Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:37 pm BST

PDB ID	:	6ERD
Title	:	Crystal structure of a putative acetyltransferase from Bacillus cereus species.
Authors	:	Silvestre, H.L.; Bolanos-Garcia, V.M.; Asensio, J.L.; Blundell, T.L.; Bastida, A.
Deposited on	:	2017-10-18
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 following versions of software and data (see references ①) were used in the production of this report:

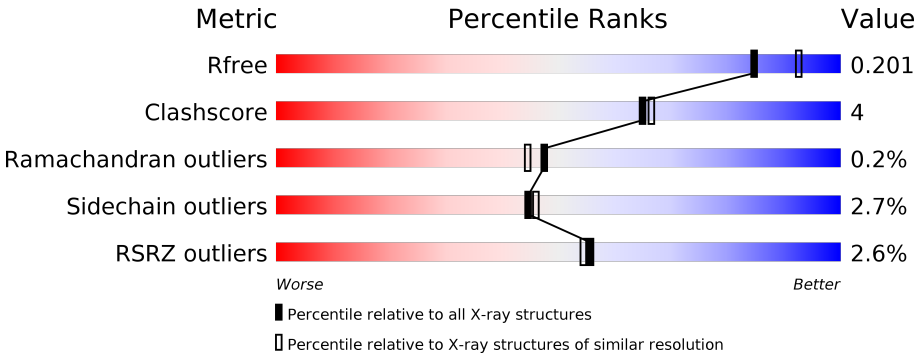
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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 <=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	211	2% 69% 9% • 21%
1	B	211	2% 68% 7% • 24%
2	C	211	% 65% 11% • 22%
2	D	211	2% 70% 9% • 19%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	D	301	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6149 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 Aminoglycoside N6'-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	Se	0	8	0
			1424	917	233	268	2	4			
1	B	161	Total	C	N	O	S	Se	0	6	0
			1354	879	218	251	2	4			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q81D84
A	2	GLY	-	expression tag	UNP Q81D84
A	3	SER	-	expression tag	UNP Q81D84
A	4	SER	-	expression tag	UNP Q81D84
A	5	HIS	-	expression tag	UNP Q81D84
A	6	HIS	-	expression tag	UNP Q81D84
A	7	HIS	-	expression tag	UNP Q81D84
A	8	HIS	-	expression tag	UNP Q81D84
A	9	HIS	-	expression tag	UNP Q81D84
A	10	HIS	-	expression tag	UNP Q81D84
A	11	SER	-	expression tag	UNP Q81D84
A	12	SER	-	expression tag	UNP Q81D84
A	13	GLY	-	expression tag	UNP Q81D84
A	14	LEU	-	expression tag	UNP Q81D84
A	15	VAL	-	expression tag	UNP Q81D84
A	16	PRO	-	expression tag	UNP Q81D84
A	17	ARG	-	expression tag	UNP Q81D84
A	18	GLY	-	expression tag	UNP Q81D84
A	19	SER	-	expression tag	UNP Q81D84
A	20	HIS	-	expression tag	UNP Q81D84
A	21	MSE	-	expression tag	UNP Q81D84
A	22	ALA	-	expression tag	UNP Q81D84
A	23	SER	-	expression tag	UNP Q81D84
A	24	MSE	-	expression tag	UNP Q81D84
A	25	THR	-	expression tag	UNP Q81D84

