



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:19 AM UTC

PDB ID : 7DOL / pdb_00007dol
Title : Mycoplasma genitalium RNase R in complex with double-stranded RNA
Authors : Abula, A.; Quan, X.; Li, X.; Yang, T.; Li, T.; Chen, Q.; Ji, X.
Deposited on : 2020-12-14
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 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

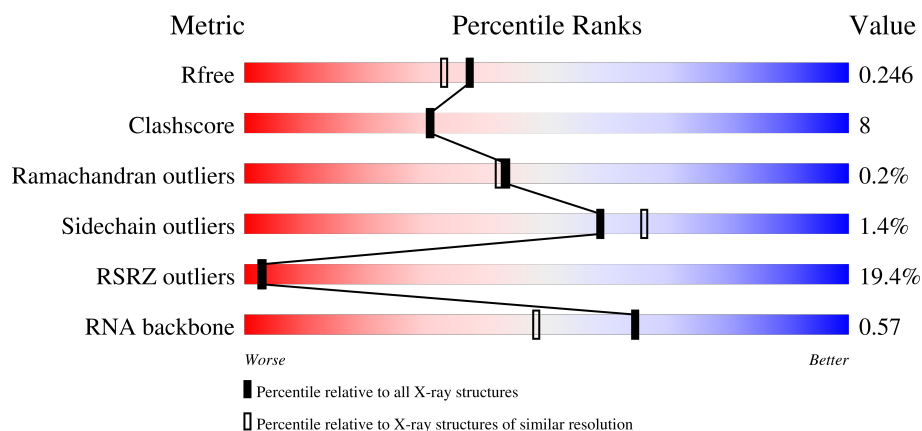
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)
RNA backbone	3983	1000 (2.36-1.64)

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	747	15% 62% 13% 24%
2	C	6	33% 67%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4914 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 Ribonuclease R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4546	2901	765	866	14			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P47350
A	-20	GLY	-	expression tag	UNP P47350
A	-19	HIS	-	expression tag	UNP P47350
A	-18	HIS	-	expression tag	UNP P47350
A	-17	HIS	-	expression tag	UNP P47350
A	-16	HIS	-	expression tag	UNP P47350
A	-15	HIS	-	expression tag	UNP P47350
A	-14	HIS	-	expression tag	UNP P47350
A	-13	HIS	-	expression tag	UNP P47350
A	-12	HIS	-	expression tag	UNP P47350
A	-11	HIS	-	expression tag	UNP P47350
A	-10	HIS	-	expression tag	UNP P47350
A	-9	SER	-	expression tag	UNP P47350
A	-8	SER	-	expression tag	UNP P47350
A	-7	GLY	-	expression tag	UNP P47350
A	-6	HIS	-	expression tag	UNP P47350
A	-5	ILE	-	expression tag	UNP P47350
A	-4	ASP	-	expression tag	UNP P47350
A	-3	ASP	-	expression tag	UNP P47350
A	-2	ASP	-	expression tag	UNP P47350
A	-1	ASP	-	expression tag	UNP P47350
A	0	LYS	-	expression tag	UNP P47350
A	284	ALA	ASP	engineered mutation	UNP P47350

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	6	Total	C	N	O	P	0	0	0
			132	60	30	36	6			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

