WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 15, 2024 – 01:31 pm GMT

PDB ID	:	6Z3O
Title	:	The E74Q mutant of Small Alarmone Hydrolase SAH from Pseudomonas aeruginosa PAO1
Authors	:	Jin, Y.; Rizkallah, P.; Bell, H.
Deposited on	:	2020-05-21
Resolution	:	1.74 Å(reported)

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

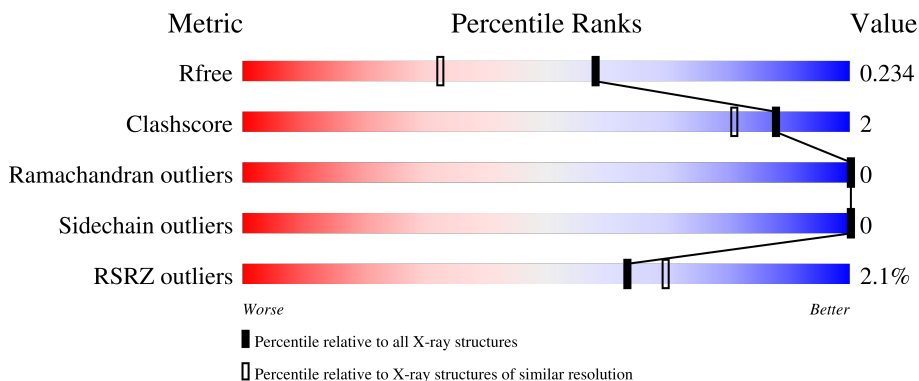|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	: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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
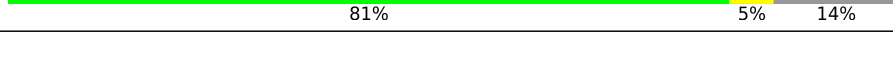*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.74 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	Percentile Ranks	Value
Rfree		0.234
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0
RSRZ outliers		2.1%

Worse ▮ *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	AAA	205	2% — 81% 5% 13%
1	BBB	205	83% • 14%
1	CCC	205	2% — 79% 7% 14%
1	DDD	205	2% — 81% 5% 14%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6242 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 Small Alarmone Hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	178	Total	C	N	O	S	0	1	0
			1422	888	264	267	3			
1	BBB	177	Total	C	N	O	S	0	2	0
			1429	893	269	264	3			
1	CCC	177	Total	C	N	O	S	0	4	0
			1439	899	269	268	3			
1	DDD	177	Total	C	N	O	S	0	1	0
			1417	886	264	264	3			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-20	MET	-	initiating methionine	UNP Q9I686
AAA	-19	GLY	-	expression tag	UNP Q9I686
AAA	-18	SER	-	expression tag	UNP Q9I686
AAA	-17	SER	-	expression tag	UNP Q9I686
AAA	-16	HIS	-	expression tag	UNP Q9I686
AAA	-15	HIS	-	expression tag	UNP Q9I686
AAA	-14	HIS	-	expression tag	UNP Q9I686
AAA	-13	HIS	-	expression tag	UNP Q9I686
AAA	-12	HIS	-	expression tag	UNP Q9I686
AAA	-11	HIS	-	expression tag	UNP Q9I686
AAA	-10	SER	-	expression tag	UNP Q9I686
AAA	-9	SER	-	expression tag	UNP Q9I686
AAA	-8	GLY	-	expression tag	UNP Q9I686
AAA	-7	GLU	-	expression tag	UNP Q9I686
AAA	-6	ASN	-	expression tag	UNP Q9I686
AAA	-5	LEU	-	expression tag	UNP Q9I686
AAA	-4	TYR	-	expression tag	UNP Q9I686
AAA	-3	PHE	-	expression tag	UNP Q9I686
AAA	-2	GLN	-	expression tag	UNP Q9I686
AAA	-1	SER	-	expression tag	UNP Q9I686
AAA	0	HIS	-	expression tag	UNP Q9I686

