



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:45 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 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

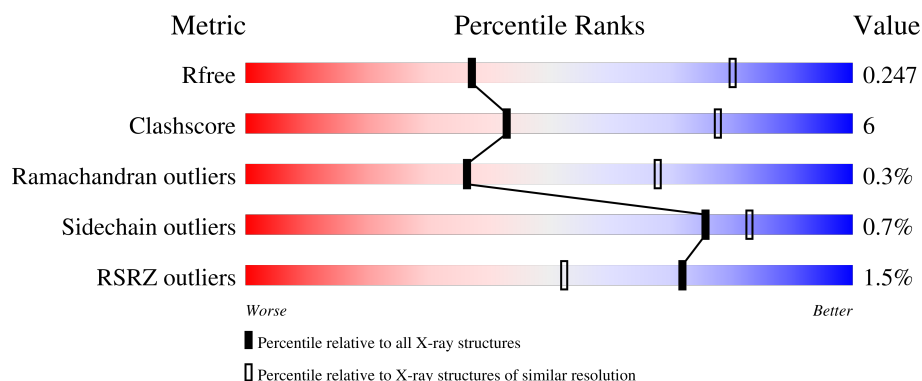
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	0.2% 65% 11% 23%
1	B	571	0.2% 66% 10% 24%
1	C	571	2% 66% 11% 23%
1	D	571	0.2% 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

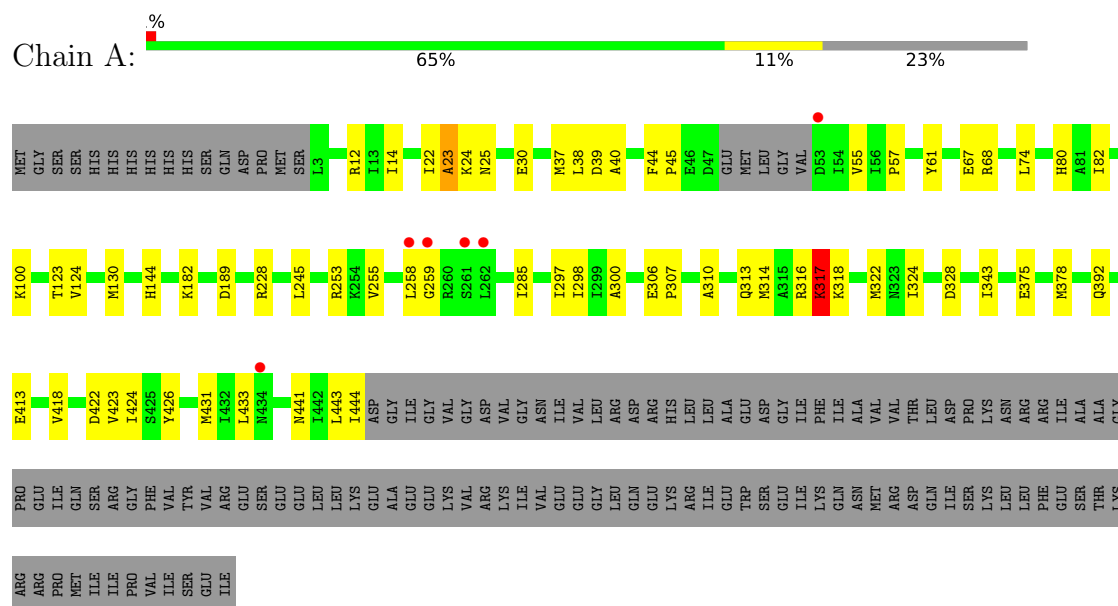
Continued from previous page...

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

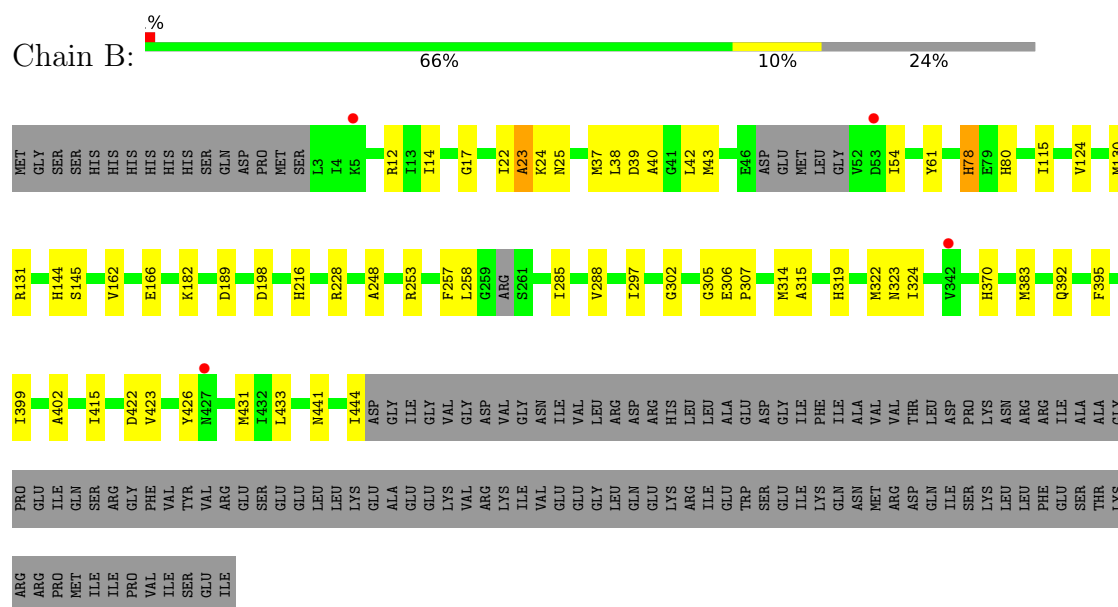
3 Residue-property plots [i](#)