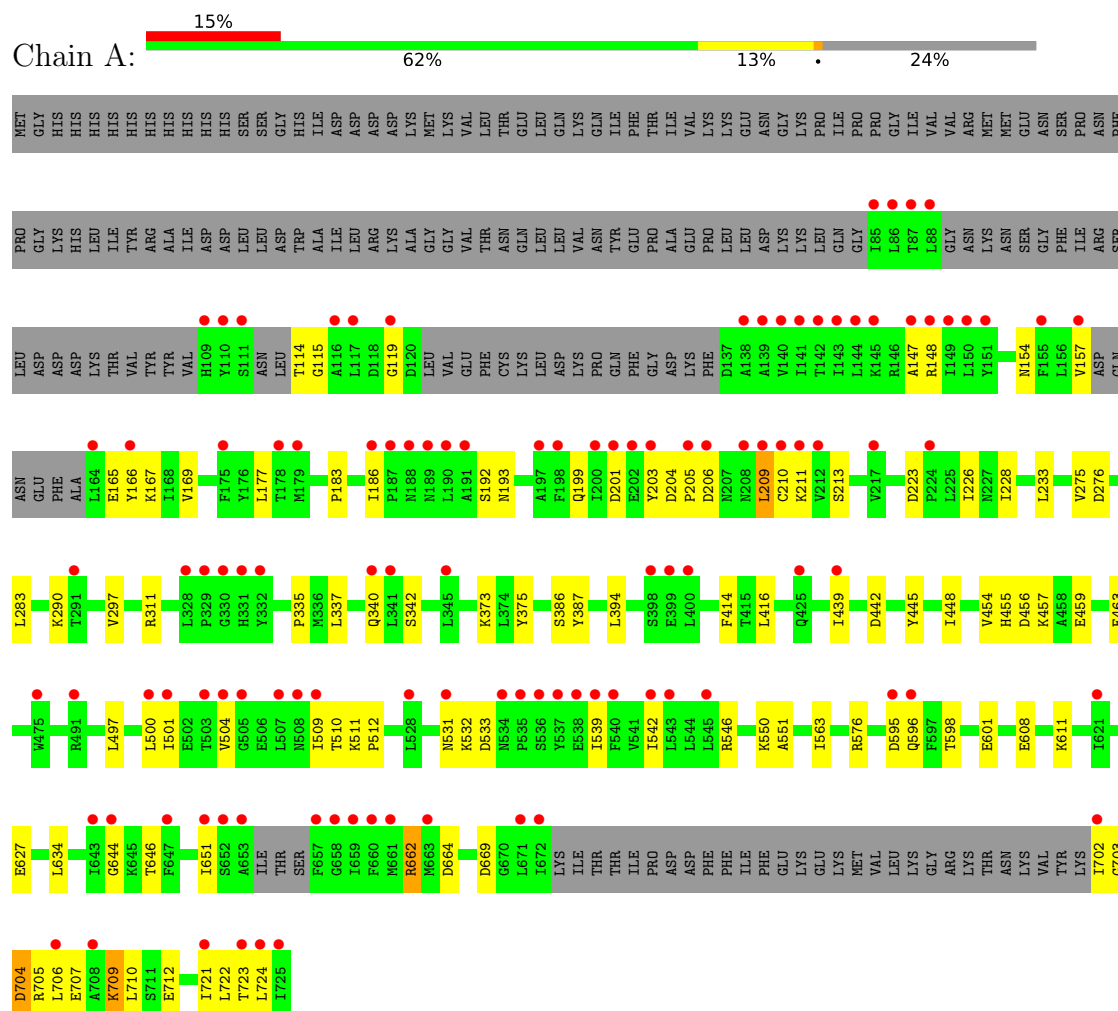
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	C	12	Total	O	0	0
			12	12		

3 Residue-property plots

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: Ribonuclease R



• Molecule 2: RNA (5'-R(P*AP*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.41Å 96.08Å 117.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.29 – 2.00 38.29 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.29-2.00) 94.7 (38.29-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10_2148	Depositor
R, R_{free}	0.220 , 0.242 0.222 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (3.45%)	wwPDB-VP
Wilson B-factor (Å ²)	39.3	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4914	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: 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	0.38	5/4629 (0.1%)	0.65	1/6279 (0.0%)
2	C	0.14	0/149	0.27	0/230
All	All	0.38	5/4778 (0.1%)	0.64	1/6509 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	ARG	NE-CZ	-10.23	1.21	1.33
1	A	662	ARG	CZ-NH1	-10.00	1.18	1.32
1	A	662	ARG	CZ-NH2	-6.23	1.25	1.33
1	A	662	ARG	CD-NE	-5.48	1.38	1.46
1	A	709	LYS	CD-CE	-5.10	1.37	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	PRO	CB-CA-C	5.07	119.08	111.68

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	4546	0	4553	77	0
2	C	132	0	67	5	0
3	A	1	0	0	0	0
4	A	223	0	0	7	0
4	C	12	0	0	0	0
All	All	4914	0	4620	77	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 8.