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP Q81D84
A	27	GLY	-	expression tag	UNP Q81D84
A	28	GLN	-	expression tag	UNP Q81D84
A	29	GLN	-	expression tag	UNP Q81D84
A	30	MSE	-	expression tag	UNP Q81D84
A	31	GLY	-	expression tag	UNP Q81D84
A	32	ARG	-	expression tag	UNP Q81D84
A	33	ASP	-	expression tag	UNP Q81D84
A	34	PRO	-	expression tag	UNP Q81D84
A	35	ASN	-	expression tag	UNP Q81D84
A	36	SER	-	expression tag	UNP Q81D84
A	37	SER	-	expression tag	UNP Q81D84
A	38	SER	-	expression tag	UNP Q81D84
A	39	VAL	-	expression tag	UNP Q81D84
A	40	ASP	-	expression tag	UNP Q81D84
A	41	LYS	-	expression tag	UNP Q81D84
A	42	LEU	-	expression tag	UNP Q81D84
A	43	VAL	-	expression tag	UNP Q81D84
B	1	MSE	-	initiating methionine	UNP Q81D84
B	2	GLY	-	expression tag	UNP Q81D84
B	3	SER	-	expression tag	UNP Q81D84
B	4	SER	-	expression tag	UNP Q81D84
B	5	HIS	-	expression tag	UNP Q81D84
B	6	HIS	-	expression tag	UNP Q81D84
B	7	HIS	-	expression tag	UNP Q81D84
B	8	HIS	-	expression tag	UNP Q81D84
B	9	HIS	-	expression tag	UNP Q81D84
B	10	HIS	-	expression tag	UNP Q81D84
B	11	SER	-	expression tag	UNP Q81D84
B	12	SER	-	expression tag	UNP Q81D84
B	13	GLY	-	expression tag	UNP Q81D84
B	14	LEU	-	expression tag	UNP Q81D84
B	15	VAL	-	expression tag	UNP Q81D84
B	16	PRO	-	expression tag	UNP Q81D84
B	17	ARG	-	expression tag	UNP Q81D84
B	18	GLY	-	expression tag	UNP Q81D84
B	19	SER	-	expression tag	UNP Q81D84
B	20	HIS	-	expression tag	UNP Q81D84
B	21	MSE	-	expression tag	UNP Q81D84
B	22	ALA	-	expression tag	UNP Q81D84
B	23	SER	-	expression tag	UNP Q81D84
B	24	MSE	-	expression tag	UNP Q81D84

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	THR	-	expression tag	UNP Q81D84
B	26	GLY	-	expression tag	UNP Q81D84
B	27	GLY	-	expression tag	UNP Q81D84
B	28	GLN	-	expression tag	UNP Q81D84
B	29	GLN	-	expression tag	UNP Q81D84
B	30	MSE	-	expression tag	UNP Q81D84
B	31	GLY	-	expression tag	UNP Q81D84
B	32	ARG	-	expression tag	UNP Q81D84
B	33	ASP	-	expression tag	UNP Q81D84
B	34	PRO	-	expression tag	UNP Q81D84
B	35	ASN	-	expression tag	UNP Q81D84
B	36	SER	-	expression tag	UNP Q81D84
B	37	SER	-	expression tag	UNP Q81D84
B	38	SER	-	expression tag	UNP Q81D84
B	39	VAL	-	expression tag	UNP Q81D84
B	40	ASP	-	expression tag	UNP Q81D84
B	41	LYS	-	expression tag	UNP Q81D84
B	42	LEU	-	expression tag	UNP Q81D84
B	43	VAL	-	expression tag	UNP Q81D84

- Molecule 2 is a protein called Aminoglycoside N6'-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	164	Total	C	N	O	S	Se	0	5	0
			1378	888	228	257	1	4			
2	D	170	Total	C	N	O	S	Se	0	5	0
			1415	918	233	258	1	5			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MSE	-	initiating methionine	UNP Q81D84
C	2	GLY	-	expression tag	UNP Q81D84
C	3	SER	-	expression tag	UNP Q81D84
C	4	SER	-	expression tag	UNP Q81D84
C	5	HIS	-	expression tag	UNP Q81D84
C	6	HIS	-	expression tag	UNP Q81D84
C	7	HIS	-	expression tag	UNP Q81D84
C	8	HIS	-	expression tag	UNP Q81D84
C	9	HIS	-	expression tag	UNP Q81D84
C	10	HIS	-	expression tag	UNP Q81D84
C	11	SER	-	expression tag	UNP Q81D84

