



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 11:29 PM GMT

PDB ID : 1XCO
Title : Crystal Structure of a Phosphotransacetylase from *Bacillus subtilis* in complex with acetylphosphate
Authors : Xu, Q.S.; Jancarik, J.; Lou, Y.; Yokota, H.; Adams, P.; Kim, R.; Kim, S.-H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-09-02
Resolution : 2.85 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

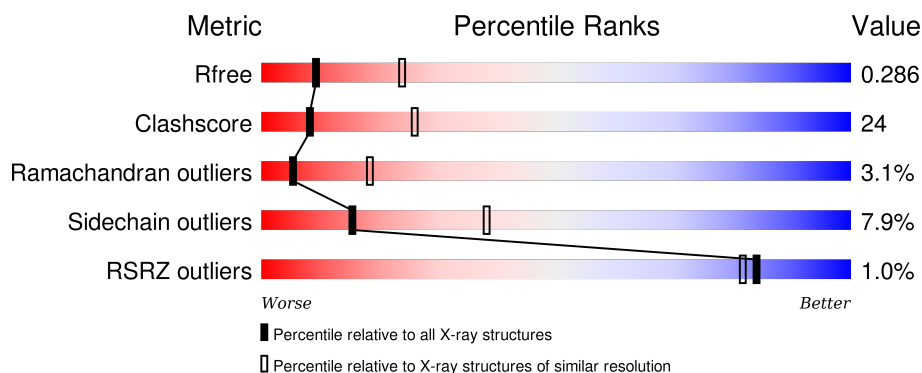
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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.



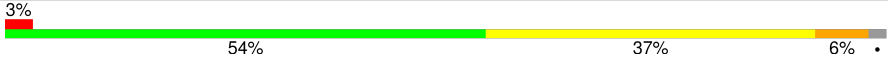
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	329	<div> <div></div> <div>58% 34% 6% •</div> </div>
1	B	329	<div> <div></div> <div>57% 36% 5% •</div> </div>
1	C	329	<div> <div></div> <div>56% 36% 6% •</div> </div>
1	D	329	<div> <div></div> <div>54% 40% 5% •</div> </div>
1	E	329	<div> <div></div> <div>57% 35% 6% •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	329	 A horizontal bar chart showing the quality of chain 1. The bar is divided into four segments: a small red segment at the beginning labeled '3%', followed by a large green segment labeled '54%', then a yellow segment labeled '37%', and a small grey segment at the end labeled '6%'. A small black dot is visible at the far right end of the bar.

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UVW	D	410	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15000 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 Phosphate acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2449	1547	408	485	9			
1	B	324	Total	C	N	O	S	0	0	0
			2449	1547	408	485	9			
1	C	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			
1	D	325	Total	C	N	O	S	0	0	0
			2453	1549	409	486	9			
1	E	324	Total	C	N	O	S	0	1	0
			2458	1552	409	488	9			
1	F	323	Total	C	N	O	S	0	0	0
			2445	1545	407	484	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP P39646
A	-4	GLY	-	CLONING ARTIFACT	UNP P39646
A	-3	GLY	-	CLONING ARTIFACT	UNP P39646
A	-2	GLY	-	CLONING ARTIFACT	UNP P39646
A	-1	GLY	-	CLONING ARTIFACT	UNP P39646
A	0	GLY	-	CLONING ARTIFACT	UNP P39646
A	1	MET	-	INITIATING METHIONINE	UNP P39646
B	-5	GLY	-	CLONING ARTIFACT	UNP P39646
B	-4	GLY	-	CLONING ARTIFACT	UNP P39646
B	-3	GLY	-	CLONING ARTIFACT	UNP P39646
B	-2	GLY	-	CLONING ARTIFACT	UNP P39646
B	-1	GLY	-	CLONING ARTIFACT	UNP P39646
B	0	GLY	-	CLONING ARTIFACT	UNP P39646
B	1	MET	-	INITIATING METHIONINE	UNP P39646
C	-5	GLY	-	CLONING ARTIFACT	UNP P39646
C	-4	GLY	-	CLONING ARTIFACT	UNP P39646
C	-3	GLY	-	CLONING ARTIFACT	UNP P39646

