



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:44 AM UTC

PDB ID : 8YYK / pdb_00008yyk
Title : Structure of RNase J2 wild type at room temperature
Authors : Singh, A.K.; Chinnasamy, K.; Gopal, B.
Deposited on : 2024-04-03
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

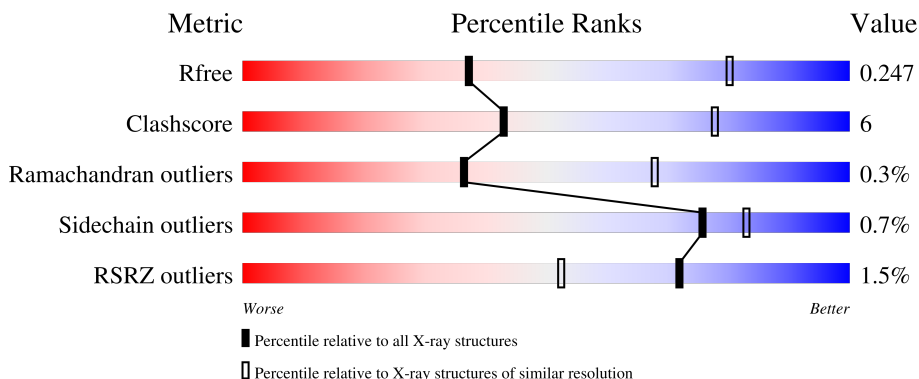
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	571	65% 11% 23%
1	B	571	66% 10% 24%
1	C	571	66% 11% 23%
1	D	571	67% 9% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13038 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 J 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3263	2094	540	608	21			
1	B	436	Total	C	N	O	S	0	0	0
			3248	2084	537	606	21			
1	C	437	Total	C	N	O	S	0	0	0
			3261	2093	540	608	20			
1	D	438	Total	C	N	O	S	0	0	0
			3262	2092	541	609	20			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q5HPR6
A	-12	GLY	-	expression tag	UNP Q5HPR6
A	-11	SER	-	expression tag	UNP Q5HPR6
A	-10	SER	-	expression tag	UNP Q5HPR6
A	-9	HIS	-	expression tag	UNP Q5HPR6
A	-8	HIS	-	expression tag	UNP Q5HPR6
A	-7	HIS	-	expression tag	UNP Q5HPR6
A	-6	HIS	-	expression tag	UNP Q5HPR6
A	-5	HIS	-	expression tag	UNP Q5HPR6
A	-4	HIS	-	expression tag	UNP Q5HPR6
A	-3	SER	-	expression tag	UNP Q5HPR6
A	-2	GLN	-	expression tag	UNP Q5HPR6
A	-1	ASP	-	expression tag	UNP Q5HPR6
A	0	PRO	-	expression tag	UNP Q5HPR6
B	-13	MET	-	initiating methionine	UNP Q5HPR6
B	-12	GLY	-	expression tag	UNP Q5HPR6
B	-11	SER	-	expression tag	UNP Q5HPR6
B	-10	SER	-	expression tag	UNP Q5HPR6
B	-9	HIS	-	expression tag	UNP Q5HPR6
B	-8	HIS	-	expression tag	UNP Q5HPR6
B	-7	HIS	-	expression tag	UNP Q5HPR6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP Q5HPR6
B	-5	HIS	-	expression tag	UNP Q5HPR6
B	-4	HIS	-	expression tag	UNP Q5HPR6
B	-3	SER	-	expression tag	UNP Q5HPR6
B	-2	GLN	-	expression tag	UNP Q5HPR6
B	-1	ASP	-	expression tag	UNP Q5HPR6
B	0	PRO	-	expression tag	UNP Q5HPR6
C	-13	MET	-	initiating methionine	UNP Q5HPR6
C	-12	GLY	-	expression tag	UNP Q5HPR6
C	-11	SER	-	expression tag	UNP Q5HPR6
C	-10	SER	-	expression tag	UNP Q5HPR6
C	-9	HIS	-	expression tag	UNP Q5HPR6
C	-8	HIS	-	expression tag	UNP Q5HPR6
C	-7	HIS	-	expression tag	UNP Q5HPR6
C	-6	HIS	-	expression tag	UNP Q5HPR6
C	-5	HIS	-	expression tag	UNP Q5HPR6
C	-4	HIS	-	expression tag	UNP Q5HPR6
C	-3	SER	-	expression tag	UNP Q5HPR6
C	-2	GLN	-	expression tag	UNP Q5HPR6
C	-1	ASP	-	expression tag	UNP Q5HPR6
C	0	PRO	-	expression tag	UNP Q5HPR6
D	-13	MET	-	initiating methionine	UNP Q5HPR6
D	-12	GLY	-	expression tag	UNP Q5HPR6
D	-11	SER	-	expression tag	UNP Q5HPR6
D	-10	SER	-	expression tag	UNP Q5HPR6
D	-9	HIS	-	expression tag	UNP Q5HPR6
D	-8	HIS	-	expression tag	UNP Q5HPR6
D	-7	HIS	-	expression tag	UNP Q5HPR6
D	-6	HIS	-	expression tag	UNP Q5HPR6
D	-5	HIS	-	expression tag	UNP Q5HPR6
D	-4	HIS	-	expression tag	UNP Q5HPR6
D	-3	SER	-	expression tag	UNP Q5HPR6
D	-2	GLN	-	expression tag	UNP Q5HPR6
D	-1	ASP	-	expression tag	UNP Q5HPR6
D	0	PRO	-	expression tag	UNP Q5HPR6