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	SER	-	expression tag	UNP Q81D84
C	13	GLY	-	expression tag	UNP Q81D84
C	14	LEU	-	expression tag	UNP Q81D84
C	15	VAL	-	expression tag	UNP Q81D84
C	16	PRO	-	expression tag	UNP Q81D84
C	17	ARG	-	expression tag	UNP Q81D84
C	18	GLY	-	expression tag	UNP Q81D84
C	19	SER	-	expression tag	UNP Q81D84
C	20	HIS	-	expression tag	UNP Q81D84
C	21	MSE	-	expression tag	UNP Q81D84
C	22	ALA	-	expression tag	UNP Q81D84
C	23	SER	-	expression tag	UNP Q81D84
C	24	MSE	-	expression tag	UNP Q81D84
C	25	THR	-	expression tag	UNP Q81D84
C	26	GLY	-	expression tag	UNP Q81D84
C	27	GLY	-	expression tag	UNP Q81D84
C	28	GLN	-	expression tag	UNP Q81D84
C	29	GLN	-	expression tag	UNP Q81D84
C	30	MSE	-	expression tag	UNP Q81D84
C	31	GLY	-	expression tag	UNP Q81D84
C	32	ARG	-	expression tag	UNP Q81D84
C	33	ASP	-	expression tag	UNP Q81D84
C	34	PRO	-	expression tag	UNP Q81D84
C	35	ASN	-	expression tag	UNP Q81D84
C	36	SER	-	expression tag	UNP Q81D84
C	37	SER	-	expression tag	UNP Q81D84
C	38	SER	-	expression tag	UNP Q81D84
C	39	VAL	-	expression tag	UNP Q81D84
C	40	ASP	-	expression tag	UNP Q81D84
C	41	LYS	-	expression tag	UNP Q81D84
C	42	LEU	-	expression tag	UNP Q81D84
C	43	VAL	-	expression tag	UNP Q81D84
D	1	MSE	-	initiating methionine	UNP Q81D84
D	2	GLY	-	expression tag	UNP Q81D84
D	3	SER	-	expression tag	UNP Q81D84
D	4	SER	-	expression tag	UNP Q81D84
D	5	HIS	-	expression tag	UNP Q81D84
D	6	HIS	-	expression tag	UNP Q81D84
D	7	HIS	-	expression tag	UNP Q81D84
D	8	HIS	-	expression tag	UNP Q81D84
D	9	HIS	-	expression tag	UNP Q81D84
D	10	HIS	-	expression tag	UNP Q81D84

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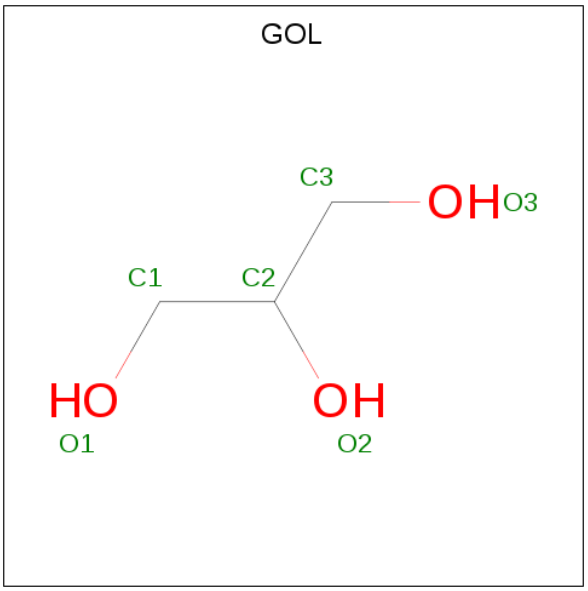
Chain	Residue	Modelled	Actual	Comment	Reference
D	11	SER	-	expression tag	UNP Q81D84
D	12	SER	-	expression tag	UNP Q81D84
D	13	GLY	-	expression tag	UNP Q81D84
D	14	LEU	-	expression tag	UNP Q81D84
D	15	VAL	-	expression tag	UNP Q81D84
D	16	PRO	-	expression tag	UNP Q81D84
D	17	ARG	-	expression tag	UNP Q81D84
D	18	GLY	-	expression tag	UNP Q81D84
D	19	SER	-	expression tag	UNP Q81D84
D	20	HIS	-	expression tag	UNP Q81D84
D	21	MSE	-	expression tag	UNP Q81D84
D	22	ALA	-	expression tag	UNP Q81D84
D	23	SER	-	expression tag	UNP Q81D84
D	24	MSE	-	expression tag	UNP Q81D84
D	25	THR	-	expression tag	UNP Q81D84
D	26	GLY	-	expression tag	UNP Q81D84
D	27	GLY	-	expression tag	UNP Q81D84
D	28	GLN	-	expression tag	UNP Q81D84
D	29	GLN	-	expression tag	UNP Q81D84
D	30	MSE	-	expression tag	UNP Q81D84
D	31	GLY	-	expression tag	UNP Q81D84
D	32	ARG	-	expression tag	UNP Q81D84
D	33	ASP	-	expression tag	UNP Q81D84
D	34	PRO	-	expression tag	UNP Q81D84
D	35	ASN	-	expression tag	UNP Q81D84
D	36	SER	-	expression tag	UNP Q81D84
D	37	SER	-	expression tag	UNP Q81D84
D	38	SER	-	expression tag	UNP Q81D84
D	39	VAL	-	expression tag	UNP Q81D84
D	40	ASP	-	expression tag	UNP Q81D84
D	41	LYS	-	expression tag	UNP Q81D84
D	42	LEU	-	expression tag	UNP Q81D84
D	43	VAL	-	expression tag	UNP Q81D84

