Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 08:30 PM JST

PDB ID	:	7DOL
Title	:	Mycoplasma genitalium RNase R in complex with double-stranded RNA
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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 (i) 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 (1)) were used in the production of this report:

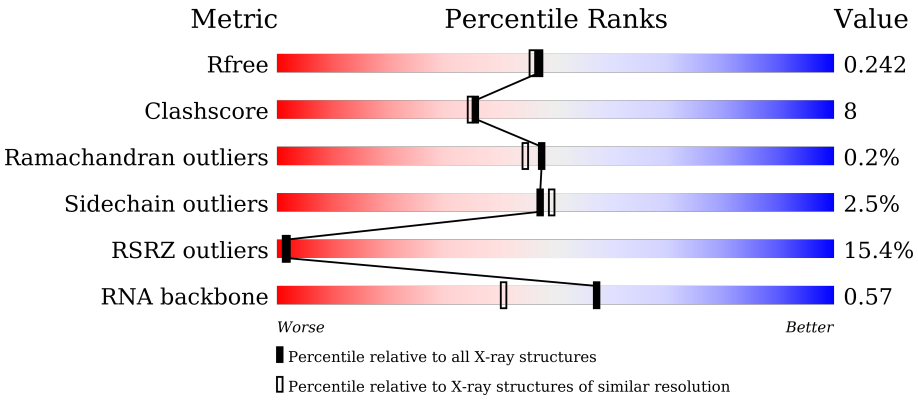
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)
RNA backbone	3102	1079 (2.50-1.50)

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 >=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 <=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	12% 62% 12% · 24%
2	C	6	33% 67%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	565	4546	2901	765	866	14	0	0	0

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*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 (three-letter code: 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.

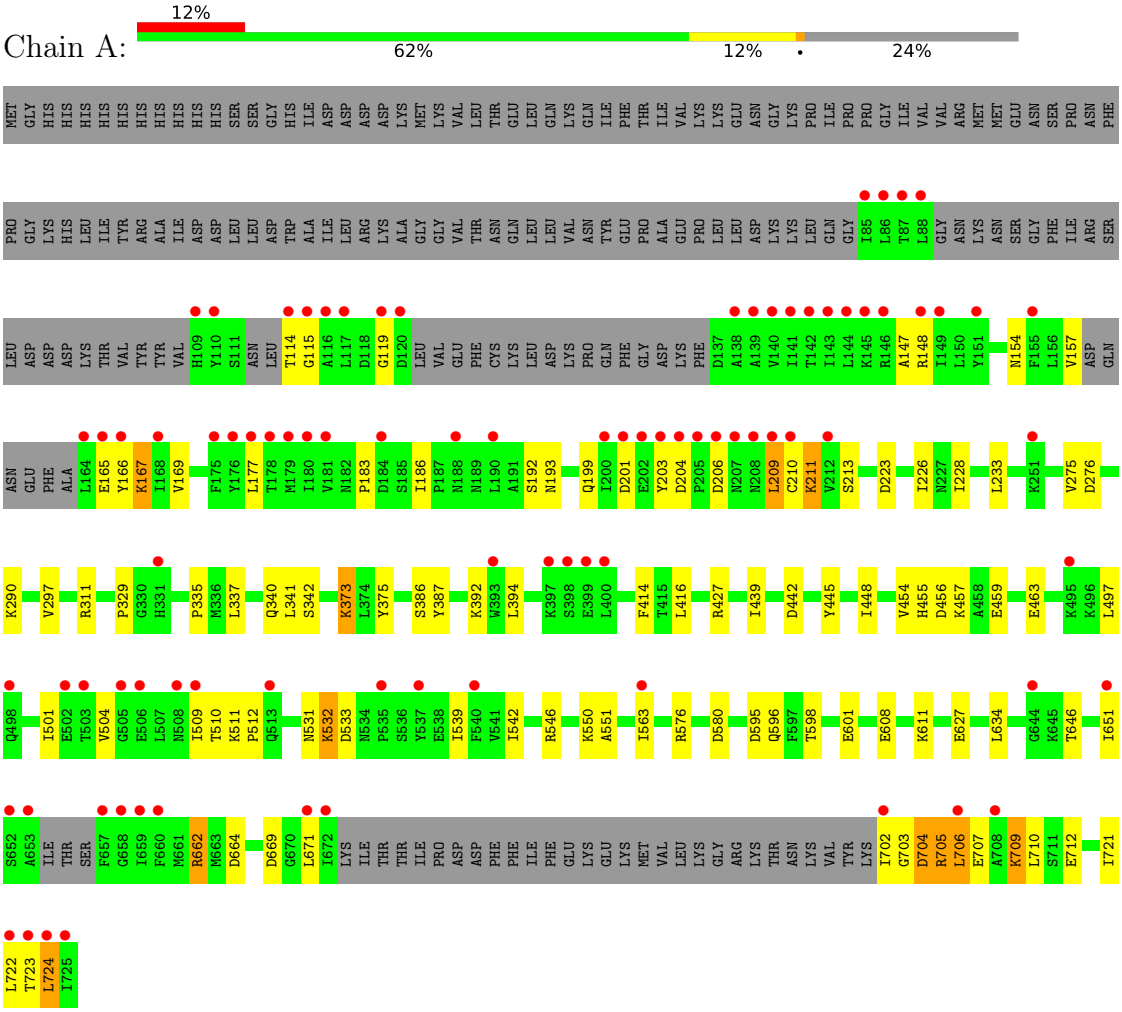
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	223	Total	O	0	0
			223	223		
4	C	12	Total	O	0	0
			12	12		