- Molecule 2 is MANGANESE (II) ION (CCD ID: 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

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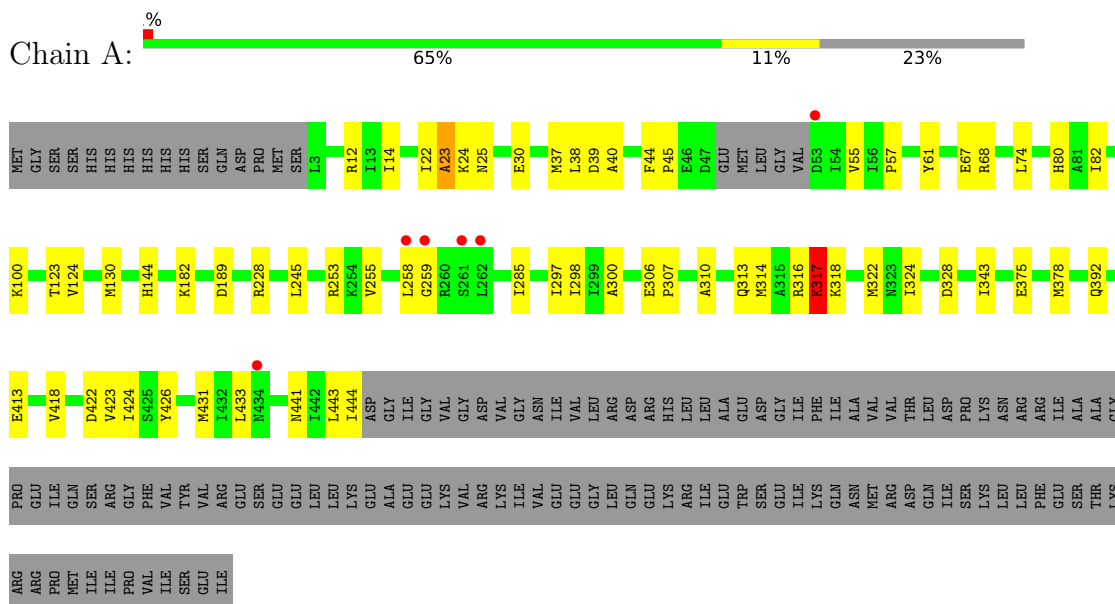
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

