



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 6, 2023 – 01:51 am GMT

PDB ID : 5AA1  
Title : Crystal structure of MltF from *Pseudomonas aeruginosa* in complex with NA  
G-anhNAM-pentapeptide  
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.  
Deposited on : 2015-07-23  
Resolution : 2.89 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](mailto: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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

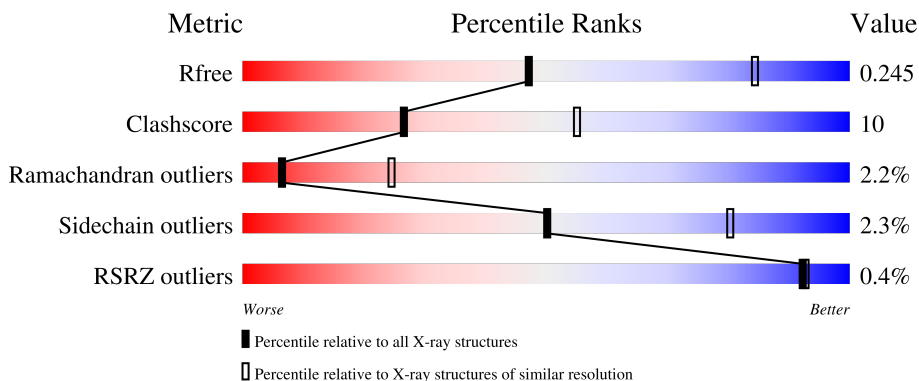
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	499	 60% 22% 16%
1	B	499	 66% 16% 17%
1	C	499	 65% 17% 16%
1	D	499	 63% 18% 16%
2	E	6	 17% 17% 50% 33%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	FGA	E	3	-	-	X	-
2	API	E	4	-	-	X	-
2	DAL	E	5	-	-	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 13551 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	418	3360	2118	597	636	9	0	1	0
1	B	413	3313	2089	591	624	9	0	0	0
1	C	419	3360	2119	598	634	9	0	0	0
1	D	417	3342	2108	595	630	9	0	0	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP Q9HYN1
A	-7	ALA	-	expression tag	UNP Q9HYN1
A	-6	PRO	-	expression tag	UNP Q9HYN1
A	-5	SER	-	expression tag	UNP Q9HYN1
A	-4	ARG	-	expression tag	UNP Q9HYN1
A	-3	LEU	-	expression tag	UNP Q9HYN1
A	-2	CYS	-	expression tag	UNP Q9HYN1
A	-1	VAL	-	expression tag	UNP Q9HYN1
A	0	TYR	-	expression tag	UNP Q9HYN1
A	1	CYS	-	expression tag	UNP Q9HYN1
A	2	ALA	-	expression tag	UNP Q9HYN1
A	3	ASP	-	expression tag	UNP Q9HYN1
A	4	VAL	-	expression tag	UNP Q9HYN1
A	5	CYS	-	expression tag	UNP Q9HYN1
A	6	PRO	-	expression tag	UNP Q9HYN1
A	7	ASP	-	expression tag	UNP Q9HYN1
A	281	THR	ALA	conflict	UNP Q9HYN1
A	302	LYS	LEU	conflict	UNP Q9HYN1
B	-8	MET	-	expression tag	UNP Q9HYN1
B	-7	ALA	-	expression tag	UNP Q9HYN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PRO	-	expression tag	UNP Q9HXN1
B	-5	SER	-	expression tag	UNP Q9HXN1
B	-4	ARG	-	expression tag	UNP Q9HXN1
B	-3	LEU	-	expression tag	UNP Q9HXN1
B	-2	CYS	-	expression tag	UNP Q9HXN1
B	-1	VAL	-	expression tag	UNP Q9HXN1
B	0	TYR	-	expression tag	UNP Q9HXN1
B	1	CYS	-	expression tag	UNP Q9HXN1
B	2	ALA	-	expression tag	UNP Q9HXN1
B	3	ASP	-	expression tag	UNP Q9HXN1
B	4	VAL	-	expression tag	UNP Q9HXN1
B	5	CYS	-	expression tag	UNP Q9HXN1
B	6	PRO	-	expression tag	UNP Q9HXN1
B	7	ASP	-	expression tag	UNP Q9HXN1
B	281	THR	ALA	conflict	UNP Q9HXN1
B	302	LYS	LEU	conflict	UNP Q9HXN1
C	-8	MET	-	expression tag	UNP Q9HXN1
C	-7	ALA	-	expression tag	UNP Q9HXN1
C	-6	PRO	-	expression tag	UNP Q9HXN1
C	-5	SER	-	expression tag	UNP Q9HXN1
C	-4	ARG	-	expression tag	UNP Q9HXN1
C	-3	LEU	-	expression tag	UNP Q9HXN1
C	-2	CYS	-	expression tag	UNP Q9HXN1
C	-1	VAL	-	expression tag	UNP Q9HXN1
C	0	TYR	-	expression tag	UNP Q9HXN1
C	1	CYS	-	expression tag	UNP Q9HXN1
C	2	ALA	-	expression tag	UNP Q9HXN1
C	3	ASP	-	expression tag	UNP Q9HXN1
C	4	VAL	-	expression tag	UNP Q9HXN1
C	5	CYS	-	expression tag	UNP Q9HXN1
C	6	PRO	-	expression tag	UNP Q9HXN1
C	7	ASP	-	expression tag	UNP Q9HXN1
C	281	THR	ALA	conflict	UNP Q9HXN1
C	302	LYS	LEU	conflict	UNP Q9HXN1
D	-8	MET	-	expression tag	UNP Q9HXN1
D	-7	ALA	-	expression tag	UNP Q9HXN1
D	-6	PRO	-	expression tag	UNP Q9HXN1
D	-5	SER	-	expression tag	UNP Q9HXN1
D	-4	ARG	-	expression tag	UNP Q9HXN1
D	-3	LEU	-	expression tag	UNP Q9HXN1
D	-2	CYS	-	expression tag	UNP Q9HXN1
D	-1	VAL	-	expression tag	UNP Q9HXN1