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Chain	Residue	Modelled	Actual	Comment	Reference
AAA	74	GLN	GLU	engineered mutation	UNP Q9I686
BBB	-20	MET	-	initiating methionine	UNP Q9I686
BBB	-19	GLY	-	expression tag	UNP Q9I686
BBB	-18	SER	-	expression tag	UNP Q9I686
BBB	-17	SER	-	expression tag	UNP Q9I686
BBB	-16	HIS	-	expression tag	UNP Q9I686
BBB	-15	HIS	-	expression tag	UNP Q9I686
BBB	-14	HIS	-	expression tag	UNP Q9I686
BBB	-13	HIS	-	expression tag	UNP Q9I686
BBB	-12	HIS	-	expression tag	UNP Q9I686
BBB	-11	HIS	-	expression tag	UNP Q9I686
BBB	-10	SER	-	expression tag	UNP Q9I686
BBB	-9	SER	-	expression tag	UNP Q9I686
BBB	-8	GLY	-	expression tag	UNP Q9I686
BBB	-7	GLU	-	expression tag	UNP Q9I686
BBB	-6	ASN	-	expression tag	UNP Q9I686
BBB	-5	LEU	-	expression tag	UNP Q9I686
BBB	-4	TYR	-	expression tag	UNP Q9I686
BBB	-3	PHE	-	expression tag	UNP Q9I686
BBB	-2	GLN	-	expression tag	UNP Q9I686
BBB	-1	SER	-	expression tag	UNP Q9I686
BBB	0	HIS	-	expression tag	UNP Q9I686
BBB	74	GLN	GLU	engineered mutation	UNP Q9I686
CCC	-20	MET	-	initiating methionine	UNP Q9I686
CCC	-19	GLY	-	expression tag	UNP Q9I686
CCC	-18	SER	-	expression tag	UNP Q9I686
CCC	-17	SER	-	expression tag	UNP Q9I686
CCC	-16	HIS	-	expression tag	UNP Q9I686
CCC	-15	HIS	-	expression tag	UNP Q9I686
CCC	-14	HIS	-	expression tag	UNP Q9I686
CCC	-13	HIS	-	expression tag	UNP Q9I686
CCC	-12	HIS	-	expression tag	UNP Q9I686
CCC	-11	HIS	-	expression tag	UNP Q9I686
CCC	-10	SER	-	expression tag	UNP Q9I686
CCC	-9	SER	-	expression tag	UNP Q9I686
CCC	-8	GLY	-	expression tag	UNP Q9I686
CCC	-7	GLU	-	expression tag	UNP Q9I686
CCC	-6	ASN	-	expression tag	UNP Q9I686
CCC	-5	LEU	-	expression tag	UNP Q9I686
CCC	-4	TYR	-	expression tag	UNP Q9I686
CCC	-3	PHE	-	expression tag	UNP Q9I686
CCC	-2	GLN	-	expression tag	UNP Q9I686

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Chain	Residue	Modelled	Actual	Comment	Reference
CCC	-1	SER	-	expression tag	UNP Q9I686
CCC	0	HIS	-	expression tag	UNP Q9I686
CCC	74	GLN	GLU	engineered mutation	UNP Q9I686
DDD	-20	MET	-	initiating methionine	UNP Q9I686
DDD	-19	GLY	-	expression tag	UNP Q9I686
DDD	-18	SER	-	expression tag	UNP Q9I686
DDD	-17	SER	-	expression tag	UNP Q9I686
DDD	-16	HIS	-	expression tag	UNP Q9I686
DDD	-15	HIS	-	expression tag	UNP Q9I686
DDD	-14	HIS	-	expression tag	UNP Q9I686
DDD	-13	HIS	-	expression tag	UNP Q9I686
DDD	-12	HIS	-	expression tag	UNP Q9I686
DDD	-11	HIS	-	expression tag	UNP Q9I686
DDD	-10	SER	-	expression tag	UNP Q9I686
DDD	-9	SER	-	expression tag	UNP Q9I686
DDD	-8	GLY	-	expression tag	UNP Q9I686
DDD	-7	GLU	-	expression tag	UNP Q9I686
DDD	-6	ASN	-	expression tag	UNP Q9I686
DDD	-5	LEU	-	expression tag	UNP Q9I686
DDD	-4	TYR	-	expression tag	UNP Q9I686
DDD	-3	PHE	-	expression tag	UNP Q9I686
DDD	-2	GLN	-	expression tag	UNP Q9I686
DDD	-1	SER	-	expression tag	UNP Q9I686
DDD	0	HIS	-	expression tag	UNP Q9I686
DDD	74	GLN	GLU	engineered mutation	UNP Q9I686

