



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 03:44 am GMT

PDB ID : 5AA4
Title : Crystal structure of MltF from Pseudomonas aeruginosa in complex with cell-wall tetrapeptide
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.
Deposited on : 2015-07-23
Resolution : 2.40 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
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

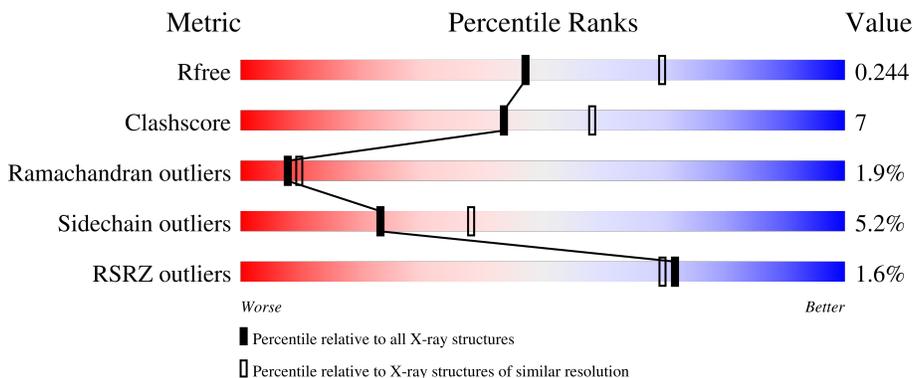
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	451	 77% 13% •• 7%
1	C	451	 78% 11% • 8%
2	B	451	 82% 10% • 8%
2	D	451	 71% 19% • 8%

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	6X4	A	1458	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26643 atoms, of which 13107 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	H	N	O	S			
1	A	418	6623	2112	3274	596	632	9	0	0	0
1	C	413	6552	2087	3240	591	625	9	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	LYS	LEU	conflict	UNP A0A077JMS
C	302	LYS	LEU	conflict	UNP A0A077JMS

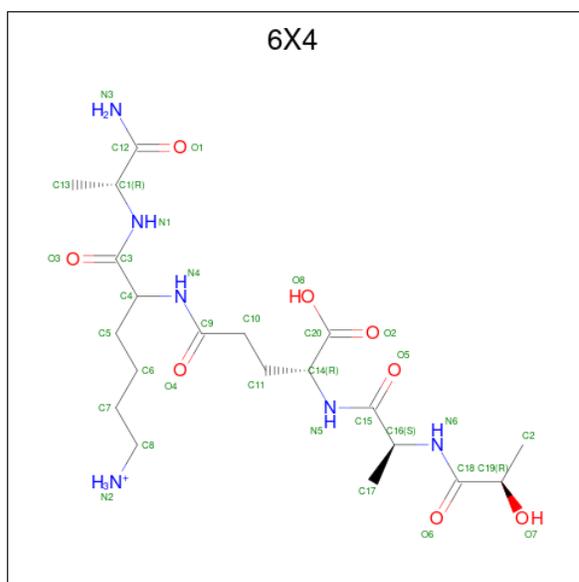
- Molecule 2 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	417	6632	2108	3288	595	632	9	0	0	0
2	D	417	6609	2102	3272	594	632	9	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	281	THR	ALA	conflict	UNP A0A077JMS
B	302	LYS	LEU	conflict	UNP A0A077JMS
D	281	THR	ALA	conflict	UNP A0A077JMS
D	302	LYS	LEU	conflict	UNP A0A077JMS

- Molecule 3 is [6-[[[(2 {R})-1-azanyl-1-oxidanylidene-propan-2-yl]amino]-6-oxidanylidene-5-[[[(4 {R})-5-oxidanyl-5-oxidanylidene-4-[[[(2 {S})-2-[[[(2 {R})-2-oxidanylpropanoyl]amino]propanoyl]amino]pentanoyl]amino]hexyl]azanium (three-letter code: 6X4) (formula: C₂₀H₃₇N₆O₈).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	67	20	33	6	8	0	0

- Molecule 4 is water.

