



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 12:42 PM UTC

PDB ID : 1XCO / pdb_00001xco
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

<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

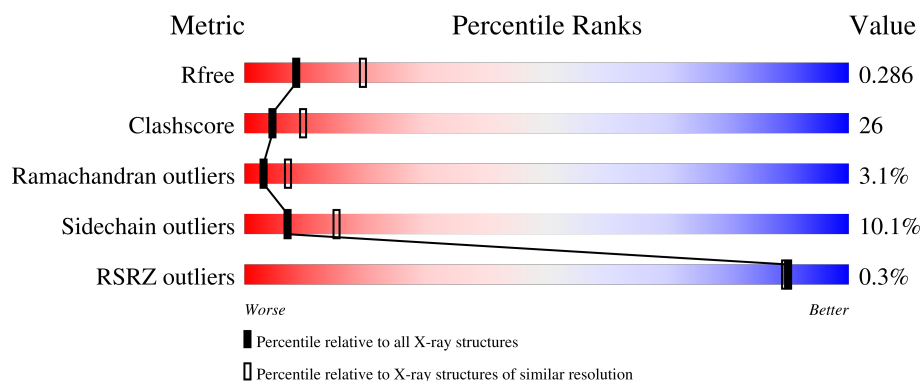
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	329	
1	B	329	
1	C	329	
1	D	329	
1	E	329	

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Mol	Chain	Length	Quality of chain
1	F	329	% 53% 35% 10% ••

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

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:

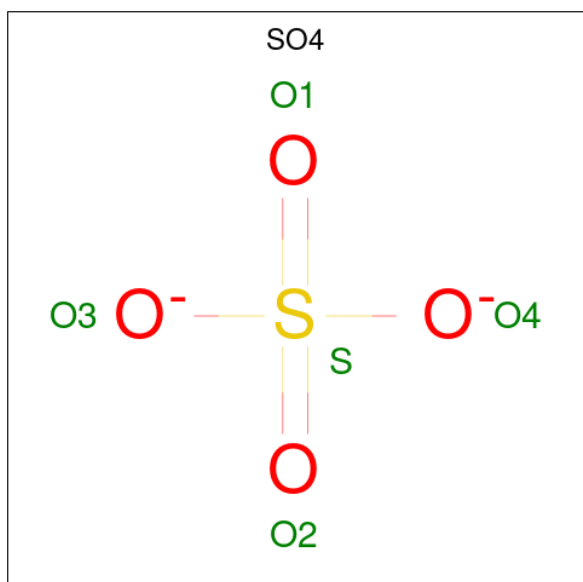
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	cloning artifact	UNP P39646
A	-4	GLY	-	cloning artifact	UNP P39646
A	-3	GLY	-	cloning artifact	UNP P39646
A	-2	GLY	-	cloning artifact	UNP P39646
A	-1	GLY	-	cloning artifact	UNP P39646
A	0	GLY	-	cloning artifact	UNP P39646
A	1	MET	-	initiating 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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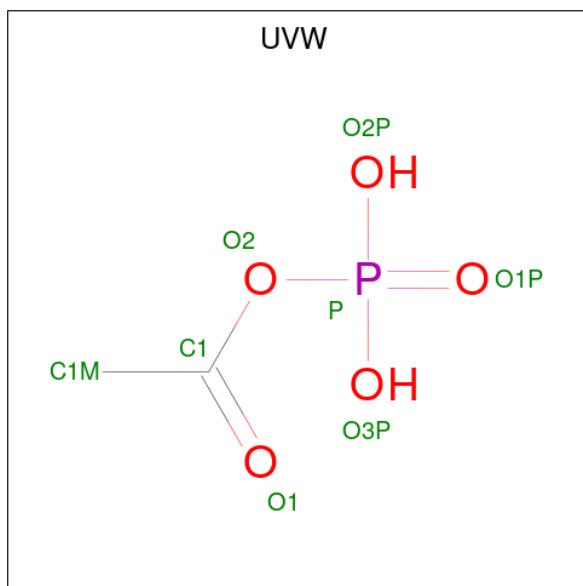
Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	cloning artifact	UNP P39646
C	-1	GLY	-	cloning artifact	UNP P39646
C	0	GLY	-	cloning artifact	UNP P39646
C	1	MET	-	initiating methionine	UNP P39646
D	-5	GLY	-	cloning artifact	UNP P39646
D	-4	GLY	-	cloning artifact	UNP P39646
D	-3	GLY	-	cloning 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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is ACETYLPHOSPHATE (CCD ID: UVW) (formula: $C_2H_5O_5P$).