All (77) 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:595:ASP:OD2	1:A:596:GLN:NE2	1.87	1.06
1:A:201:ASP:HB2	1:A:211:LYS:HE3	1.45	0.96
1:A:706:LEU:HD11	1:A:724:LEU:HD21	1.49	0.91
1:A:456:ASP:OD2	1:A:457:LYS:N	2.12	0.79
1:A:706:LEU:HD11	1:A:724:LEU:CD2	2.12	0.78
1:A:709:LYS:HB3	1:A:723:THR:HG23	1.65	0.77
1:A:201:ASP:HB2	1:A:211:LYS:CE	2.17	0.75
1:A:706:LEU:HD13	1:A:707:GLU:N	2.02	0.74
1:A:563:ILE:HD11	2:C:6:A:H4'	1.69	0.74
1:A:154:ASN:HD21	1:A:193:ASN:HA	1.60	0.67
1:A:627:GLU:OE1	4:A:901:HOH:O	2.12	0.66
1:A:211:LYS:C	1:A:211:LYS:HD2	2.20	0.66
1:A:439:ILE:HD13	1:A:634:LEU:HB3	1.76	0.66
1:A:209:LEU:HD12	1:A:209:LEU:O	1.97	0.64
1:A:595:ASP:CG	1:A:596:GLN:NE2	2.56	0.64
1:A:463:GLU:HG3	2:C:7:A:O4'	1.97	0.64
1:A:311:ARG:NH1	1:A:608:GLU:OE1	2.30	0.61
1:A:442:ASP:HB3	1:A:448:ILE:HD11	1.83	0.60
1:A:710:LEU:HA	1:A:722:LEU:HD23	1.82	0.60
1:A:204:ASP:HB3	1:A:209:LEU:HG	1.84	0.59
1:A:209:LEU:HD12	1:A:209:LEU:C	2.28	0.58
1:A:510:THR:HG23	1:A:531:ASN:HD21	1.69	0.58
1:A:183:PRO:O	1:A:186:ILE:HG12	2.05	0.57
1:A:148:ARG:NH1	4:A:911:HOH:O	2.38	0.57
1:A:199:GLN:NE2	1:A:201:ASP:OD1	2.38	0.56
1:A:651:ILE:HD12	1:A:704:ASP:O	2.06	0.56
1:A:335:PRO:HB2	1:A:337:LEU:O	2.06	0.56
1:A:165:GLU:HG2	1:A:167:LYS:HE3	1.87	0.55
1:A:550:LYS:HD2	2:C:4:A:H3'	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LYS:NZ	1:A:213:SER:OG	2.39	0.55
1:A:340:GLN:H	1:A:340:GLN:CD	2.15	0.54
1:A:664:ASP:OD2	1:A:705:ARG:NH2	2.42	0.53
1:A:204:ASP:HB3	1:A:209:LEU:CD1	2.41	0.51
1:A:275:VAL:HG12	1:A:387:TYR:CD1	2.44	0.51
1:A:576:ARG:HG2	4:A:1060:HOH:O	2.10	0.51
1:A:373:LYS:HG3	1:A:375:TYR:HD1	1.76	0.51
1:A:598:THR:OG1	1:A:601:GLU:HG3	2.10	0.51
1:A:233:LEU:O	4:A:902:HOH:O	2.19	0.50
1:A:550:LYS:HD2	2:C:5:A:OP1	2.11	0.50
1:A:703:GLY:O	4:A:903:HOH:O	2.19	0.50