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	TYR	-	expression tag	UNP Q9HXN1
D	1	CYS	-	expression tag	UNP Q9HXN1
D	2	ALA	-	expression tag	UNP Q9HXN1
D	3	ASP	-	expression tag	UNP Q9HXN1
D	4	VAL	-	expression tag	UNP Q9HXN1
D	5	CYS	-	expression tag	UNP Q9HXN1
D	6	PRO	-	expression tag	UNP Q9HXN1
D	7	ASP	-	expression tag	UNP Q9HXN1
D	281	THR	ALA	conflict	UNP Q9HXN1
D	302	LYS	LEU	conflict	UNP Q9HXN1

- Molecule 2 is a protein called N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-ALA-D-GLU-M-DAP-D-ALA-D-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	6	42	24	6	12	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

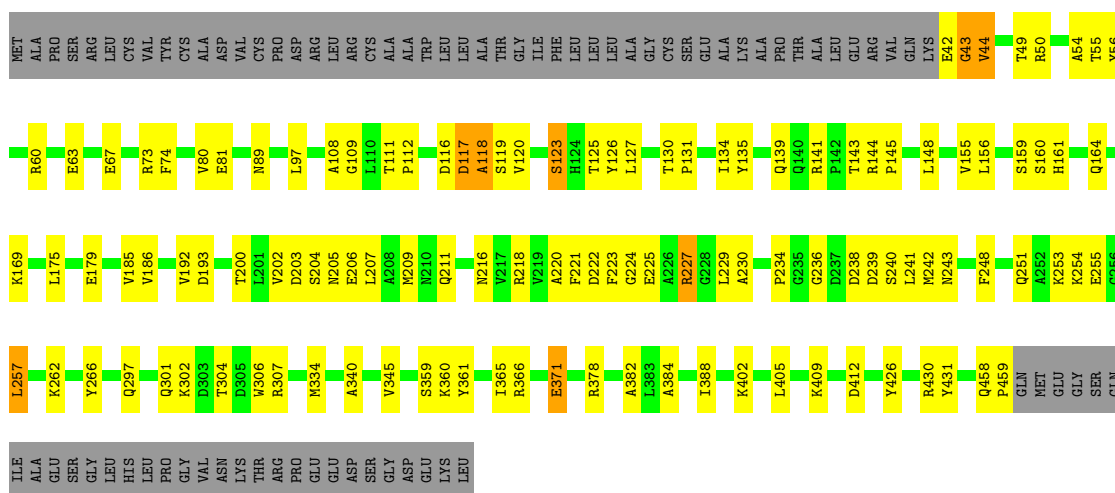
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	52	52	52	0	0
4	B	28	28	28	0	0
4	C	35	35	35	0	0
4	D	14	14	14	0	0

### 3 Residue-property plots [i](#)

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.