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

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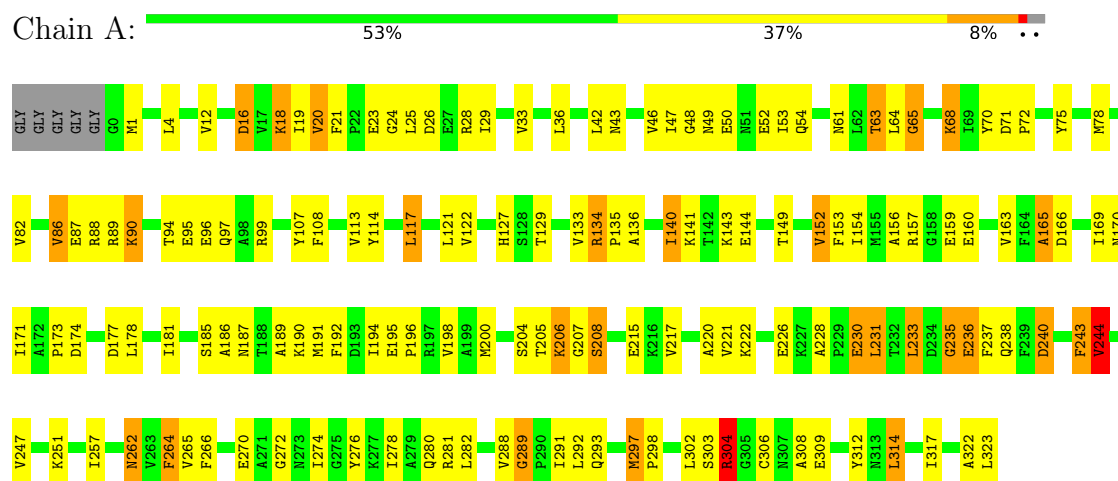
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	8	Total	O	0	0
			8	8		

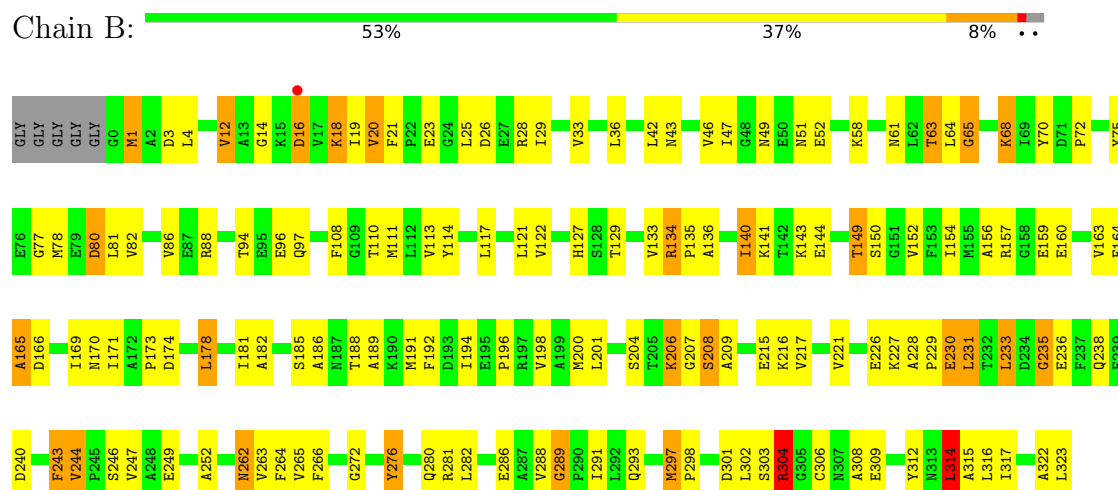
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: Phosphate acetyltransferase

