



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 6, 2016 – 08:02 AM EDT

PDB ID : 4Z38
Title : Crystal structure of enoyl reductase domain of MlnA from the macrolactin biosynthesis cluster from *Bacillus amyloliquefaciens*
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Deposited on : 2015-03-31
Resolution : 2.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

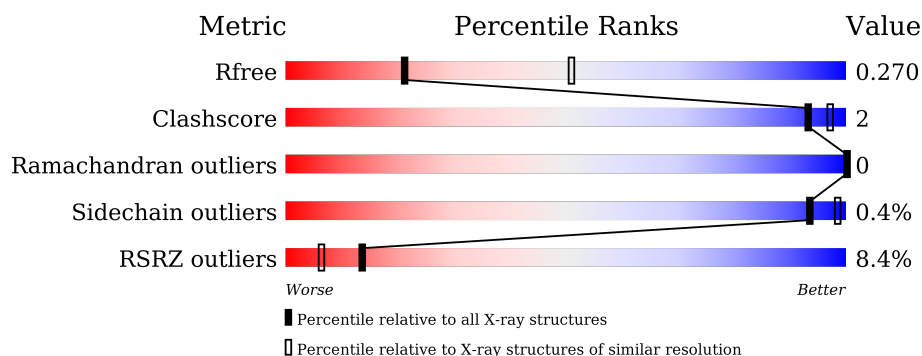
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	470	<div> <div>11%</div> <div>89%</div> <div>7%</div> </div>
1	B	470	<div> <div>5%</div> <div>90%</div> <div>7%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 14180 atoms, of which 7021 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.

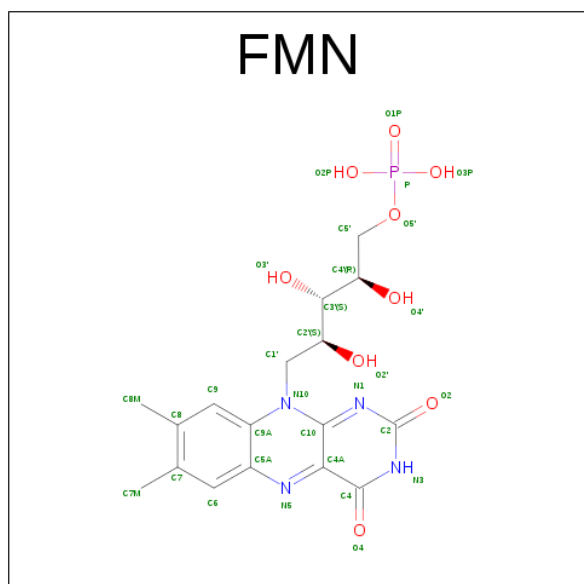
- Molecule 1 is a protein called MlnA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	437	Total	C	H	N	O	S	0	0	0
			6986	2222	3497	597	650	20			
1	B	439	Total	C	H	N	O	S	0	0	0
			7001	2224	3506	599	652	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	299	SER	-	expression tag	UNP A7Z470
A	300	MET	-	expression tag	UNP A7Z470
B	299	SER	-	expression tag	UNP A7Z470
B	300	MET	-	expression tag	UNP A7Z470

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			40	17	9	4	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			40	17	9	4	9	1		

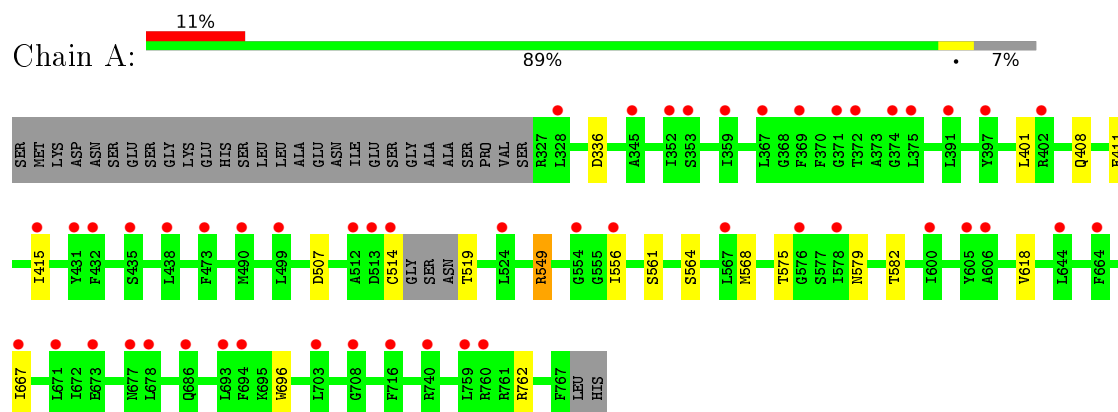
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	43	Total	O	0	0
			43	43		
3	B	70	Total	O	0	0
			70	70		

