



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:55 AM EDT

PDB ID : 7XJV / pdb_00007xjv
Title : Crystal Structure of Alpha-1,3-mannosyltransferase MNT2 from *Saccharomyces cerevisiae*, Mn/GDP-mannose form
Authors : Hira, D.; Kadooka, C.; Oka, T.
Deposited on : 2022-04-18
Resolution : 2.80 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

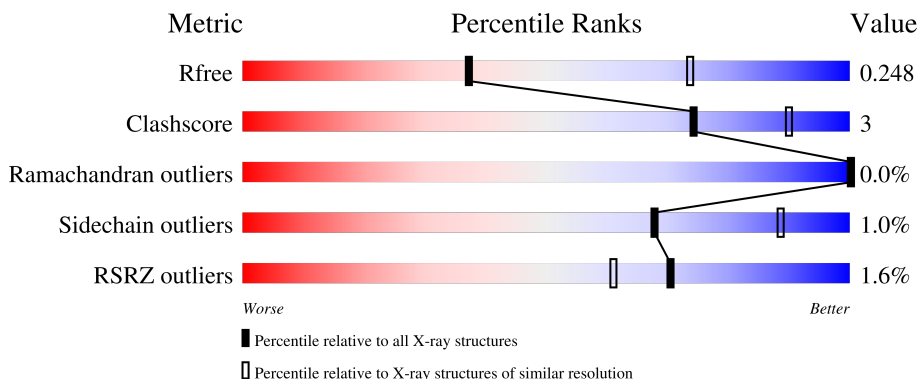
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	548	86% 6% 7%
1	B	548	86% 8% 6%
1	C	548	86% 8% 7%
1	D	548	83% 9% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17178 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 Alpha-1,3-mannosyltransferase MNT2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			4200	2725	684	778	13			
1	B	514	Total	C	N	O	S	0	0	0
			4247	2752	693	789	13			
1	C	511	Total	C	N	O	S	0	0	0
			4227	2741	688	786	12			
1	D	509	Total	C	N	O	S	0	0	0
			4208	2729	684	782	13			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-29	MET	-	initiating methionine	UNP P53059
A	-28	GLY	-	expression tag	UNP P53059
A	-27	SER	-	expression tag	UNP P53059
A	-26	SER	-	expression tag	UNP P53059
A	-25	HIS	-	expression tag	UNP P53059
A	-24	HIS	-	expression tag	UNP P53059
A	-23	HIS	-	expression tag	UNP P53059
A	-22	HIS	-	expression tag	UNP P53059
A	-21	HIS	-	expression tag	UNP P53059
A	-20	HIS	-	expression tag	UNP P53059
A	-19	SER	-	expression tag	UNP P53059
A	-18	SER	-	expression tag	UNP P53059
A	-17	GLY	-	expression tag	UNP P53059
A	-16	HIS	-	expression tag	UNP P53059
A	-15	SER	-	expression tag	UNP P53059
A	247	LYS	GLU	conflict	UNP P53059
B	-29	MET	-	initiating methionine	UNP P53059
B	-28	GLY	-	expression tag	UNP P53059
B	-27	SER	-	expression tag	UNP P53059
B	-26	SER	-	expression tag	UNP P53059
B	-25	HIS	-	expression tag	UNP P53059

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	HIS	-	expression tag	UNP P53059
B	-23	HIS	-	expression tag	UNP P53059
B	-22	HIS	-	expression tag	UNP P53059
B	-21	HIS	-	expression tag	UNP P53059
B	-20	HIS	-	expression tag	UNP P53059
B	-19	SER	-	expression tag	UNP P53059
B	-18	SER	-	expression tag	UNP P53059
B	-17	GLY	-	expression tag	UNP P53059
B	-16	HIS	-	expression tag	UNP P53059
B	-15	SER	-	expression tag	UNP P53059
B	247	LYS	GLU	conflict	UNP P53059
C	-29	MET	-	initiating methionine	UNP P53059
C	-28	GLY	-	expression tag	UNP P53059
C	-27	SER	-	expression tag	UNP P53059
C	-26	SER	-	expression tag	UNP P53059
C	-25	HIS	-	expression tag	UNP P53059
C	-24	HIS	-	expression tag	UNP P53059
C	-23	HIS	-	expression tag	UNP P53059
C	-22	HIS	-	expression tag	UNP P53059
C	-21	HIS	-	expression tag	UNP P53059
C	-20	HIS	-	expression tag	UNP P53059
C	-19	SER	-	expression tag	UNP P53059
C	-18	SER	-	expression tag	UNP P53059
C	-17	GLY	-	expression tag	UNP P53059
C	-16	HIS	-	expression tag	UNP P53059
C	-15	SER	-	expression tag	UNP P53059
C	247	LYS	GLU	conflict	UNP P53059
D	-29	MET	-	initiating methionine	UNP P53059
D	-28	GLY	-	expression tag	UNP P53059
D	-27	SER	-	expression tag	UNP P53059
D	-26	SER	-	expression tag	UNP P53059
D	-25	HIS	-	expression tag	UNP P53059
D	-24	HIS	-	expression tag	UNP P53059
D	-23	HIS	-	expression tag	UNP P53059
D	-22	HIS	-	expression tag	UNP P53059
D	-21	HIS	-	expression tag	UNP P53059
D	-20	HIS	-	expression tag	UNP P53059
D	-19	SER	-	expression tag	UNP P53059
D	-18	SER	-	expression tag	UNP P53059
D	-17	GLY	-	expression tag	UNP P53059
D	-16	HIS	-	expression tag	UNP P53059
D	-15	SER	-	expression tag	UNP P53059