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.

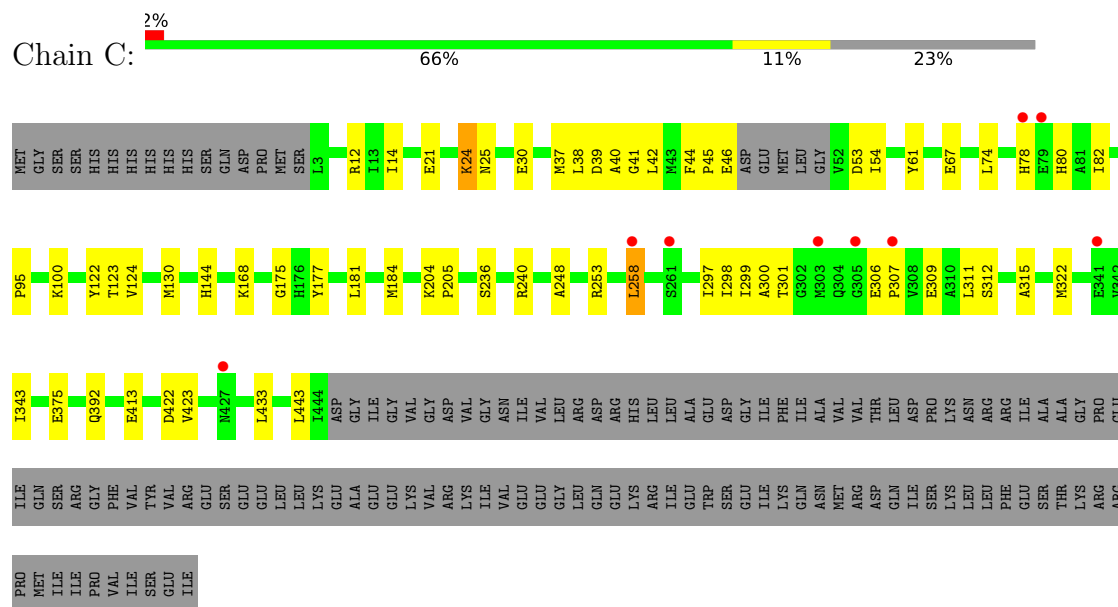
• Molecule 1: Ribonuclease J 2



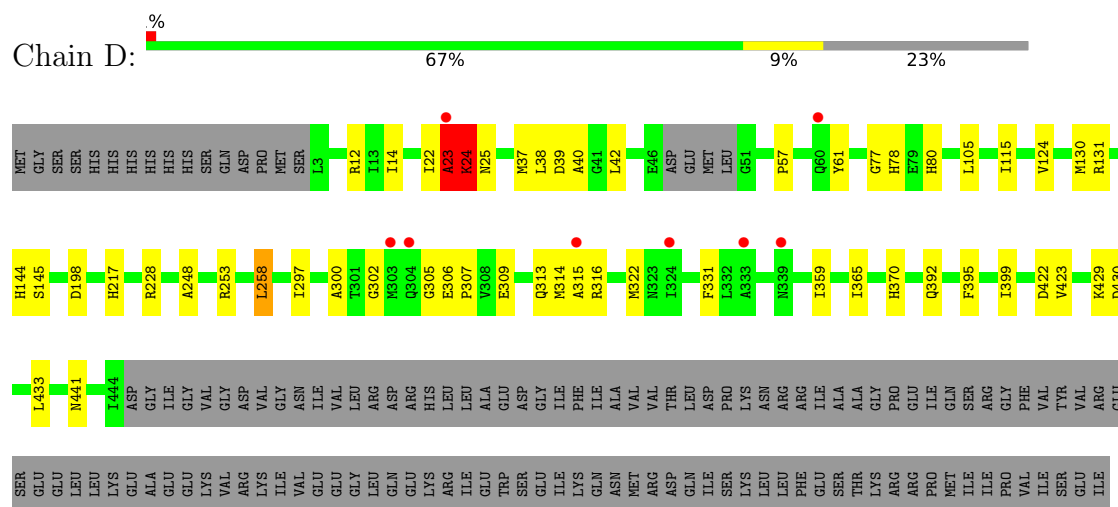
• Molecule 1: Ribonuclease J 2



- Molecule 1: Ribonuclease J 2



- Molecule 1: Ribonuclease J 2



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 [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	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

All (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
1	B	80	HIS	CE1-NE2	7.23	1.39	1.32
1	A	144	HIS	CE1-NE2	6.11	1.38	1.32
1	C	144	HIS	CE1-NE2	5.53	1.38	1.32
1	B	216	HIS	CE1-NE2	5.38	1.38	1.32
1	B	166	GLU	CD-OE1	5.09	1.35	1.25
1	B	78	HIS	CE1-NE2	5.04	1.37	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
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.