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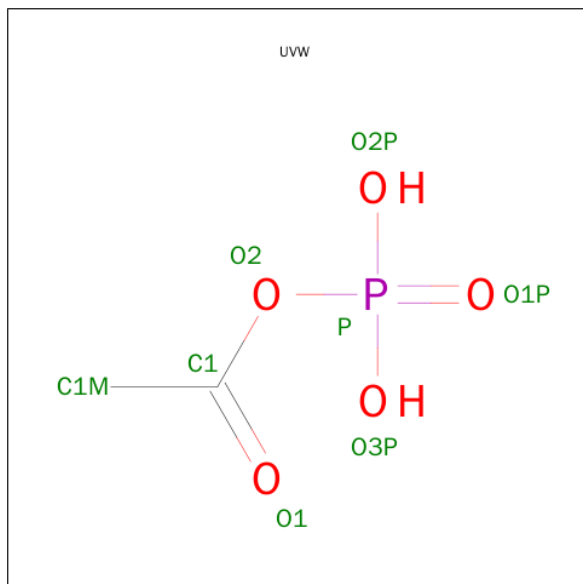
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	CLONING ARTIFACT	UNP P39646
C	-1	GLY	-	CLONING ARTIFACT	UNP P39646
C	0	GLY	-	CLONING ARTIFACT	UNP P39646
C	1	MET	-	INITIATING METHIONINE	UNP P39646
D	-5	GLY	-	CLONING ARTIFACT	UNP P39646
D	-4	GLY	-	CLONING ARTIFACT	UNP P39646
D	-3	GLY	-	CLONING ARTIFACT	UNP P39646
D	-2	GLY	-	CLONING ARTIFACT	UNP P39646
D	-1	GLY	-	CLONING ARTIFACT	UNP P39646
D	0	GLY	-	CLONING ARTIFACT	UNP P39646
D	1	MET	-	INITIATING METHIONINE	UNP P39646
E	-5	GLY	-	CLONING ARTIFACT	UNP P39646
E	-4	GLY	-	CLONING ARTIFACT	UNP P39646
E	-3	GLY	-	CLONING ARTIFACT	UNP P39646
E	-2	GLY	-	CLONING ARTIFACT	UNP P39646
E	-1	GLY	-	CLONING ARTIFACT	UNP P39646
E	0	GLY	-	CLONING ARTIFACT	UNP P39646
E	1	MET	-	INITIATING METHIONINE	UNP P39646
F	-5	GLY	-	CLONING ARTIFACT	UNP P39646
F	-4	GLY	-	CLONING ARTIFACT	UNP P39646
F	-3	GLY	-	CLONING ARTIFACT	UNP P39646
F	-2	GLY	-	CLONING ARTIFACT	UNP P39646
F	-1	GLY	-	CLONING ARTIFACT	UNP P39646
F	0	GLY	-	CLONING ARTIFACT	UNP P39646
F	1	MET	-	INITIATING METHIONINE	UNP P39646

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ACETYLPHOSPHATE (three-letter code: UVW) (formula: $C_2H_5O_5P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			8	2	5	1		
3	A	1	Total	C	O	P	0	0
			8	2	5	1		
3	B	1	Total	C	O	P	0	0
			8	2	5	1		
3	B	1	Total	C	O	P	0	0
			8	2	5	1		
3	B	1	Total	C	O	P	0	0
			8	2	5	1		
3	A	1	Total	C	O	P	0	0
			8	2	5	1		
3	C	1	Total	C	O	P	0	0
			8	2	5	1		
3	C	1	Total	C	O	P	0	0
			8	2	5	1		
3	D	1	Total	C	O	P	0	0
			8	2	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total 8	C 2	O 5	P 1	0	0
3	D	1	Total 8	C 2	O 5	P 1	0	0
3	C	1	Total 8	C 2	O 5	P 1	0	0
3	E	1	Total 8	C 2	O 5	P 1	0	0
3	E	1	Total 8	C 2	O 5	P 1	0	0
3	E	1	Total 8	C 2	O 5	P 1	0	0
3	F	1	Total 8	C 2	O 5	P 1	0	0
3	F	1	Total 8	C 2	O 5	P 1	0	0
3	A	1	Total 8	C 2	O 5	P 1	0	0
3	B	1	Total 8	C 2	O 5	P 1	0	0
3	C	1	Total 8	C 2	O 5	P 1	0	0
3	D	1	Total 8	C 2	O 5	P 1	0	0
3	E	1	Total 8	C 2	O 5	P 1	0	0
3	F	1	Total 8	C 2	O 5	P 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total 23	O 23	0	0
4	B	11	Total 11	O 11	0	0
4	C	21	Total 21	O 21	0	0
4	D	16	Total 16	O 16	0	0
4	E	23	Total 23	O 23	0	0