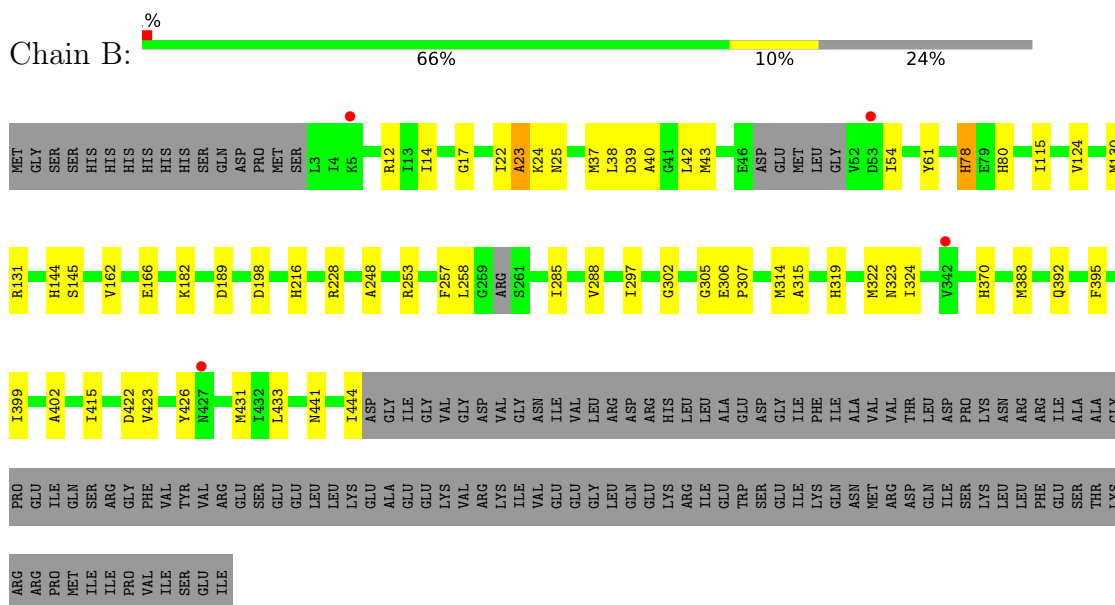
3 Residue-property plots [i](#)

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: Ribonuclease J 2



• Molecule 1: Ribonuclease J 2



Chain C:

Position	Amino Acid	Background Color	Red Dot
1	ILE	Grey	No
2	GLN	Green	No
3	SER	Green	No
4	ILE	Green	No
5	ARG	Green	No
6	GLY	Green	No
7	PHE	Green	No
8	VAL	Green	No
9	ILE	Green	No
10	SER	Green	No
11	GLU	Green	No
12	ILE	Green	No
13	SER	Green	No
14	GLN	Green	No
15	ASP	Green	No
16	GLU	Green	No
17	GLU	Green	No
18	LEU	Green	No
19	LYS	Green	No
20	ASP	Green	No
21	ALA	Green	No
22	ILE	Green	No
23	GLU	Green	No
24	GLU	Green	No
25	LYS	Green	No
26	VAL	Green	No
27	GLY	Green	No
28	VAL	Green	No
29	GLU	Green	No
30	GLY	Green	No
31	LEU	Green	No
32	ARG	Green	No
33	LYS	Green	No
34	ILE	Green	No
35	VAL	Green	No
36	GLU	Green	No
37	GLY	Green	No
38	LEU	Green	No
39	GLN	Green	No
40	GLU	Green	No
41	LYS	Green	No
42	ARG	Green	No
43	LEU	Green	No
44	ALA	Green	No
45	GLU	Green	No
46	TRP	Green	No
47	ASP	Green	No
48	GLY	Green	No
49	ILE	Green	No
50	LYS	Green	No
51	GLN	Green	No
52	ASN	Green	No
53	MET	Green	No
54	ARG	Green	No
55	ASP	Green	No
56	GLN	Green	No
57	ILE	Green	No
58	SER	Green	No
59	LYS	Green	No
60	LEU	Green	No
61	LEU	Green	No
62	PHE	Green	No
63	GLU	Green	No
64	SER	Green	No
65	THR	Green	No
66	LYS	Green	No
67	ARG	Green	No
68	PRO	Green	No
69	CTU	Green	No
70	ILE	Green	No
71	ALA	Green	No
72	ALA	Green	No
73	THR	Green	No
74	LYS	Green	No
75	GLY	Green	No
76	ARG	Green	No
77	PRO	Green	No
78	ASP	Green	No
79	LEU	Green	No
80	GLY	Green	No
81	ASP	Green	No
82	THR	Green	No
83	GLY	Green	No
84	VAL	Green	No
85	LEU	Green	No
86	ASP	Green	No
87	GLY	Green	No
88	LEU	Green	No
89	GLY	Green	No
90	ASP	Green	No
91	GLU	Green	No
92	ASP	Green	No
93	GLU	Green	No
94	ASP	Green	No
95	P45	Green	No
96	P45	Green	No
97	F44	Green	No
98	M43	Green	No
99	L42	Green	No
100	G41	Green	No
101	A40	Green	No
102	D39	Green	No
103	L38	Green	No
104	M37	Green	No
105	E30	Green	No
106	N25	Green	No
107	K24	Green	No
108	E21	Green	No
109	I14	Green	No
110	I13	Green	No
111	R12	Green	No
112	L3	Green	No
113	SER	Green	No
114	GLN	Green	No
115	ASP	Green	No
116	PRO	Green	No
117	MET	Green	No
118	MET	Green	No
119	Y177	Green	No
120	H176	Green	No
121	G175	Green	No
122	K168	Green	No
123	H144	Green	No
124	M130	Green	No
125	HIS	Green	No
126	V124	Green	No
127	T123	Green	No
128	Y122	Green	No
129	SER	Green	No
130	K100	Green	No
131	P95	Green	No
132	I343	Green	No
133	E413	Green	No
134	V422	Green	No
135	D422	Green	No
136	H427	Green	Yes
137	L444	Green	No