- 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	AAA	1	Total 1	Mn 1	0	0
2	BBB	1	Total 1	Mn 1	0	0
2	CCC	1	Total 1	Mn 1	0	0
2	DDD	1	Total 1	Mn 1	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	144	Total 146	O 146	0	2
3	BBB	125	Total 125	O 125	0	0
3	CCC	124	Total 127	O 127	0	3
3	DDD	133	Total 133	O 133	0	0

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.
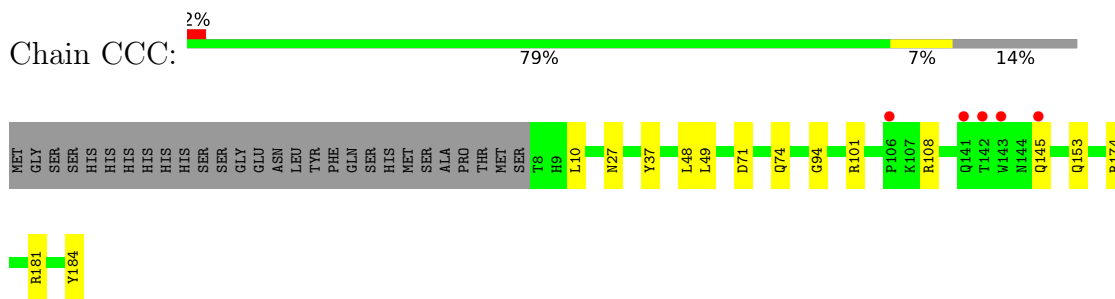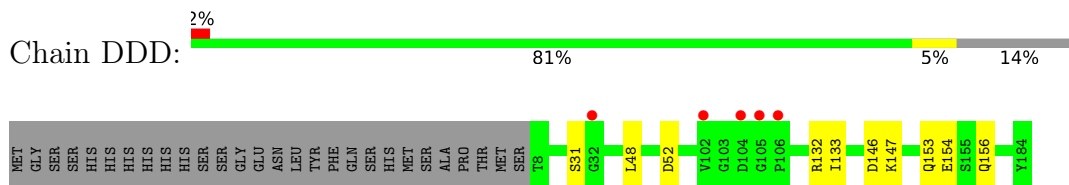
• Molecule 1: Small Alarmone Hydrolase
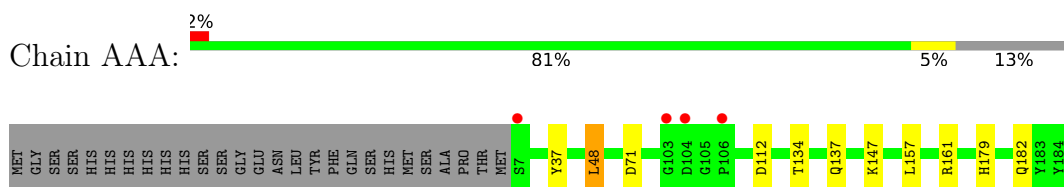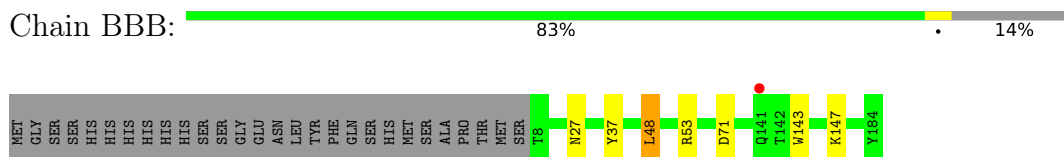
Chain AAA:

• Molecule 1: Small Alarmone Hydrolase

Chain BBB:

• Molecule 1: Small Alarmone Hydrolase

Chain CCC:

• Molecule 1: Small Alarmone Hydrolase

Chain DDD:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.15Å 86.05Å 122.58Å 90.00° 101.77° 90.00°	Depositor
Resolution (Å)	43.06 – 1.74 57.28 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.3 (43.06-1.74) 99.3 (57.28-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.152 , 0.227 0.166 , 0.234	Depositor DCC
R_{free} test set	4527 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 50.2	EDS
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6242	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	AAA	0.84	0/1453	0.92	2/1973 (0.1%)
1	BBB	0.84	0/1461	0.90	1/1983 (0.1%)
1	CCC	0.84	1/1476 (0.1%)	0.96	3/2003 (0.1%)
1	DDD	0.89	3/1448 (0.2%)	0.95	3/1966 (0.2%)
All	All	0.85	4/5838 (0.1%)	0.93	9/7925 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	DDD	133	ILE	C-O	5.46	1.33	1.23
1	DDD	31	SER	C-O	5.35	1.33	1.23
1	DDD	154	GLU	CD-OE2	-5.16	1.20	1.25
1	CCC	94	GLY	C-O	5.12	1.31	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	CCC	174[A]	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	CCC	174[B]	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	DDD	146	ASP	N-CA-CB	-6.03	99.74	110.60
1	DDD	132	ARG	NE-CZ-NH2	5.87	123.24	120.30
1	CCC	108	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	AAA	48	LEU	CA-CB-CG	-5.30	103.12	115.30
1	AAA	161	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	DDD	48	LEU	CA-CB-CG	-5.13	103.50	115.30
1	BBB	48	LEU	CA-CB-CG	-5.10	103.57	115.30

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	AAA	1422	0	1385	8	0
1	BBB	1429	0	1395	5	0
1	CCC	1439	0	1408	11	0
1	DDD	1417	0	1384	6	0
2	AAA	1	0	0	0	0
2	BBB	1	0	0	0	0
2	CCC	1	0	0	0	0
2	DDD	1	0	0	0	0
3	AAA	146	0	0	0	0
3	BBB	125	0	0	0	0
3	CCC	127	0	0	0	0
3	DDD	133	0	0	0	0
All	All	6242	0	5572	23	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 2.

All (23) 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:BBB:37:TYR:OH	1:BBB:71:ASP:OD2	2.05	0.68
1:AAA:37:TYR:OH	1:AAA:71:ASP:OD2	2.09	0.67
1:AAA:112[B]:ASP:OD1	1:CCC:181:ARG:NH2	2.28	0.66
1:CCC:37:TYR:OH	1:CCC:71:ASP:OD2	2.13	0.64
1:AAA:157:LEU:HD13	1:CCC:153[A]:GLN:HE21	1.65	0.60
1:CCC:74:GLN:HG2	1:CCC:101:ARG:O	2.02	0.59
1:CCC:145:GLN:NE2	1:CCC:184:TYR:HA	2.18	0.59
1:DDD:153[B]:GLN:NE2	1:DDD:156:GLN:HE22	2.02	0.57
1:DDD:153[B]:GLN:HE22	1:DDD:156:GLN:HE22	1.53	0.57
1:BBB:53:ARG:NH1	1:DDD:52:ASP:OD2	2.45	0.49
1:AAA:134:THR:O	1:AAA:137:GLN:HG2	2.13	0.48
1:CCC:145:GLN:HE22	1:CCC:184:TYR:HA	1.77	0.48
1:CCC:10:LEU:HD21	1:CCC:49:LEU:HD11	1.98	0.46
1:AAA:147:LYS:HD3	1:BBB:27:ASN:HB3	1.98	0.46
1:AAA:179:HIS:O	1:AAA:182:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:27:ASN:HB3	1:DDD:147:LYS:HD3	2.01	0.42
1:BBB:48:LEU:O	1:BBB:48:LEU:HG	2.15	0.42
1:CCC:27:ASN:CB	1:DDD:147:LYS:HD3	2.50	0.42
1:DDD:153[B]:GLN:NE2	1:DDD:156:GLN:NE2	2.67	0.42
1:CCC:48:LEU:HD13	1:CCC:48:LEU:C	2.40	0.41
1:AAA:48:LEU:O	1:AAA:48:LEU:HG	2.21	0.40
1:AAA:112[B]:ASP:CG	1:CCC:181:ARG:HH22	2.25	0.40
1:BBB:143:TRP:CE2	1:BBB:147:LYS:HE3	2.57	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	AAA	177/205 (86%)	174 (98%)	3 (2%)	0	100	100
1	BBB	177/205 (86%)	174 (98%)	3 (2%)	0	100	100
1	CCC	179/205 (87%)	176 (98%)	3 (2%)	0	100	100
1	DDD	176/205 (86%)	173 (98%)	3 (2%)	0	100	100
All	All	709/820 (86%)	697 (98%)	12 (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	AAA	146/169 (86%)	146 (100%)	0	100	100
1	BBB	146/169 (86%)	146 (100%)	0	100	100
1	CCC	148/169 (88%)	148 (100%)	0	100	100
1	DDD	145/169 (86%)	145 (100%)	0	100	100
All	All	585/676 (86%)	585 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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, 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(Å²)	Q<0.9
1	AAA	178/205 (86%)	0.06	4 (2%)	62	68	21, 27, 53, 84	0
1	BBB	177/205 (86%)	0.11	1 (0%)	89	92	20, 27, 51, 67	0
1	CCC	177/205 (86%)	0.08	5 (2%)	53	58	20, 27, 50, 73	0
1	DDD	177/205 (86%)	0.08	5 (2%)	53	58	20, 27, 54, 84	0
All	All	709/820 (86%)	0.08	15 (2%)	63	70	20, 27, 52, 84	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	104	ASP	4.6
1	AAA	7	SER	3.7
1	CCC	141	GLN	3.6
1	AAA	104	ASP	3.4
1	DDD	32	GLY	3.3
1	DDD	106	PRO	3.3
1	BBB	141	GLN	2.9
1	CCC	143	TRP	2.8
1	DDD	102	VAL	2.6
1	CCC	142	THR	2.4
1	DDD	105	GLY	2.4
1	CCC	106	PRO	2.3
1	CCC	145	GLN	2.2
1	AAA	106	PRO	2.0
1	AAA	103	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