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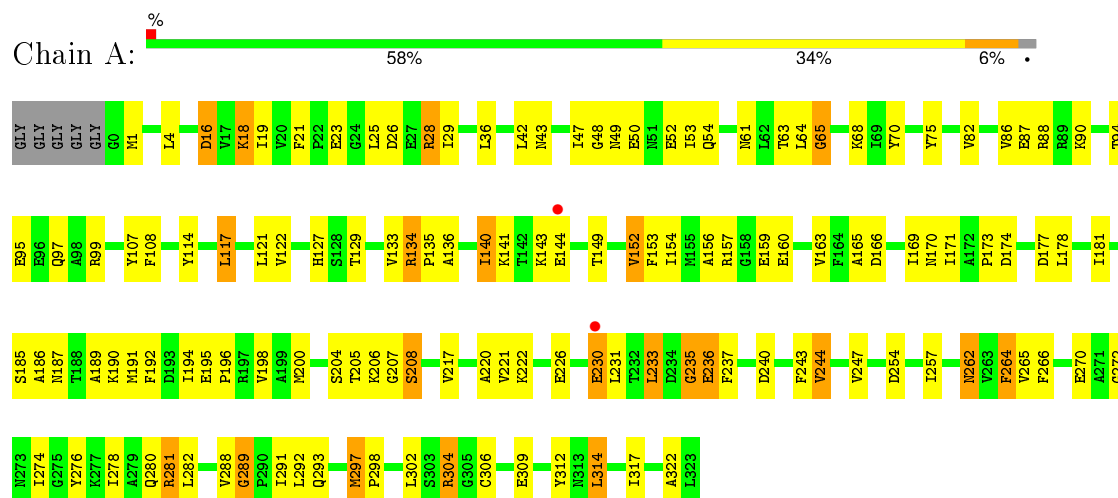
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	8	Total	O	0	0
			8	8		

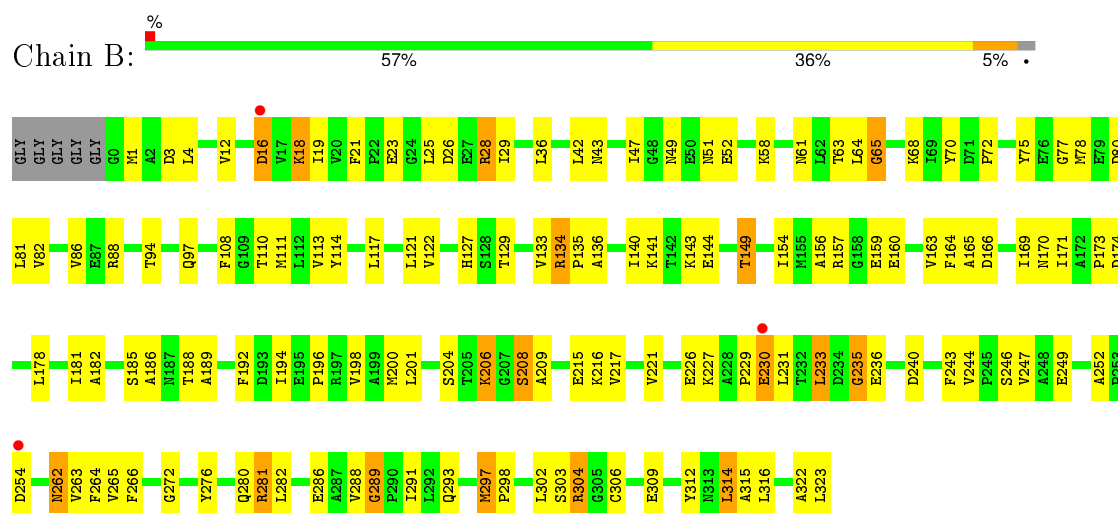
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phosphate acetyltransferase