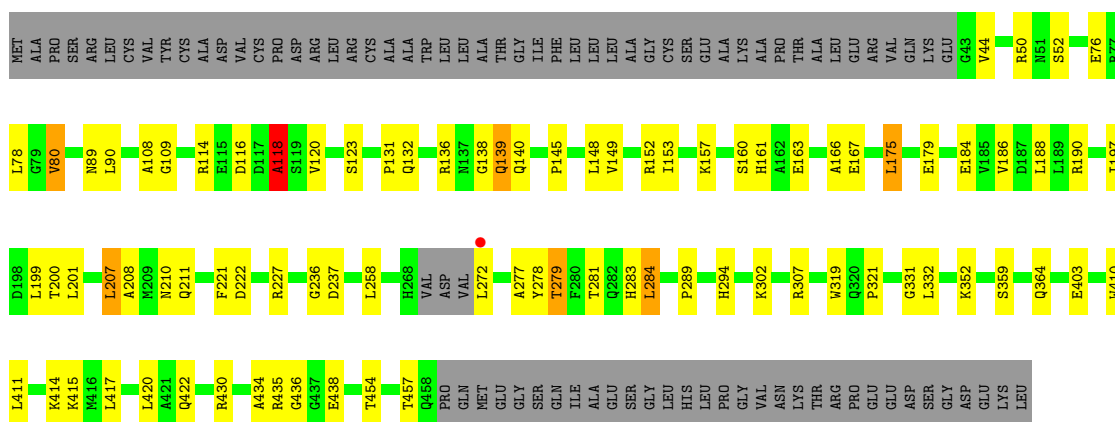
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain A: 



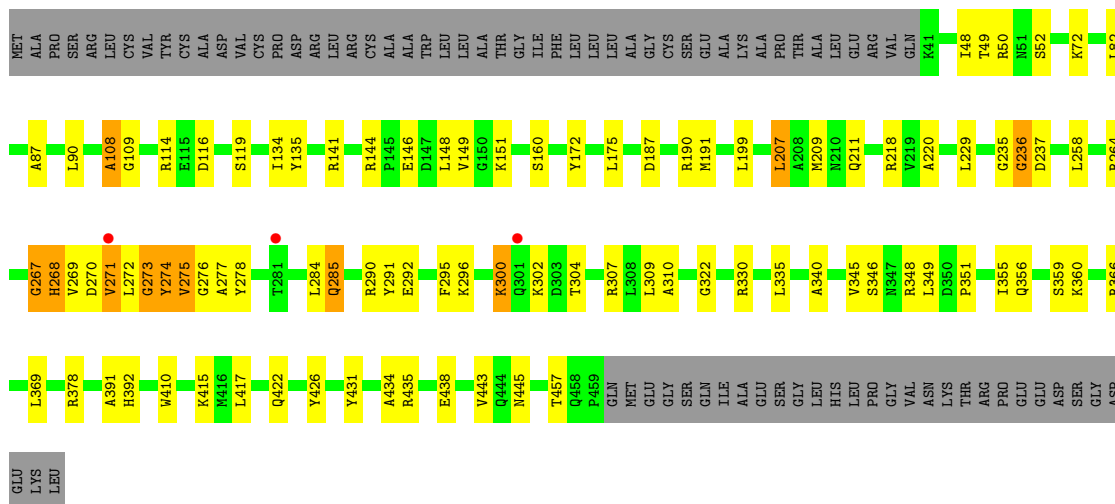
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain B: 