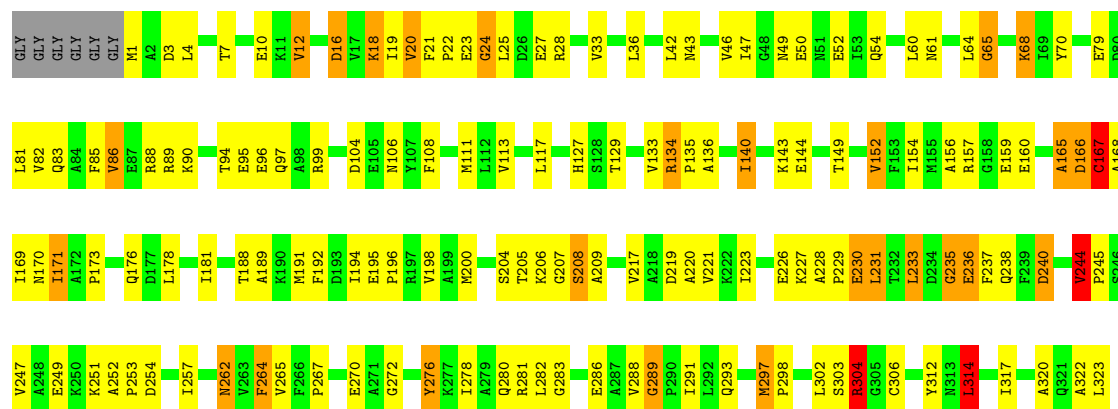


• Molecule 1: Phosphate acetyltransferase



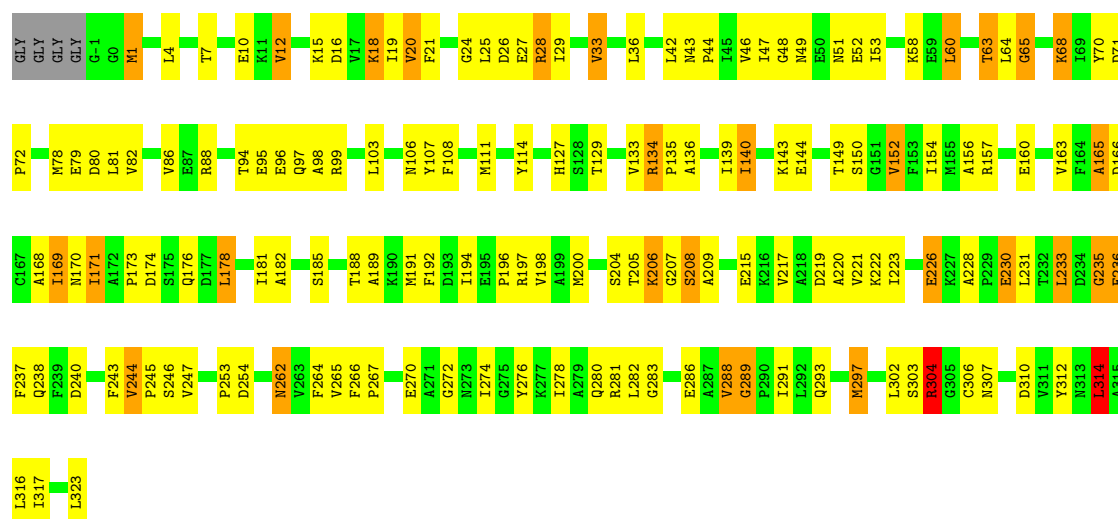
• Molecule 1: Phosphate acetyltransferase