Chain D:

Amino Acid	Count
MET	1
GLY	1
SER	1
SER	1
HIS	1
HIS	1
HIS	1
HIS	1
HIS	1
SER	1
GLN	1
ASP	1
PRO	1
PRO	1
MET	1
SER	1
L3	1
R12	1
I13	1
I14	1
T22	1
K23	1
K24	1
N25	1
K37	1
L38	1
D39	1
A40	1
G41	1
L42	1
F46	1
ASP	1
GLU	1
MET	1
LEU	1
G51	1
P57	1
Q60	1
Y61	1
G77	1
H78	1
E79	1
H80	1
L105	1
I115	1
V124	1
M130	1
R131	1
H144	1
S145	1
D198	1
H217	1
R228	1
A248	1
R253	1
L258	1
L297	1
A300	1
T301	1
G302	1
K303	1
K304	1
G305	1
E306	1
P307	1
V308	1
E309	1
G313	1
K314	1
A315	1
R316	1
K322	1
K323	1
T324	1
F331	1
L332	1
A333	1
K339	1
L359	1
L365	1
H370	1
Q392	1
F395	1
L399	1
D422	1
V423	1
K429	1
D430	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.30Å 133.38Å 117.75Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	58.60 – 3.20 58.60 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.7 (58.60-3.20) 89.7 (58.60-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0350	Depositor
R, R_{free}	0.205 , 0.248 0.208 , 0.247	Depositor DCC
R_{free} test set	1392 reflections (4.17%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.139 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13038	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

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	0.61	2/3325 (0.1%)	0.94	3/4513 (0.1%)
1	B	0.62	5/3309 (0.2%)	0.95	0/4492
1	C	0.59	2/3323 (0.1%)	0.93	0/4512
1	D	0.61	2/3324 (0.1%)	0.93	2/4513 (0.0%)
All	All	0.60	11/13281 (0.1%)	0.94	5/18030 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	D	0	3
All	All	0	6

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	HIS	CE1-NE2	7.56	1.40	1.32
1	C	80	HIS	CE1-NE2	7.44	1.40	1.32
1	B	144	HIS	CE1-NE2	7.40	1.40	1.32
1	D	144	HIS	CE1-NE2	7.35	1.39	1.32
1	A	80	HIS	CE1-NE2	7.29	1.39	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	LYS	CB-CA-C	8.67	127.67	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	LYS	N-CA-C	-6.77	94.84	107.71
1	A	317	LYS	N-CA-C	-6.41	97.15	110.80
1	D	23	ALA	N-CA-C	5.86	123.28	110.80
1	A	318	LYS	N-CA-C	5.78	120.28	113.23

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	68	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	228	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	24	LYS	Mainchain

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	3263	0	3140	40	0
1	B	3248	0	3112	42	0
1	C	3261	0	3134	43	0
1	D	3262	0	3128	36	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
All	All	13038	0	12514	159	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 6.

The worst 5 of 159 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:C:258:LEU:HD23	1:C:300:ALA:HA	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LYS:O	1:D:430:ASP:OD1	1.91	0.88
1:B:24:LYS:NZ	1:B:441:ASN:OD1	2.09	0.86
1:D:37:MET:HE3	1:D:40:ALA:HB2	1.60	0.84
1:A:258:LEU:HD23	1:A:300:ALA:HA	1.59	0.82

