Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2021 – 09:13 am BST

PDB ID	:	6YVC
Title	:	Crystal structure of the small alarmone hydrolase (SAH) of Pseudomonas aeruginosa
Authors	:	Altegoer, F.; Bange, G.
Deposited on	:	2020-04-28
Resolution	:	1.85 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 following versions of software and data (see references ⓘ) were used in the production of this report:

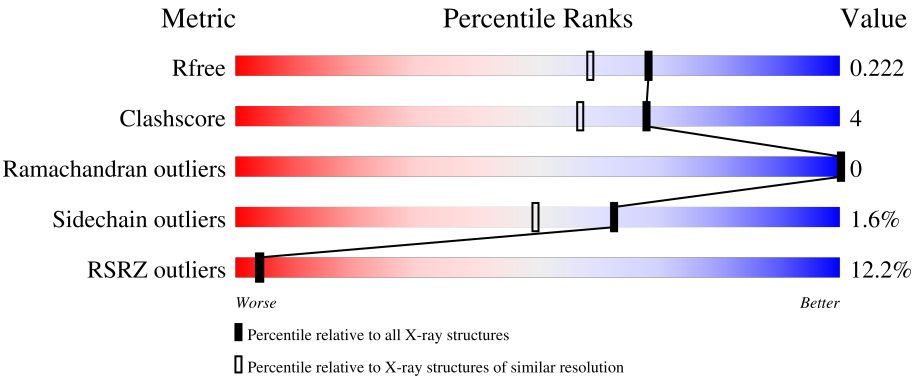
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	191	11% 85% 6% 8%
1	B	191	12% 83% 8% 9%
1	C	191	12% 85% 6% 8%
1	D	191	10% 81% 8% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6411 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 Bifunctional (P)ppGpp synthetase/guanosine-3',5'-bis(Diphosphate) 3'-pyrophosphohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	175	Total	C	N	O	S	0	0	0
			1398	876	260	259	3			
1	B	173	Total	C	N	O	S	0	0	0
			1385	868	258	256	3			
1	C	175	Total	C	N	O	S	0	0	0
			1396	875	260	258	3			
1	D	172	Total	C	N	O	S	0	0	0
			1374	862	254	255	3			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A071L0I0
A	-5	GLY	-	expression tag	UNP A0A071L0I0
A	-4	HIS	-	expression tag	UNP A0A071L0I0
A	-3	HIS	-	expression tag	UNP A0A071L0I0
A	-2	HIS	-	expression tag	UNP A0A071L0I0
A	-1	HIS	-	expression tag	UNP A0A071L0I0
A	0	HIS	-	expression tag	UNP A0A071L0I0
A	1	HIS	-	expression tag	UNP A0A071L0I0
A	5	MET	THR	conflict	UNP A0A071L0I0
B	-6	MET	-	initiating methionine	UNP A0A071L0I0
B	-5	GLY	-	expression tag	UNP A0A071L0I0
B	-4	HIS	-	expression tag	UNP A0A071L0I0
B	-3	HIS	-	expression tag	UNP A0A071L0I0
B	-2	HIS	-	expression tag	UNP A0A071L0I0
B	-1	HIS	-	expression tag	UNP A0A071L0I0
B	0	HIS	-	expression tag	UNP A0A071L0I0
B	1	HIS	-	expression tag	UNP A0A071L0I0
B	5	MET	THR	conflict	UNP A0A071L0I0
C	-6	MET	-	initiating methionine	UNP A0A071L0I0
C	-5	GLY	-	expression tag	UNP A0A071L0I0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP A0A071L0I0
C	-3	HIS	-	expression tag	UNP A0A071L0I0
C	-2	HIS	-	expression tag	UNP A0A071L0I0
C	-1	HIS	-	expression tag	UNP A0A071L0I0
C	0	HIS	-	expression tag	UNP A0A071L0I0
C	1	HIS	-	expression tag	UNP A0A071L0I0
C	5	MET	THR	conflict	UNP A0A071L0I0
D	-6	MET	-	initiating methionine	UNP A0A071L0I0
D	-5	GLY	-	expression tag	UNP A0A071L0I0
D	-4	HIS	-	expression tag	UNP A0A071L0I0
D	-3	HIS	-	expression tag	UNP A0A071L0I0
D	-2	HIS	-	expression tag	UNP A0A071L0I0
D	-1	HIS	-	expression tag	UNP A0A071L0I0
D	0	HIS	-	expression tag	UNP A0A071L0I0
D	1	HIS	-	expression tag	UNP A0A071L0I0
D	5	MET	THR	conflict	UNP A0A071L0I0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is water.