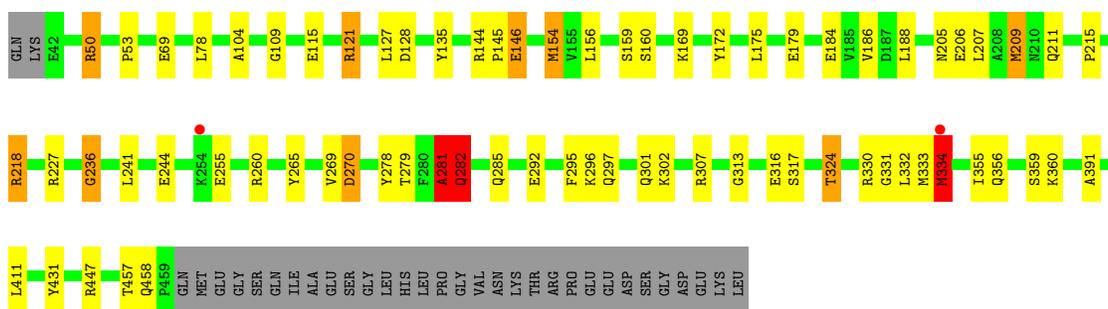
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		
4	B	46	Total	O	0	0
			46	46		
4	C	33	Total	O	0	0
			33	33		
4	D	8	Total	O	0	0
			8	8		

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.

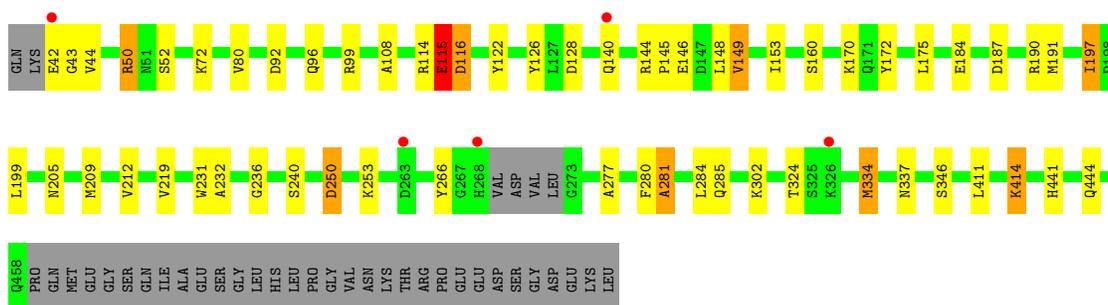
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain A: 



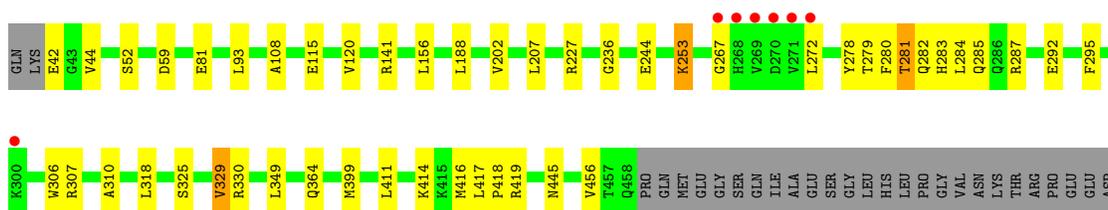
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain C: 



- Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain B: 



SER
GLY
ASP
GLU
LYS
LEU

● Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain D:  3% 71% 19% 8%

GLN
LYS
E42
C43
V44
L45
R46
V47
I48
T49
R50
T55
H56
T64
G65
R73
F74
L78
G79
W80
F81
L82
L93
Y94
R99
E100
G101
L105
A108
T111
P112
G113
R114
E115
D116
D117
A118
S119
V120
R121
Y122
S123
H124
T125
Y126
Y135
R141
P142
T143

R144
P145
E146
D147
S160
E167
K170
Q171
Y172
V185
V186
D187
R190
D198
V202
M209
M210
R218
E225
A226
R227
L233
P234
G235
G236
D237
D238
D239
M242
R243
E244
V245
M246
A247
F248
L249
K254
E255
G256
K262
Y266
G267
H268
Y274

V275
G276
A277
Y278
T279
F280
T281
Q282
H283
L284
L288
P289
Q297
Q301
K302
T324
R330
S346
Q353
S359
K360
S372
A391
K423
Y426
R430
Y431
G432
Y433
A434
R435
R448
I452
V456
T457
Q458
PRO
GLN
MET
GLU
GLY
SER
GLN
ILE