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	433/571 (76%)	416 (96%)	15 (4%)	2 (0%)	24	59
1	B	430/571 (75%)	407 (95%)	22 (5%)	1 (0%)	43	73
1	C	433/571 (76%)	416 (96%)	16 (4%)	1 (0%)	43	73
1	D	434/571 (76%)	417 (96%)	16 (4%)	1 (0%)	43	73
All	All	1730/2284 (76%)	1656 (96%)	69 (4%)	5 (0%)	36	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	ALA
1	B	23	ALA
1	A	317	LYS
1	D	23	ALA
1	C	24	LYS

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	330/496 (66%)	328 (99%)	2 (1%)	78	84
1	B	327/496 (66%)	325 (99%)	2 (1%)	78	84
1	C	329/496 (66%)	326 (99%)	3 (1%)	70	81
1	D	328/496 (66%)	326 (99%)	2 (1%)	78	84
All	All	1314/1984 (66%)	1305 (99%)	9 (1%)	76	83

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	115	ILE
1	D	258	LEU
1	B	444	ILE
1	C	258	LEU
1	C	343	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	349	ASN
1	C	392	GLN
1	D	392	GLN
1	D	134	ASN
1	D	357	HIS

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 oligosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	437/571 (76%)	-0.05	6 (1%) 73 54	12, 34, 72, 115	0
1	B	436/571 (76%)	0.04	4 (0%) 81 64	15, 38, 82, 112	0
1	C	437/571 (76%)	0.05	9 (2%) 63 43	18, 39, 74, 118	0
1	D	438/571 (76%)	0.23	8 (1%) 67 48	21, 45, 98, 121	0
All	All	1748/2284 (76%)	0.07	27 (1%) 72 52	12, 39, 81, 121	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	53	ASP	3.9
1	D	333	ALA	3.5
1	C	427	ASN	3.3
1	A	259	GLY	3.0
1	C	261	SER	2.9

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](#)

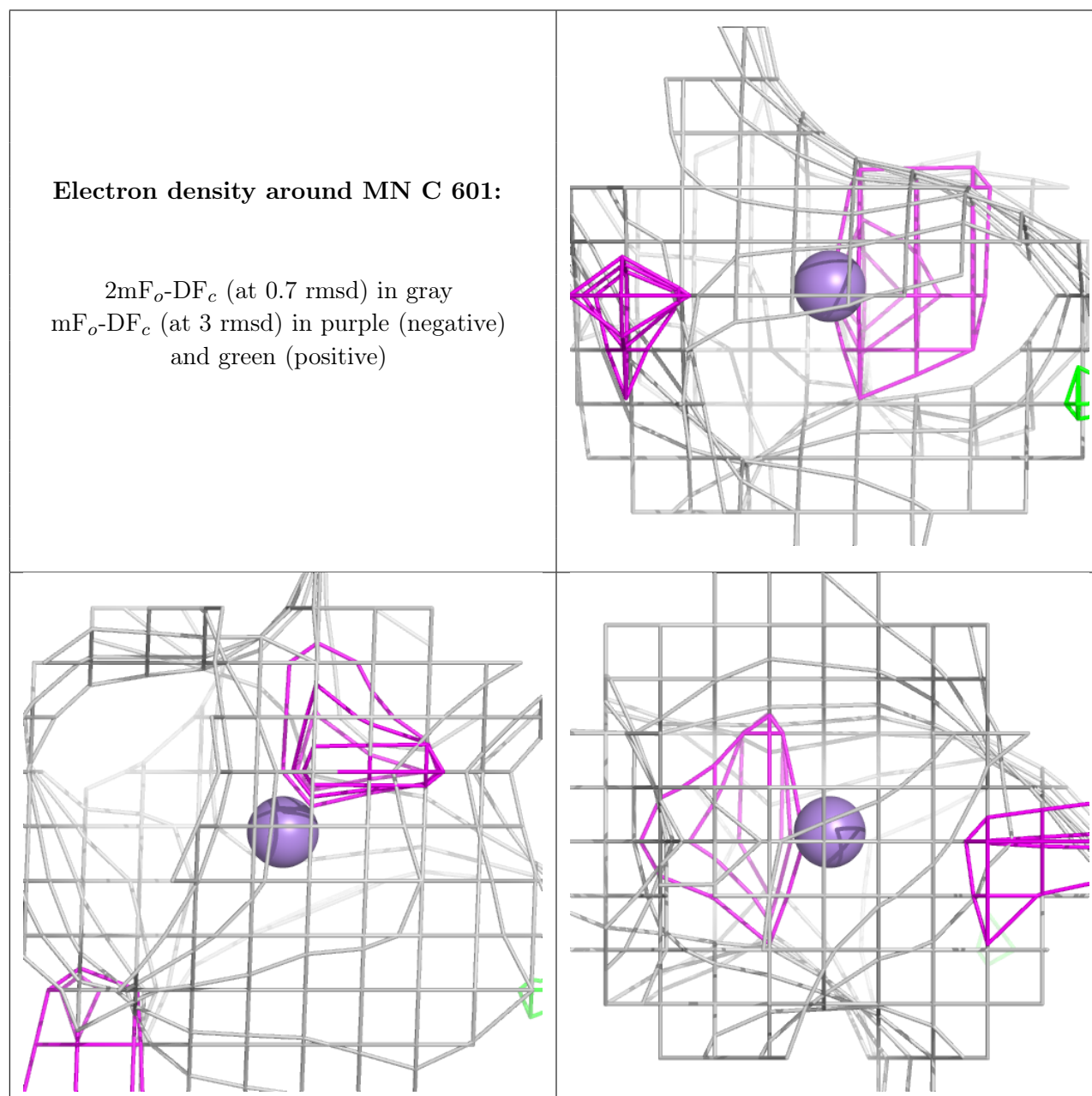
There are no oligosaccharides in this entry.