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	2	Total Cl 2 2	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is water.

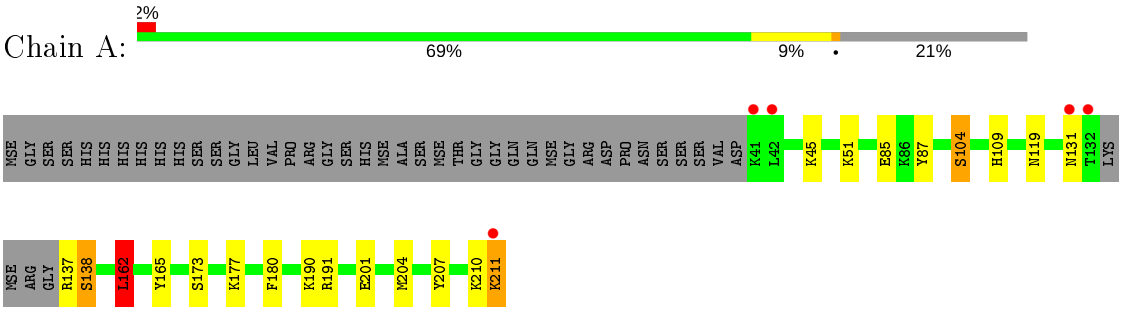
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	136	Total O 136 136	0	0
5	B	122	Total O 122 122	0	0
5	C	122	Total O 122 122	0	0
5	D	147	Total O 147 147	0	0

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 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.

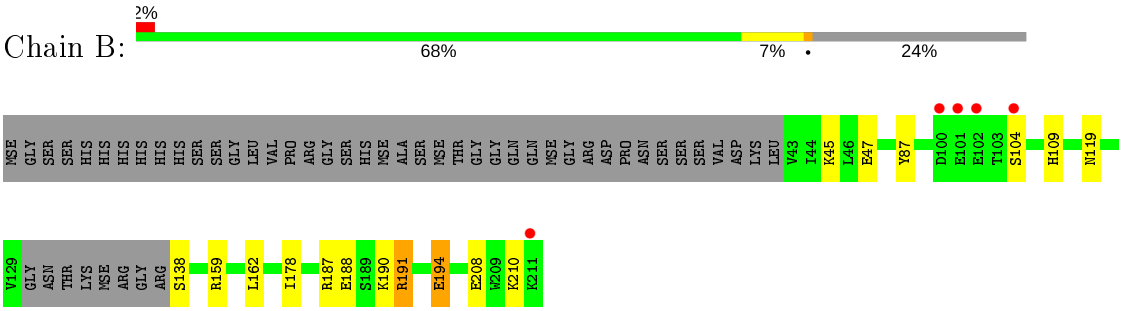
- Molecule 1: Aminoglycoside N6'-acetyltransferase