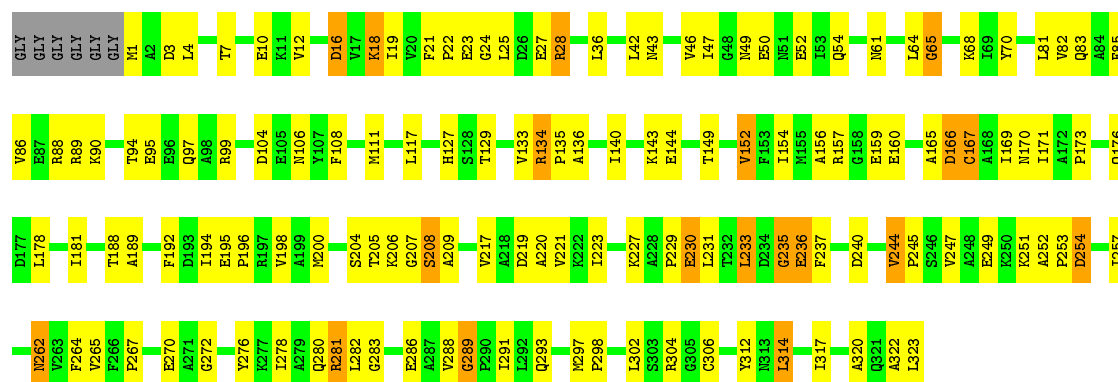


• Molecule 1: Phosphate acetyltransferase

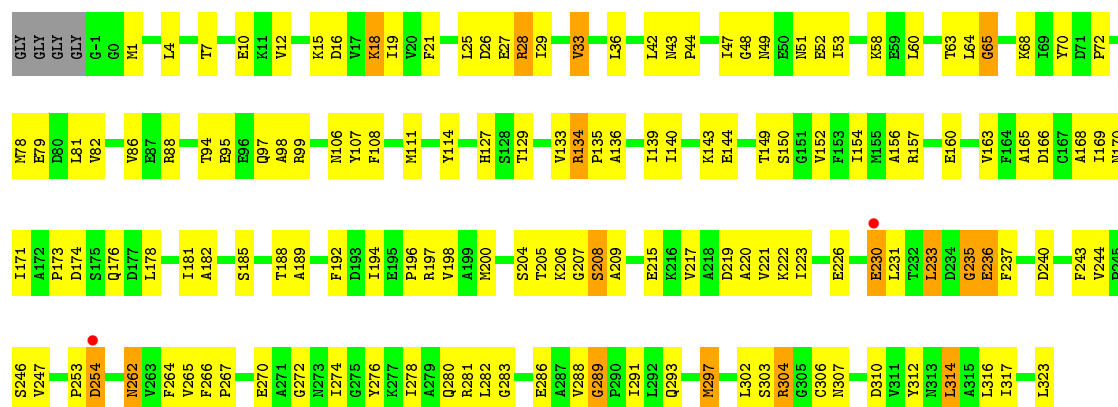


• Molecule 1: Phosphate acetyltransferase

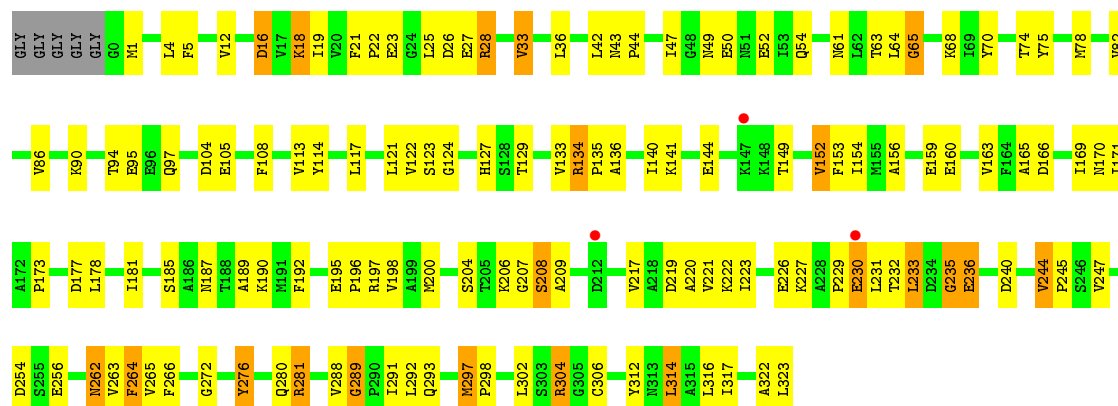




• Molecule 1: Phosphate acetyltransferase

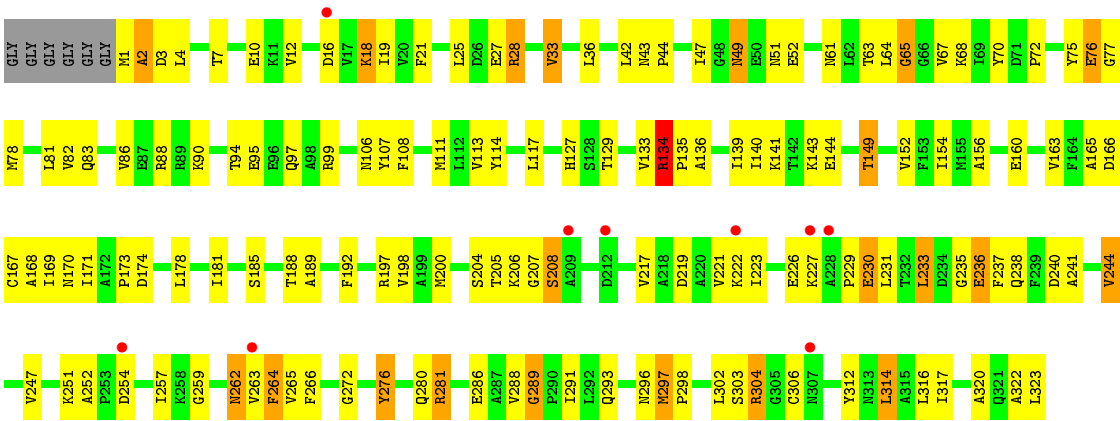


• Molecule 1: Phosphate acetyltransferase



• Molecule 1: Phosphate acetyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.66 Å 184.66 Å 259.46 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.85 19.99 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.99-2.85) 99.8 (19.99-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.83 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.288 0.243 , 0.286	Depositor DCC
R_{free} test set	1665 reflections (2.73%)	DCC
Wilson B-factor (Å ²)	47.6	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	8 of 61173 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15000	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 54.17 % 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 3.7951e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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, UVW

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	0.56	0/2483	0.79	2/3351 (0.1%)
1	B	0.55	0/2483	0.80	1/3351 (0.0%)
1	C	0.57	0/2479	0.78	1/3346 (0.0%)
1	D	0.53	0/2487	0.77	1/3356 (0.0%)
1	E	0.58	0/2492	0.79	1/3363 (0.0%)
1	F	0.50	0/2479	0.75	1/3346 (0.0%)
All	All	0.55	0/14903	0.78	7/20113 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	GLY	N-CA-C	5.77	127.52	113.10
1	A	235	GLY	N-CA-C	5.64	127.20	113.10
1	C	235	GLY	N-CA-C	5.45	126.71	113.10
1	B	235	GLY	N-CA-C	5.31	126.37	113.10
1	F	238	GLN	N-CA-C	-5.19	96.99	111.00