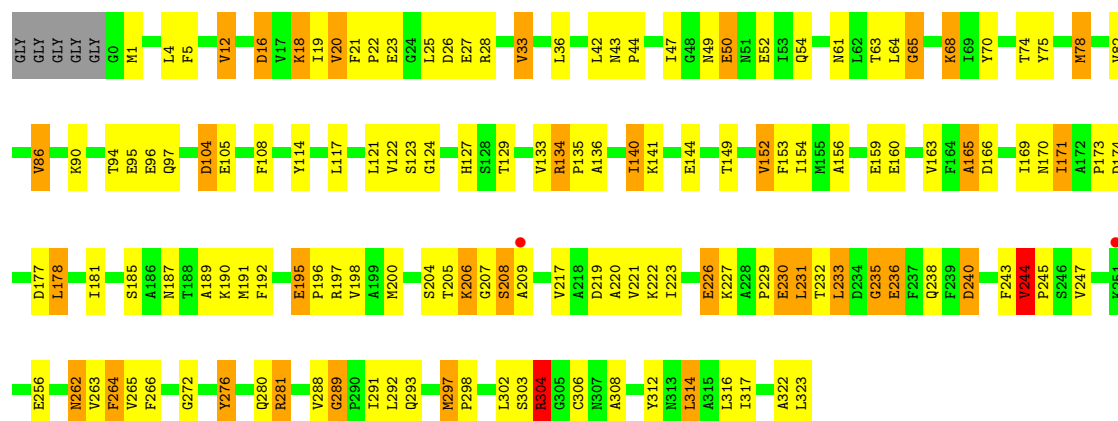
• Molecule 1: Phosphate acetyltransferase

Chain D: 51% 39% 9% ..

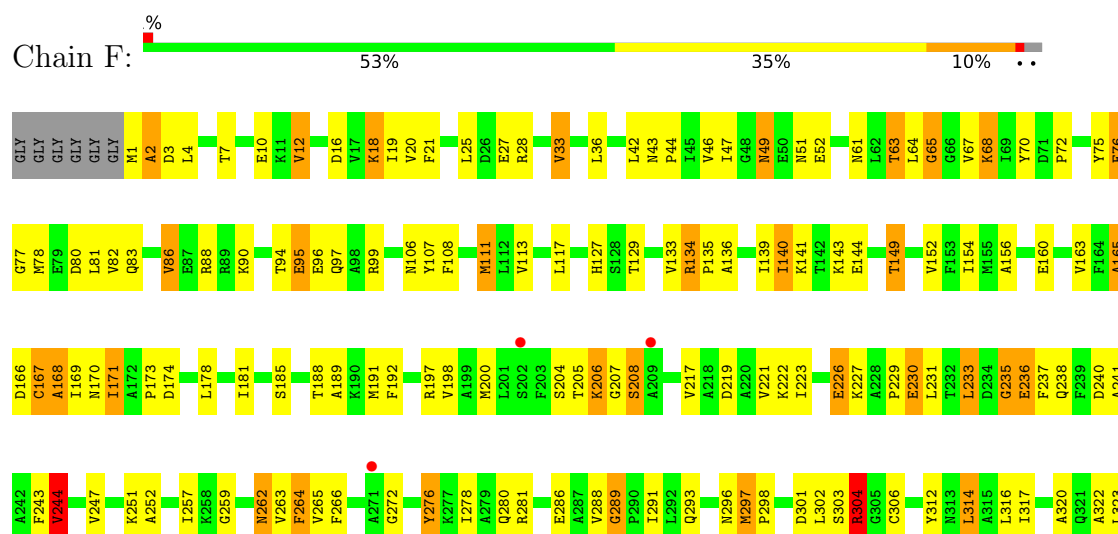


• Molecule 1: Phosphate acetyltransferase

Chain E: 55% 33% 10% ..



