



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2021 – 06:15 PM JST

PDB ID : 6M48  
Title : Crystal structure of pilus adhesin, SpaC from *Lactobacillus rhamnosus* GG - P21212 form  
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Deposited on : 2020-03-05  
Resolution : 2.50 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](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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
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)	:	2.23.1

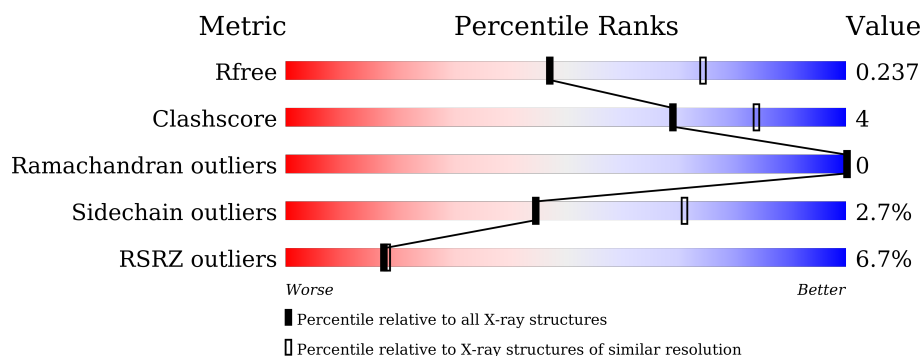
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	836	
1	B	836	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12506 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 SpaC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	813	Total	C	N	O	S	0	0	0
			6118	3803	1041	1261	13			
1	B	812	Total	C	N	O	S	0	0	0
			6081	3779	1045	1244	13			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	MET	-	initiating methionine	UNP A0A1Y0DVK9
A	?	GLY	-	expression tag	UNP A0A1Y0DVK9
A	?	ARG	-	expression tag	UNP A0A1Y0DVK9
A	?	ASP	-	expression tag	UNP A0A1Y0DVK9
A	?	PRO	-	expression tag	UNP A0A1Y0DVK9
A	?	ASN	-	expression tag	UNP A0A1Y0DVK9
A	?	SER	-	expression tag	UNP A0A1Y0DVK9
A	?	LEU	-	expression tag	UNP A0A1Y0DVK9
A	?	GLU	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
A	?	HIS	-	expression tag	UNP A0A1Y0DVK9
B	?	MET	-	initiating methionine	UNP A0A1Y0DVK9
B	?	GLY	-	expression tag	UNP A0A1Y0DVK9
B	?	ARG	-	expression tag	UNP A0A1Y0DVK9
B	?	ASP	-	expression tag	UNP A0A1Y0DVK9
B	?	PRO	-	expression tag	UNP A0A1Y0DVK9
B	?	ASN	-	expression tag	UNP A0A1Y0DVK9
B	?	SER	-	expression tag	UNP A0A1Y0DVK9
B	?	LEU	-	expression tag	UNP A0A1Y0DVK9
B	?	GLU	-	expression tag	UNP A0A1Y0DVK9
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9
B	?	HIS	-	expression tag	UNP A0A1Y0DVK9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0

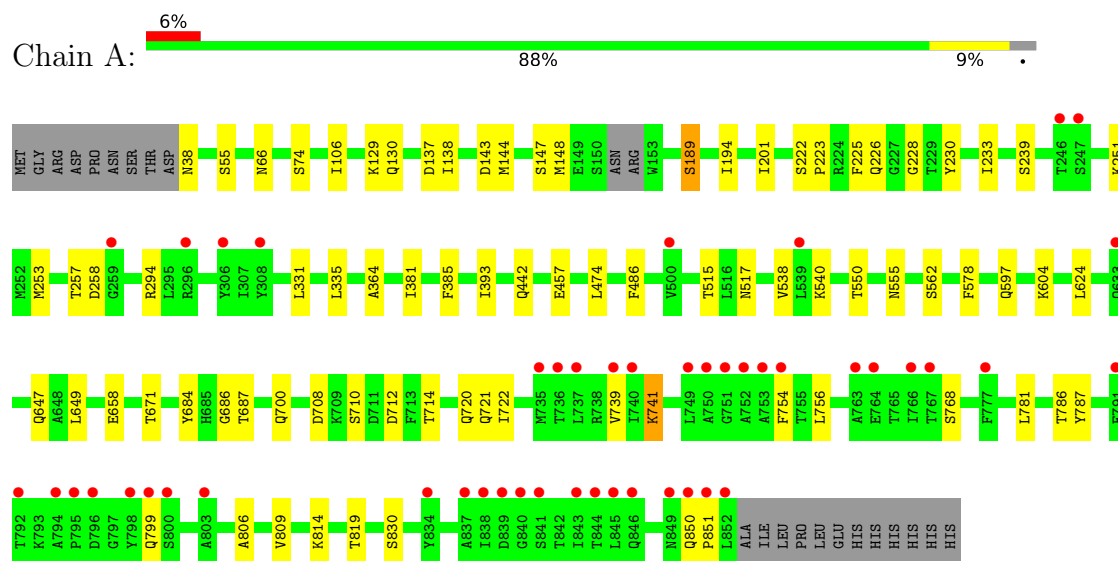
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	177	Total O 177 177	0	0
4	B	126	Total O 126 126	0	0