All (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	228	ARG	Sidechain
1	D	24	LYS	Mainchain

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	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.

All (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
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
1:B:54:ILE:O	1:B:54:ILE:HG13	1.85	0.77
1:D:258:LEU:HD23	1:D:300:ALA:HA	1.69	0.75
1:B:24:LYS:NZ	1:B:441:ASN:CG	2.46	0.74
1:C:37:MET:HE3	1:C:40:ALA:HB2	1.68	0.73
1:D:24:LYS:NZ	1:D:441:ASN:OD1	2.21	0.73
1:C:14:ILE:HG12	1:C:423:VAL:HG22	1.72	0.71
1:A:310:ALA:O	1:A:314:MET:HG3	1.91	0.71
1:A:37:MET:HE3	1:A:40:ALA:HB2	1.74	0.70
1:A:316:ARG:O	1:A:317:LYS:C	2.34	0.69
1:C:53:ASP:O	1:C:54:ILE:HD13	1.92	0.69
1:D:24:LYS:NZ	1:D:441:ASN:CG	2.51	0.68
1:C:53:ASP:O	1:C:54:ILE:HG12	1.93	0.68
1:C:53:ASP:O	1:C:54:ILE:CD1	2.42	0.68
1:D:23:ALA:O	1:D:42:LEU:O	2.12	0.68
1:B:24:LYS:HG3	1:B:43:MET:HB2	1.76	0.67
1:A:316:ARG:C	1:A:317:LYS:O	2.32	0.67
1:B:314:MET:HB3	1:B:324:ILE:HG23	1.78	0.65
1:B:258:LEU:HA	1:B:285:ILE:CD1	2.26	0.64
1:C:309:GLU:O	1:C:312:SER:HB3	1.96	0.64
1:C:53:ASP:O	1:C:54:ILE:CG1	2.46	0.64
1:A:14:ILE:HG12	1:A:423:VAL:HG22	1.79	0.64
1:A:189:ASP:OD2	1:B:182:LYS:HD3	1.98	0.64
1:D:12:ARG:NH1	1:D:61:TYR:OH	2.31	0.62
1:A:45:PRO:HD3	1:A:55:VAL:HG23	1.82	0.61
1:C:24:LYS:O	1:C:24:LYS:HG3	2.00	0.61
1:B:422:ASP:HB3	1:B:433:LEU:HD11	1.83	0.61
1:D:24:LYS:HZ3	1:D:441:ASN:CG	2.08	0.60
1:C:124:VAL:HG12	1:C:130:MET:CE	2.30	0.60
1:D:14:ILE:HG12	1:D:423:VAL:HG22	1.83	0.60
1:D:253:ARG:HD3	1:D:297:ILE:HG13	1.84	0.60
1:B:124:VAL:HG12	1:B:130:MET:HE2	1.83	0.60
1:B:14:ILE:HG12	1:B:423:VAL:HG22	1.82	0.60
1:B:37:MET:HE3	1:B:40:ALA:HB2	1.85	0.59
1:A:124:VAL:HG12	1:A:130:MET:HE2	1.85	0.59
1:C:124:VAL:HG12	1:C:130:MET:HE2	1.85	0.58
1:B:22:ILE:O	1:B:23:ALA:HB2	2.02	0.58
1:C:38:LEU:O	1:C:39:ASP:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:GLY:HA3	1:B:307:PRO:HD3	1.87	0.56
1:B:124:VAL:HG12	1:B:130:MET:CE	2.36	0.56
1:A:24:LYS:HG2	1:A:57:PRO:HG3	1.88	0.56
1:D:314:MET:O	1:D:316:ARG:O	2.24	0.56
1:C:298:ILE:HG12	1:C:322:MET:HE1	1.88	0.56
1:A:74:LEU:HD13	1:A:82:ILE:HG22	1.89	0.55
1:B:258:LEU:HA	1:B:285:ILE:HD12	1.87	0.55
1:C:253:ARG:HD3	1:C:297:ILE:HG13	1.89	0.55
1:B:12:ARG:NH1	1:B:61:TYR:OH	2.34	0.55
1:B:395:PHE:CE2	1:B:399:ILE:HD11	2.42	0.55
1:D:302:GLY:HA3	1:D:307:PRO:HD3	1.89	0.53
1:A:100:LYS:HD2	1:A:123:THR:HG21	1.91	0.53
1:A:313:GLN:O	1:A:317:LYS:O	2.27	0.52
1:D:248:ALA:HB2	1:D:297:ILE:HD12	1.91	0.52
1:A:24:LYS:CG	1:A:57:PRO:HG3	2.40	0.52
1:C:25:ASN:OD1	1:C:392:GLN:NE2	2.43	0.52
1:B:25:ASN:OD1	1:B:392:GLN:NE2	2.42	0.52
1:B:302:GLY:CA	1:B:307:PRO:HD3	2.40	0.52
1:D:422:ASP:HB3	1:D:433:LEU:HD11	1.91	0.52
1:A:258:LEU:HD23	1:A:300:ALA:CA	2.36	0.51
1:A:426:TYR:HB2	1:A:431:MET:HE3	1.91	0.51
1:C:12:ARG:NH1	1:C:61:TYR:OH	2.40	0.51
1:B:38:LEU:O	1:B:39:ASP:HB2	2.11	0.51
1:D:306:GLU:N	1:D:307:PRO:CD	2.74	0.51
1:D:314:MET:HG2	1:D:322:MET:O	2.11	0.51
1:C:21:GLU:OE2	1:C:24:LYS:CE	2.59	0.50
1:D:38:LEU:O	1:D:39:ASP:HB2	2.11	0.50
1:B:24:LYS:HZ2	1:B:441:ASN:CG	2.20	0.50
1:A:298:ILE:HG12	1:A:322:MET:HE1	1.93	0.50
1:D:306:GLU:N	1:D:307:PRO:HD2	2.26	0.50
1:D:306:GLU:O	1:D:309:GLU:N	2.45	0.49
1:D:305:GLY:C	1:D:307:PRO:HD2	2.38	0.49
1:A:253:ARG:HD3	1:A:297:ILE:HG13	1.94	0.49
1:C:21:GLU:OE2	1:C:24:LYS:HE2	2.12	0.49
1:D:198:ASP:OD2	1:D:370:HIS:ND1	2.33	0.49
1:D:124:VAL:HG12	1:D:130:MET:HE2	1.94	0.49
1:B:17:GLY:HA3	1:B:24:LYS:O	2.11	0.49