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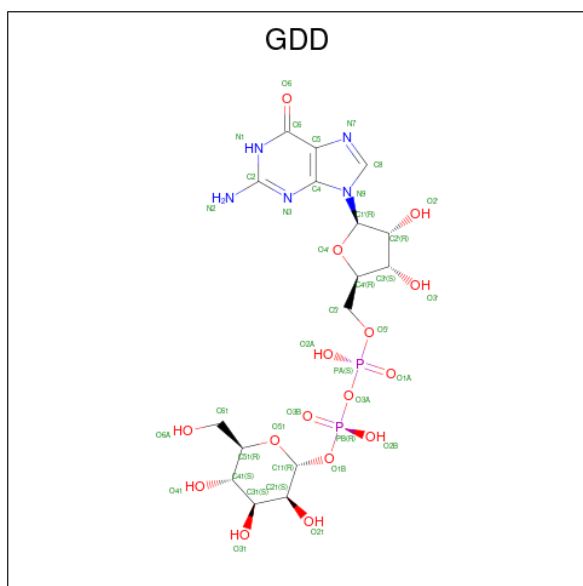
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Chain	Residue	Modelled	Actual	Comment	Reference
D	247	LYS	GLU	conflict	UNP P53059

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

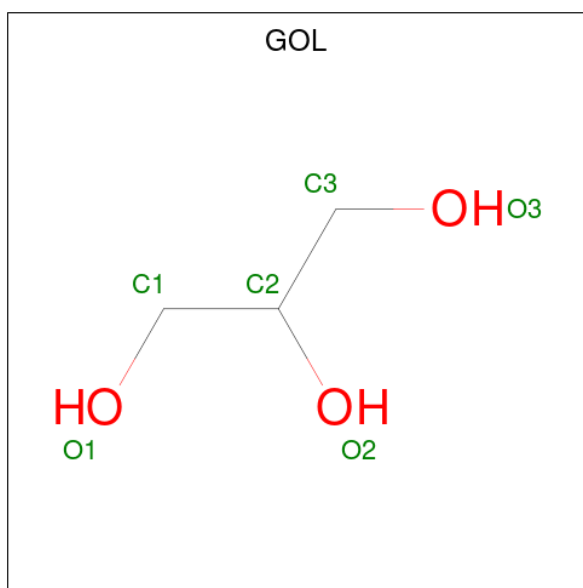
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (CCD ID: GDD) (formula: C₁₆H₂₅N₅O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 39 16 5 16 2	0	0
3	B	1	Total C N O P 39 16 5 16 2	0	0
3	C	1	Total C N O P 39 16 5 16 2	0	0
3	D	1	Total C N O P 39 16 5 16 2	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

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

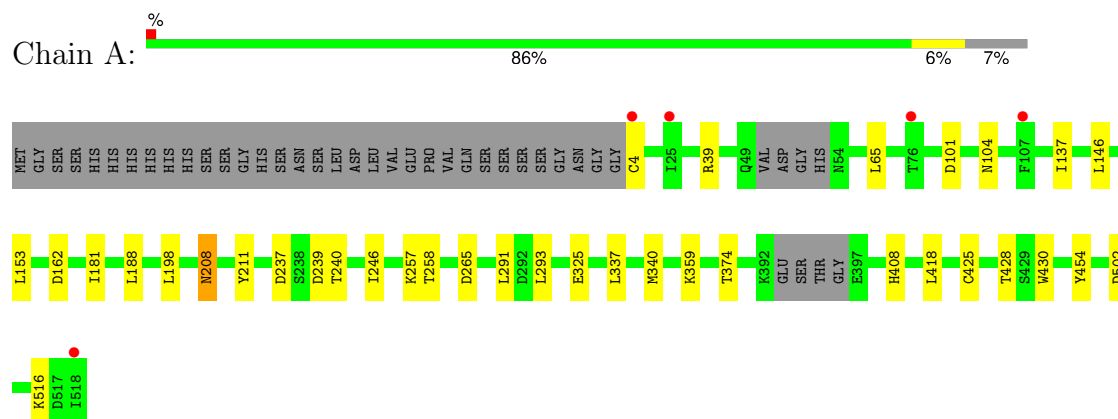
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total	O	0	0
			12	12		
6	B	5	Total	O	0	0
			5	5		
6	C	6	Total	O	0	0
			6	6		
6	D	6	Total	O	0	0
			6	6		