Chain A:



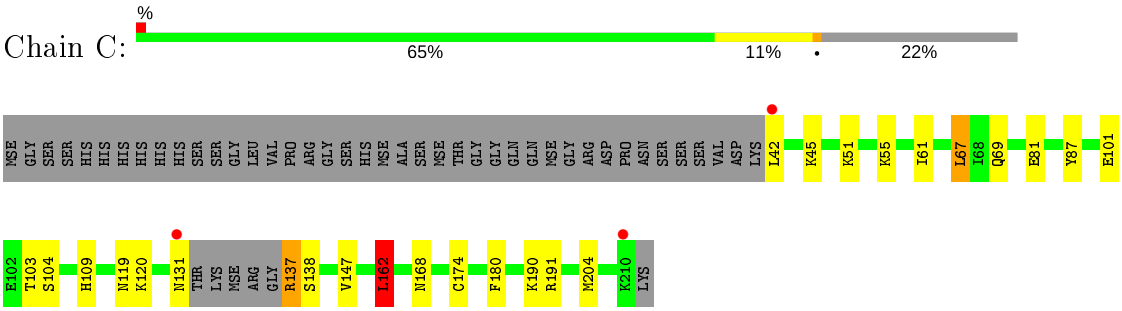
- Molecule 1: Aminoglycoside N6'-acetyltransferase

Chain B:



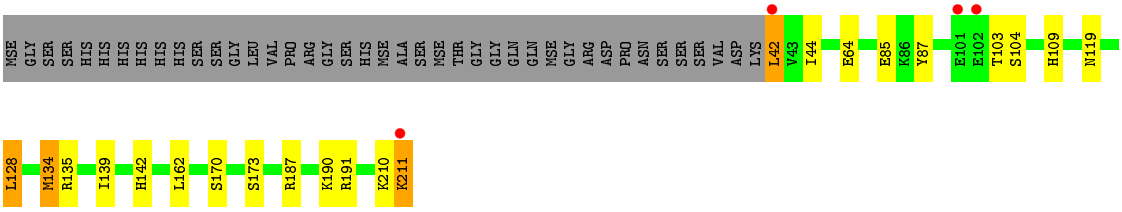
- Molecule 2: Aminoglycoside N6'-acetyltransferase

Chain C:



- Molecule 2: Aminoglycoside N6'-acetyltransferase

Chain D:


MSE GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MSE ALA SER MSE THR GLY GLY GLN GLN MSE GLY ARG ASP PRO ASN SER SER SER VAL ASP LYS L42 V43 I44 E64 E85 K86 Y87 E101 E102 T103 S104 H109 N119
L128 M134 R135 I139 H142 L162 S170 S173 R187 K190 R191 K210 K211

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.52Å 84.17Å 72.08Å 90.00° 98.49° 90.00°	Depositor
Resolution (Å)	44.97 – 2.00 44.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.97-2.00) 99.7 (44.97-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.164 , 0.201 0.164 , 0.201	Depositor DCC
R_{free} test set	2770 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	23.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6149	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CME, CL

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	1.12	4/1442 (0.3%)	1.04	4/1929 (0.2%)
1	B	1.06	1/1378 (0.1%)	1.05	5/1845 (0.3%)
2	C	1.08	0/1401	1.02	4/1878 (0.2%)
2	D	1.18	5/1450 (0.3%)	1.13	6/1940 (0.3%)
All	All	1.11	10/5671 (0.2%)	1.06	19/7592 (0.3%)