• 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	184.66Å 184.66Å 259.46Å 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) 99.4 (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 2.83Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.245 , 0.288 0.243 , 0.286	Depositor DCC
R_{free} test set	1666 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å ²)	47.6	Xtrriage
Anisotropy	0.486	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15000	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage'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.*

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: UVW, 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	A	0.73	0/2483	1.19	19/3351 (0.6%)
1	B	0.70	0/2483	1.20	18/3351 (0.5%)
1	C	0.73	0/2479	1.18	20/3346 (0.6%)
1	D	0.68	0/2487	1.20	22/3356 (0.7%)
1	E	0.73	1/2492 (0.0%)	1.20	17/3363 (0.5%)
1	F	0.65	0/2479	1.15	17/3346 (0.5%)
All	All	0.70	1/14903 (0.0%)	1.19	113/20113 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	78	MET	SD-CE	5.11	1.92	1.79

The worst 5 of 113 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ILE	N-CA-C	-11.26	97.49	110.21
1	A	235	GLY	N-CA-C	10.40	127.20	111.18
1	C	235	GLY	N-CA-C	10.09	126.71	111.18
1	E	235	GLY	N-CA-C	9.90	127.52	111.38
1	B	235	GLY	N-CA-C	9.86	126.37	111.18

There are no chirality outliers.

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	2449	0	2471	131	0
1	B	2449	0	2471	131	0
1	C	2445	0	2468	133	0
1	D	2453	0	2474	135	0
1	E	2458	0	2476	121	0
1	F	2445	0	2468	134	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	774	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 26.

The worst 5 of 774 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:C1	3:B:403:UVW:O2	1.65	1.44
3:C:420:UVW:O2	3:C:420:UVW:C1	1.64	1.44
3:D:421:UVW:C1	3:D:421:UVW:O2	1.64	1.43
3:D:410:UVW:C1	3:D:410:UVW:O2	1.64	1.42
3:E:413:UVW:C1	3:E:413:UVW:O2	1.63	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%)	3	7
1	B	322/329 (98%)	283 (88%)	31 (10%)	8 (2%)	4	10
1	C	321/329 (98%)	289 (90%)	22 (7%)	10 (3%)	3	7
1	D	323/329 (98%)	288 (89%)	26 (8%)	9 (3%)	4	9
1	E	323/329 (98%)	284 (88%)	30 (9%)	9 (3%)	4	9
1	F	321/329 (98%)	280 (87%)	28 (9%)	13 (4%)	2	4
All	All	1932/1974 (98%)	1716 (89%)	157 (8%)	59 (3%)	3	7

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%)	231 (90%)	26 (10%)	7	15
1	B	257/257 (100%)	230 (90%)	27 (10%)	6	13
1	C	257/257 (100%)	232 (90%)	25 (10%)	8	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	257/257 (100%)	234 (91%)	23 (9%)	9	20
1	E	258/257 (100%)	232 (90%)	26 (10%)	7	15
1	F	257/257 (100%)	229 (89%)	28 (11%)	6	12
All	All	1543/1542 (100%)	1388 (90%)	155 (10%)	7	16

5 of 155 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	178	LEU
1	F	167	CYS
1	E	233	LEU
1	F	25	LEU
1	F	264	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	43	ASN
1	F	161	GLN
1	D	161	GLN
1	F	127	HIS
1	F	9	GLN