1:A:157:VAL:HG22	1:A:166:TYR:HD1	1.76	0.50
1:A:662:ARG:HB2	1:A:669:ASP:OD1	2.11	0.50
1:A:709:LYS:HB3	1:A:723:THR:CG2	2.39	0.50
1:A:119:GLY:C	1:A:147:ALA:HB2	2.37	0.49
1:A:203:TYR:HD1	1:A:210:CYS:HB2	1.77	0.49
1:A:550:LYS:HG3	1:A:551:ALA:O	2.12	0.49
1:A:290:LYS:HG2	1:A:297:VAL:HB	1.95	0.48
1:A:201:ASP:OD2	1:A:211:LYS:NZ	2.39	0.47
1:A:154:ASN:HB3	1:A:169:VAL:HG13	1.96	0.47
1:A:276:ASP:O	1:A:386:SER:HA	2.13	0.47
1:A:209:LEU:C	1:A:209:LEU:CD1	2.88	0.46
1:A:497:LEU:O	1:A:501:ILE:HG12	2.16	0.46
1:A:454:VAL:O	1:A:456:ASP:N	2.48	0.46
1:A:228:ILE:HG13	1:A:445:TYR:CE1	2.50	0.46
1:A:206:ASP:OD2	1:A:206:ASP:N	2.48	0.46
1:A:154:ASN:HB3	1:A:169:VAL:CG1	2.46	0.45
1:A:394:LEU:HD11	1:A:414:PHE:CE1	2.50	0.45
1:A:542:ILE:CG2	1:A:546:ARG:HH11	2.29	0.45
1:A:511:LYS:HD3	1:A:512:PRO:O	2.16	0.45
1:A:504:VAL:HB	1:A:509:ILE:HG21	1.99	0.45
1:A:724:LEU:HD23	1:A:724:LEU:HA	1.53	0.44
1:A:644:GLY:C	1:A:709:LYS:NZ	2.76	0.44
1:A:387:TYR:CD2	1:A:459:GLU:HG3	2.53	0.43
1:A:646:THR:HG22	1:A:709:LYS:HD3	2.00	0.43
1:A:204:ASP:HB3	1:A:209:LEU:CG	2.49	0.43
1:A:611:LYS:HG3	4:A:906:HOH:O	2.18	0.43
1:A:712:GLU:HG2	1:A:721:ILE:HB	2.00	0.42
1:A:706:LEU:HD13	1:A:707:GLU:H	1.82	0.42
1:A:114:THR:N	4:A:931:HOH:O	2.53	0.42
1:A:223:ASP:OD2	1:A:226:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:LYS:HD2	1:A:533:ASP:OD1	2.20	0.41
1:A:115:GLY:HA2	1:A:177:LEU:HD21	2.03	0.41
1:A:595:ASP:CG	1:A:596:GLN:HE21	2.26	0.41
1:A:539:ILE:HG12	1:A:702:ILE:CG2	2.50	0.41
1:A:662:ARG:HB2	1:A:662:ARG:HE	1.63	0.41
1:A:542:ILE:HG22	1:A:546:ARG:HE	1.86	0.41
1:A:550:LYS:HB2	2:C:4:A:H5'	2.03	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	551/747 (74%)	542 (98%)	8 (2%)	1 (0%)	43 42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	455	HIS