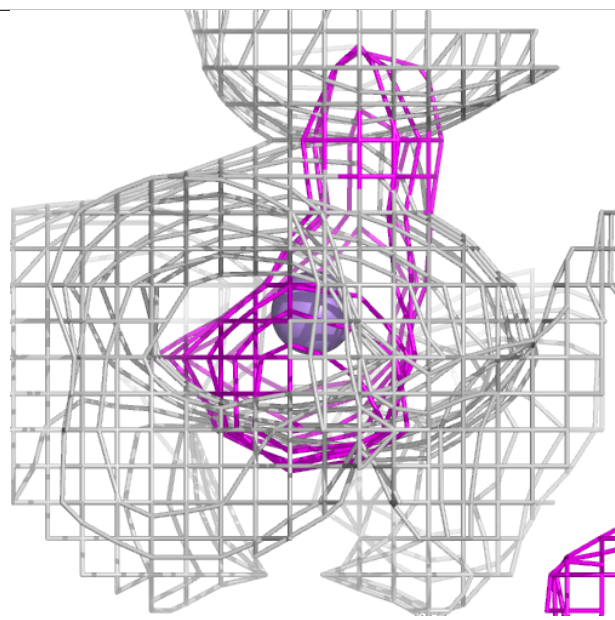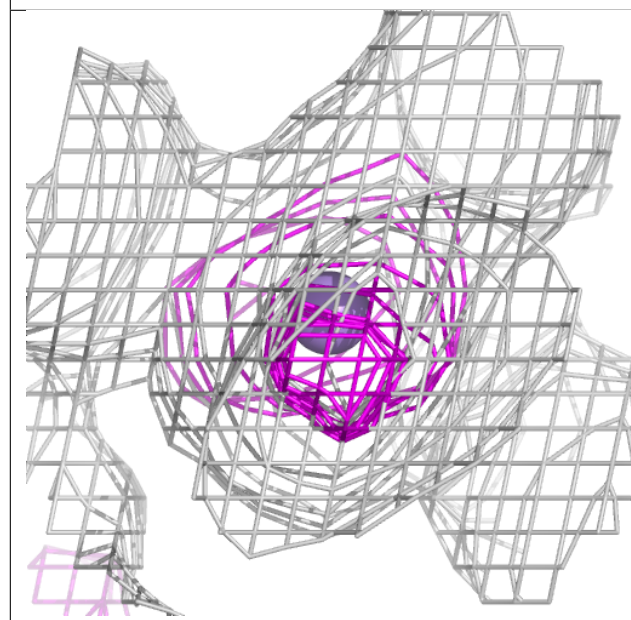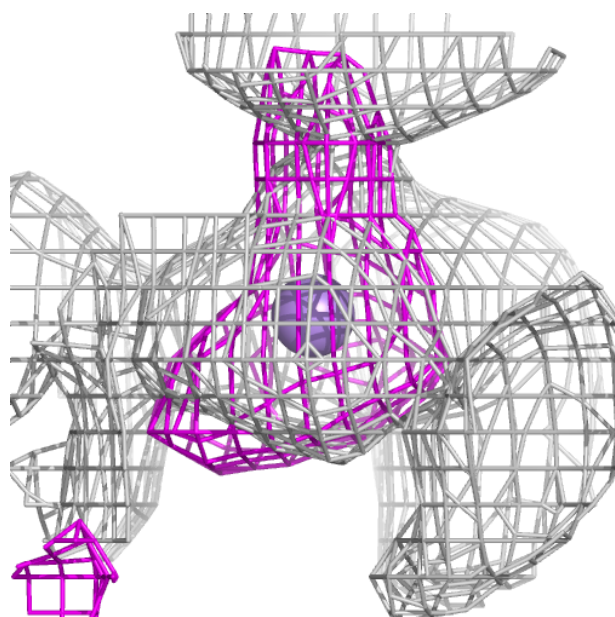There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