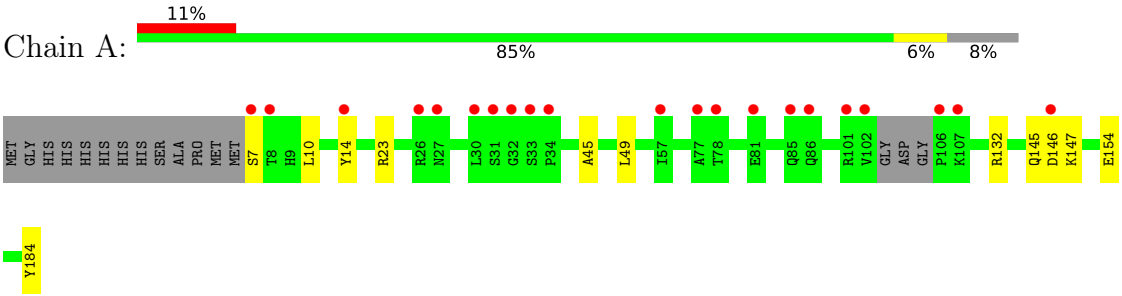
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	223	Total O 223 223	0	0
3	B	216	Total O 216 216	0	0
3	C	225	Total O 225 225	0	0
3	D	190	Total O 190 190	0	0

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.

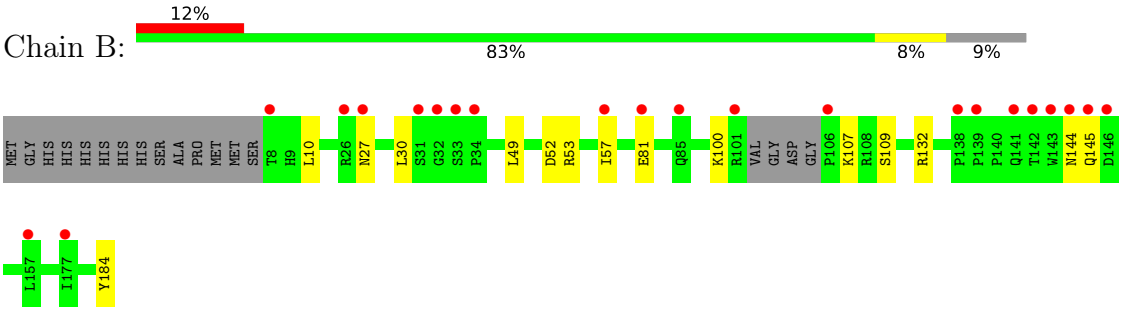
• Molecule 1: Bifunctional (P)ppGpp synthetase/guanosine-3',5'-bis(Diphosphate) 3'-pyrophosph ohydrolase

Chain A:



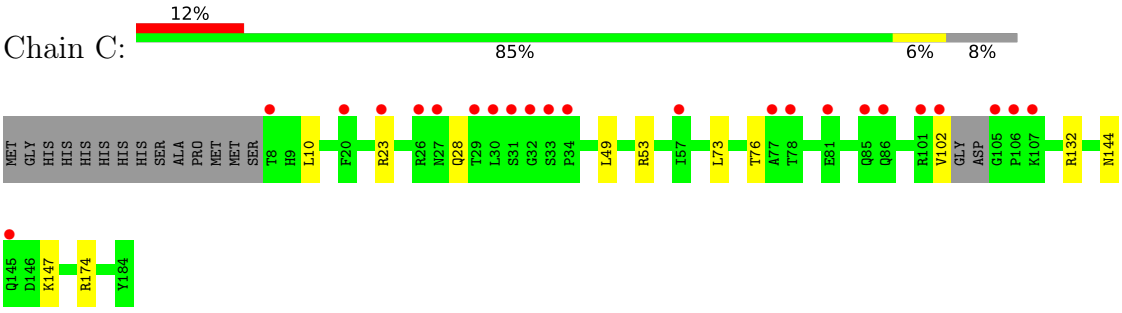
• Molecule 1: Bifunctional (P)ppGpp synthetase/guanosine-3',5'-bis(Diphosphate) 3'-pyrophosph ohydrolase

Chain B:



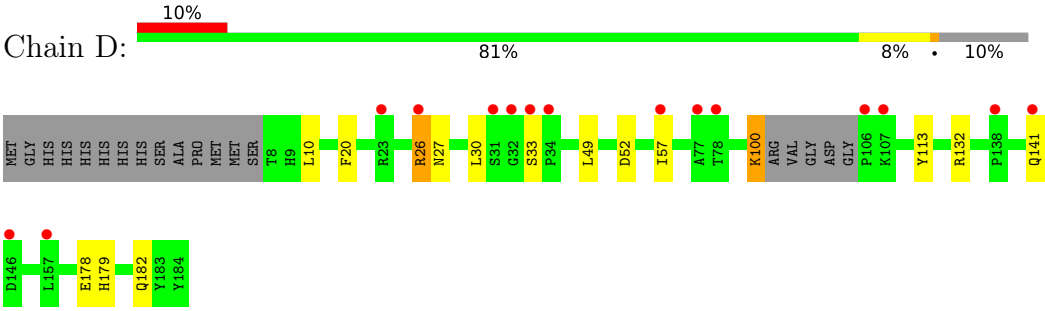
• Molecule 1: Bifunctional (P)ppGpp synthetase/guanosine-3',5'-bis(Diphosphate) 3'-pyrophosph ohydrolase

Chain C:



• Molecule 1: Bifunctional (P)ppGpp synthetase/guanosine-3',5'-bis(Diphosphate) 3'-pyrophosph ohydrolase

Chain D:


10%
81%
8%
10%
MET GLY HIS HIS HIS HIS HIS SER ALA PRO MET MET SER T8 H9 L10 F20 R23 R26 N27 L30 S31 G32 S33 P34 L49 D52 I57 A77 T78 K100 ARG VAL GLY ASP GLY P106 K107 Y113 R132 P138 Q141 T142 W143 N144 Q145
D146 L157 E178 H179 Q182 Y183 Y184

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.33Å 85.38Å 122.17Å 90.00° 102.06° 90.00°	Depositor
Resolution (Å)	45.78 – 1.85 45.78 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.1 (45.78-1.85) 98.0 (45.78-1.79)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.66 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.191 , 0.222 0.191 , 0.222	Depositor DCC
R_{free} test set	3627 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6411	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.90% 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: MN

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	0.31	0/1427	0.49	0/1936
1	B	0.31	0/1414	0.50	0/1918
1	C	0.32	0/1425	0.51	0/1934
1	D	0.32	0/1403	0.49	0/1904
All	All	0.31	0/5669	0.50	0/7692

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	1398	0	1376	8	0
1	B	1385	0	1362	14	0
1	C	1396	0	1373	10	0
1	D	1374	0	1349	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	223	0	0	2	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	216	0	0	3	3
3	C	225	0	0	5	1
3	D	190	0	0	3	1
All	All	6411	0	5460	42	4

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 (42) 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:D:26:ARG:HA	1:D:26:ARG:HE	1.37	0.89
1:D:178:GLU:OE1	3:D:301:HOH:O	2.08	0.72
1:D:27:ASN:ND2	3:D:302:HOH:O	2.17	0.70
1:A:145:GLN:HG2	1:A:184:TYR:HB2	1.74	0.68
1:C:174:ARG:NH1	3:C:303:HOH:O	2.29	0.63
1:B:27:ASN:HD22	1:C:144:ASN:HD21	1.46	0.61
1:A:10:LEU:HD21	1:A:49:LEU:HD11	1.82	0.61
1:D:26:ARG:HE	1:D:26:ARG:CA	2.14	0.60
1:B:144:ASN:ND2	3:B:310:HOH:O	2.37	0.58
1:A:147:LYS:HB2	1:D:27:ASN:HB3	1.87	0.56
1:B:53:ARG:NH2	3:B:311:HOH:O	2.38	0.56
1:C:53:ARG:NH2	3:C:308:HOH:O	2.38	0.56
1:C:10:LEU:HD21	1:C:49:LEU:HD11	1.89	0.54
1:B:107:LYS:HZ3	1:B:109:SER:HA	1.72	0.54
1:B:27:ASN:HA	1:C:144:ASN:ND2	2.23	0.54
1:A:14:TYR:HE2	1:A:45:ALA:HB1	1.73	0.53
1:A:23:ARG:NH2	3:A:305:HOH:O	2.40	0.52
1:D:27:ASN:OD1	3:D:303:HOH:O	2.19	0.52
1:B:30:LEU:O	3:B:301:HOH:O	2.19	0.51
1:D:52:ASP:HB2	1:D:57:ILE:HD12	1.94	0.50
1:A:49:LEU:HD23	1:B:49:LEU:HD23	1.94	0.50
1:C:28:GLN:HB2	3:C:383:HOH:O	2.11	0.49
1:D:30:LEU:HB2	1:D:33:SER:HB3	1.94	0.49
1:D:142:THR:HG23	1:D:143:TRP:CD1	2.48	0.48
1:B:10:LEU:HD21	1:B:49:LEU:HD11	1.96	0.47
1:B:107:LYS:NZ	1:B:109:SER:HA	2.30	0.47
1:A:154:GLU:OE2	3:A:302:HOH:O	2.20	0.46
1:D:100:LYS:HG3	1:D:113:TYR:CD1	2.51	0.46
1:B:52:ASP:HB2	1:B:57:ILE:HD12	1.98	0.45
1:D:26:ARG:HA	1:D:26:ARG:NE	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLN:H	1:D:141:GLN:CD	2.20	0.45
1:B:27:ASN:HB3	1:C:147:LYS:HB2	1.97	0.45
1:D:179:HIS:O	1:D:182:GLN:HG2	2.16	0.45
1:D:10:LEU:HD21	1:D:49:LEU:HD11	1.99	0.44
1:C:76:THR:HG22	3:C:301:HOH:O	2.17	0.44
1:B:81:GLU:H	1:B:81:GLU:CD	2.20	0.44
1:A:14:TYR:HE2	1:A:45:ALA:CB	2.30	0.43
1:B:145:GLN:HG2	1:B:184:TYR:HB2	2.01	0.42
1:C:23:ARG:NH1	3:C:314:HOH:O	2.52	0.42
1:C:73:LEU:HB3	1:C:102:VAL:HG13	2.02	0.41
1:D:142:THR:HG23	1:D:143:TRP:HD1	1.84	0.41
1:B:100:LYS:HE2	1:B:107:LYS:HE2	2.02	0.40