3 Residue-property plots (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: Ribonuclease R

Chain A:



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

Chain C:

4 Data and refinement statistics (i)

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 40.52 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.29-2.00) 94.8 (40.52-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10_2148	Depositor
R, R_{free}	0.220 , 0.242 0.220 , 0.242	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)	0.33 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.41	4/4629 (0.1%)	0.67	8/6279 (0.1%)
2	C	0.24	0/149	0.61	0/230
All	All	0.41	4/4778 (0.1%)	0.67	8/6509 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	662	ARG	CZ-NH1	-11.00	1.18	1.33
1	A	662	ARG	NE-CZ	-8.66	1.21	1.33
1	A	662	ARG	CZ-NH2	-5.92	1.25	1.33
1	A	709	LYS	CD-CE	-5.64	1.37	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	724	LEU	CB-CG-CD2	-7.93	97.51	111.00
1	A	724	LEU	CA-CB-CG	-6.85	99.56	115.30
1	A	392	LYS	CD-CE-NZ	-6.27	97.29	111.70
1	A	341	LEU	CA-CB-CG	6.17	129.48	115.30
1	A	671	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	671	LEU	CB-CG-CD2	5.59	120.50	111.00
1	A	706	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	A	662	ARG	NE-CZ-NH1	-5.19	117.70	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	4546	0	4553	75	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	75	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 (75) 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: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:463:GLU:HG3	2:C:7:A:O4'	1.97	0.64
1:A:211:LYS:C	1:A:211:LYS:HD2	2.20	0.61
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:595:ASP:CG	1:A:596:GLN:NE2	2.56	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:211:LYS:NZ	1:A:213:SER:OG	2.39	0.55
1:A:209:LEU:HD12	1:A:209:LEU:C	2.28	0.53
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:340:GLN:H	1:A:340:GLN:CD	2.15	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: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: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:119:GLY:C	1:A:147:ALA:HB2	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:209:LEU:C	1:A:209:LEU:CD1	2.88	0.42
1:A:223:ASP:OD2	1:A:226:ILE:HG12	2.20	0.42
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: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%)	47 44