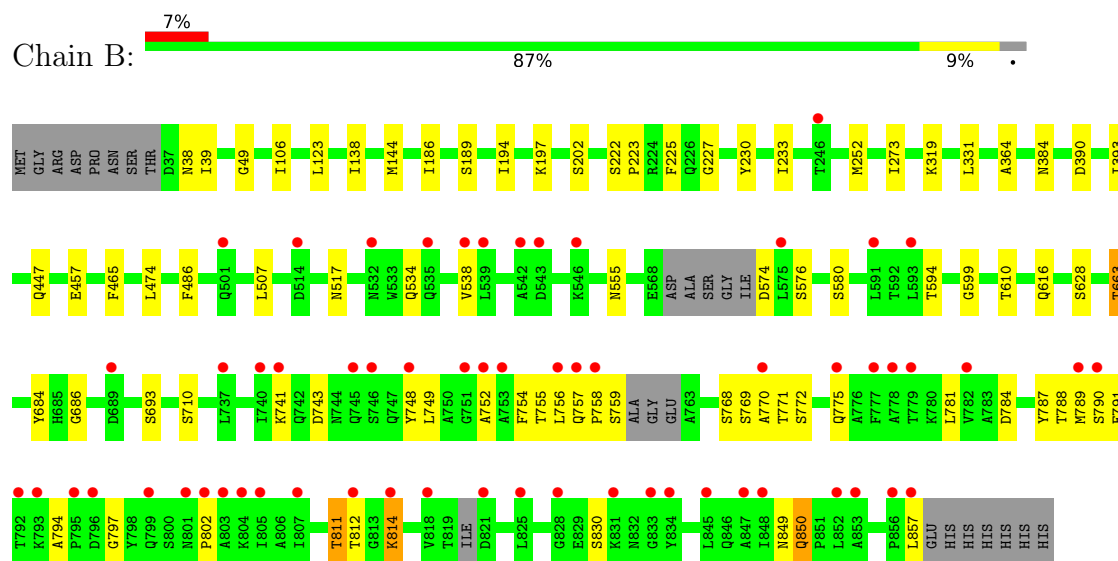
### 3 Residue-property plots [i](#)

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: SpaC



#### • Molecule 1: SpaC



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.18Å 128.13Å 136.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.26 – 2.50 44.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.26-2.50) 99.7 (44.22-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.192 , 0.235 0.195 , 0.237	Depositor DCC
$R_{free}$ test set	3635 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.4	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 36.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12506	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% 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

### 5.1 Standard geometry

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

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	0.77	0/6236	0.91	0/8500
1	B	0.76	0/6198	0.92	0/8450
All	All	0.77	0/12434	0.91	0/16950

There are no bond length outliers.

There are no bond angle outliers.