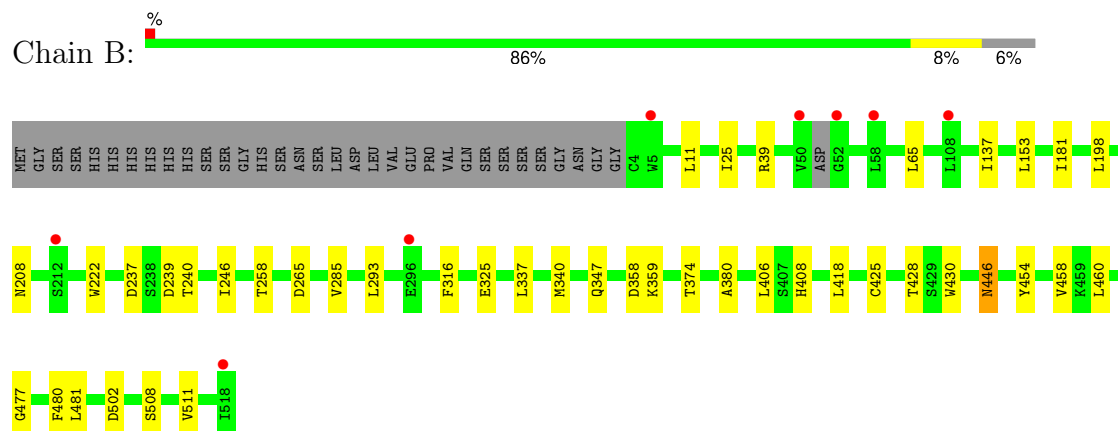
3 Residue-property plots [i](#)

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.

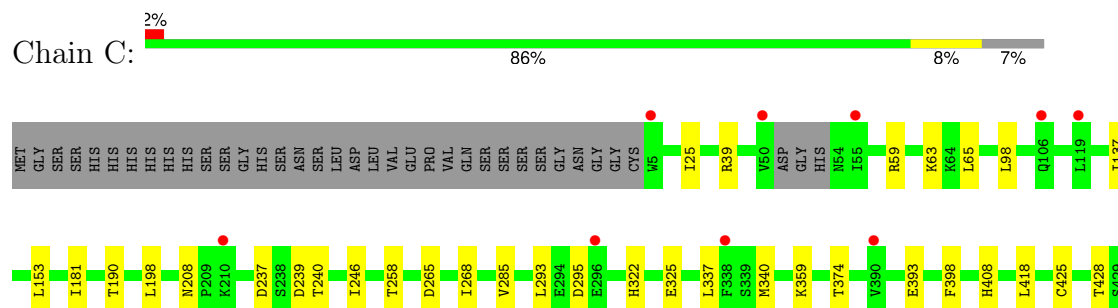
• Molecule 1: Alpha-1,3-mannosyltransferase MNT2



• Molecule 1: Alpha-1,3-mannosyltransferase MNT2

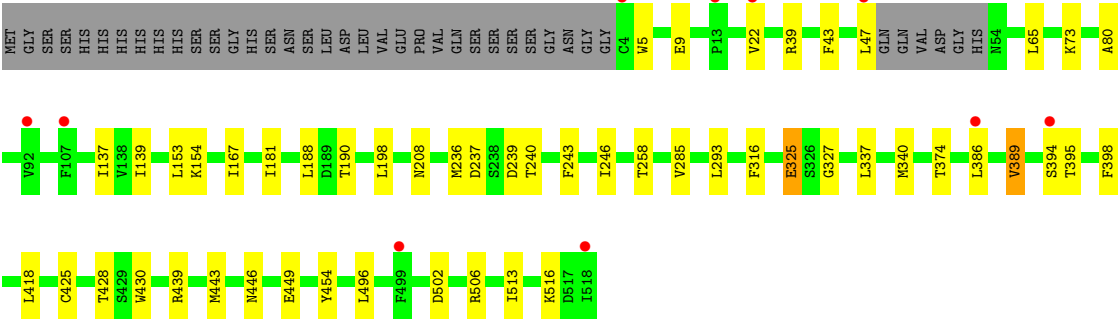
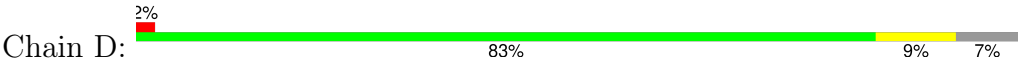


• Molecule 1: Alpha-1,3-mannosyltransferase MNT2





● Molecule 1: Alpha-1,3-mannosyltransferase MNT2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	130.85Å 131.19Å 169.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 40.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-2.80) 99.9 (40.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.251 0.216 , 0.248	Depositor DCC
R_{free} test set	3516 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17178	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.69% 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: GOL, GDD, MN, NA

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	0.97	0/4310	1.40	0/5832
1	B	0.98	0/4359	1.42	0/5900
1	C	0.98	0/4338	1.41	0/5872
1	D	0.98	0/4319	1.41	2/5846 (0.0%)
All	All	0.98	0/17326	1.41	2/23450 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	TRP	CA-C-N	5.08	127.33	120.38
1	D	5	TRP	C-N-CA	5.08	127.33	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4200	0	4101	25	0
1	B	4247	0	4142	28	0
1	C	4227	0	4129	23	0
1	D	4208	0	4107	31	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	39	0	23	0	0
3	B	39	0	23	0	0
3	C	39	0	23	0	0
3	D	39	0	23	1	0
4	A	30	0	40	0	0
4	B	24	0	32	0	0
4	C	24	0	32	0	0
4	D	24	0	32	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	0	0	0
6	B	5	0	0	0	0
6	C	6	0	0	0	0
6	D	6	0	0	0	0
All	All	17178	0	16707	105	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 3.