1:C:24:LYS:HA	1:C:41:GLY:C	2.38	0.48
1:C:42:LEU:C	1:C:42:LEU:HD12	2.37	0.48
1:A:22:ILE:O	1:A:23:ALA:HB2	2.14	0.48
1:A:306:GLU:O	1:A:307:PRO:C	2.56	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:MET:CE	1:D:40:ALA:HB2	2.37	0.48
1:B:24:LYS:HG3	1:B:43:MET:CB	2.43	0.47
1:C:74:LEU:HD13	1:C:82:ILE:HG22	1.96	0.47
1:B:24:LYS:HZ3	1:B:441:ASN:CG	2.22	0.47
1:A:375:GLU:HA	1:A:378:MET:HE3	1.96	0.47
1:B:314:MET:HG3	1:B:319:HIS:CD2	2.50	0.47
1:C:67:GLU:H	1:C:67:GLU:CD	2.22	0.47
1:C:168:LYS:HG2	1:C:375:GLU:OE2	2.15	0.47
1:D:22:ILE:O	1:D:23:ALA:HB3	2.15	0.47
1:C:306:GLU:N	1:C:307:PRO:CD	2.78	0.47
1:C:45:PRO:O	1:C:46:GLU:C	2.58	0.46
1:B:306:GLU:N	1:B:307:PRO:HD2	2.30	0.46
1:B:257:PHE:O	1:B:258:LEU:C	2.59	0.46
1:A:418:VAL:HG11	1:A:424:ILE:HD11	1.98	0.46
1:A:245:LEU:HD23	1:A:255:VAL:HG21	1.98	0.46
1:D:315:ALA:O	1:D:316:ARG:C	2.58	0.46
1:B:198:ASP:OD2	1:B:370:HIS:ND1	2.36	0.45
1:D:217:HIS:ND1	1:D:365:ILE:HD11	2.31	0.45
1:C:422:ASP:HB3	1:C:433:LEU:HD11	1.98	0.45
1:B:315:ALA:HA	1:B:324:ILE:CG1	2.46	0.45
1:B:288:VAL:HG11	1:B:322:MET:CE	2.47	0.45
1:B:322:MET:HG2	1:B:323:ASN:N	2.32	0.45
1:C:12:ARG:NH1	1:C:30:GLU:OE1	2.49	0.45
1:A:24:LYS:NZ	1:A:441:ASN:OD1	2.50	0.45
1:D:313:GLN:O	1:D:316:ARG:O	2.35	0.44
1:A:38:LEU:O	1:A:39:ASP:HB2	2.18	0.44
1:C:306:GLU:O	1:C:307:PRO:C	2.60	0.44
1:B:319:HIS:HB3	1:B:322:MET:O	2.17	0.44
1:C:248:ALA:HB2	1:C:297:ILE:HD12	2.00	0.44
1:A:306:GLU:N	1:A:307:PRO:CD	2.81	0.44
1:A:25:ASN:OD1	1:A:392:GLN:NE2	2.47	0.43
1:C:299:ILE:HG22	1:C:301:THR:HG23	1.99	0.43
1:C:306:GLU:O	1:C:309:GLU:N	2.52	0.43
1:D:77:GLY:HA3	1:D:105:LEU:HD12	2.00	0.43
1:A:12:ARG:NH1	1:A:30:GLU:OE1	2.51	0.43
1:B:78:HIS:HE1	1:B:145:SER:OG	2.00	0.43
1:B:253:ARG:HD3	1:B:297:ILE:HG13	2.01	0.43
1:C:78:HIS:CD2	1:C:236:SER:HB2	2.54	0.43
1:D:24:LYS:HG2	1:D:57:PRO:HG3	2.00	0.43
1:C:53:ASP:C	1:C:54:ILE:HG12	2.42	0.43
1:D:306:GLU:O	1:D:307:PRO:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ALA:HB2	1:B:297:ILE:HD12	2.00	0.43
1:C:44:PHE:O	1:C:45:PRO:C	2.62	0.42
1:A:124:VAL:HG12	1:A:130:MET:CE	2.48	0.42
1:B:258:LEU:HA	1:B:285:ILE:HD13	1.98	0.42
1:B:402:ALA:HB1	1:B:415:ILE:HG21	2.01	0.42
1:C:181:LEU:HA	1:C:184:MET:HE3	2.02	0.42
1:D:25:ASN:HD21	1:D:392:GLN:NE2	2.18	0.42
1:A:422:ASP:HB3	1:A:433:LEU:HD11	2.00	0.42
1:B:162:VAL:HG11	1:B:383:MET:HE3	2.01	0.42
1:C:311:LEU:O	1:C:315:ALA:HB2	2.19	0.42
1:C:175:GLY:C	1:C:177:TYR:H	2.27	0.42
1:A:306:GLU:N	1:A:307:PRO:HD2	2.35	0.42
1:B:426:TYR:HB2	1:B:431:MET:HE3	2.02	0.41
1:A:314:MET:HB3	1:A:324:ILE:HG13	2.03	0.41
1:C:306:GLU:N	1:C:307:PRO:HD2	2.35	0.41
1:C:95:PRO:HB3	1:C:122:TYR:HE2	1.85	0.41
1:D:258:LEU:CD2	1:D:300:ALA:HA	2.47	0.41
1:A:228:ARG:HB3	1:A:328:ASP:OD1	2.20	0.41
1:C:204:LYS:HA	1:C:205:PRO:HD3	1.93	0.41
1:A:44:PHE:O	1:A:45:PRO:C	2.63	0.41
1:A:67:GLU:H	1:A:67:GLU:CD	2.29	0.41
1:A:443:LEU:HD23	1:A:444:ILE:N	2.35	0.41
1:B:42:LEU:C	1:B:42:LEU:HD12	2.46	0.41
1:D:24:LYS:HZ1	1:D:441:ASN:CG	2.27	0.41
1:D:331:PHE:HB2	1:D:359:ILE:HD12	2.01	0.41
1:A:258:LEU:HD13	1:A:258:LEU:HA	1.91	0.41
1:C:443:LEU:N	1:C:443:LEU:HD12	2.35	0.41
1:A:12:ARG:NH1	1:A:61:TYR:OH	2.41	0.40
1:A:182:LYS:HD3	1:B:189:ASP:OD2	2.21	0.40
1:A:259:GLY:HA3	1:A:285:ILE:HG21	2.04	0.40
1:B:305:GLY:O	1:B:306:GLU:C	2.64	0.40
1:C:240:ARG:HH11	1:C:240:ARG:HD3	1.75	0.40
1:D:78:HIS:HE1	1:D:145:SER:OG	2.04	0.40
1:C:100:LYS:HD2	1:C:123:THR:HG21	2.03	0.40
1:D:395:PHE:CE2	1:D:399:ILE:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