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	6118	0	5777	41	0
1	B	6081	0	5711	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
4	A	177	0	0	0	0
4	B	126	0	0	0	0
All	All	12506	0	11488	88	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 (88) 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:B:756:LEU:HA	1:B:789:MET:HA	1.47	0.96
1:A:258:ASP:O	1:A:335:LEU:HD12	1.78	0.83
1:A:799:GLN:NE2	1:A:851:PRO:O	2.26	0.69
1:B:789:MET:HG2	1:B:790:SER:N	2.09	0.68
1:A:258:ASP:O	1:A:335:LEU:CD1	2.41	0.67
1:B:756:LEU:CB	1:B:789:MET:HB2	2.26	0.65
1:A:130:GLN:HG3	1:A:385:PHE:O	1.96	0.64
1:B:755:THR:C	1:B:789:MET:HG3	2.18	0.63
1:B:784:ASP:OD1	1:B:811:THR:HA	2.00	0.61
1:B:755:THR:O	1:B:789:MET:HG3	2.00	0.61
1:A:604:LYS:HE2	1:A:658:GLU:OE2	2.03	0.58
1:B:743:ASP:HB3	1:B:749:LEU:HD21	1.86	0.57
1:B:748:TYR:CB	1:B:770:ALA:HA	2.35	0.57
1:B:743:ASP:HA	1:B:849:ASN:O	2.05	0.56
1:A:739:VAL:HG11	1:A:754:PHE:CE2	2.42	0.55
1:B:812:THR:HB	1:B:814:LYS:HD2	1.88	0.54
1:B:189:SER:HB3	1:B:194:ILE:HB	1.90	0.53
1:B:769:SER:CB	1:B:771:THR:HG22	2.40	0.53
1:B:144:MET:HA	1:B:225:PHE:CD2	2.45	0.52
1:B:794:ALA:HB3	1:B:797:GLY:HA2	1.91	0.52
1:A:578:PHE:CE2	1:A:597:GLN:HB2	2.45	0.51
1:A:781:LEU:HB3	1:A:809:VAL:HG21	1.92	0.51
1:B:616:GLN:HA	1:B:663:THR:HG23	1.92	0.51
1:A:194:ILE:HG23	1:A:201:ILE:HG23	1.93	0.51
1:B:138:ILE:HD13	1:B:252:MET:HE3	1.91	0.51
1:A:144:MET:HA	1:A:225:PHE:CD2	2.46	0.51
1:B:781:LEU:HD12	1:B:781:LEU:N	2.25	0.51
1:B:791:GLU:O	1:B:802:PRO:HB3	2.12	0.50
1:A:624:LEU:HD23	1:A:647:GLN:NE2	2.27	0.49
1:B:189:SER:OG	1:B:227:GLY:HA3	2.13	0.49
1:A:700:GLN:CG	1:A:714:THR:HG22	2.43	0.49
1:A:515:THR:HG22	1:A:540:LYS:HG2	1.95	0.49
1:A:138:ILE:HD11	1:A:381:ILE:HD13	1.95	0.48
1:A:239:SER:N	1:A:253:MET:HE1	2.28	0.48
1:B:757:GLN:N	1:B:788:THR:O	2.42	0.48
1:B:752:ALA:HB3	1:B:768:SER:CB	2.44	0.47
1:B:273:ILE:CD1	1:B:319:LYS:HE2	2.44	0.47
1:A:756:LEU:HD11	1:A:787:TYR:HB3	1.97	0.47
1:B:331:LEU:HD11	1:B:364:ALA:HB2	1.97	0.46
1:A:806:ALA:HB3	1:A:819:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:GLU:OE2	1:B:555:ASN:HB2	2.16	0.46