All (105) 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:B:477:GLY:HA2	1:B:481:LEU:HD23	1.65	0.76
1:D:243:PHE:O	1:D:506:ARG:NH2	2.21	0.73
1:D:513:ILE:HD12	1:D:516:LYS:HD3	1.73	0.69
1:D:43:PHE:O	1:D:47:LEU:HD23	1.94	0.67
1:C:237:ASP:HB3	1:C:239:ASP:OD1	1.98	0.64
1:D:325:GLU:OE1	1:D:327:GLY:N	2.30	0.63
1:D:237:ASP:HB3	1:D:239:ASP:OD1	1.97	0.63
1:A:237:ASP:HB3	1:A:239:ASP:OD1	1.98	0.62
1:B:237:ASP:HB3	1:B:239:ASP:OD1	1.98	0.62
1:A:146:LEU:C	1:A:146:LEU:HD23	2.24	0.62
1:A:208:ASN:OD1	1:A:211:TYR:HD1	1.86	0.59
1:B:458:VAL:HG13	1:B:460:LEU:CD1	2.33	0.58
1:A:137:ILE:HD11	1:A:246:ILE:HG13	1.88	0.55
1:D:386:LEU:HD23	1:D:496:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ILE:HD11	1:B:246:ILE:HG13	1.89	0.55
1:D:137:ILE:HD11	1:D:246:ILE:HG13	1.90	0.54
1:C:98:LEU:N	1:C:98:LEU:HD12	2.23	0.54
1:B:325:GLU:OE1	1:B:408:HIS:NE2	2.38	0.53
1:D:73:LYS:HE2	1:D:80:ALA:HB1	1.90	0.53
1:D:167:ILE:HD12	1:D:167:ILE:N	2.23	0.53
1:D:394:SER:O	1:D:395:THR:HG22	2.09	0.53
1:C:325:GLU:OE1	1:C:408:HIS:NE2	2.37	0.52
1:C:137:ILE:HD11	1:C:246:ILE:HG13	1.90	0.52
1:B:446:ASN:N	1:B:446:ASN:OD1	2.42	0.52
1:A:265:ASP:OD2	1:A:359:LYS:NZ	2.43	0.52
1:A:208:ASN:OD1	1:A:208:ASN:O	2.27	0.52
1:C:265:ASP:OD2	1:C:359:LYS:NZ	2.42	0.52
1:D:139:ILE:CD1	1:D:236:MET:HB2	2.40	0.51
1:B:222:TRP:HE1	1:B:347:GLN:HE21	1.58	0.51
1:A:257:LYS:HE3	1:B:480:PHE:CD2	2.46	0.51
1:D:237:ASP:HB2	1:D:240:THR:OG1	2.11	0.51
1:A:188:LEU:HD22	1:A:188:LEU:N	2.26	0.51
1:A:237:ASP:HB2	1:A:240:THR:OG1	2.11	0.50
1:B:237:ASP:HB2	1:B:240:THR:OG1	2.11	0.50
1:C:337:LEU:HD12	1:C:340:MET:HE3	1.93	0.50
1:C:98:LEU:N	1:C:98:LEU:CD1	2.75	0.50
1:B:25:ILE:HD12	1:D:9:GLU:HB3	1.94	0.50
1:C:237:ASP:HB2	1:C:240:THR:OG1	2.11	0.50
1:B:337:LEU:HD12	1:B:340:MET:HE3	1.94	0.48
1:D:428:THR:HA	1:D:430:TRP:CZ3	2.49	0.48
1:C:25:ILE:H	1:C:25:ILE:HD12	1.78	0.48
1:C:398:PHE:CD2	1:C:489:LYS:HD3	2.49	0.47
1:A:258:THR:HG21	1:A:374:THR:HG22	1.97	0.46
1:A:325:GLU:OE1	1:A:408:HIS:NE2	2.37	0.46
1:D:188:LEU:HD12	1:D:188:LEU:N	2.30	0.46
1:C:393:GLU:O	1:C:393:GLU:HG3	2.15	0.46
1:A:146:LEU:C	1:A:146:LEU:CD2	2.89	0.46
1:A:293:LEU:HD22	1:A:293:LEU:N	2.30	0.46
1:D:386:LEU:H	1:D:386:LEU:HD12	1.81	0.46
1:A:428:THR:HA	1:A:430:TRP:CZ3	2.51	0.46
1:B:39:ARG:HB3	1:B:65:LEU:HD21	1.99	0.45
1:B:285:VAL:HG11	1:B:293:LEU:HD11	1.99	0.45
1:C:428:THR:HA	1:C:430:TRP:CZ3	2.51	0.45
1:A:257:LYS:HE3	1:B:480:PHE:CE2	2.52	0.45
1:D:39:ARG:HB3	1:D:65:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LEU:HD21	1:D:198:LEU:HD12	1.98	0.45
1:B:153:LEU:HD21	1:B:198:LEU:HD12	1.98	0.45
1:C:153:LEU:HD21	1:C:198:LEU:HD12	1.98	0.45
1:C:258:THR:HG21	1:C:374:THR:HG22	1.99	0.45