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	515/680 (76%)	508 (99%)	7 (1%)	59 66

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	SER
1	A	209	LEU
1	A	283	LEU
1	A	342	SER
1	A	416	LEU
1	A	500	LEU
1	A	704	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	250	ASN
1	A	260	HIS
1	A	343	ASN
1	A	383	ASN
1	A	421	GLN
1	A	425	GLN
1	A	444	HIS
1	A	498	GLN
1	A	531	ASN
1	A	584	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is 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, 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	565/747 (75%)	1.11	111 (19%)  	30, 56, 122, 211	0
2	C	6/6 (100%)	-0.60	0  	42, 43, 50, 98	0
All	All	571/753 (75%)	1.10	111 (19%)  	30, 56, 122, 211	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	659	ILE	7.9
1	A	652	SER	6.6
1	A	144	LEU	6.2
1	A	210	CYS	6.1
1	A	660	PHE	6.0
1	A	672	ILE	5.9
1	A	702	ILE	5.6
1	A	164	LEU	5.5
1	A	139	ALA	5.0
1	A	671	LEU	5.0
1	A	140	VAL	5.0
1	A	657	PHE	5.0
1	A	87	THR	4.9
1	A	157	VAL	4.8
1	A	189	ASN	4.7
1	A	205	PRO	4.7
1	A	190	LEU	4.6
1	A	88	LEU	4.5
1	A	166	TYR	4.5
1	A	188	ASN	4.5
1	A	116	ALA	4.4
1	A	110	TYR	4.3
1	A	708	ALA	4.2
1	A	653	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	ILE	4.1
1	A	535	PRO	4.1
1	A	400	LEU	4.0
1	A	531	ASN	4.0
1	A	209	LEU	3.9
1	A	149	ILE	3.9
1	A	509	ILE	3.9
1	A	503	THR	3.7
1	A	706	LEU	3.7
1	A	155	PHE	3.7
1	A	505	GLY	3.7
1	A	201	ASP	3.6
1	A	643	ILE	3.6
1	A	539	ILE	3.5
1	A	142	THR	3.5
1	A	191	ALA	3.5
1	A	86	LEU	3.4
1	A	109	HIS	3.4
1	A	331	HIS	3.3
1	A	504	VAL	3.2
1	A	85	ILE	3.2
1	A	203	TYR	3.2
1	A	651	ILE	3.2
1	A	536	SER	3.1
1	A	212	VAL	3.1
1	A	329	PRO	3.1
1	A	425	GLN	3.1
1	A	187	PRO	3.0
1	A	141	ILE	3.0
1	A	507	LEU	3.0
1	A	725	ILE	3.0
1	A	595	ASP	3.0
1	A	537	TYR	2.9
1	A	138	ALA	2.9
1	A	328	LEU	2.9
1	A	119	GLY	2.9
1	A	543	LEU	2.8
1	A	217	VAL	2.8
1	A	658	GLY	2.8
1	A	596	GLN	2.8
1	A	540	PHE	2.8
1	A	206	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	151	TYR	2.7
1	A	528	LEU	2.7
1	A	208	ASN	2.7
1	A	143	ILE	2.7
1	A	111	SER	2.7
1	A	724	LEU	2.7
1	A	202	GLU	2.7
1	A	186	ILE	2.7
1	A	538	GLU	2.6
1	A	439	ILE	2.6
1	A	644	GLY	2.6
1	A	197	ALA	2.6
1	A	150	LEU	2.6
1	A	175	PHE	2.5
1	A	398	SER	2.5
1	A	542	ILE	2.5
1	A	148	ARG	2.4
1	A	117	LEU	2.4
1	A	345	LEU	2.4
1	A	198	PHE	2.4
1	A	147	ALA	2.4
1	A	341	LEU	2.4
1	A	491	ARG	2.4
1	A	508	ASN	2.3
1	A	661	MET	2.3
1	A	721	ILE	2.3
1	A	475	TRP	2.3
1	A	145	LYS	2.3
1	A	291	THR	2.3
1	A	332	TYR	2.2
1	A	340	GLN	2.2
1	A	179	MET	2.2
1	A	500	LEU	2.2
1	A	224	PRO	2.1
1	A	399	GLU	2.1
1	A	647	PHE	2.1
1	A	545	LEU	2.1
1	A	723	THR	2.1
1	A	211	LYS	2.1
1	A	501	ILE	2.1
1	A	534	ASN	2.0
1	A	330	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	621	ILE	2.0
1	A	663	MET	2.0
1	A	178	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