1:A:624:LEU:HD21	1:A:649:LEU:HD21	1.97	0.46
1:B:748:TYR:HB3	1:B:770:ALA:HA	1.97	0.46
1:B:769:SER:HB3	1:B:771:THR:HG22	1.98	0.46
1:B:222:SER:N	1:B:223:PRO:CD	2.78	0.46
1:A:137:ASP:HB2	1:A:251:LYS:HD3	1.97	0.45
1:B:580:SER:HA	1:B:594:THR:O	2.16	0.45
1:B:769:SER:HB2	1:B:771:THR:HG22	1.99	0.45
1:B:230:TYR:O	1:B:233:ILE:HG22	2.16	0.45
1:A:138:ILE:CD1	1:A:381:ILE:HD13	2.46	0.44
1:A:393:ILE:HA	1:A:474:LEU:O	2.18	0.44
1:B:138:ILE:CD1	1:B:252:MET:HE3	2.48	0.44
1:B:393:ILE:HA	1:B:474:LEU:O	2.17	0.44
1:B:789:MET:CG	1:B:790:SER:N	2.80	0.44
1:A:721:GLN:HG2	1:A:722:ILE:HG13	1.99	0.44
1:B:517:ASN:OD1	1:B:538:VAL:HG22	2.18	0.43
1:A:106:ILE:HB	1:A:486:PHE:CE2	2.53	0.43
1:A:457:GLU:OE2	1:A:555:ASN:HB2	2.18	0.43
1:A:230:TYR:O	1:A:233:ILE:HG22	2.18	0.43
1:A:799:GLN:HG2	1:A:850:GLN:O	2.19	0.43
1:B:754:PHE:HA	1:B:791:GLU:HA	2.00	0.43
1:B:758:PRO:HA	1:B:787:TYR:CD2	2.54	0.43
1:A:517:ASN:OD1	1:A:538:VAL:HG22	2.18	0.43
1:B:106:ILE:HB	1:B:486:PHE:CE2	2.54	0.43
1:B:756:LEU:HA	1:B:788:THR:O	2.19	0.43
1:A:55:SER:HA	1:A:66:ASN:O	2.19	0.43
1:A:194:ILE:CG2	1:A:201:ILE:HG23	2.49	0.43
1:A:189:SER:HB2	1:A:194:ILE:HD12	2.01	0.42
1:B:574:ASP:OD1	1:B:576:SER:HB3	2.18	0.42
1:A:147:SER:OG	1:A:258:ASP:OD2	2.37	0.42
1:B:186:ILE:HD13	1:B:202:SER:HB3	2.02	0.42
1:A:143:ASP:HB3	1:A:257:THR:HA	2.01	0.42
1:A:129:LYS:HE3	1:A:442:GLN:OE1	2.19	0.42
1:A:222:SER:N	1:A:223:PRO:CD	2.82	0.42
1:A:700:GLN:HG2	1:A:714:THR:HG22	2.01	0.42
1:A:684:TYR:CZ	1:A:686:GLY:HA2	2.53	0.42
1:A:671:THR:O	1:A:687:THR:HA	2.20	0.42
1:B:507:LEU:HD13	1:B:599:GLY:HA3	2.01	0.41
1:A:331:LEU:HD11	1:A:364:ALA:HB2	2.02	0.41
1:A:700:GLN:HG3	1:A:714:THR:HG22	2.01	0.41
1:A:741:LYS:HB2	1:A:768:SER:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:TYR:CZ	1:B:686:GLY:HA2	2.55	0.41
1:B:756:LEU:HA	1:B:789:MET:CA	2.33	0.41
1:B:748:TYR:HB2	1:B:770:ALA:C	2.40	0.41
1:B:850:GLN:H	1:B:850:GLN:HG2	1.56	0.40
1:A:228:GLY:HA2	1:B:857:LEU:O	2.21	0.40
1:B:49:GLY:HA2	1:B:465:PHE:CZ	2.56	0.40
1:B:123:LEU:O	1:B:447:GLN:HA	2.22	0.40