1:D:258:THR:HG21	1:D:374:THR:HG22	1.99	0.45
1:D:425:CYS:HB3	1:D:454:TYR:CG	2.52	0.45
1:B:258:THR:HG21	1:B:374:THR:HG22	1.98	0.45
1:B:428:THR:HA	1:B:430:TRP:CZ3	2.52	0.44
1:B:458:VAL:HG13	1:B:460:LEU:HD11	2.00	0.44
1:C:39:ARG:HB3	1:C:65:LEU:HD21	1.98	0.44
1:C:425:CYS:HB3	1:C:454:TYR:CG	2.52	0.44
1:B:265:ASP:OD2	1:B:359:LYS:NZ	2.42	0.44
1:B:425:CYS:HB3	1:B:454:TYR:CG	2.53	0.44
1:D:446:ASN:OD1	1:D:449:GLU:HG3	2.17	0.44
1:A:153:LEU:HD21	1:A:198:LEU:HD12	1.99	0.44
1:A:337:LEU:HD12	1:A:340:MET:HE2	2.00	0.44
1:A:153:LEU:HD11	1:A:181:ILE:HG23	1.99	0.44
1:A:39:ARG:HB3	1:A:65:LEU:HD21	1.99	0.43
1:A:425:CYS:HB3	1:A:454:TYR:CG	2.52	0.43
1:C:59:ARG:HG3	1:C:63:LYS:HE2	2.00	0.43
1:D:293:LEU:HD13	1:D:316:PHE:CE2	2.54	0.43
1:D:337:LEU:HD12	1:D:340:MET:HE2	2.00	0.43
1:D:389:VAL:HG13	1:D:398:PHE:C	2.44	0.43
1:B:293:LEU:HD13	1:B:316:PHE:CE2	2.54	0.43
1:D:73:LYS:HE2	1:D:80:ALA:CB	2.48	0.43
1:D:285:VAL:HG11	1:D:293:LEU:HD11	2.00	0.43
1:B:347:GLN:NE2	1:B:358:ASP:HA	2.34	0.42
1:C:153:LEU:HD11	1:C:181:ILE:HG23	2.01	0.42
1:C:489:LYS:HG2	1:C:492:GLU:HG3	2.00	0.42
1:B:347:GLN:HE22	1:B:358:ASP:HA	1.84	0.42
1:C:285:VAL:HG11	1:C:293:LEU:HD11	2.02	0.42
1:D:153:LEU:HD11	1:D:181:ILE:HG23	2.01	0.42
1:A:291:LEU:HD22	1:A:293:LEU:HD11	2.02	0.41
1:B:153:LEU:HD11	1:B:181:ILE:HG23	2.01	0.41
1:D:418:LEU:C	1:D:418:LEU:HD12	2.45	0.41
1:B:418:LEU:C	1:B:418:LEU:HD12	2.46	0.41
1:C:268:ILE:HD12	1:C:322:HIS:CD2	2.56	0.41
1:C:418:LEU:HD12	1:C:418:LEU:C	2.46	0.41
3:D:602:GDD:O1A	4:D:605:GOL:O3	2.32	0.41
1:C:508:SER:HA	1:C:511:VAL:HG22	2.03	0.41
1:B:460:LEU:HD13	1:B:511:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:HB3	1:A:104:ASN:OD1	2.21	0.40
1:A:418:LEU:C	1:A:418:LEU:HD12	2.46	0.40
1:B:508:SER:HA	1:B:511:VAL:HG22	2.04	0.40
1:D:340:MET:HE2	1:D:340:MET:HB3	1.94	0.40
1:D:439:ARG:NH1	1:D:443:MET:HE1	2.36	0.40
1:A:162:ASP:OD1	1:A:162:ASP:N	2.54	0.40
1:A:340:MET:HE2	1:A:340:MET:HB3	1.94	0.40
1:B:380:ALA:HB1	1:B:406:LEU:HD11	2.03	0.40
1:D:154:LYS:HB3	1:D:513:ILE:HG13	2.03	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	A	501/548 (91%)	485 (97%)	15 (3%)	1 (0%)	43	72
1	B	510/548 (93%)	492 (96%)	18 (4%)	0	100	100
1	C	507/548 (92%)	490 (97%)	17 (3%)	0	100	100
1	D	505/548 (92%)	490 (97%)	15 (3%)	0	100	100
All	All	2023/2192 (92%)	1957 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	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	469/503 (93%)	466 (99%)	3 (1%)	78	92
1	B	474/503 (94%)	470 (99%)	4 (1%)	73	90
1	C	472/503 (94%)	467 (99%)	5 (1%)	65	87
1	D	470/503 (93%)	464 (99%)	6 (1%)	61	86
All	All	1885/2012 (94%)	1867 (99%)	18 (1%)	68	88