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
1	A	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	GLU	CD-OE2	6.53	1.32	1.25
2	D	64	GLU	CD-OE1	-6.29	1.18	1.25
2	D	85	GLU	CD-OE1	5.55	1.31	1.25
2	D	170	SER	CB-OG	-5.37	1.35	1.42
1	A	104	SER	CB-OG	-5.31	1.35	1.42
1	A	165	TYR	CG-CD1	-5.29	1.32	1.39
1	B	208	GLU	CD-OE2	5.26	1.31	1.25
2	D	173[A]	SER	CB-OG	-5.17	1.35	1.42
2	D	173[B]	SER	CB-OG	-5.17	1.35	1.42
1	A	201	GLU	CD-OE1	5.12	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	135	ARG	NE-CZ-NH2	10.67	125.64	120.30
1	B	187	ARG	NE-CZ-NH2	9.06	124.83	120.30
2	C	137	ARG	NE-CZ-NH1	7.51	124.06	120.30
2	C	162	LEU	CA-CB-CG	7.41	132.35	115.30
1	A	162	LEU	CA-CB-CG	6.72	130.75	115.30
2	D	128[A]	LEU	CB-CG-CD1	6.65	122.31	111.00
2	D	128[B]	LEU	CB-CG-CD1	6.65	122.31	111.00
2	C	147	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	B	159	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	C	67	LEU	CA-CB-CG	5.68	128.36	115.30
2	D	187	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	D	42	LEU	CA-CB-CG	5.52	128.01	115.30
1	A	138	SER	CA-C-N	-5.29	105.57	117.20
2	D	135	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	A	104	SER	N-CA-CB	5.26	118.39	110.50
1	B	188	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	B	162	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	45	LYS	CD-CE-NZ	5.10	123.44	111.70
1	B	191	ARG	NE-CZ-NH2	-5.06	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	ARG	Peptide
1	A	210	LYS	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	1424	0	1424	12	0
1	B	1354	0	1367	11	0
2	C	1378	0	1370	18	0
2	D	1415	0	1445	17	0
3	A	18	0	24	0	0
3	B	18	0	24	0	0
3	C	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	6	0	8	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	136	0	0	1	0
5	B	122	0	0	2	0
5	C	122	0	0	3	0
5	D	147	0	0	0	0
All	All	6149	0	5670	46	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 4.