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	809/836 (97%)	784 (97%)	25 (3%)	0	100	100
1	B	804/836 (96%)	773 (96%)	31 (4%)	0	100	100
All	All	1613/1672 (96%)	1557 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	648/693 (94%)	632 (98%)	16 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	636/693 (92%)	617 (97%)	19 (3%)	41 68
All	All	1284/1386 (93%)	1249 (97%)	35 (3%)	44 71

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	74	SER
1	A	148	MET
1	A	189	SER
1	A	226	GLN
1	A	294	ARG
1	A	550	THR
1	A	562	SER
1	A	708	ASP
1	A	710	SER
1	A	712	ASP
1	A	720	GLN
1	A	741	LYS
1	A	786	THR
1	A	814	LYS
1	A	830	SER
1	B	38	ASN
1	B	39	ILE
1	B	197	LYS
1	B	384	ASN
1	B	390	ASP
1	B	534	GLN
1	B	610	THR
1	B	628	SER
1	B	663	THR
1	B	693	SER
1	B	710	SER
1	B	741	LYS
1	B	759	SER
1	B	772	SER
1	B	775	GLN
1	B	811	THR
1	B	814	LYS
1	B	830	SER
1	B	850	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

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, 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	813/836 (97%)	0.25	48 (5%)	22 23	29, 57, 105, 162	0
1	B	812/836 (97%)	0.33	61 (7%)	14 14	29, 56, 132, 182	0
All	All	1625/1672 (97%)	0.29	109 (6%)	17 18	29, 56, 116, 182	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	PRO	9.0
1	A	800	SER	8.0
1	A	852	LEU	7.3
1	B	803	ALA	6.8
1	B	825	LEU	6.8
1	B	853	ALA	6.6
1	B	802	PRO	6.1
1	A	792	THR	6.1
1	B	804	LYS	6.0
1	B	792	THR	5.5
1	A	766	ILE	5.4
1	B	751	GLY	5.4
1	B	789	MET	5.3
1	A	752	ALA	5.2
1	B	833	GLY	5.1
1	B	779	THR	5.1
1	A	791	GLU	5.0
1	A	850	GLN	4.8
1	B	777	PHE	4.6
1	A	840	GLY	4.6
1	B	778	ALA	4.3
1	A	851	PRO	4.3
1	A	296	ARG	4.3
1	A	798	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	746	SER	4.1
1	A	794	ALA	4.0
1	B	532	ASN	3.9
1	A	837	ALA	3.9
1	B	805	ILE	3.9
1	B	796	ASP	3.8
1	B	790	SER	3.7
1	A	838	ILE	3.7
1	B	793	LYS	3.7
1	A	737	LEU	3.6
1	A	799	GLN	3.6
1	B	795	PRO	3.5
1	A	754	PHE	3.5
1	B	740	ILE	3.5
1	B	745	GLN	3.5
1	A	753	ALA	3.4
1	B	752	ALA	3.4
1	A	796	ASP	3.4
1	B	818	VAL	3.3
1	B	246	THR	3.2
1	B	848	ILE	3.2
1	B	757	GLN	3.2
1	B	737	LEU	3.2
1	A	767	THR	3.1
1	A	843	ILE	3.1
1	B	775	GLN	3.0
1	B	828	GLY	3.0
1	A	846	GLN	2.9
1	A	777	PHE	2.9
1	B	543	ASP	2.9
1	A	246	THR	2.9
1	A	803	ALA	2.8
1	B	845	LEU	2.8
1	B	801	ASN	2.8
1	B	542	ALA	2.8
1	A	841	SER	2.8
1	B	575	LEU	2.7
1	B	799	GLN	2.7
1	B	689	ASP	2.7
1	A	750	ALA	2.6
1	A	845	LEU	2.6
1	B	834	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	821	ASP	2.6
1	A	259	GLY	2.6
1	A	739	VAL	2.5
1	B	514	ASP	2.5
1	A	844	THR	2.5
1	B	546	LYS	2.5
1	B	591	LEU	2.5
1	B	847	ALA	2.4
1	B	770	ALA	2.4
1	A	736	THR	2.4
1	A	539	LEU	2.4
1	B	753	ALA	2.3
1	B	852	LEU	2.3
1	B	807	ILE	2.3
1	B	812	THR	2.2
1	A	500	VAL	2.2
1	B	756	LEU	2.2
1	A	849	ASN	2.2
1	A	308	TYR	2.2
1	B	748	TYR	2.2
1	A	749	LEU	2.2
1	A	839	ASP	2.2
1	B	538	VAL	2.2
1	B	782	VAL	2.2
1	B	501	GLN	2.2
1	A	751	GLY	2.2
1	B	856	PRO	2.2
1	B	535	GLN	2.2
1	B	758	PRO	2.2
1	B	741	LYS	2.1
1	A	735	MET	2.1
1	A	740	ILE	2.1
1	A	306	TYR	2.1
1	A	764	GLU	2.1
1	B	539	LEU	2.1
1	A	763	ALA	2.1
1	B	831	LYS	2.1
1	B	857	LEU	2.1
1	A	633	GLN	2.1
1	A	834	TYR	2.0
1	B	814	LYS	2.0
1	B	593	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	247	SER	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 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.