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%)	502 (98%)	13 (2%)	47 49

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	167	LYS
1	A	192	SER
1	A	209	LEU
1	A	211	LYS
1	A	329	PRO
1	A	342	SER
1	A	373	LYS
1	A	416	LEU
1	A	427	ARG
1	A	532	LYS
1	A	580	ASP
1	A	704	ASP
1	A	705	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	ASN
1	A	421	GLN
1	A	425	GLN
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

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 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, 95^{th} 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%)	0.91	88 (15%) 2 1	30, 56, 122, 211	0
2	C	6/6 (100%)	-0.43	0 100 100	42, 43, 50, 98	0
All	All	571/753 (75%)	0.90	88 (15%) 2 1	30, 56, 122, 211	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	VAL	12.5
1	A	201	ASP	9.9
1	A	144	LEU	9.8
1	A	725	ILE	9.8
1	A	139	ALA	9.7
1	A	657	PHE	9.1
1	A	659	ILE	7.5
1	A	116	ALA	7.3
1	A	210	CYS	7.1
1	A	702	ILE	7.0
1	A	164	LEU	6.9
1	A	87	THR	6.7
1	A	206	ASP	6.2
1	A	203	TYR	6.1
1	A	143	ILE	5.9
1	A	138	ALA	5.7
1	A	142	THR	5.7
1	A	145	LYS	5.7
1	A	209	LEU	5.5
1	A	85	ILE	5.5
1	A	141	ILE	5.4
1	A	671	LEU	5.1
1	A	400	LEU	4.9
1	A	115	GLY	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	188	ASN	4.9
1	A	653	ALA	4.8
1	A	652	SER	4.7
1	A	114	THR	4.5
1	A	644	GLY	4.3
1	A	205	PRO	4.2
1	A	176	TYR	3.9
1	A	86	LEU	3.9
1	A	88	LEU	3.7
1	A	149	ILE	3.7
1	A	166	TYR	3.7
1	A	208	ASN	3.6
1	A	177	LEU	3.6
1	A	110	TYR	3.5
1	A	660	PHE	3.5
1	A	202	GLU	3.5
1	A	513	GLN	3.5
1	A	505	GLY	3.5
1	A	723	THR	3.5
1	A	503	THR	3.4
1	A	207	ASN	3.4
1	A	658	GLY	3.3
1	A	398	SER	3.3
1	A	190	LEU	3.2
1	A	535	PRO	3.2
1	A	724	LEU	3.2
1	A	119	GLY	3.1
1	A	175	PHE	3.0
1	A	495	LYS	3.0
1	A	168	ILE	3.0
1	A	397	LYS	2.9
1	A	200	ILE	2.9
1	A	165	GLU	2.9
1	A	155	PHE	2.8
1	A	146	ARG	2.8
1	A	109	HIS	2.6
1	A	151	TYR	2.6
1	A	331	HIS	2.5
1	A	204	ASP	2.5
1	A	178	THR	2.5
1	A	179	MET	2.5
1	A	212	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	509	ILE	2.4
1	A	540	PHE	2.4
1	A	722	LEU	2.4
1	A	708	ALA	2.4
1	A	563	ILE	2.4
1	A	393	TRP	2.4
1	A	651	ILE	2.3
1	A	251	LYS	2.3
1	A	706	LEU	2.3
1	A	498	GLN	2.2
1	A	120	ASP	2.2
1	A	537	TYR	2.2
1	A	117	LEU	2.1
1	A	672	ILE	2.1
1	A	502	GLU	2.1
1	A	181	VAL	2.1
1	A	180	ILE	2.0
1	A	508	ASN	2.0
1	A	399	GLU	2.0
1	A	506	GLU	2.0
1	A	148	ARG	2.0
1	A	184	ASP	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)