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	A	2449	0	2471	121	0
1	B	2449	0	2471	126	0
1	C	2445	0	2468	123	0
1	D	2453	0	2474	127	0
1	E	2458	0	2476	114	0
1	F	2445	0	2468	129	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
2	E	5	0	0	0	0
3	A	32	0	12	3	0
3	B	32	0	12	6	0
3	C	32	0	12	3	0
3	D	32	0	12	6	0
3	E	32	0	12	8	0
3	F	24	0	9	1	0
4	A	23	0	0	1	0
4	B	11	0	0	2	0
4	C	21	0	0	2	0
4	D	16	0	0	1	0
4	E	23	0	0	2	0
4	F	8	0	0	0	0
All	All	15000	0	14897	728	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 24.

The worst 5 of 728 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)
3:B:403:UVW:O2	3:B:403:UVW:C1	1.65	1.44
3:C:420:UVW:C1	3:C:420:UVW:O2	1.64	1.44
3:D:421:UVW:C1	3:D:421:UVW:O2	1.64	1.43
3:E:413:UVW:C1	3:E:413:UVW:O2	1.63	1.42
3:D:410:UVW:C1	3:D:410:UVW:O2	1.64	1.42

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	322/329 (98%)	292 (91%)	20 (6%)	10 (3%)	5	18
1	B	322/329 (98%)	283 (88%)	31 (10%)	8 (2%)	7	24
1	C	321/329 (98%)	289 (90%)	22 (7%)	10 (3%)	5	18
1	D	323/329 (98%)	288 (89%)	26 (8%)	9 (3%)	6	21
1	E	323/329 (98%)	284 (88%)	30 (9%)	9 (3%)	6	21
1	F	321/329 (98%)	280 (87%)	28 (9%)	13 (4%)	4	12
All	All	1932/1974 (98%)	1716 (89%)	157 (8%)	59 (3%)	5	18

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	65	GLY
1	A	144	GLU
1	A	289	GLY
1	B	65	GLY
1	B	144	GLU

5.3.2 Protein sidechains [i](#)

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	257/257 (100%)	238 (93%)	19 (7%)	17	42
1	B	257/257 (100%)	237 (92%)	20 (8%)	16	39
1	C	257/257 (100%)	236 (92%)	21 (8%)	14	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	257/257 (100%)	240 (93%)	17 (7%)	21	48
1	E	258/257 (100%)	236 (92%)	22 (8%)	13	34
1	F	257/257 (100%)	234 (91%)	23 (9%)	12	32
All	All	1543/1542 (100%)	1421 (92%)	122 (8%)	15	38

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	276	TYR
1	D	230	GLU
1	F	233	LEU
1	C	281	ARG
1	D	25	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	262	ASN
1	D	127	HIS
1	F	161	GLN
1	C	293	GLN
1	D	49	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 carbohydrates in this entry.