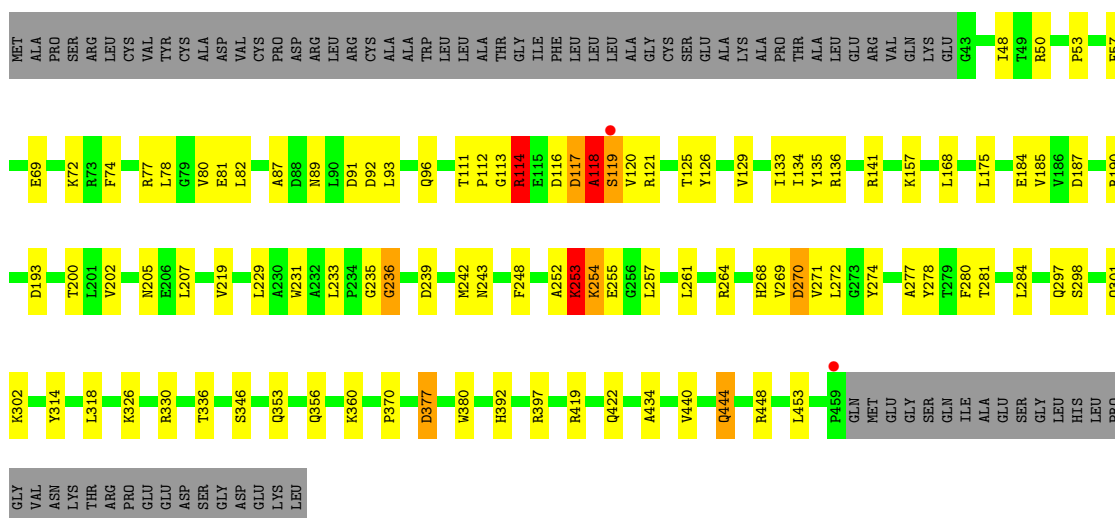
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain C: 



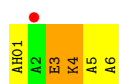
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain D: 63% 18% 16%



• Molecule 2: N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-A LA-D-GLU-M-DAP-D-ALA-D-ALA

Chain E: 17% 17% 50% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.85Å 135.75Å 138.03Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	47.25 – 2.89 47.25 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.25-2.89) 91.7 (47.25-2.89)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.168 , 0.243 0.170 , 0.245	Depositor DCC
$R_{free}$ test set	2025 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.3	Xtrriage
Anisotropy	0.186	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 45.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.001 for -h,l,k 0.014 for -h,-l,-k 0.034 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13551	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: AH0, FGA, API, CL, DAL

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	0.49	0/3431	0.66	2/4639 (0.0%)
1	B	0.44	0/3382	0.66	2/4569 (0.0%)
1	C	0.48	0/3431	0.66	0/4638
1	D	0.42	0/3413	0.63	3/4615 (0.1%)
2	E	0.85	0/4	0.70	0/4
All	All	0.46	0/13661	0.65	7/18465 (0.0%)

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	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

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	D	118	ALA	N-CA-C	5.78	126.60	111.00
1	D	114	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	257	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	43	GLY	C-N-CA	5.55	135.57	121.70
1	D	253	LYS	C-N-CA	5.36	135.09	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	GLN	Peptide
1	C	273	GLY	Peptide
1	D	253	LYS	Peptide
1	D	270	ASP	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	3360	0	3300	84	0
1	B	3313	0	3259	50	0
1	C	3360	0	3308	59	0
1	D	3342	0	3289	81	0
2	E	42	0	31	18	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	52	0	0	5	1
4	B	28	0	0	2	0
4	C	35	0	0	0	1
4	D	14	0	0	3	0
All	All	13551	0	13187	274	1

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 10.

The worst 5 of 274 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:D:114:ARG:HD3	1:D:117:ASP:HB3	1.40	1.02
1:D:118:ALA:HA	1:D:119:SER:HB3	1.53	0.88
1:A:185:VAL:HG11	1:A:206:GLU:HG2	1.60	0.84
1:B:50:ARG:NH1	1:B:184:GLU:OE2	2.11	0.83
1:D:114:ARG:HD3	1:D:117:ASP:CB	2.08	0.83

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2016:HOH:O	4:C:2025:HOH:O[1_455]	2.16	0.04