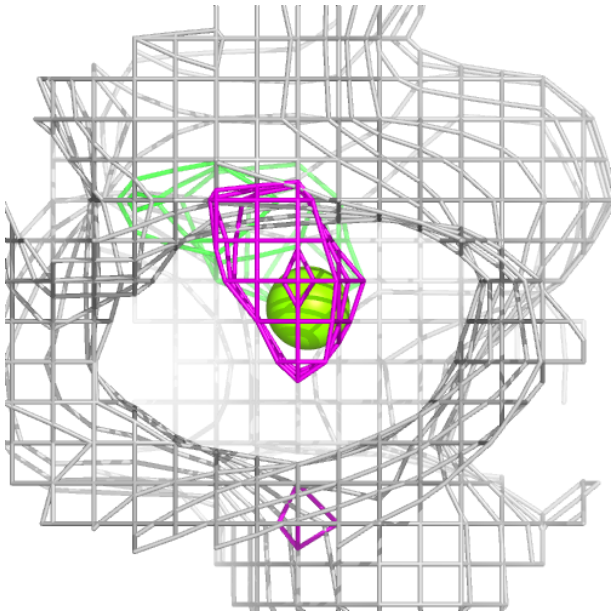
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

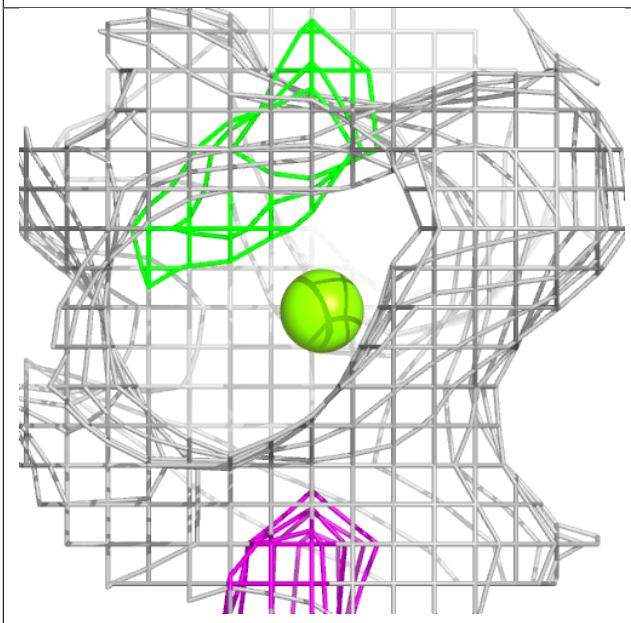
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	A	801	1/1	0.94	0.16	25,25,25,25	0

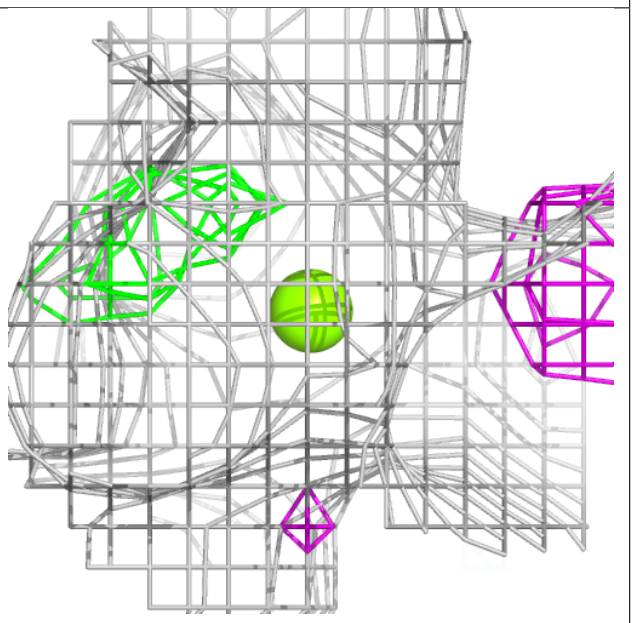
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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