5.6 Ligand geometry

26 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	UVW	A	401	-	5,7,7	3.15	2 (40%)	7,10,10	3.18	2 (28%)
3	UVW	A	402	-	5,7,7	3.13	3 (60%)	7,10,10	3.40	2 (28%)
3	UVW	A	406	-	5,7,7	3.14	4 (80%)	7,10,10	4.01	2 (28%)
3	UVW	A	418	-	5,7,7	3.08	2 (40%)	7,10,10	3.61	2 (28%)
2	SO4	A	501	-	4,4,4	3.45	2 (50%)	6,6,6	0.98	0
3	UVW	B	403	-	5,7,7	3.20	3 (60%)	7,10,10	3.23	2 (28%)
3	UVW	B	404	-	5,7,7	3.27	2 (40%)	7,10,10	3.20	2 (28%)
3	UVW	B	405	-	5,7,7	3.17	2 (40%)	7,10,10	3.43	2 (28%)
3	UVW	B	419	-	5,7,7	3.22	3 (60%)	7,10,10	3.77	2 (28%)
3	UVW	C	407	-	5,7,7	3.08	2 (40%)	7,10,10	3.37	2 (28%)
3	UVW	C	408	-	5,7,7	3.22	3 (60%)	7,10,10	3.26	2 (28%)
3	UVW	C	412	-	5,7,7	3.10	2 (40%)	7,10,10	3.47	2 (28%)
3	UVW	C	420	-	5,7,7	3.06	2 (40%)	7,10,10	3.46	2 (28%)
2	SO4	C	502	-	4,4,4	3.52	2 (50%)	6,6,6	1.03	1 (16%)
3	UVW	D	409	-	5,7,7	3.13	2 (40%)	7,10,10	3.43	2 (28%)
3	UVW	D	410	-	5,7,7	3.21	3 (60%)	7,10,10	3.04	2 (28%)
3	UVW	D	411	-	5,7,7	3.28	2 (40%)	7,10,10	3.79	2 (28%)
3	UVW	D	421	-	5,7,7	3.27	3 (60%)	7,10,10	3.49	2 (28%)
3	UVW	E	413	-	5,7,7	3.14	3 (60%)	7,10,10	3.39	2 (28%)
3	UVW	E	414	-	5,7,7	3.17	2 (40%)	7,10,10	3.27	2 (28%)
3	UVW	E	415	-	5,7,7	3.19	3 (60%)	7,10,10	3.29	2 (28%)
3	UVW	E	422	-	5,7,7	3.19	3 (60%)	7,10,10	4.03	2 (28%)
2	SO4	E	503	-	4,4,4	3.56	2 (50%)	6,6,6	0.86	0
3	UVW	F	416	-	5,7,7	3.02	2 (40%)	7,10,10	3.62	2 (28%)
3	UVW	F	417	-	5,7,7	3.25	2 (40%)	7,10,10	2.92	2 (28%)
3	UVW	F	423	-	5,7,7	3.29	3 (60%)	7,10,10	3.34	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UVW	A	401	-	-	0/3/5/5	0/0/0/0
3	UVW	A	402	-	-	0/3/5/5	0/0/0/0
3	UVW	A	406	-	-	0/3/5/5	0/0/0/0
3	UVW	A	418	-	-	0/3/5/5	0/0/0/0
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
3	UVW	B	403	-	-	0/3/5/5	0/0/0/0
3	UVW	B	404	-	-	0/3/5/5	0/0/0/0
3	UVW	B	405	-	-	0/3/5/5	0/0/0/0
3	UVW	B	419	-	-	0/3/5/5	0/0/0/0
3	UVW	C	407	-	-	0/3/5/5	0/0/0/0
3	UVW	C	408	-	-	0/3/5/5	0/0/0/0
3	UVW	C	412	-	-	0/3/5/5	0/0/0/0
3	UVW	C	420	-	-	0/3/5/5	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
3	UVW	D	409	-	-	0/3/5/5	0/0/0/0
3	UVW	D	410	-	-	0/3/5/5	0/0/0/0
3	UVW	D	411	-	-	0/3/5/5	0/0/0/0
3	UVW	D	421	-	-	0/3/5/5	0/0/0/0
3	UVW	E	413	-	-	0/3/5/5	0/0/0/0
3	UVW	E	414	-	-	0/3/5/5	0/0/0/0
3	UVW	E	415	-	-	0/3/5/5	0/0/0/0
3	UVW	E	422	-	-	0/3/5/5	0/0/0/0
2	SO4	E	503	-	-	0/0/0/0	0/0/0/0
3	UVW	F	416	-	-	0/3/5/5	0/0/0/0
3	UVW	F	417	-	-	0/3/5/5	0/0/0/0
3	UVW	F	423	-	-	0/3/5/5	0/0/0/0

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	UVW	C1M-C1	-6.47	1.26	1.49
3	D	411	UVW	C1M-C1	-6.35	1.26	1.49
3	A	401	UVW	C1M-C1	-6.33	1.26	1.49
3	F	417	UVW	C1M-C1	-6.32	1.26	1.49
3	F	423	UVW	C1M-C1	-6.26	1.26	1.49