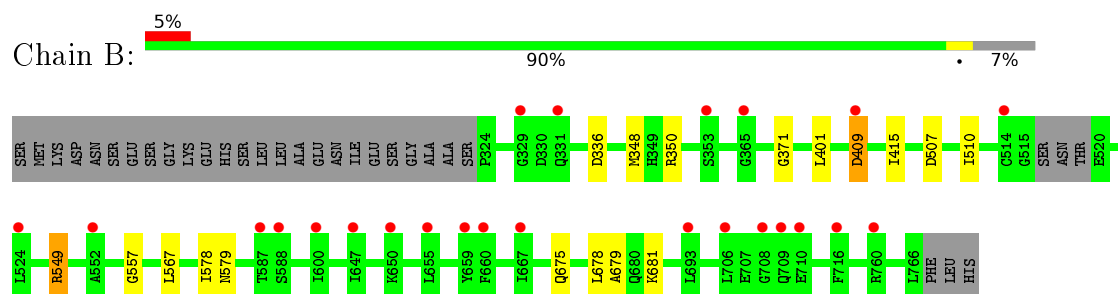
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MlnA



• Molecule 1: MlnA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.17Å 104.67Å 216.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.05 – 2.80 108.05 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (108.05-2.80) 99.7 (108.05-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.246 , 0.263 0.259 , 0.270	Depositor DCC
R_{free} test set	1213 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	79.6	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 98.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 23587 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14180	wwPDB-VP
Average B, all atoms (Å ²)	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3558	0.59	0/4788
1	B	0.42	0/3564	0.62	1/4796 (0.0%)
All	All	0.43	0/7122	0.60	1/9584 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	409	ASP	CB-CG-OD2	5.26	123.03	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3489	3497	3497	15	0
1	B	3495	3506	3506	12	2
2	A	31	9	19	0	0
2	B	31	9	19	0	0
3	A	43	0	0	0	0
3	B	70	0	0	0	0
All	All	7159	7021	7041	26	2

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 2.

All (26) 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:507:ASP:OD1	1:A:549:ARG:HD3	1.83	0.78
1:B:348:MET:HE1	1:B:579:ASN:HB2	1.69	0.72
1:A:514:CYS:HG	1:A:519:THR:N	1.86	0.71
1:A:564:SER:O	1:A:568:MET:HG3	2.05	0.57
1:B:348:MET:O	1:B:371:GLY:HA3	2.05	0.56
1:A:762:ARG:NH1	1:B:567:LEU:O	2.40	0.54
1:A:667:ILE:HD11	1:A:696:TRP:CD1	2.43	0.54
1:B:336:ASP:OD2	1:B:549:ARG:NH2	2.43	0.52
1:A:336:ASP:OD2	1:A:549:ARG:NH2	2.40	0.51
1:B:350:ARG:HG2	1:B:350:ARG:HH11	1.74	0.50
1:B:675:GLN:O	1:B:678:LEU:HG	2.14	0.48
1:A:667:ILE:HD11	1:A:696:TRP:NE1	2.29	0.47
1:A:575:THR:O	1:A:579:ASN:OD1	2.34	0.46
1:A:579:ASN:O	1:A:582:THR:HG22	2.16	0.45
1:B:678:LEU:HD12	1:B:679:ALA:N	2.32	0.45
1:B:557:GLY:HA2	1:B:578:ILE:HD11	1.98	0.44
1:A:408:GLN:NE2	1:A:411:GLU:OE1	2.52	0.43
1:B:507:ASP:OD1	1:B:549:ARG:HD3	2.17	0.43
1:A:519:THR:HG22	1:A:618:VAL:HG23	2.00	0.43
1:B:401:LEU:HD21	1:B:415:ILE:HD11	2.02	0.42
1:A:401:LEU:HD21	1:A:415:ILE:HD11	2.02	0.41
1:A:401:LEU:CD2	1:A:415:ILE:HD11	2.50	0.41
1:B:348:MET:CE	1:B:579:ASN:HB2	2.44	0.41
1:A:549:ARG:CD	1:A:549:ARG:N	2.84	0.41
1:B:401:LEU:CD2	1:B:415:ILE:HD11	2.50	0.41
1:A:556:ILE:HA	1:A:561:SER:HB3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:ASP:OD1	1:B:681:LYS:HZ2[3_455]	1.32	0.28
1:B:409:ASP:OD1	1:B:681:LYS:NZ[3_455]	2.09	0.11