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.

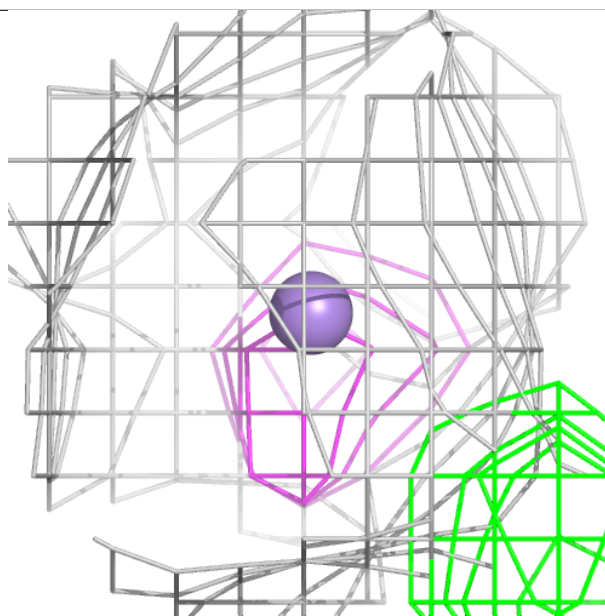
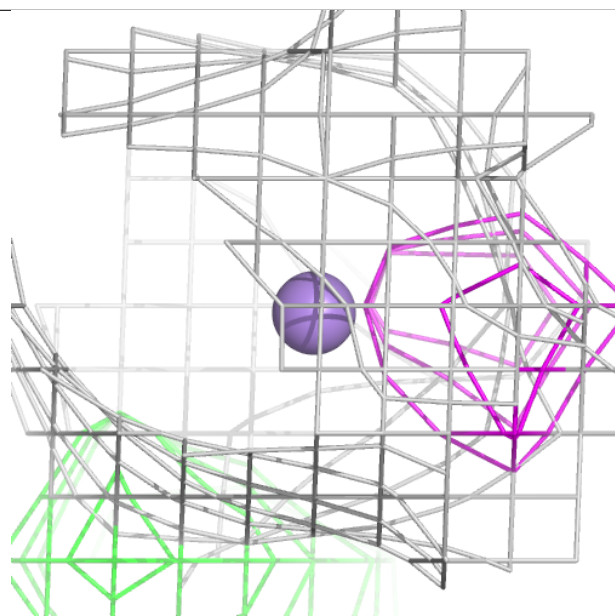
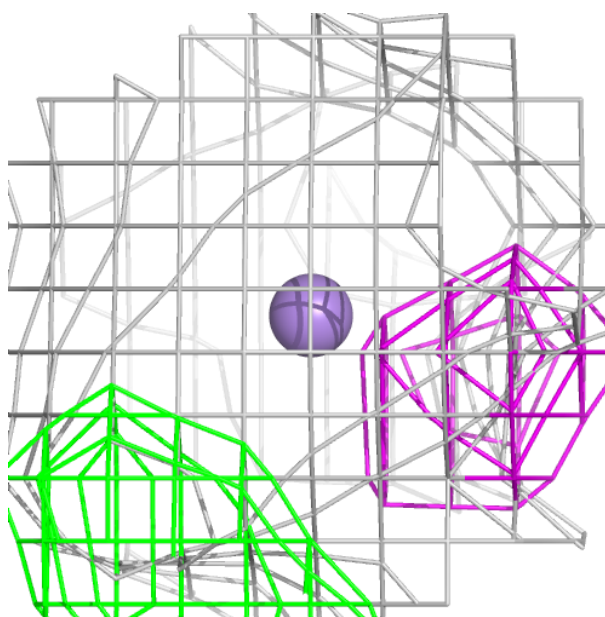
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MN	C	601	1/1	0.93	0.14	85,85,85,85	0
2	MN	B	601	1/1	0.95	0.07	36,36,36,36	0
2	MN	D	601	1/1	0.97	0.05	55,55,55,55	0
2	MN	A	601	1/1	0.99	0.10	47,47,47,47	0