Mol	Chain	Res	Type
1	A	343	ILE
1	A	413	GLU
1	B	115	ILE
1	B	444	ILE
1	C	258	LEU
1	C	343	ILE
1	C	413	GLU
1	D	115	ILE
1	D	258	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	392	GLN
1	B	60	GLN
1	B	141	ASN
1	B	319	HIS
1	B	392	GLN
1	C	141	ASN
1	C	349	ASN
1	C	392	GLN
1	C	398	GLN
1	D	25	ASN
1	D	134	ASN
1	D	357	HIS
1	D	392	GLN

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 ⓘ

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	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

All (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
1	A	53	ASP	2.9
1	A	261	SER	2.8
1	A	262	LEU	2.8
1	D	303	MET	2.7
1	D	23	ALA	2.7
1	A	434	ASN	2.5
1	D	315	ALA	2.5
1	D	339	ASN	2.4
1	D	60	GLN	2.4
1	C	303	MET	2.4
1	C	341	GLU	2.3
1	B	342	VAL	2.3
1	D	304	GLN	2.3
1	C	305	GLY	2.2
1	A	258	LEU	2.2
1	C	78	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	324	ILE	2.2
1	C	79	GLU	2.2
1	B	427	ASN	2.1
1	C	307	PRO	2.1
1	B	5	LYS	2.1
1	C	258	LEU	2.1

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](#)