All (46) 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:42:LEU:HD13	2:D:142:HIS:ND1	1.97	0.80
1:A:119:ASN:HD22	1:B:191:ARG:H	1.30	0.79
1:A:191:ARG:H	1:B:119:ASN:HD22	1.29	0.77
2:C:119:ASN:HD22	2:D:191:ARG:H	1.35	0.75
2:C:69:GLN:HE21	2:C:168[B]:ASN:HD21	1.36	0.71
2:C:191:ARG:H	2:D:119:ASN:HD22	1.36	0.70
1:A:207:TYR:HB2	1:A:211:LYS:HE2	1.77	0.66
1:B:45:LYS:HE3	1:B:47:GLU:OE2	1.96	0.65
2:D:134:MSE:HG2	2:D:139[B]:ILE:HD11	1.79	0.63
2:C:174:CYS:SG	5:C:507:HOH:O	2.56	0.61
1:A:87:TYR:OH	1:A:109:HIS:HE1	1.84	0.61
1:B:87:TYR:OH	1:B:109:HIS:HE1	1.84	0.61
2:C:87:TYR:OH	2:C:109:HIS:HE1	1.84	0.60
2:D:87:TYR:OH	2:D:109:HIS:HE1	1.84	0.60
2:C:119:ASN:HD21	2:D:190:LYS:NZ	2.00	0.59
2:D:162:LEU:HD12	2:D:162:LEU:C	2.23	0.58
1:B:178[B]:ILE:HD13	1:B:178[B]:ILE:N	2.13	0.58
2:C:190:LYS:NZ	2:D:119:ASN:HD21	2.03	0.56
2:C:42:LEU:HD23	2:C:101:GLU:OE1	2.05	0.56
3:C:301:GOL:H12	5:C:505:HOH:O	2.07	0.55
2:C:103:THR:O	2:C:104:SER:HB3	2.08	0.53
2:D:139[B]:ILE:HD13	2:D:139[B]:ILE:N	2.23	0.53
2:D:42:LEU:HD12	2:D:44:ILE:H	1.75	0.52
2:C:51:LYS:HE3	2:C:81:GLU:OE1	2.10	0.52
1:A:173:SER:O	1:A:177:LYS:HG3	2.09	0.51
1:A:190:LYS:NZ	1:B:119:ASN:HD21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:HG3	5:A:470:HOH:O	2.12	0.49
1:A:119:ASN:ND2	1:B:191:ARG:H	2.05	0.48
2:C:120:LYS:HE3	5:C:474:HOH:O	2.13	0.48
2:C:61:ILE:HG21	2:C:67:LEU:HD23	1.95	0.48
2:C:190:LYS:HZ3	2:D:119:ASN:HD21	1.63	0.47
2:D:103:THR:O	2:D:104:SER:HB2	2.15	0.46
1:B:194:GLU:CD	1:B:194:GLU:H	2.19	0.46
1:A:119:ASN:HD21	1:B:190:LYS:NZ	2.14	0.46
2:D:210:LYS:O	2:D:211:LYS:HB2	2.16	0.45
1:A:162:LEU:HD23	1:A:162:LEU:C	2.37	0.45
2:D:134:MSE:CG	2:D:139[B]:ILE:HD11	2.47	0.44
2:C:162:LEU:HD23	2:C:162:LEU:C	2.38	0.44
2:C:119:ASN:ND2	2:D:191:ARG:H	2.10	0.44
1:A:180:PHE:CE1	1:A:204:MSE:HE3	2.54	0.43
1:A:191:ARG:H	1:B:119:ASN:ND2	2.07	0.43
2:D:211:LYS:NZ	2:D:211:LYS:HB2	2.34	0.42
1:B:138:SER:N	5:B:408:HOH:O	2.52	0.41
2:C:119:ASN:HD21	2:D:190:LYS:HZ2	1.68	0.41
2:C:180:PHE:CE1	2:C:204:MSE:HE3	2.56	0.41
5:B:429:HOH:O	2:C:55:LYS:HE2	2.21	0.41

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	170/211 (81%)	168 (99%)	1 (1%)	1 (1%)	25	19
1	B	162/211 (77%)	161 (99%)	1 (1%)	0	100	100
2	C	165/211 (78%)	164 (99%)	1 (1%)	0	100	100
2	D	173/211 (82%)	172 (99%)	1 (1%)	0	100	100
All	All	670/844 (79%)	665 (99%)	4 (1%)	1 (0%)	47	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER

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	157/176 (89%)	152 (97%)	5 (3%)	39	38
1	B	150/176 (85%)	147 (98%)	3 (2%)	55	58
2	C	152/177 (86%)	147 (97%)	5 (3%)	38	37
2	D	157/177 (89%)	153 (98%)	4 (2%)	47	49
All	All	616/706 (87%)	599 (97%)	17 (3%)	44	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	104	SER
1	A	131	ASN
1	A	162	LEU
1	A	211	LYS
1	B	104	SER
1	B	194	GLU
1	B	210	LYS
2	C	45	LYS
2	C	131	ASN
2	C	137	ARG
2	C	138	SER
2	C	162	LEU
2	D	128[A]	LEU
2	D	128[B]	LEU
2	D	134	MSE
2	D	211	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	109	HIS
1	A	119	ASN
1	B	59	ASN
1	B	109	HIS
1	B	119	ASN
2	C	56	GLN
2	C	69	GLN
2	C	109	HIS
2	C	119	ASN
2	D	59	ASN
2	D	109	HIS
2	D	119	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CME	B	174	1	8,9,10	0.94	0	5,9,11	1.21	0
1	CME	A	174	1	8,9,10	0.86	0	5,9,11	0.94	0

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
1	CME	B	174	1	-	1/5/8/10	-
1	CME	A	174	1	-	2/5/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	174	CME	SD-CE-CZ-OH
1	A	174	CME	SD-CE-CZ-OH
1	A	174	CME	CZ-CE-SD-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 for Mogul analysis.