ALA
GLU
SER
GLY
LEU
HIS
LEU
PRO
GLY
VAL
ASN
LYS
THR
ARG
PRO
GLU
GLU
ASP
SER
GLY
ASP
GLU
LYS
LEU

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.12Å 136.77Å 138.10Å 90.00° 92.34° 90.00°	Depositor
Resolution (Å)	48.57 – 2.40 48.72 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.57-2.40) 93.6 (48.72-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.39Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.185 , 0.239 0.191 , 0.244	Depositor DCC
R_{free} test set	4681 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k 0.022 for -h,-l,-k 0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26643	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6X4

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	0.82	0/3420	0.86	8/4624 (0.2%)
1	C	0.73	0/3381	0.77	2/4567 (0.0%)
2	B	0.80	1/3414 (0.0%)	0.79	2/4615 (0.0%)
2	D	0.59	0/3407	0.72	0/4607
All	All	0.74	1/13622 (0.0%)	0.78	12/18413 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	VAL	CB-CG2	-5.03	1.42	1.52

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	154	MET	CG-SD-CE	-8.74	86.21	100.20
1	A	334	MET	CG-SD-CE	-7.50	88.21	100.20
1	A	281	ALA	C-N-CA	7.42	140.26	121.70
2	B	419	ARG	NE-CZ-NH2	-7.42	116.59	120.30

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	3349	3274	3293	63	0
1	C	3312	3240	3252	36	0
2	B	3344	3288	3288	28	0
2	D	3337	3272	3268	58	0
3	A	34	33	0	9	0
4	A	73	0	0	7	0
4	B	46	0	0	5	0
4	C	33	0	0	1	0
4	D	8	0	0	2	0
All	All	13536	13107	13101	177	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 7.

The worst 5 of 177 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:A:333:MET:SD	4:A:2050:HOH:O	2.00	1.20
1:A:281:ALA:HB1	1:C:285:GLN:HB2	1.55	0.87
1:A:179:GLU:OE1	4:A:2019:HOH:O	1.93	0.86
2:D:117:ASP:O	2:D:119:SER:N	2.09	0.86
1:A:281:ALA:HB3	1:A:282:GLN:HB2	1.58	0.85

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	416/451 (92%)	395 (95%)	15 (4%)	6 (1%)	11 15
1	C	409/451 (91%)	381 (93%)	21 (5%)	7 (2%)	9 11
2	B	415/451 (92%)	397 (96%)	14 (3%)	4 (1%)	15 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	415/451 (92%)	379 (91%)	21 (5%)	15 (4%)	3	3
All	All	1655/1804 (92%)	1552 (94%)	71 (4%)	32 (2%)	8	10

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	GLU
1	A	282	GLN
2	B	281	THR
1	C	149	VAL
2	D	113	GLY

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	348/376 (93%)	333 (96%)	15 (4%)	29	46
1	C	343/376 (91%)	321 (94%)	22 (6%)	17	28
2	B	348/377 (92%)	335 (96%)	13 (4%)	34	53
2	D	346/377 (92%)	324 (94%)	22 (6%)	17	28
All	All	1385/1506 (92%)	1313 (95%)	72 (5%)	23	38

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	105	LEU
2	D	430	ARG
2	D	160	SER
2	D	262	LYS
2	B	329	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	GLN
2	B	282	GLN
2	B	285	GLN
1	C	140	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	6X4	A	1458	-	33,33,33	2.54	8 (24%)	43,43,43	3.59	22 (51%)

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	6X4	A	1458	-	1/1/15/15	15/46/46/46	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1458	6X4	C15-N5	7.35	1.50	1.34
3	A	1458	6X4	O7-C19	-6.50	1.20	1.42
3	A	1458	6X4	C18-N6	5.35	1.45	1.34
3	A	1458	6X4	C9-N4	5.13	1.45	1.34
3	A	1458	6X4	C3-N1	4.37	1.43	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1458	6X4	C11-C10-C9	8.27	131.52	113.04
3	A	1458	6X4	C10-C11-C14	7.75	127.64	113.16
3	A	1458	6X4	C4-C3-N1	7.67	133.53	116.70
3	A	1458	6X4	C5-C4-C3	7.54	127.81	110.20
3	A	1458	6X4	C14-N5-C15	7.44	137.62	121.67