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	UVW	O2-C1-O1	-9.57	114.88	122.07
3	E	422	UVW	O2-C1-O1	-9.53	114.91	122.07
3	D	411	UVW	O2-C1-O1	-9.07	115.25	122.07
3	A	418	UVW	O2-C1-O1	-8.79	115.46	122.07
3	F	416	UVW	O2-C1-O1	-8.76	115.48	122.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	UVW	3	0
3	B	403	UVW	2	0
3	B	404	UVW	3	0
3	B	419	UVW	1	0
3	C	407	UVW	1	0
3	C	420	UVW	2	0
3	D	410	UVW	4	0
3	D	421	UVW	2	0
3	E	413	UVW	3	0
3	E	415	UVW	3	0
3	E	422	UVW	2	0
3	F	416	UVW	1	0

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	324/329 (98%)	-0.47	2 (0%) 90 89	13, 37, 67, 89	0
1	B	324/329 (98%)	-0.28	3 (0%) 85 84	19, 43, 74, 97	0
1	C	323/329 (98%)	-0.46	0 100 100	9, 37, 71, 95	0
1	D	325/329 (98%)	-0.27	2 (0%) 90 89	15, 43, 78, 105	0
1	E	324/329 (98%)	-0.35	3 (0%) 85 84	12, 39, 72, 93	0
1	F	323/329 (98%)	0.21	9 (2%) 56 51	24, 65, 95, 108	0
All	All	1943/1974 (98%)	-0.27	19 (0%) 84 81	9, 43, 82, 108	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	254	ASP	3.5
1	F	227	LYS	3.2
1	F	228	ALA	2.8
1	D	254	ASP	2.8
1	D	230	GLU	2.6

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(Å ²)	Q<0.9
3	UVW	A	406	8/8	0.91	0.21	1.18	25,42,52,57	8
3	UVW	B	419	8/8	0.87	0.23	1.08	27,45,49,55	8
3	UVW	C	420	8/8	0.78	0.28	1.05	40,50,62,75	8
3	UVW	D	421	8/8	0.87	0.27	0.98	8,39,47,54	8
3	UVW	C	412	8/8	0.94	0.19	0.89	22,35,41,50	8
3	UVW	E	422	8/8	0.89	0.24	0.84	34,43,58,58	8
3	UVW	F	423	8/8	0.83	0.26	0.68	19,36,49,57	8
3	UVW	E	415	8/8	0.91	0.21	0.67	15,33,45,52	8
3	UVW	A	418	8/8	0.91	0.22	0.54	37,44,55,63	8
3	UVW	B	403	8/8	0.94	0.18	0.45	38,52,58,68	8
3	UVW	D	409	8/8	0.94	0.17	0.24	27,36,46,49	8
3	UVW	A	401	8/8	0.94	0.22	-	37,42,47,50	8
3	UVW	F	417	8/8	0.90	0.19	-	17,29,43,45	8
2	SO4	A	501	5/5	0.94	0.22	-	39,39,48,51	5
3	UVW	B	405	8/8	0.92	0.26	-	17,33,49,50	8
3	UVW	A	402	8/8	0.95	0.21	-	24,37,40,46	8
3	UVW	F	416	8/8	0.93	0.21	-	39,44,49,51	8
3	UVW	C	407	8/8	0.95	0.16	-	23,35,41,46	8
3	UVW	D	410	8/8	0.95	0.26	-	31,41,48,48	8
3	UVW	B	404	8/8	0.92	0.22	-	36,41,49,50	8
3	UVW	E	413	8/8	0.88	0.28	-	28,48,58,60	8
3	UVW	E	414	8/8	0.92	0.28	-	21,32,49,50	8
3	UVW	D	411	8/8	0.92	0.26	-	28,35,43,44	8
2	SO4	C	502	5/5	0.94	0.26	-	42,45,47,49	5
2	SO4	E	503	5/5	0.94	0.19	-	33,34,46,53	5
3	UVW	C	408	8/8	0.94	0.20	-	33,43,53,55	8

6.5 Other polymers [i](#)

There are no such residues in this entry.