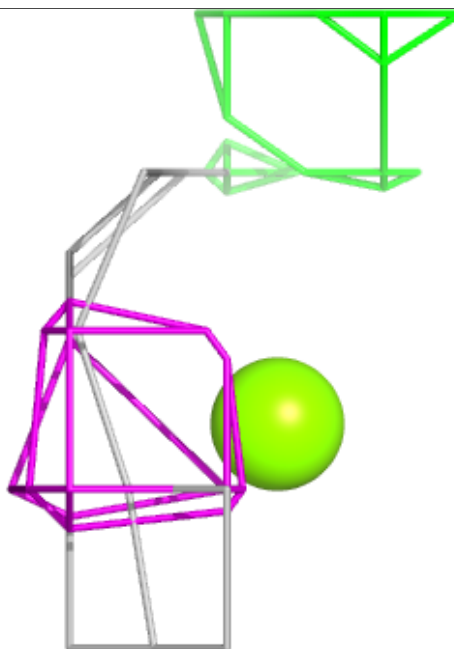
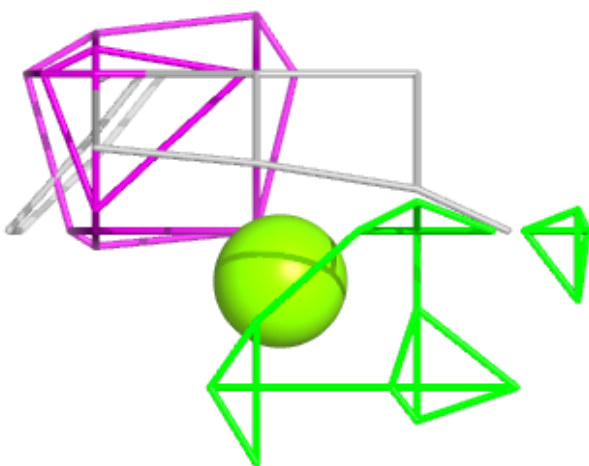
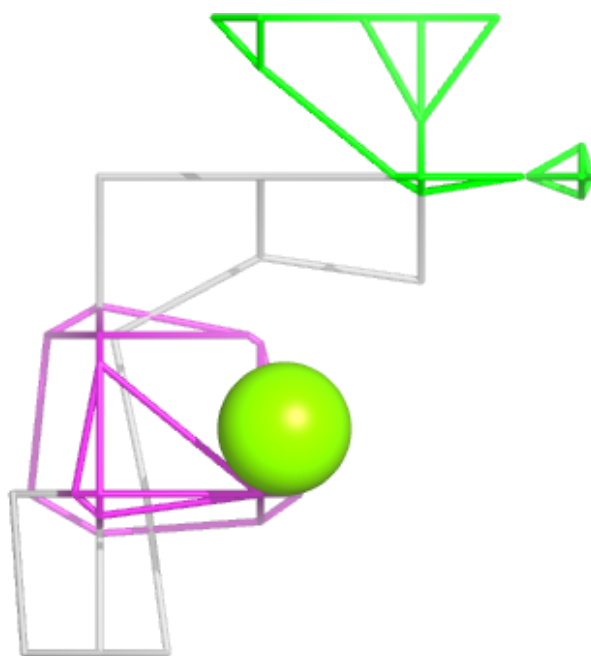
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	A	901	1/1	0.78	0.10	69,69,69,69	0
3	CL	A	903	1/1	0.88	0.15	85,85,85,85	0
3	CL	A	902	1/1	0.95	0.11	67,67,67,67	0
2	MG	B	901	1/1	0.98	0.09	40,40,40,40	0

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.



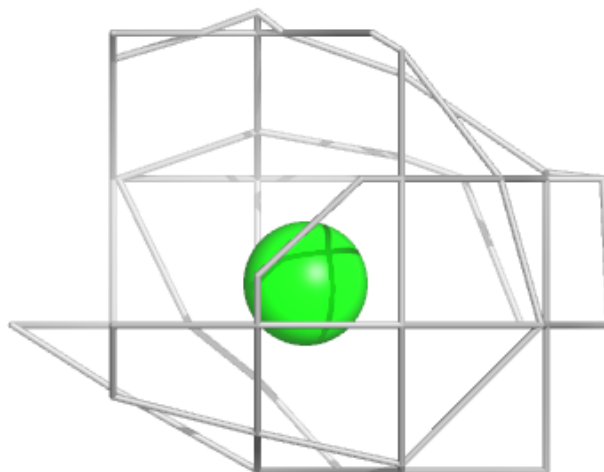
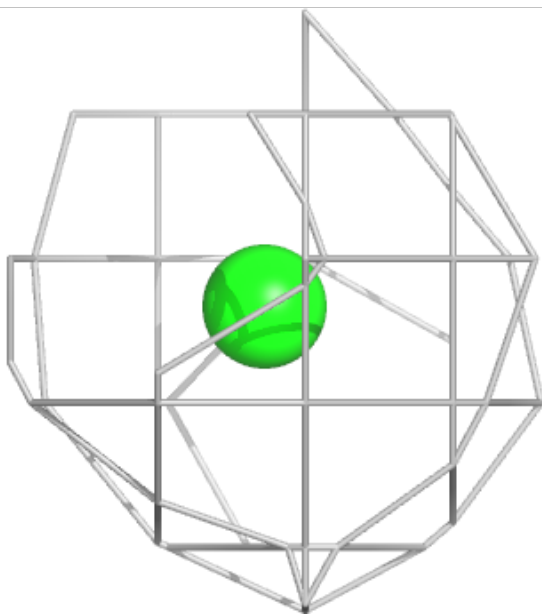
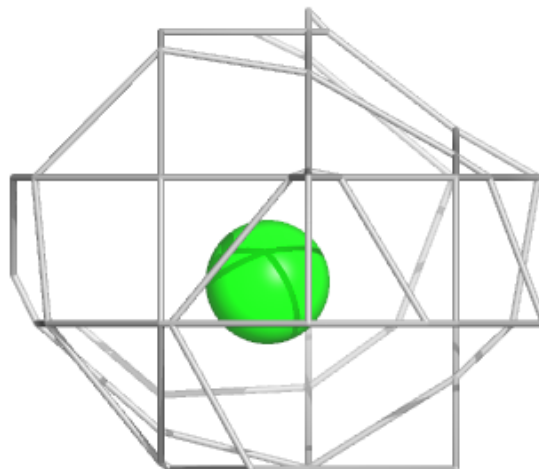
**Electron density around MG A 901:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