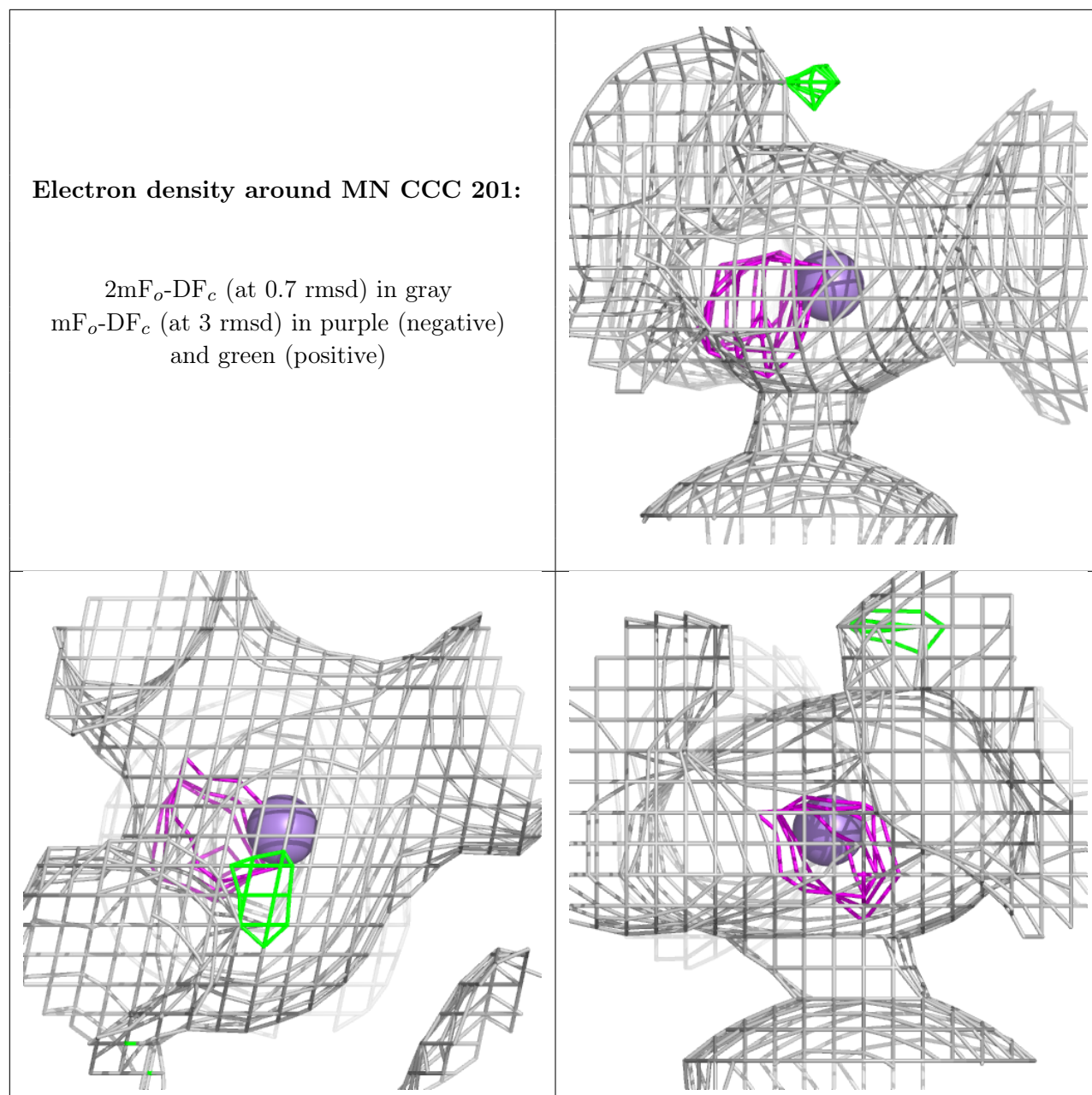
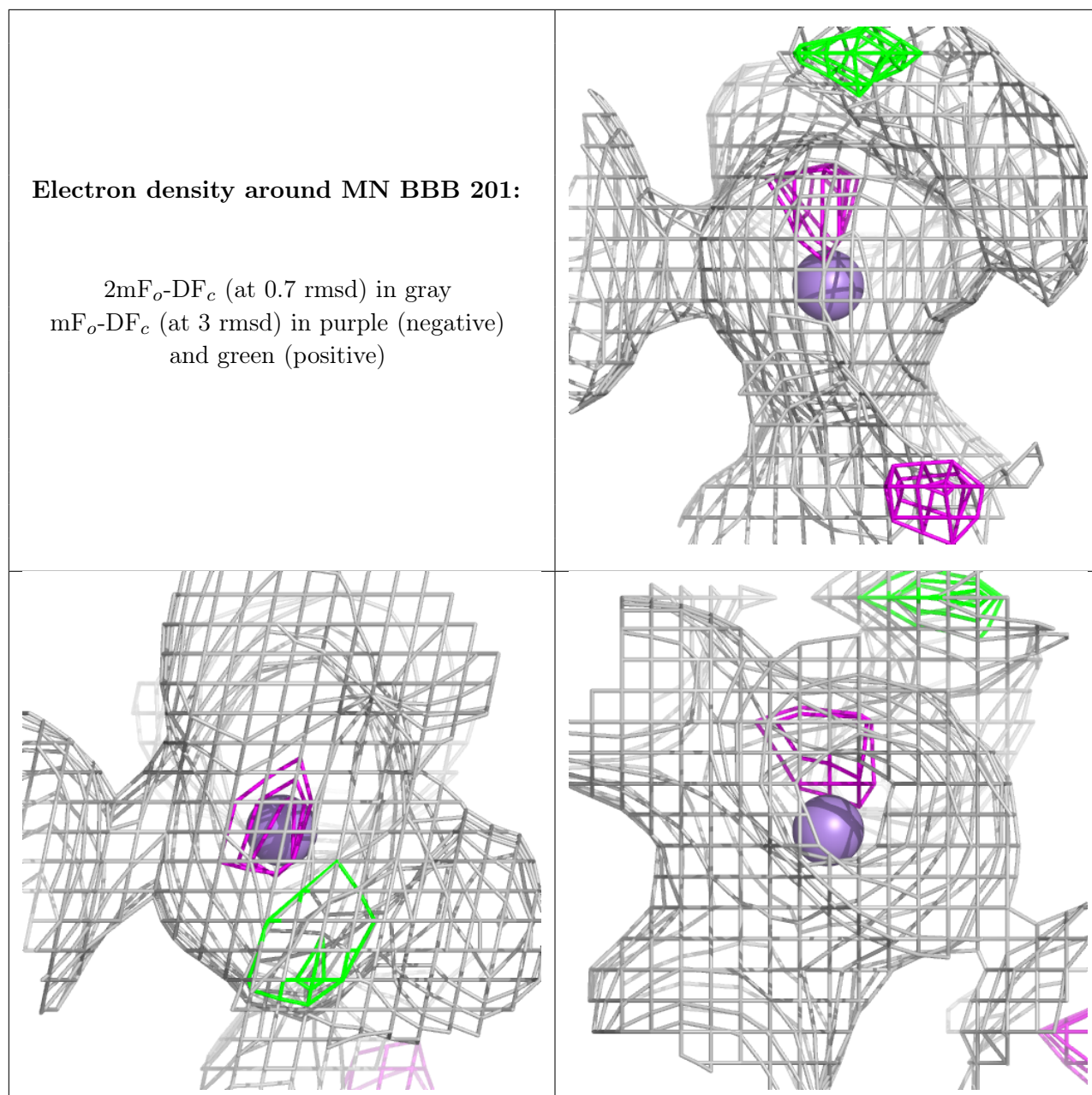| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MN	AAA	201	1/1	0.99	0.07	46,46,46,46	0
2	MN	CCC	201	1/1	0.99	0.05	46,46,46,46	0
2	MN	BBB	201	1/1	1.00	0.05	43,43,43,43	0
2	MN	DDD	201	1/1	1.00	0.10	46,46,46,46	0