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1458	6X4	C4

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1458	6X4	O6-C18-C19-O7
3	A	1458	6X4	N6-C18-C19-O7
3	A	1458	6X4	C19-C18-N6-C16
3	A	1458	6X4	C3-C4-C5-C6
3	A	1458	6X4	C17-C16-N6-C18

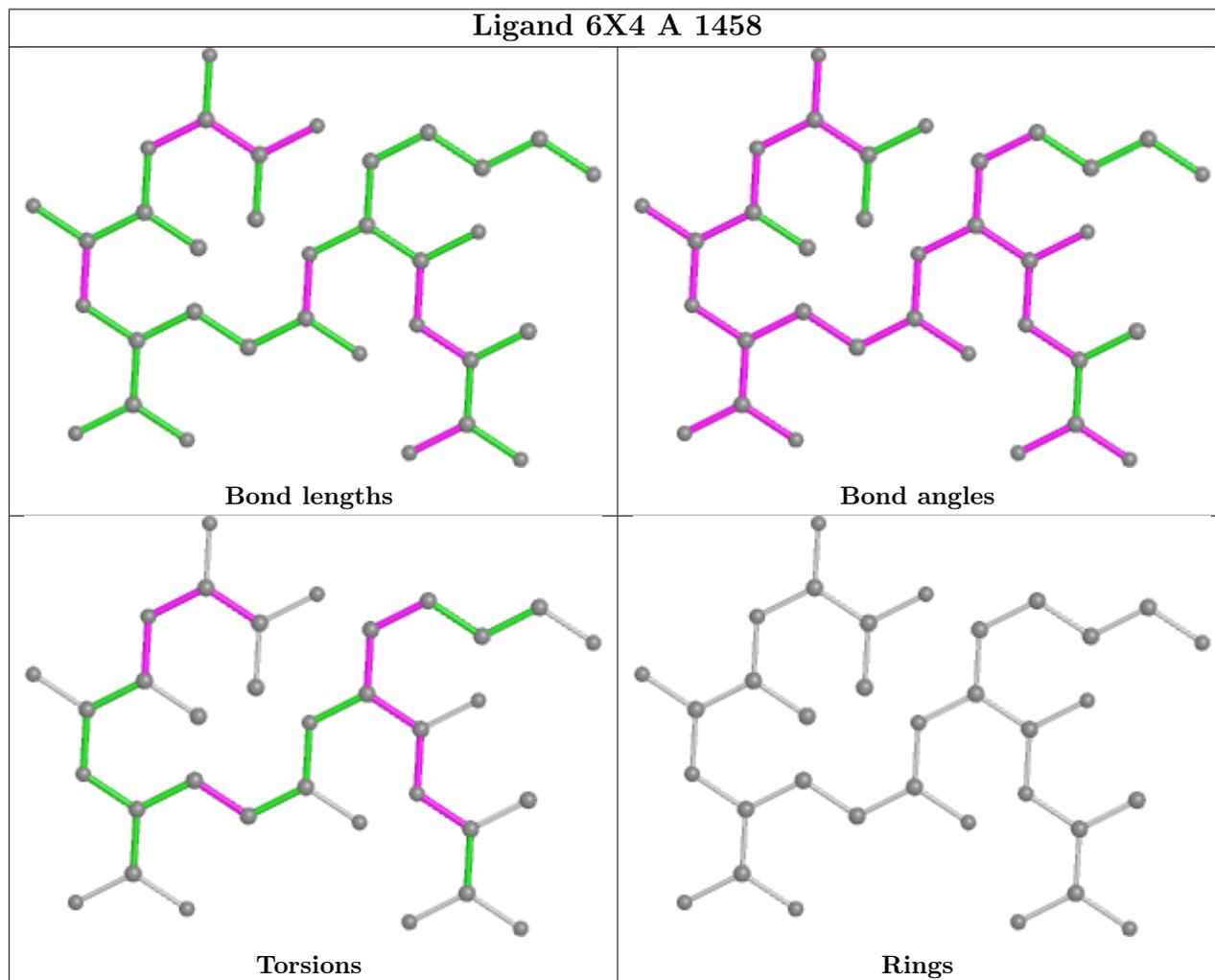
There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1458	6X4	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	418/451 (92%)	-0.08	2 (0%) 91 89	37, 55, 90, 148	0
1	C	413/451 (91%)	-0.04	5 (1%) 79 77	40, 67, 100, 148	0
2	B	417/451 (92%)	0.00	7 (1%) 70 68	40, 63, 96, 186	0
2	D	417/451 (92%)	0.21	13 (3%) 49 47	56, 80, 109, 128	0
All	All	1665/1804 (92%)	0.02	27 (1%) 72 70	37, 68, 102, 186	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	270	ASP	8.0
2	B	271	VAL	7.0
2	B	269	VAL	5.7
1	A	254	LYS	3.6
2	B	272	LEU	3.4