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	208	ASN
1	A	502	ASP
1	B	11	LEU
1	B	208	ASN
1	B	446	ASN
1	B	502	ASP
1	C	190	THR
1	C	208	ASN
1	C	295	ASP
1	C	446	ASN
1	C	502	ASP
1	D	22	VAL
1	D	190	THR
1	D	208	ASN
1	D	325	GLU
1	D	389	VAL
1	D	502	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	114	ASN
1	A	310	GLN
1	B	24	GLN
1	B	106	GLN

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Mol	Chain	Res	Type
1	B	169	HIS
1	B	310	GLN
1	B	347	GLN
1	C	106	GLN
1	C	169	HIS
1	C	310	GLN
1	C	322	HIS
1	C	385	GLN
1	C	441	ASN
1	C	515	ASN
1	D	310	GLN
1	D	445	GLN
1	D	515	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 9 are monoatomic - leaving 21 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	B	603	-	5,5,5	0.09	0	5,5,5	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	603	-	5,5,5	0.09	0	5,5,5	0.31	0
4	GOL	C	604	-	5,5,5	0.09	0	5,5,5	0.24	0
3	GDD	D	602	2	41,42,42	0.49	0	62,65,65	0.83	3 (4%)
4	GOL	B	606	-	5,5,5	0.10	0	5,5,5	0.24	0
4	GOL	D	603	-	5,5,5	0.10	0	5,5,5	0.26	0
4	GOL	D	606	-	5,5,5	0.08	0	5,5,5	0.23	0
4	GOL	C	603	-	5,5,5	0.12	0	5,5,5	0.37	0
4	GOL	A	604	-	5,5,5	0.08	0	5,5,5	0.28	0
4	GOL	D	605	-	5,5,5	0.08	0	5,5,5	0.27	0
3	GDD	C	602	2	41,42,42	0.43	0	62,65,65	0.83	3 (4%)
4	GOL	A	605	-	5,5,5	0.09	0	5,5,5	0.25	0
4	GOL	C	606	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	B	605	-	5,5,5	0.10	0	5,5,5	0.29	0
4	GOL	C	605	-	5,5,5	0.08	0	5,5,5	0.23	0
4	GOL	B	604	-	5,5,5	0.10	0	5,5,5	0.27	0
4	GOL	D	604	-	5,5,5	0.07	0	5,5,5	0.21	0
3	GDD	A	602	2	41,42,42	0.46	0	62,65,65	0.80	1 (1%)
4	GOL	A	607	-	5,5,5	0.09	0	5,5,5	0.26	0
3	GDD	B	602	2	41,42,42	0.46	0	62,65,65	0.88	3 (4%)
4	GOL	A	606	-	5,5,5	0.09	0	5,5,5	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	603	-	-	1/4/4/4	-
4	GOL	A	603	-	-	0/4/4/4	-
4	GOL	C	604	-	-	2/4/4/4	-
3	GDD	D	602	2	-	6/23/59/59	0/4/4/4
4	GOL	B	606	-	-	0/4/4/4	-
4	GOL	D	603	-	-	2/4/4/4	-
4	GOL	D	606	-	-	0/4/4/4	-
4	GOL	C	603	-	-	4/4/4/4	-
4	GOL	A	604	-	-	2/4/4/4	-
4	GOL	D	605	-	-	2/4/4/4	-
3	GDD	C	602	2	-	4/23/59/59	0/4/4/4
4	GOL	A	605	-	-	2/4/4/4	-
4	GOL	C	606	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	605	-	-	2/4/4/4	-
4	GOL	C	605	-	-	1/4/4/4	-
4	GOL	B	604	-	-	0/4/4/4	-
4	GOL	D	604	-	-	2/4/4/4	-
3	GDD	A	602	2	-	6/23/59/59	0/4/4/4
4	GOL	A	607	-	-	2/4/4/4	-
3	GDD	B	602	2	-	4/23/59/59	0/4/4/4
4	GOL	A	606	-	-	0/4/4/4	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	GDD	PB-O1B-C11	3.95	137.30	121.21
3	B	602	GDD	PB-O1B-C11	3.84	136.84	121.21
3	C	602	GDD	PB-O1B-C11	3.80	136.69	121.21
3	A	602	GDD	PB-O1B-C11	3.72	136.38	121.21
3	B	602	GDD	O51-C11-O1B	-3.03	107.40	111.36
3	D	602	GDD	O1B-C11-C21	2.20	112.41	108.38
3	C	602	GDD	O51-C11-O1B	-2.15	108.56	111.36
3	B	602	GDD	O1B-PB-O3B	2.15	116.67	109.81
3	C	602	GDD	O1B-PB-O3B	2.14	116.66	109.81
3	D	602	GDD	O1B-PB-O3B	2.06	116.39	109.81