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

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	-	6,7,7	3.28	3 (50%)	7,10,10	1.58	1 (14%)
3	UVW	B	419	-	6,7,7	3.49	4 (66%)	7,10,10	1.98	1 (14%)
3	UVW	C	420	-	6,7,7	3.20	3 (50%)	7,10,10	2.04	1 (14%)
2	SO4	E	503	-	4,4,4	2.15	1 (25%)	6,6,6	0.82	0
3	UVW	F	423	-	6,7,7	3.42	4 (66%)	7,10,10	1.89	1 (14%)
2	SO4	A	501	-	4,4,4	2.13	1 (25%)	6,6,6	0.81	0
3	UVW	A	402	-	6,7,7	3.31	4 (66%)	7,10,10	1.68	1 (14%)
3	UVW	A	406	-	6,7,7	3.07	4 (66%)	7,10,10	1.92	1 (14%)
3	UVW	C	408	-	6,7,7	3.21	3 (50%)	7,10,10	1.68	1 (14%)
3	UVW	D	409	-	6,7,7	3.30	3 (50%)	7,10,10	1.70	1 (14%)
3	UVW	D	421	-	6,7,7	3.48	4 (66%)	7,10,10	1.89	1 (14%)
3	UVW	F	416	-	6,7,7	3.24	3 (50%)	7,10,10	1.64	1 (14%)
3	UVW	B	403	-	6,7,7	3.12	3 (50%)	7,10,10	1.78	1 (14%)
3	UVW	B	404	-	6,7,7	3.52	3 (50%)	7,10,10	1.70	1 (14%)
3	UVW	C	412	-	6,7,7	3.34	3 (50%)	7,10,10	1.79	1 (14%)
3	UVW	E	414	-	6,7,7	3.41	3 (50%)	7,10,10	1.83	1 (14%)
3	UVW	D	410	-	6,7,7	3.20	3 (50%)	7,10,10	1.66	1 (14%)
3	UVW	E	413	-	6,7,7	3.20	4 (66%)	7,10,10	1.54	1 (14%)
2	SO4	C	502	-	4,4,4	2.17	1 (25%)	6,6,6	0.71	0
3	UVW	B	405	-	6,7,7	3.28	3 (50%)	7,10,10	1.87	1 (14%)
3	UVW	D	411	-	6,7,7	3.47	3 (50%)	7,10,10	1.77	1 (14%)
3	UVW	E	422	-	6,7,7	3.46	4 (66%)	7,10,10	1.94	1 (14%)
3	UVW	A	418	-	6,7,7	3.57	3 (50%)	7,10,10	1.55	1 (14%)
3	UVW	E	415	-	6,7,7	3.28	4 (66%)	7,10,10	1.70	1 (14%)
3	UVW	C	407	-	6,7,7	3.39	3 (50%)	7,10,10	1.69	1 (14%)
3	UVW	F	417	-	6,7,7	3.42	3 (50%)	7,10,10	1.83	1 (14%)

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	-
3	UVW	B	419	-	-	0/3/5/5	-
3	UVW	C	420	-	-	2/3/5/5	-
3	UVW	F	423	-	-	0/3/5/5	-
3	UVW	A	402	-	-	0/3/5/5	-
3	UVW	A	406	-	-	1/3/5/5	-
3	UVW	C	408	-	-	0/3/5/5	-
3	UVW	D	409	-	-	0/3/5/5	-
3	UVW	D	421	-	-	0/3/5/5	-
3	UVW	F	416	-	-	0/3/5/5	-
3	UVW	B	403	-	-	0/3/5/5	-
3	UVW	B	404	-	-	0/3/5/5	-
3	UVW	C	412	-	-	0/3/5/5	-
3	UVW	E	414	-	-	0/3/5/5	-
3	UVW	D	410	-	-	0/3/5/5	-
3	UVW	C	407	-	-	3/3/5/5	-
3	UVW	E	413	-	-	0/3/5/5	-
3	UVW	B	405	-	-	0/3/5/5	-
3	UVW	D	411	-	-	1/3/5/5	-
3	UVW	E	422	-	-	0/3/5/5	-
3	UVW	A	418	-	-	0/3/5/5	-
3	UVW	E	415	-	-	0/3/5/5	-
3	UVW	F	417	-	-	1/3/5/5	-

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	UVW	C1M-C1	-7.08	1.26	1.49
3	D	411	UVW	C1M-C1	-6.94	1.26	1.49
3	A	401	UVW	C1M-C1	-6.92	1.26	1.49
3	F	417	UVW	C1M-C1	-6.91	1.26	1.49
3	F	423	UVW	C1M-C1	-6.85	1.26	1.49