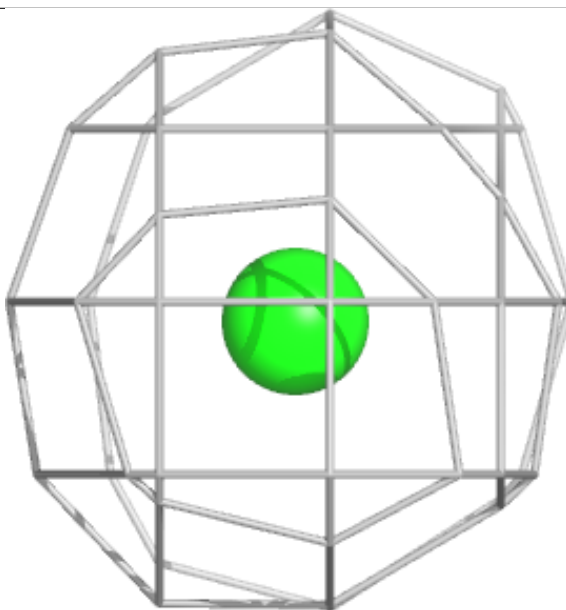
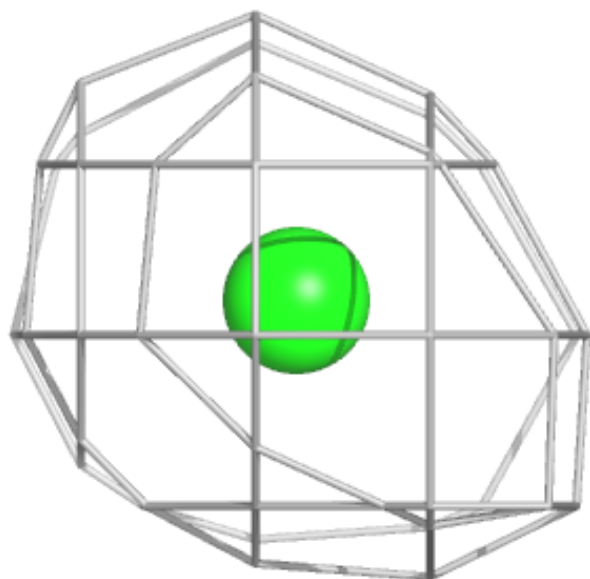
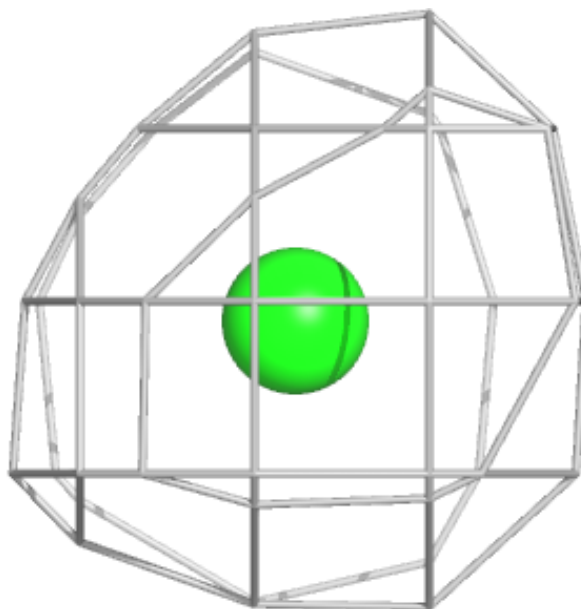
**Electron density around CL A 903:**