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GDD	C11-O1B-PB-O3A
3	A	602	GDD	C11-O1B-PB-O3B
3	A	602	GDD	O51-C11-O1B-PB
3	A	602	GDD	C21-C11-O1B-PB
3	B	602	GDD	C11-O1B-PB-O3A
3	B	602	GDD	O51-C11-O1B-PB
3	B	602	GDD	C21-C11-O1B-PB
3	C	602	GDD	C11-O1B-PB-O3A
3	C	602	GDD	O51-C11-O1B-PB
3	C	602	GDD	C21-C11-O1B-PB
3	D	602	GDD	C11-O1B-PB-O3A
3	D	602	GDD	C11-O1B-PB-O3B

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Mol	Chain	Res	Type	Atoms
3	D	602	GDD	O51-C11-O1B-PB
3	D	602	GDD	C21-C11-O1B-PB
4	A	607	GOL	O1-C1-C2-C3
4	B	605	GOL	O1-C1-C2-C3
4	C	603	GOL	O1-C1-C2-C3
4	C	603	GOL	C1-C2-C3-O3
4	D	603	GOL	C1-C2-C3-O3
4	A	604	GOL	O1-C1-C2-C3
4	A	605	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-C3
4	D	604	GOL	C1-C2-C3-O3
4	D	605	GOL	O1-C1-C2-C3
4	B	605	GOL	O1-C1-C2-O2
4	C	603	GOL	O1-C1-C2-O2
4	C	604	GOL	O1-C1-C2-O2
4	D	604	GOL	O2-C2-C3-O3
4	A	604	GOL	O1-C1-C2-O2
4	A	607	GOL	O1-C1-C2-O2
4	C	603	GOL	O2-C2-C3-O3
4	D	603	GOL	O2-C2-C3-O3
3	D	602	GDD	O4'-C4'-C5'-O5'
4	A	605	GOL	O1-C1-C2-O2
4	B	603	GOL	O2-C2-C3-O3
4	C	605	GOL	O1-C1-C2-O2
3	D	602	GDD	C3'-C4'-C5'-O5'
4	D	605	GOL	O1-C1-C2-O2
3	A	602	GDD	O4'-C4'-C5'-O5'
3	A	602	GDD	C3'-C4'-C5'-O5'
3	B	602	GDD	C3'-C4'-C5'-O5'
3	C	602	GDD	C3'-C4'-C5'-O5'

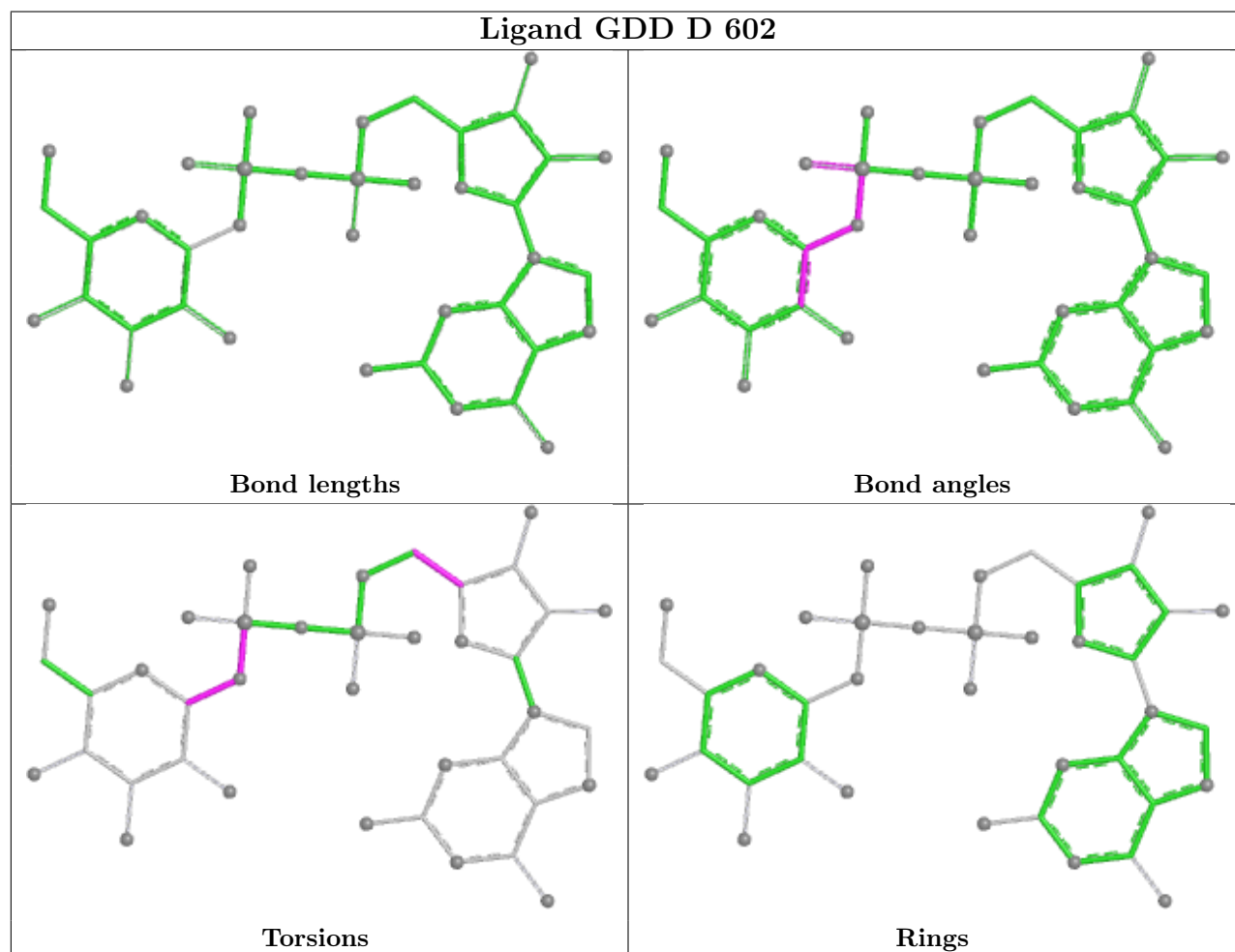
There are no ring outliers.