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.



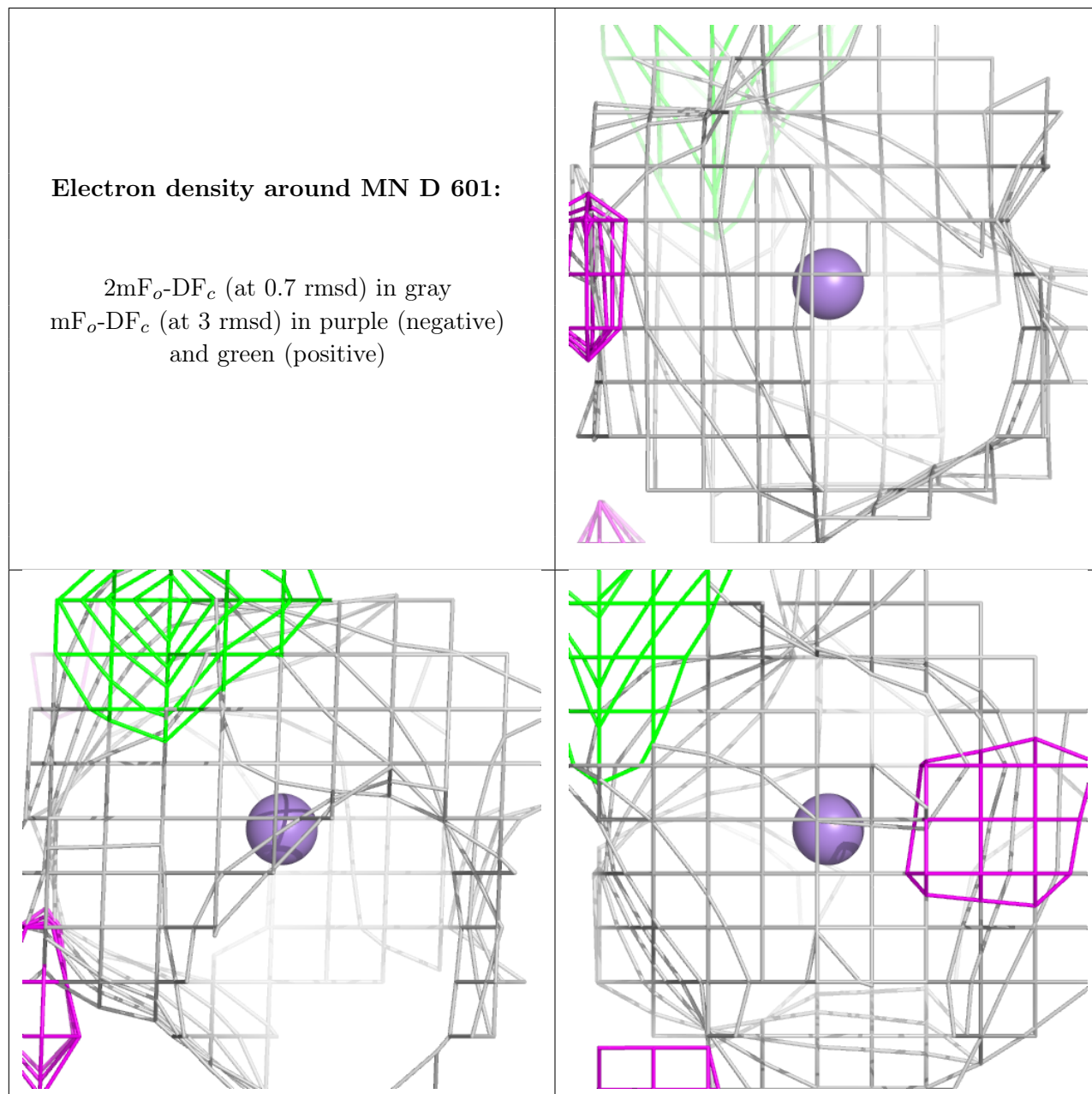
Electron density around MN B 601:

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



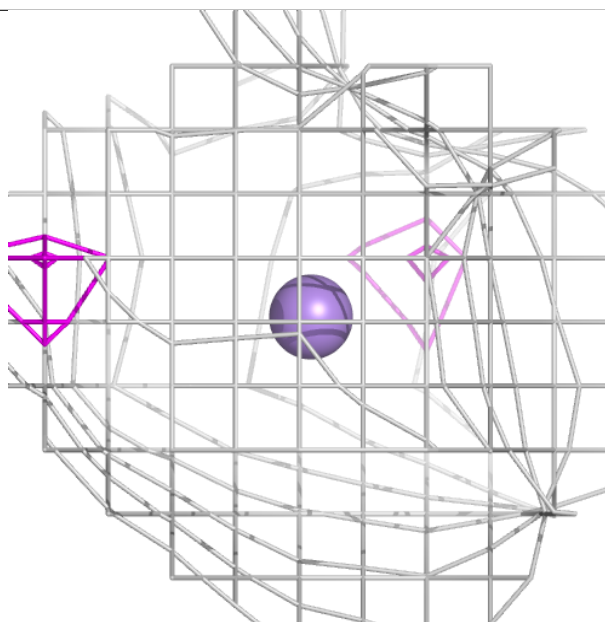
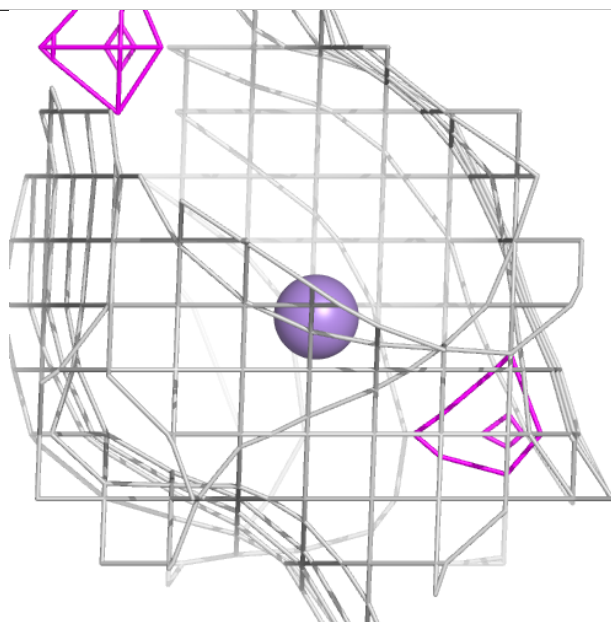
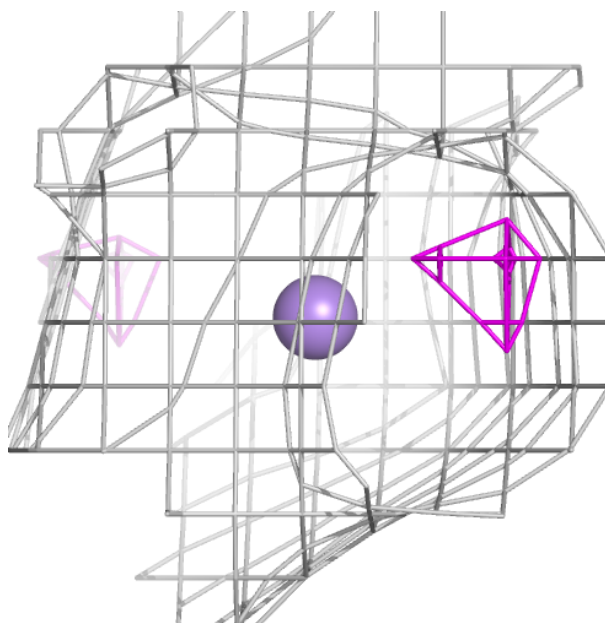
Electron density around MN D 601:

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



Electron density around MN A 601:

$2mF_o-DF_c$ (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.