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	420	UVW	O3P-P-O2	4.88	119.52	105.32
3	B	419	UVW	O3P-P-O2	4.49	118.41	105.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	422	UVW	O3P-P-O2	4.44	118.24	105.32
3	D	421	UVW	O3P-P-O2	4.40	118.14	105.32
3	F	417	UVW	O3P-P-O2	4.28	117.79	105.32

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	417	UVW	C1-O2-P-O1P
3	C	407	UVW	C1-O2-P-O2P
3	C	420	UVW	C1-O2-P-O3P
3	C	407	UVW	C1-O2-P-O3P
3	A	406	UVW	C1-O2-P-O1P

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	419	UVW	1	0
3	C	420	UVW	2	0
3	D	421	UVW	2	0
3	F	416	UVW	1	0
3	B	403	UVW	2	0
3	B	404	UVW	3	0
3	D	410	UVW	4	0
3	E	413	UVW	3	0
3	E	422	UVW	2	0
3	E	415	UVW	3	0
3	C	407	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%)	-0.54	0 100 100	13, 37, 67, 89	0
1	B	324/329 (98%)	-0.32	1 (0%) 90 89	19, 43, 74, 97	0
1	C	323/329 (98%)	-0.49	0 100 100	9, 37, 71, 95	0
1	D	325/329 (98%)	-0.31	0 100 100	15, 43, 78, 105	0
1	E	324/329 (98%)	-0.33	2 (0%) 85 82	12, 39, 72, 93	1 (0%)
1	F	323/329 (98%)	0.34	3 (0%) 81 76	24, 65, 95, 108	0
All	All	1943/1974 (98%)	-0.28	6 (0%) 90 89	9, 43, 82, 108	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	202	SER	2.7
1	F	271	ALA	2.5
1	F	209	ALA	2.4
1	B	16	ASP	2.4
1	E	251	LYS	2.3

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 ⓘ

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	UVW	C	420	8/8	0.67	0.18	40,50,62,75	8
3	UVW	E	415	8/8	0.80	0.15	15,33,45,52	8
3	UVW	E	413	8/8	0.81	0.14	28,48,58,60	8
3	UVW	B	419	8/8	0.81	0.17	27,45,49,55	8
3	UVW	F	423	8/8	0.81	0.15	19,36,49,57	8
3	UVW	A	418	8/8	0.82	0.13	37,44,55,63	8
3	UVW	A	406	8/8	0.82	0.13	25,42,52,57	8
3	UVW	D	409	8/8	0.83	0.14	27,36,46,49	8
3	UVW	C	412	8/8	0.85	0.12	22,35,41,50	8
3	UVW	A	401	8/8	0.86	0.12	37,42,47,50	8
3	UVW	E	422	8/8	0.87	0.17	34,43,58,58	8
2	SO4	C	502	5/5	0.88	0.09	42,45,47,49	5
3	UVW	B	403	8/8	0.88	0.11	38,52,58,68	8
3	UVW	D	410	8/8	0.88	0.11	31,41,48,48	8
3	UVW	F	417	8/8	0.88	0.11	17,29,43,45	8
3	UVW	D	421	8/8	0.88	0.15	8,39,47,54	8
3	UVW	B	404	8/8	0.89	0.10	36,41,49,50	8
3	UVW	A	402	8/8	0.89	0.09	24,37,40,46	8
3	UVW	C	407	8/8	0.89	0.09	23,35,41,46	8
3	UVW	D	411	8/8	0.89	0.10	28,35,43,44	8
2	SO4	E	503	5/5	0.89	0.09	33,34,46,53	5
3	UVW	F	416	8/8	0.91	0.10	39,44,49,51	8
3	UVW	E	414	8/8	0.92	0.09	21,32,49,50	8
2	SO4	A	501	5/5	0.92	0.08	39,39,48,51	5
3	UVW	C	408	8/8	0.93	0.07	33,43,53,55	8
3	UVW	B	405	8/8	0.94	0.07	17,33,49,50	8

6.5 Other polymers ⓘ

There are no such residues in this entry.