All (4) 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)
3:C:333:HOH:O	3:D:429:HOH:O[2_555]	2.10	0.10
3:A:317:HOH:O	3:B:421:HOH:O[3_545]	2.15	0.05
3:A:507:HOH:O	3:B:480:HOH:O[3_545]	2.15	0.05
3:A:317:HOH:O	3:B:302:HOH:O[3_545]	2.17	0.03

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	171/191 (90%)	168 (98%)	3 (2%)	0	100	100
1	B	169/191 (88%)	165 (98%)	4 (2%)	0	100	100
1	C	171/191 (90%)	166 (97%)	5 (3%)	0	100	100
1	D	168/191 (88%)	165 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	679/764 (89%)	664 (98%)	15 (2%)	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	144/156 (92%)	141 (98%)	3 (2%)	53 38
1	B	142/156 (91%)	141 (99%)	1 (1%)	84 79
1	C	143/156 (92%)	142 (99%)	1 (1%)	84 79
1	D	141/156 (90%)	137 (97%)	4 (3%)	43 27
All	All	570/624 (91%)	561 (98%)	9 (2%)	62 49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	132	ARG
1	A	146	ASP
1	B	132	ARG
1	C	132	ARG
1	D	20	PHE
1	D	26	ARG
1	D	100	LYS
1	D	132	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	ASN
1	D	27	ASN

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^{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	175/191 (91%)	0.94	21 (12%)	4	4	12, 21, 48, 74	0
1	B	173/191 (90%)	0.94	22 (12%)	3	3	12, 22, 49, 73	0
1	C	175/191 (91%)	1.02	23 (13%)	3	3	13, 21, 51, 79	0
1	D	172/191 (90%)	0.95	19 (11%)	5	5	13, 22, 51, 66	0
All	All	695/764 (90%)	0.96	85 (12%)	4	4	12, 21, 50, 79	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	32	GLY	15.0
1	D	32	GLY	8.9
1	C	105	GLY	7.8
1	B	32	GLY	7.6
1	A	32	GLY	7.4
1	A	102	VAL	7.2
1	C	102	VAL	6.4
1	C	106	PRO	5.8
1	A	7	SER	5.5
1	C	33	SER	4.8
1	A	33	SER	4.8
1	A	31	SER	4.7
1	D	142	THR	4.6
1	D	57	ILE	4.6
1	D	106	PRO	4.5
1	D	146	ASP	4.5
1	A	106	PRO	4.5
1	B	145	GLN	4.3
1	B	33	SER	4.2
1	B	146	ASP	4.1
1	D	31	SER	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	141	GLN	4.1
1	B	141	GLN	4.0
1	C	77	ALA	4.0
1	C	101	ARG	3.9
1	D	143	TRP	3.9
1	C	26	ARG	3.8
1	B	106	PRO	3.8
1	D	144	ASN	3.7
1	B	101	ARG	3.7
1	A	30	LEU	3.6
1	D	145	GLN	3.6
1	A	107	LYS	3.6
1	A	57	ILE	3.6
1	B	57	ILE	3.6
1	C	85	GLN	3.6
1	A	8	THR	3.6
1	B	142	THR	3.6
1	B	143	TRP	3.5
1	D	33	SER	3.5
1	A	27	ASN	3.4
1	A	101	ARG	3.4
1	C	78	THR	3.4
1	C	27	ASN	3.3
1	C	86	GLN	3.3
1	A	77	ALA	3.2
1	D	34	PRO	3.2
1	A	78	THR	3.1
1	B	31	SER	3.1
1	D	77	ALA	3.1
1	C	23	ARG	3.0
1	B	81	GLU	3.0
1	B	34	PRO	3.0
1	C	30	LEU	3.0
1	A	14	TYR	3.0
1	B	85	GLN	2.8
1	C	34	PRO	2.7
1	B	144	ASN	2.7
1	B	139	PRO	2.7
1	C	20	PHE	2.6
1	C	81	GLU	2.6
1	C	31	SER	2.6
1	D	157	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	57	ILE	2.6
1	B	138	PRO	2.4
1	D	138	PRO	2.4
1	D	23	ARG	2.4
1	A	34	PRO	2.4
1	A	86	GLN	2.4
1	C	145	GLN	2.4
1	D	107	LYS	2.3
1	B	27	ASN	2.3
1	A	81	GLU	2.3
1	A	26	ARG	2.3
1	A	146	ASP	2.3
1	C	107	LYS	2.3
1	D	26	ARG	2.2
1	C	8	THR	2.1
1	C	29	THR	2.1
1	B	26	ARG	2.1
1	B	8	THR	2.1
1	B	177	ILE	2.1
1	A	85	GLN	2.1
1	D	78	THR	2.1
1	B	157	LEU	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
2	MN	A	201	1/1	0.93	0.09	24,24,24,24	1