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](#)

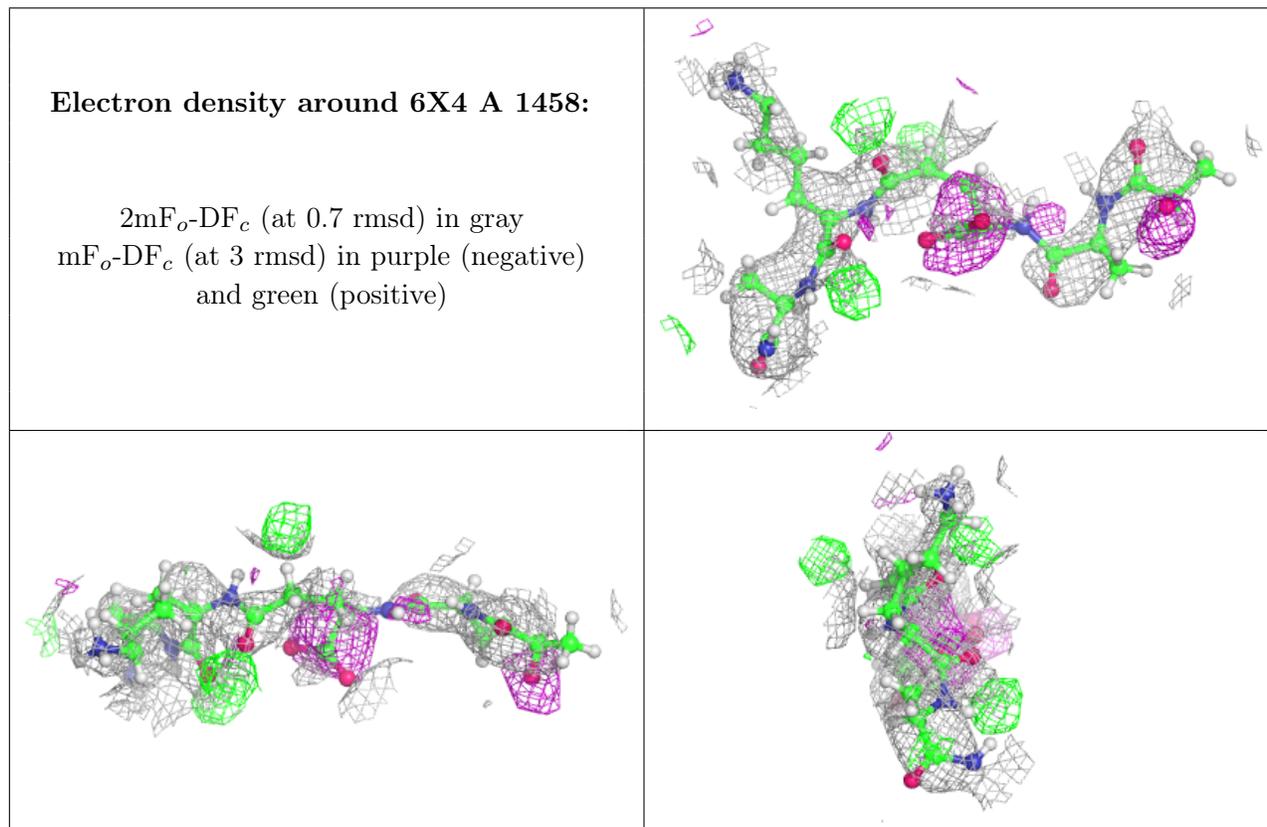
There are no monosaccharides in this entry.

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, 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(\AA^2)	Q<0.9
3	6X4	A	1458	34/34	0.77	0.44	56,77,94,104	67

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.