5.3 Torsion angles

5.3.1 Protein backbone

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	433/470 (92%)	421 (97%)	12 (3%)	0	100	100
1	B	435/470 (93%)	414 (95%)	21 (5%)	0	100	100
All	All	868/940 (92%)	835 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	374/401 (93%)	373 (100%)	1 (0%)	94	99
1	B	375/401 (94%)	373 (100%)	2 (0%)	92	98
All	All	749/802 (93%)	746 (100%)	3 (0%)	93	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	549	ARG
1	B	510	ILE
1	B	549	ARG

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

Mol	Chain	Res	Type
1	A	408	GLN
1	A	729	HIS
1	B	580	GLN
1	B	719	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	FMN	A	900	-	31,33,33	1.27	4 (12%)	32,50,50	1.52	2 (6%)
2	FMN	B	900	-	31,33,33	1.20	4 (12%)	32,50,50	1.59	3 (9%)

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	FMN	A	900	-	-	0/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FMN	B	900	-	-	0/18/18/18	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	FMN	C9A-N10	2.54	1.42	1.38
2	B	900	FMN	C4A-C10	2.55	1.45	1.40
2	B	900	FMN	C5A-N5	2.57	1.39	1.35
2	A	900	FMN	C9A-N10	3.00	1.43	1.38
2	A	900	FMN	C5A-N5	3.02	1.40	1.35
2	A	900	FMN	C4A-C10	3.03	1.46	1.40
2	A	900	FMN	C4-C4A	3.06	1.46	1.40
2	B	900	FMN	C4-C4A	3.63	1.47	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	FMN	C4A-C10-N10	-4.95	116.92	120.52
2	A	900	FMN	C4A-C10-N10	-4.80	117.03	120.52
2	B	900	FMN	O2P-P-O1P	2.04	117.27	110.63
2	A	900	FMN	C2-N1-C10	5.94	118.46	113.39
2	B	900	FMN	C2-N1-C10	6.11	118.60	113.39

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	437/470 (92%)	0.80	50 (11%) 7 3	80, 114, 208, 246	0
1	B	439/470 (93%)	0.58	24 (5%) 29 18	57, 100, 219, 245	0
All	All	876/940 (93%)	0.69	74 (8%) 14 6	57, 108, 213, 246	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	708	GLY	12.0
1	A	499	LEU	4.2
1	A	353	SER	4.1
1	B	709	GLN	4.1
1	A	513	ASP	4.0
1	B	710	GLU	3.8
1	A	760	ARG	3.8
1	A	372	THR	3.7
1	A	367	LEU	3.7
1	A	391	LEU	3.7
1	B	600	ILE	3.7
1	B	659	TYR	3.6
1	A	397	TYR	3.5
1	A	490	MET	3.5
1	A	371	GLY	3.5
1	A	708	GLY	3.5
1	A	352	ILE	3.5
1	B	655	LEU	3.4
1	B	587	THR	3.2
1	B	514	CYS	3.2
1	A	673	GLU	3.2
1	A	671	LEU	3.1
1	B	660	PHE	3.1
1	A	693	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	759	LEU	3.1
1	B	331	GLN	3.1
1	A	716	PHE	3.0
1	A	576	GLY	3.0
1	B	650	LYS	3.0
1	B	667	ILE	3.0
1	A	667	ILE	2.9
1	A	438	LEU	2.9
1	A	328	LEU	2.8
1	B	693	LEU	2.8
1	A	514	CYS	2.7
1	A	686	GLN	2.7
1	A	431	TYR	2.7
1	A	512	ALA	2.7
1	B	716	PHE	2.7
1	A	435	SER	2.6
1	A	402	ARG	2.6
1	A	567	LEU	2.5
1	B	760	ARG	2.5
1	A	359	ILE	2.5
1	A	369	PHE	2.4
1	A	345	ALA	2.4
1	A	677	ASN	2.4
1	B	329	GLY	2.4
1	A	600	ILE	2.4
1	A	524	LEU	2.4
1	A	605	TYR	2.4
1	B	409	ASP	2.3
1	A	375	LEU	2.3
1	A	740	ARG	2.3
1	A	606	ALA	2.3
1	B	588	SER	2.3
1	A	678	LEU	2.3
1	B	353	SER	2.3
1	B	552	ALA	2.3
1	A	374	GLY	2.3
1	A	415	ILE	2.2
1	A	644	LEU	2.2
1	B	706	LEU	2.2
1	B	647	ILE	2.2
1	A	578	ILE	2.2
1	B	524	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	556	ILE	2.2
1	A	703	LEU	2.1
1	B	365	GLY	2.1
1	A	432	PHE	2.1
1	A	473	PHE	2.1
1	A	664	PHE	2.1
1	A	554	GLY	2.0
1	A	694	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FMN	B	900	31/31	0.97	0.27	0.78	59,64,76,76	0
2	FMN	A	900	31/31	0.93	0.28	-0.07	99,120,131,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.