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	GOL	A	302	-	5,5,5	0.49	0	5,5,5	0.50	0
3	GOL	B	303	-	5,5,5	0.30	0	5,5,5	0.64	0
3	GOL	A	303	-	5,5,5	0.34	0	5,5,5	0.43	0
3	GOL	B	302	-	5,5,5	0.39	0	5,5,5	0.30	0
3	GOL	B	301	-	5,5,5	0.39	0	5,5,5	1.22	0
3	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	GOL	D	301	-	5,5,5	0.78	0	5,5,5	2.06	2 (40%)
3	GOL	C	301	-	5,5,5	0.42	0	5,5,5	1.34	0

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	GOL	A	302	-	-	4/4/4/4	-
3	GOL	B	303	-	-	2/4/4/4	-
3	GOL	A	303	-	-	2/4/4/4	-
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	A	301	-	-	0/4/4/4	-
3	GOL	D	301	-	-	4/4/4/4	-
3	GOL	C	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	GOL	O1-C1-C2	3.62	127.54	110.20
3	D	301	GOL	O2-C2-C1	2.15	118.61	109.12

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	GOL	C1-C2-C3-O3
3	A	303	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	B	303	GOL	O1-C1-C2-C3
3	B	301	GOL	C1-C2-C3-O3
3	D	301	GOL	C1-C2-C3-O3
3	C	301	GOL	O1-C1-C2-C3
3	A	303	GOL	O2-C2-C3-O3
3	B	301	GOL	O2-C2-C3-O3
3	D	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O2-C2-C3-O3
3	B	303	GOL	O1-C1-C2-O2
3	D	301	GOL	O2-C2-C3-O3
3	A	302	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	GOL	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	162/211 (76%)	-0.37	5 (3%) 49 48	15, 23, 50, 91	1 (0%)
1	B	156/211 (73%)	-0.23	5 (3%) 47 46	17, 25, 50, 86	0
2	C	160/211 (75%)	-0.42	3 (1%) 66 65	17, 26, 49, 68	1 (0%)
2	D	165/211 (78%)	-0.43	4 (2%) 59 57	14, 23, 44, 73	0
All	All	643/844 (76%)	-0.36	17 (2%) 56 54	14, 24, 50, 91	2 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	42	LEU	5.9
1	B	211	LYS	4.1
2	C	131	ASN	3.7
2	D	102	GLU	3.5
2	D	101	GLU	3.3
1	A	132	THR	3.2
1	B	102	GLU	3.1
1	A	42	LEU	3.0
2	C	42	LEU	2.9
1	B	101	GLU	2.9
1	A	211	LYS	2.8
1	B	104	SER	2.8
1	A	41	LYS	2.6
2	C	210	LYS	2.4
1	A	131	ASN	2.1
1	B	100	ASP	2.1
2	D	211	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CME	A	174	10/11	0.93	0.10	26,34,53,56	10
1	CME	B	174	10/11	0.96	0.11	26,37,61,66	0

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. The B-factors column lists the minimum, median, 95^{th} 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	GOL	A	303	6/6	0.72	0.14	57,60,61,64	6
3	GOL	A	302	6/6	0.89	0.18	46,50,53,58	0
3	GOL	C	301	6/6	0.89	0.16	46,47,52,54	0
3	GOL	D	301	6/6	0.90	0.14	29,40,41,44	0
3	GOL	B	303	6/6	0.90	0.13	52,56,58,59	0
4	CL	B	304	1/1	0.91	0.07	37,37,37,37	0
3	GOL	B	301	6/6	0.92	0.13	44,48,50,54	0
4	CL	A	304	1/1	0.96	0.06	33,33,33,33	0
3	GOL	B	302	6/6	0.97	0.08	24,26,28,28	0
3	GOL	A	301	6/6	0.98	0.08	16,20,20,22	0
4	CL	B	305	1/1	0.98	0.06	47,47,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.