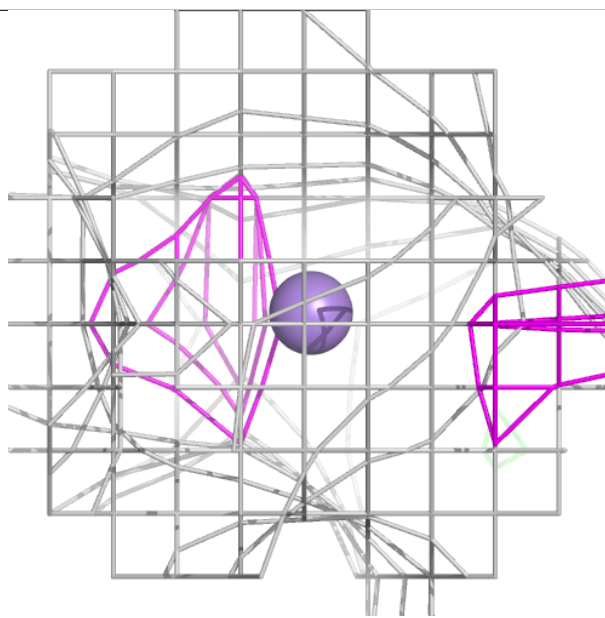
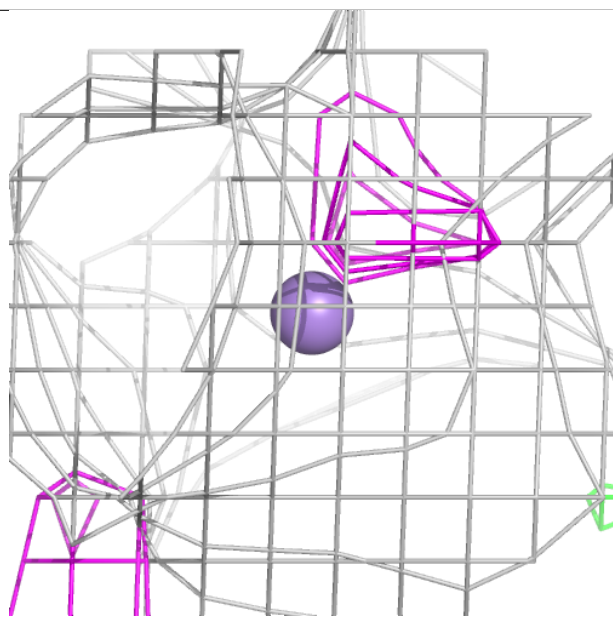
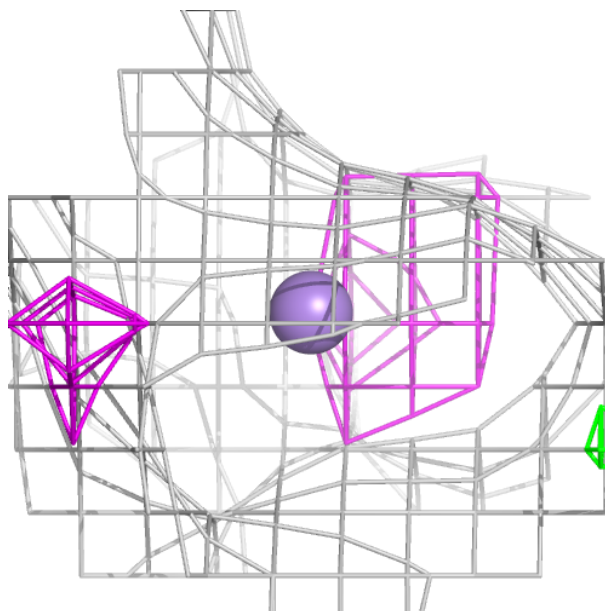
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