## 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	417/499 (84%)	387 (93%)	22 (5%)	8 (2%)	8	28
1	B	409/499 (82%)	370 (90%)	27 (7%)	12 (3%)	4	18
1	C	417/499 (84%)	389 (93%)	20 (5%)	8 (2%)	8	28
1	D	415/499 (83%)	375 (90%)	32 (8%)	8 (2%)	8	28
2	E	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1659/2002 (83%)	1522 (92%)	101 (6%)	36 (2%)	6	24

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	118	ALA
1	A	120	VAL
1	B	118	ALA
1	B	277	ALA

### 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	350/414 (84%)	342 (98%)	8 (2%)	50	80
1	B	344/414 (83%)	335 (97%)	9 (3%)	46	77
1	C	350/414 (84%)	339 (97%)	11 (3%)	40	74
1	D	348/414 (84%)	343 (99%)	5 (1%)	67	89
All	All	1392/1656 (84%)	1359 (98%)	33 (2%)	50	79

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	89	ASN
1	D	272	LEU
1	D	444	GLN
1	B	167	GLU
1	B	160	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	C	445	ASN
1	D	243	ASN
1	D	301	GLN
1	D	356	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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
2	FGA	E	3	2	7,8,9	0.92	0	7,9,11	1.49	1 (14%)
2	API	E	4	2	9,11,12	1.48	2 (22%)	7,13,15	1.48	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
2	FGA	E	3	2	-	3/7/8/9	-
2	API	E	4	2	-	6/11/12/14	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	API	O4-C7	-2.64	1.21	1.30
2	E	4	API	C3-CA	-2.15	1.50	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	FGA	CB-CA-C	-2.27	104.89	110.30
2	E	4	API	C5-C4-C3	-2.18	103.23	113.24

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	API	C4-C3-CA-C
2	E	4	API	C4-C3-CA-N
2	E	4	API	C4-C5-C6-C7
2	E	4	API	C4-C5-C6-N6
2	E	3	FGA	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	FGA	5	0
2	E	4	API	7	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	418/499 (83%)	-0.35	0 <span style="border: 1px solid blue; padding: 2px;">100</span> <span style="border: 1px solid blue; padding: 2px;">100</span>	27, 47, 94, 138	0
1	B	413/499 (82%)	-0.29	1 (0%) <span style="border: 1px solid blue; padding: 2px;">95</span> <span style="border: 1px solid blue; padding: 2px;">95</span>	31, 60, 104, 135	0
1	C	419/499 (83%)	-0.30	3 (0%) <span style="border: 1px solid blue; padding: 2px;">87</span> <span style="border: 1px solid blue; padding: 2px;">87</span>	28, 54, 96, 173	0
1	D	417/499 (83%)	-0.07	2 (0%) <span style="border: 1px solid blue; padding: 2px;">91</span> <span style="border: 1px solid blue; padding: 2px;">91</span>	42, 73, 130, 242	0
2	E	1/6 (16%)	2.38	1 (100%) <span style="border: 1px solid red; padding: 2px;">0</span> <span style="border: 1px solid red; padding: 2px;">0</span>	103, 103, 103, 103	1 (100%)
All	All	1668/2002 (83%)	-0.25	7 (0%) <span style="border: 1px solid blue; padding: 2px;">92</span> <span style="border: 1px solid blue; padding: 2px;">93</span>	27, 60, 109, 242	1 (0%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLN	4.6
1	C	271	VAL	4.2
1	D	459	PRO	3.7
1	D	119	SER	3.0
1	B	272	LEU	2.4

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	DAL	E	5	5/6	0.78	0.59	118,123,124,127	5
2	FGA	E	3	9/10	0.80	0.38	76,82,90,99	9
2	API	E	4	12/13	0.89	0.46	88,137,141,142	12
2	DAL	E	6	6/6	0.91	0.45	68,85,111,115	6



### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	CL	D	1460	1/1	0.88	0.14	92,92,92,92	0
3	CL	B	1460	1/1	0.90	0.57	120,120,120,120	0
3	CL	A	1460	1/1	0.91	0.12	68,68,68,68	0
3	CL	B	1459	1/1	0.95	0.13	76,76,76,76	0
3	CL	C	1460	1/1	0.96	0.21	58,58,58,58	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.