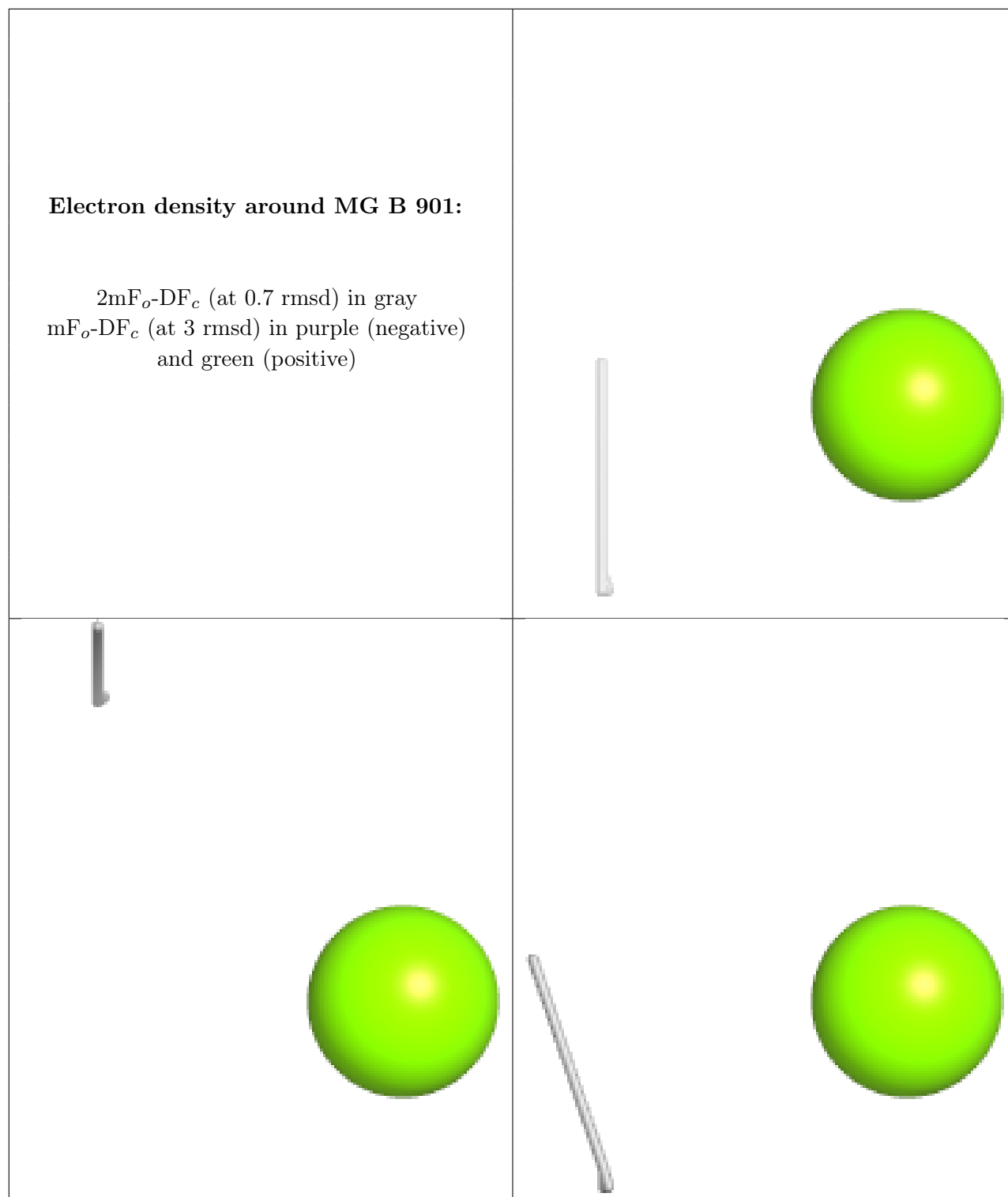
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around CL A 902:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.