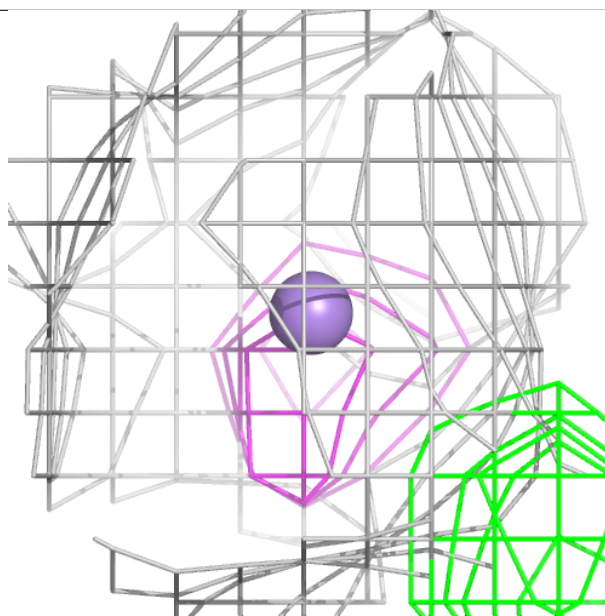
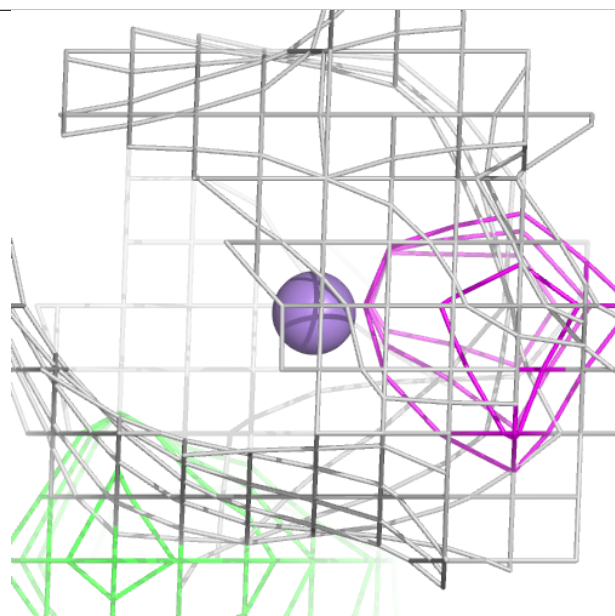
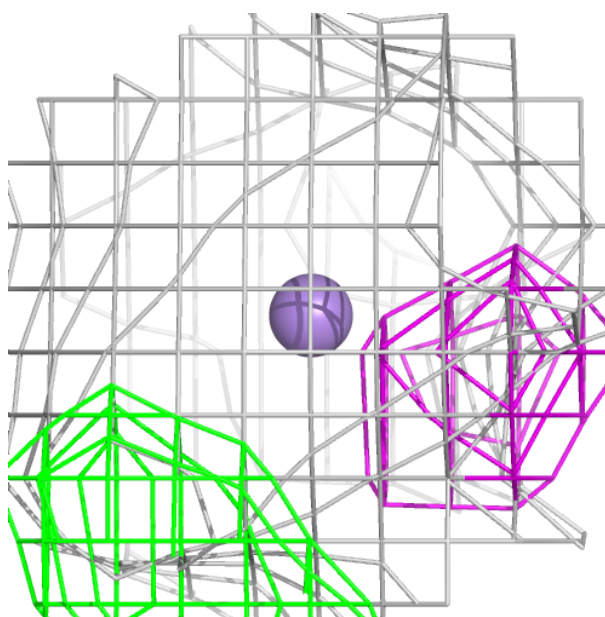
Electron density around MN C 601:

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



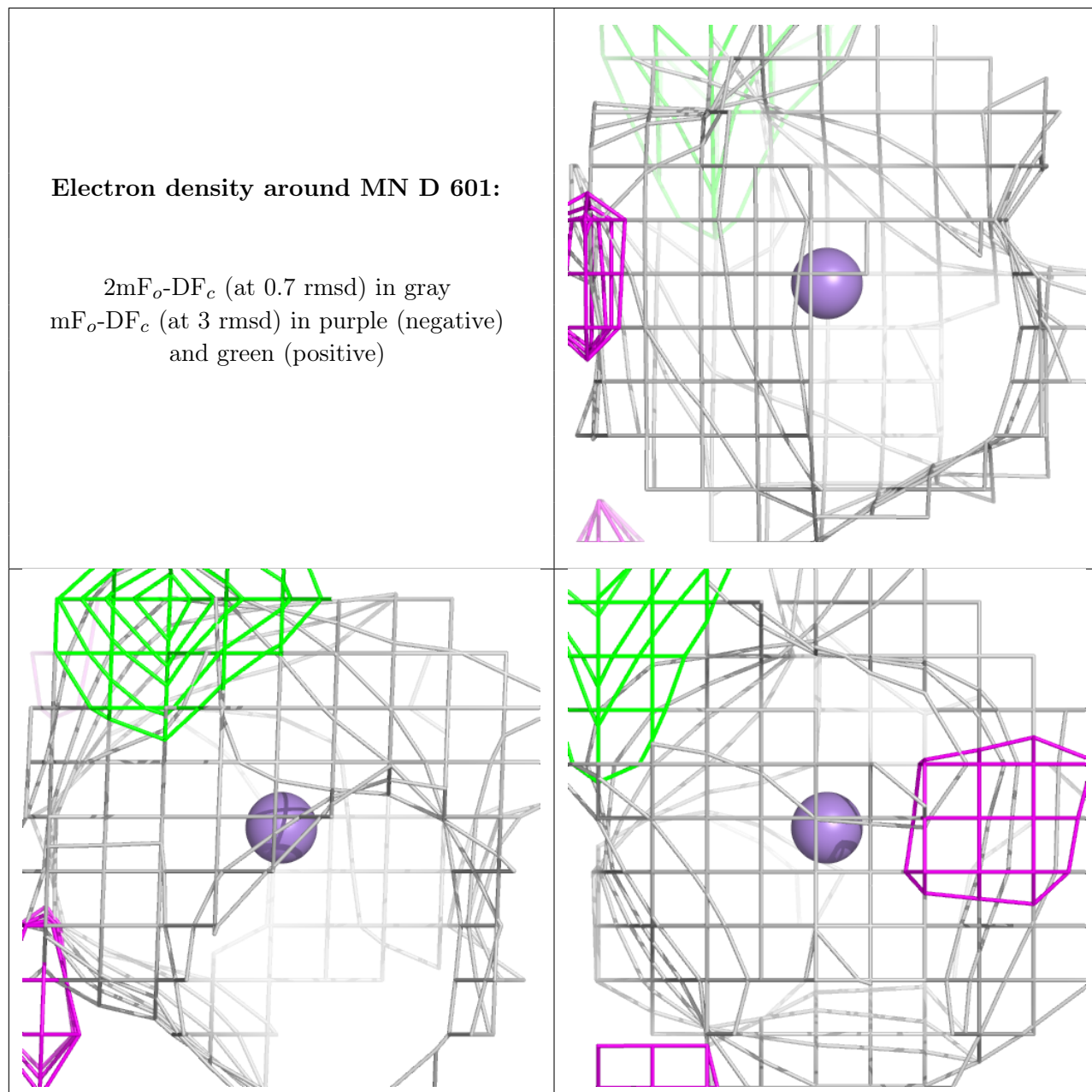
Electron density around MN B 601:

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



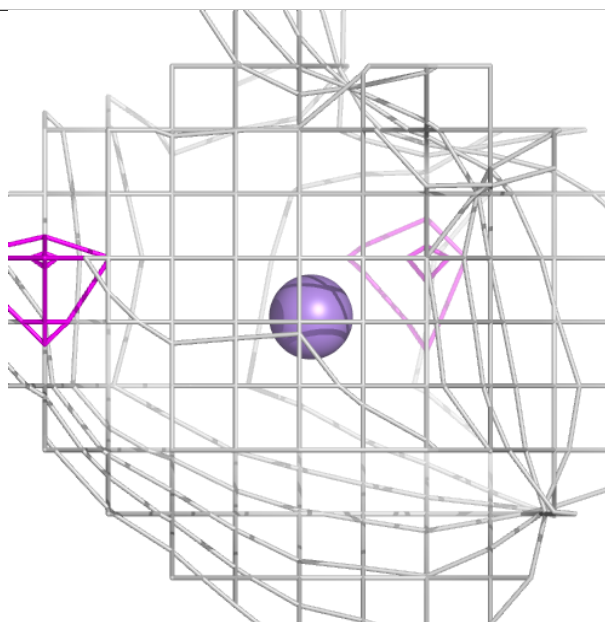
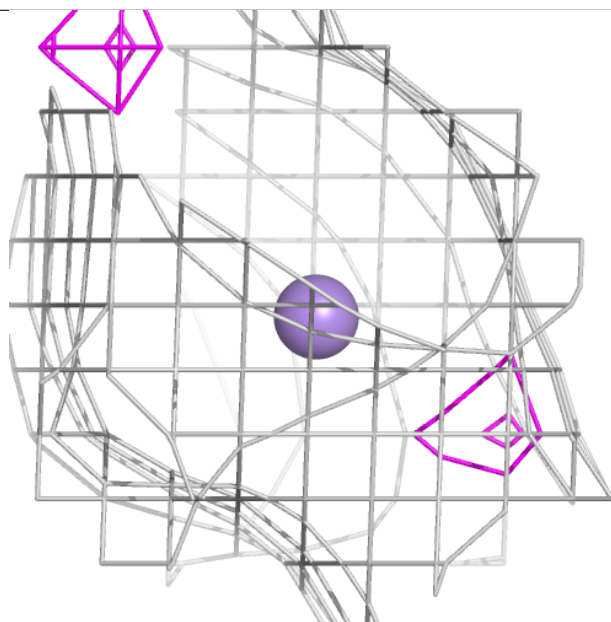
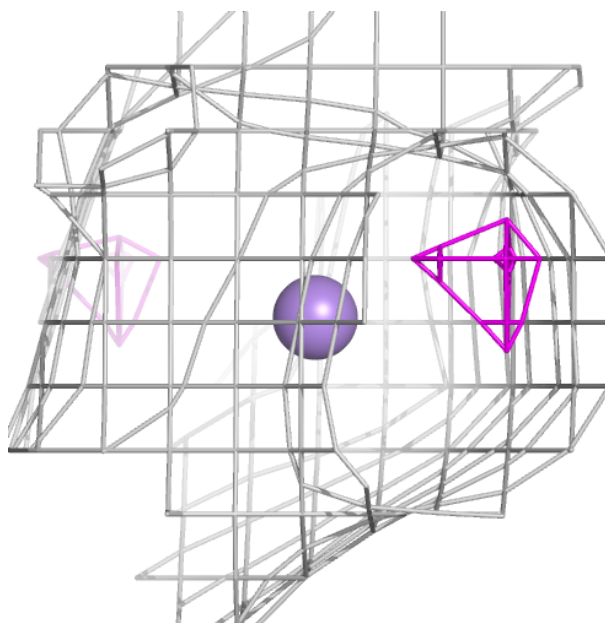
Electron density around MN D 601:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.