	R405
I254	F256	R256	F257	A260	E263	V264	L267	M271	I275	G276	Y277	Q278	P279	T280	L281	A282	T283	E284	Q287	L288	Q289	I292	T293	S294	T295	K297	A296	G298	S299	I300	Q304	V308	P309	A310	D311	D312	Y313	T314	D315	P316	A317	P318	F322	S323	H324	L325	D326	A327	T328

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	159.50Å 159.50Å 159.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20 6.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (6.00-3.20) 83.5 (6.00-3.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , 0.299 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.020 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7299	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	B	0.70	1/3716 (0.0%)	1.10	18/5035 (0.4%)
2	E	0.70	1/3692 (0.0%)	1.14	22/4998 (0.4%)
All	All	0.70	2/7408 (0.0%)	1.12	40/10033 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	65	ALA	CA-CB	-5.26	1.46	1.53
1	B	52	ALA	CA-CB	5.02	1.60	1.53

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	85	VAL	N-CA-C	9.84	117.26	109.19
2	E	217	GLN	N-CA-C	9.59	122.08	110.19
2	E	145	LEU	N-CA-C	8.46	123.38	112.89
2	E	98	VAL	CB-CA-C	-8.07	101.55	111.88
2	E	423	GLN	CA-C-N	7.82	128.23	119.32

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	B	3660	0	3718	213	0
2	E	3629	0	3644	201	0
3	B	5	0	0	0	0
3	E	5	0	0	0	0
All	All	7299	0	7362	403	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 27.

The worst 5 of 403 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:B:167:ILE:HG22	1:B:342:ILE:HB	1.40	1.02
2:E:240:ARG:HG3	2:E:299:SER:N	1.90	0.85
1:B:475:ILE:HG12	1:B:481:LEU:HD21	1.59	0.84
2:E:254:ILE:O	2:E:257:PHE:HB3	1.79	0.82
2:E:178:GLU:HG3	2:E:427:TYR:CE2	2.16	0.80

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	B	471/502 (94%)	397 (84%)	60 (13%)	14 (3%)	3	23
2	E	468/473 (99%)	407 (87%)	54 (12%)	7 (2%)	8	37
All	All	939/975 (96%)	804 (86%)	114 (12%)	21 (2%)	5	29

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	GLN

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Mol	Chain	Res	Type
1	B	310	GLY
1	B	411	ALA
1	B	499	VAL
2	E	394	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	B	391/410 (95%)	356 (91%)	35 (9%)	9	34
2	E	387/390 (99%)	351 (91%)	36 (9%)	8	33
All	All	778/800 (97%)	707 (91%)	71 (9%)	9	34

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	295	THR
2	E	354	LEU
2	E	413	ASN
1	B	262	ASP
1	B	251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
2	E	278	GLN
2	E	372	GLN
2	E	423	GLN
2	E	413	ASN
2	E	330	ASN

5.3.3 RNA ⓘ

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	E	474	-	4,4,4	0.56	0	6,6,6	0.37	0
3	SO4	B	503	-	4,4,4	0.51	0	6,6,6	0.81	0

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	B	479/502 (95%)	-0.49	2 (0%) 88 79	22, 54, 155, 249	0
2	E	470/473 (99%)	-0.61	0 100 100	26, 51, 121, 192	0
All	All	949/975 (97%)	-0.55	2 (0%) 91 85	22, 53, 152, 249	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	405	ALA	2.3
1	B	25	VAL	2.2

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(Å ²)	Q<0.9
3	SO4	E	474	5/5	0.89	0.12	135,135,135,136	0
3	SO4	B	503	5/5	0.98	0.05	63,63,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.