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.
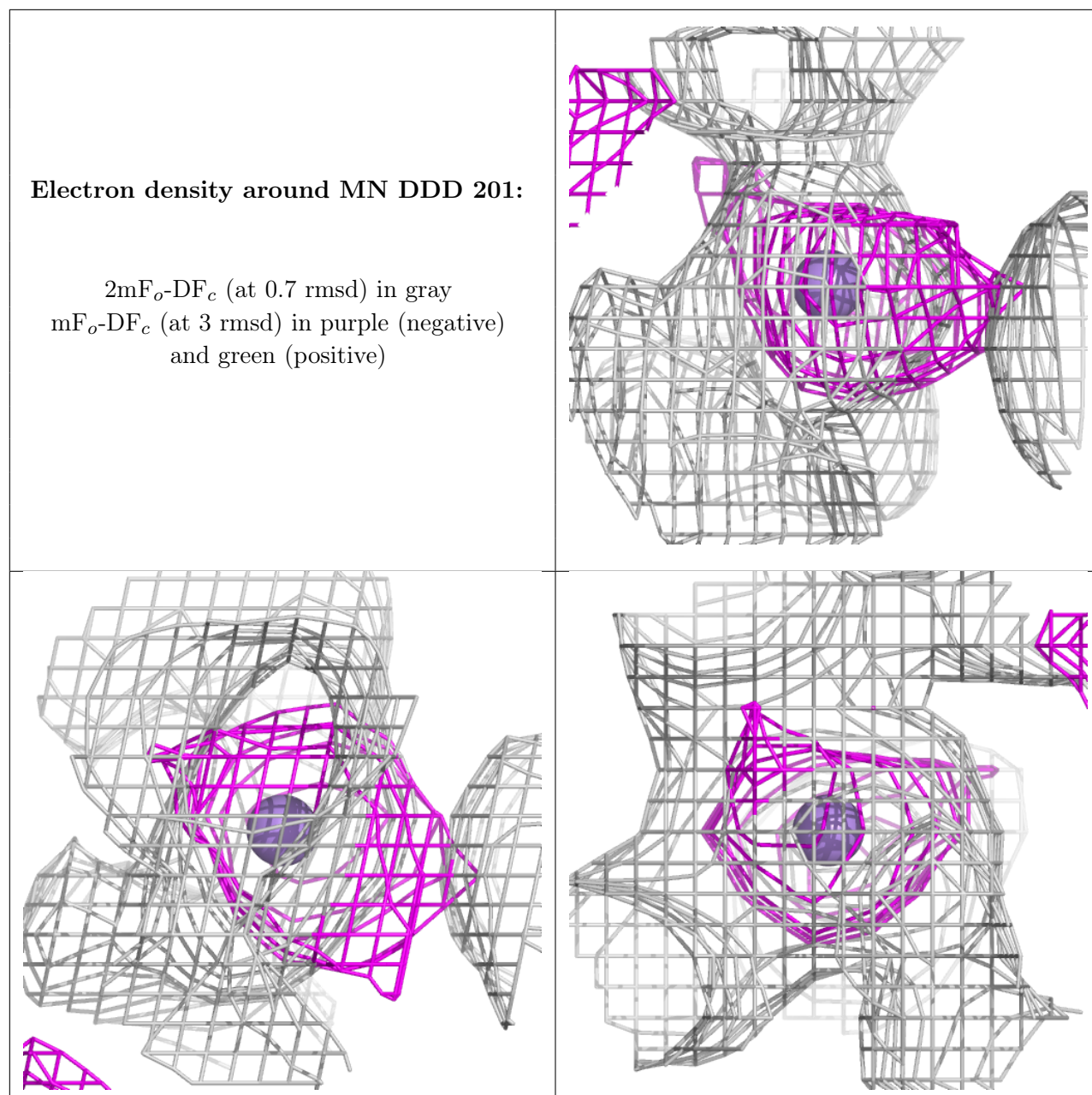
Electron density around MN AAA 201:

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

Electron density around MN CCC 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 BBB 201:

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

Electron density around MN DDD 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 ⓘ

There are no such residues in this entry.