Continued on next page...

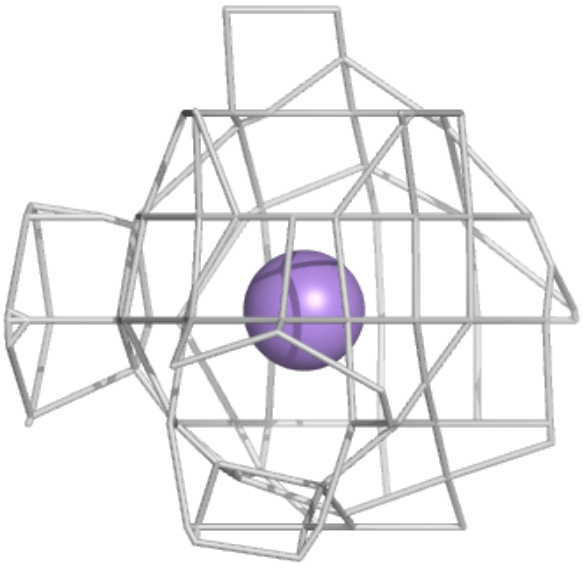
Continued from previous page...

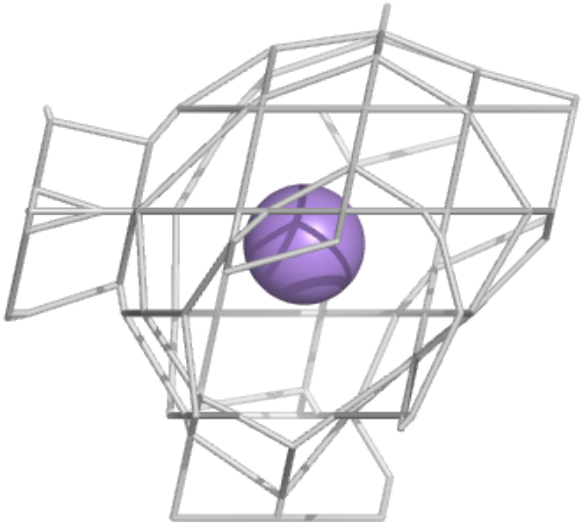
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	B	201	1/1	0.96	0.06	21,21,21,21	1
2	MN	D	201	1/1	0.96	0.08	21,21,21,21	1
2	MN	C	201	1/1	0.97	0.11	28,28,28,28	1

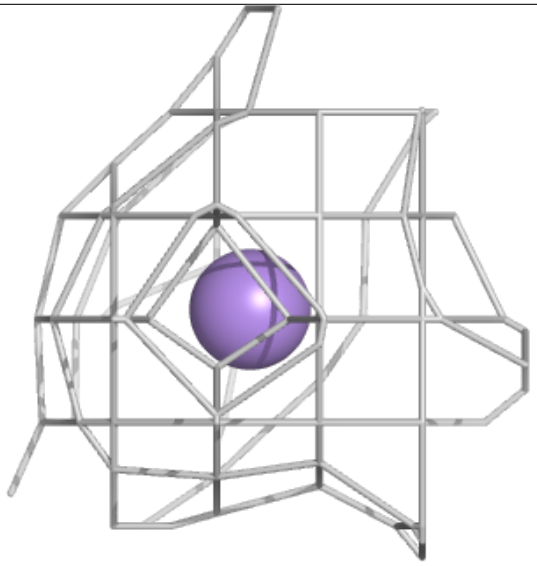
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MN A 201:

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

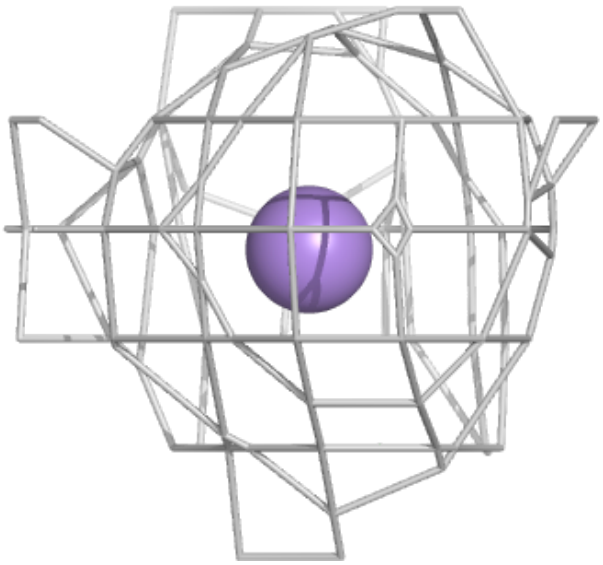


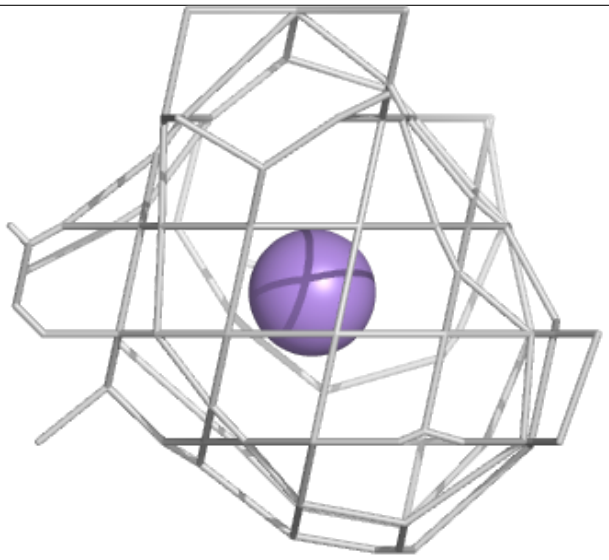


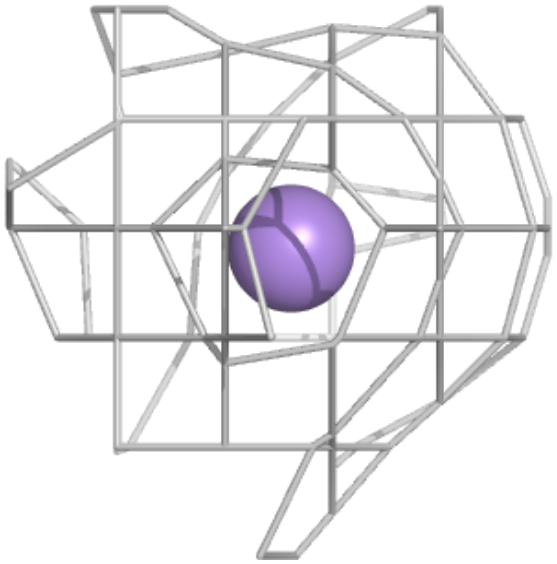


Electron density around MN B 201:

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

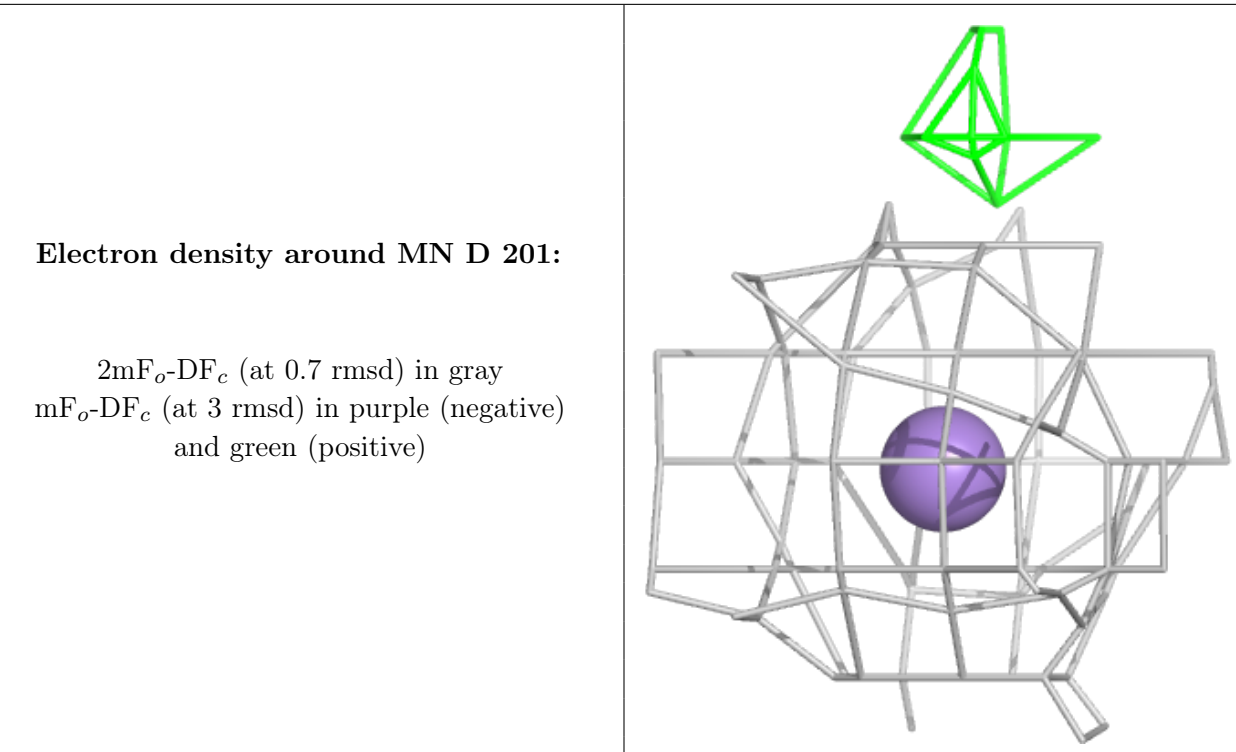


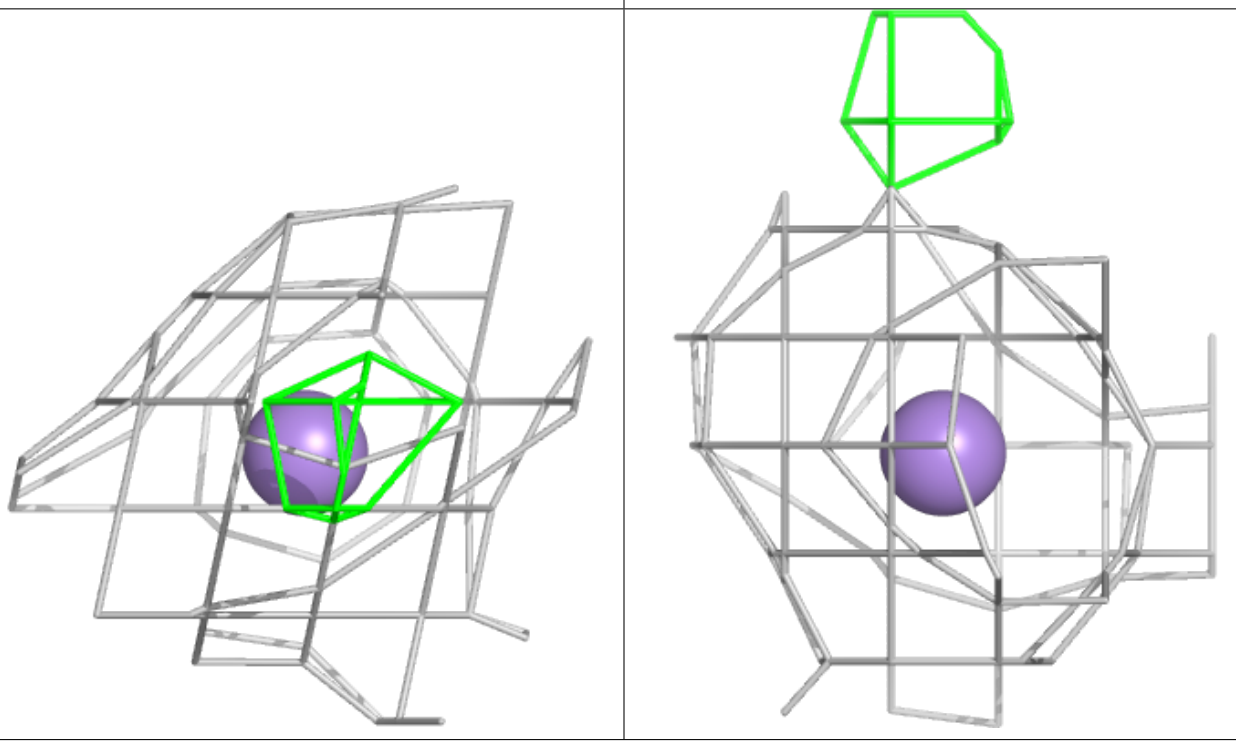




Electron density around MN D 201:

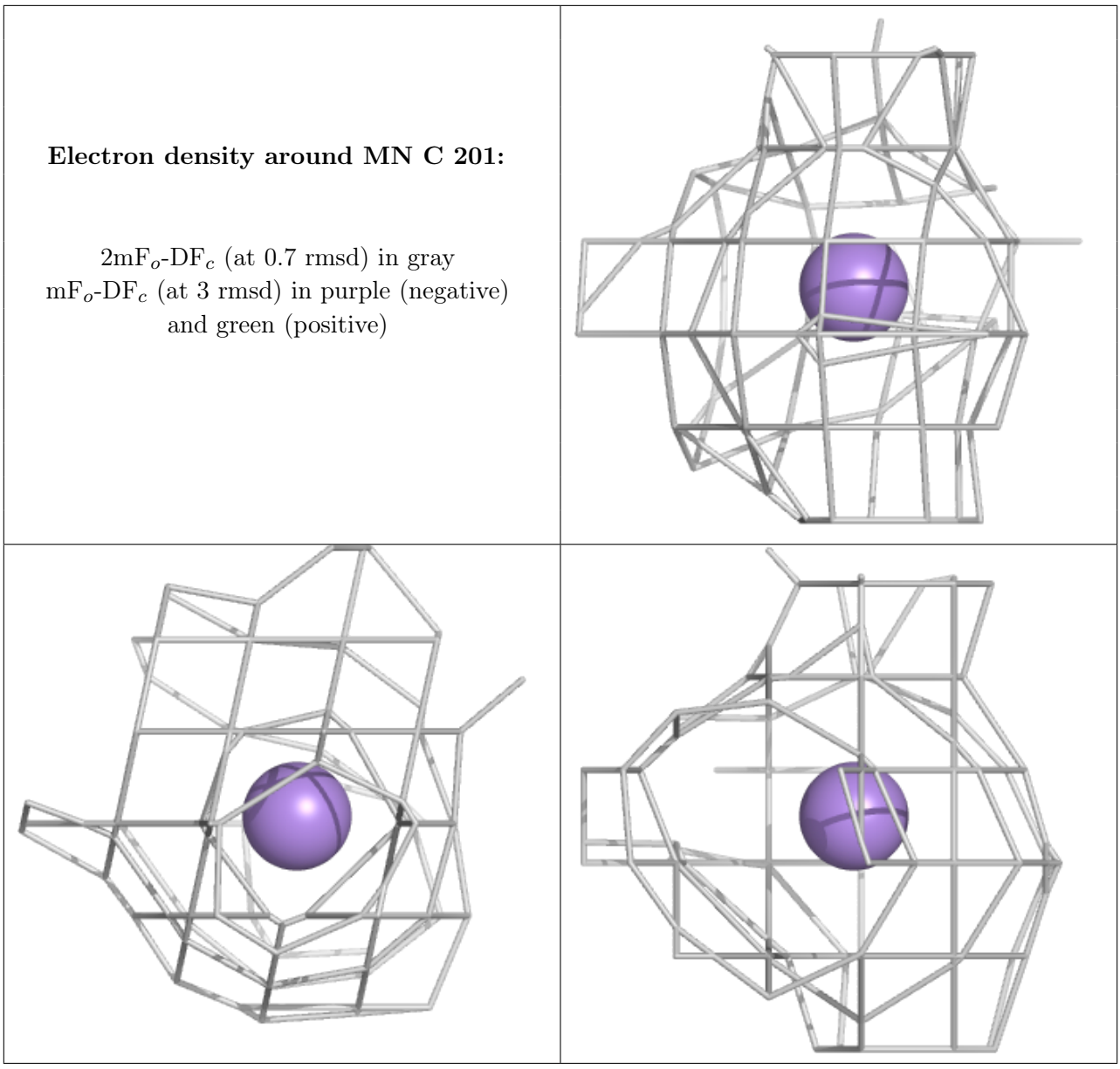
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around MN C 201:

$2mF_o$-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.