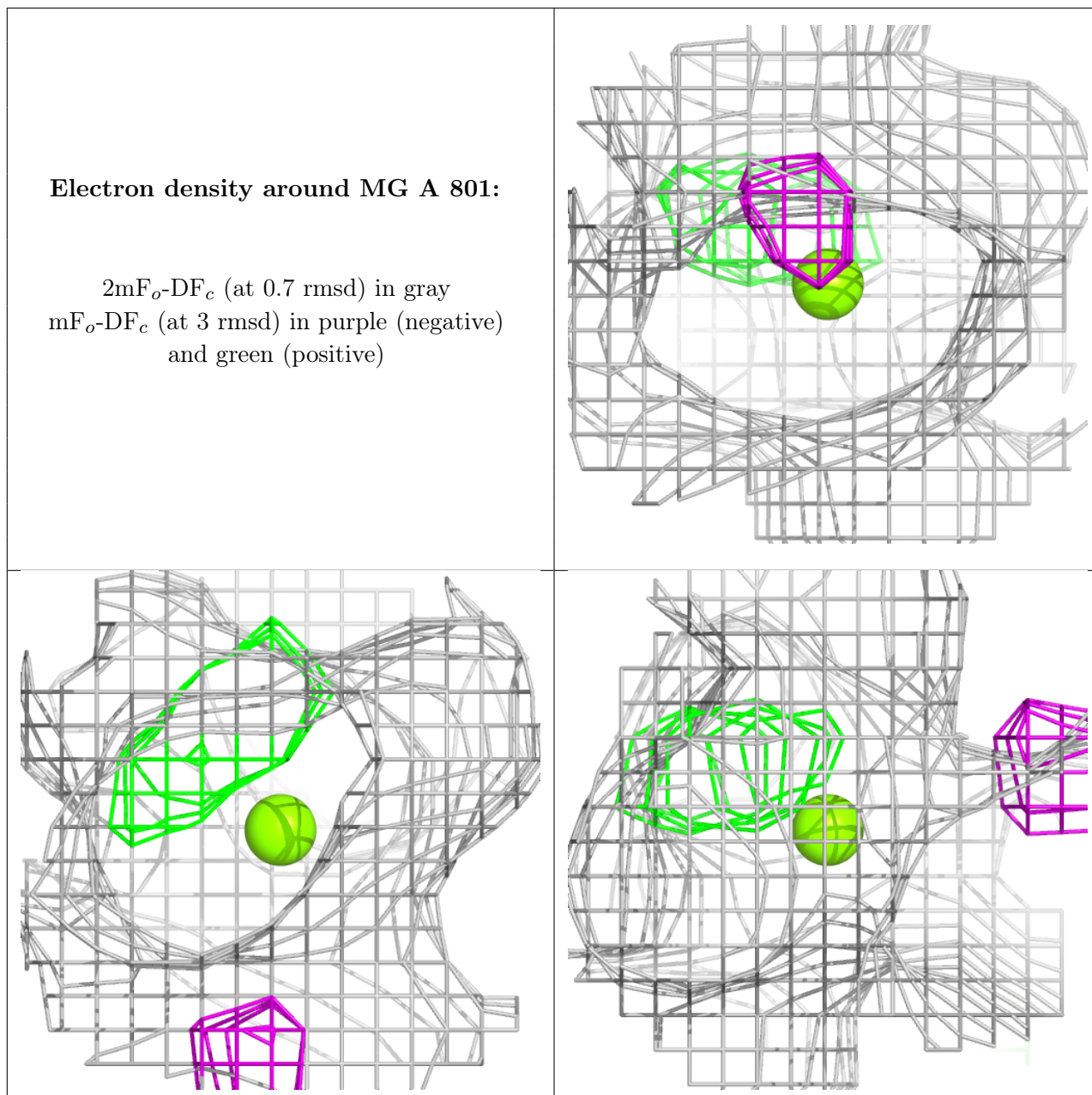
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	801	1/1	0.98	0.04	25,25,25,25	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 801:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.