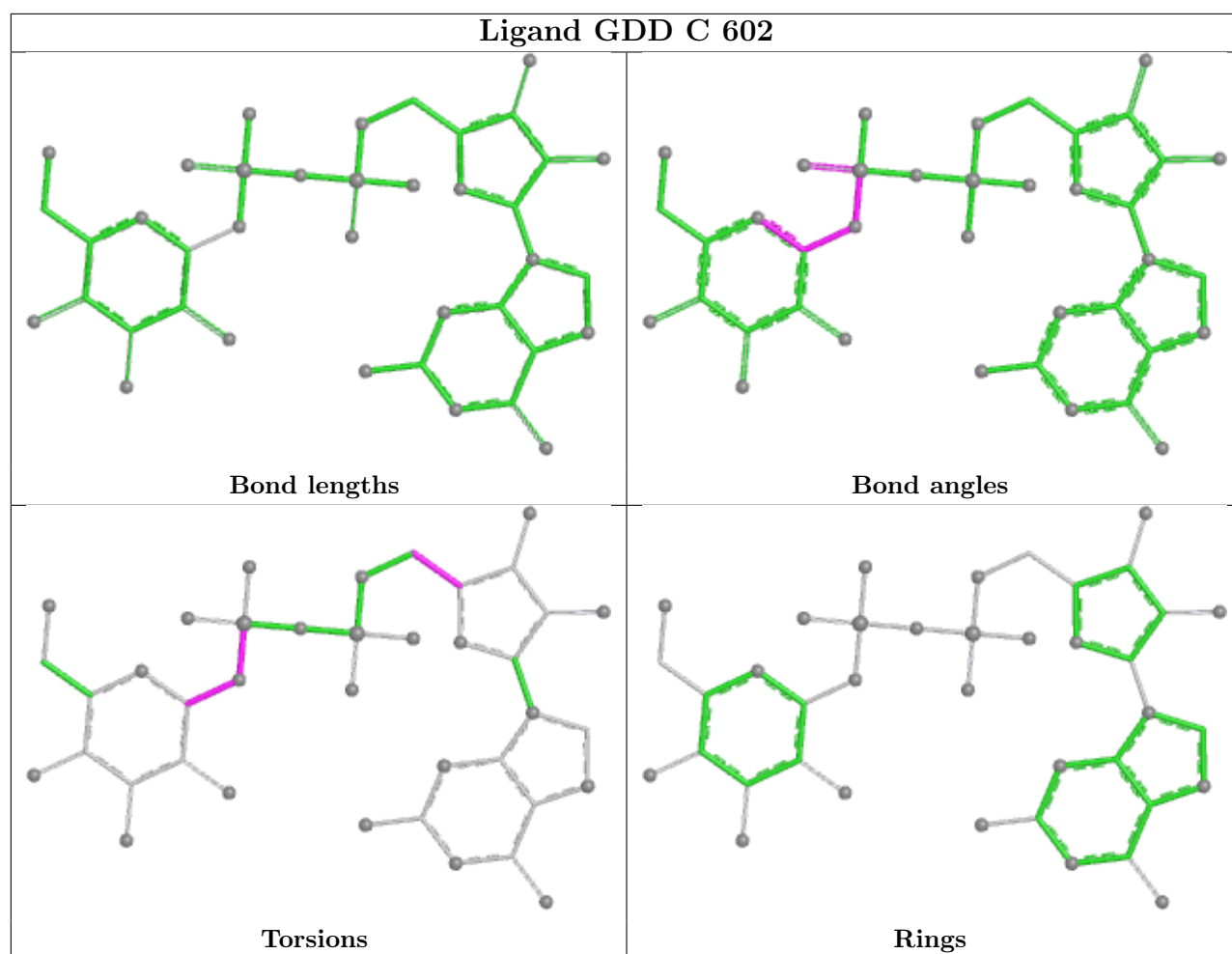
2 monomers are involved in 1 short contact:

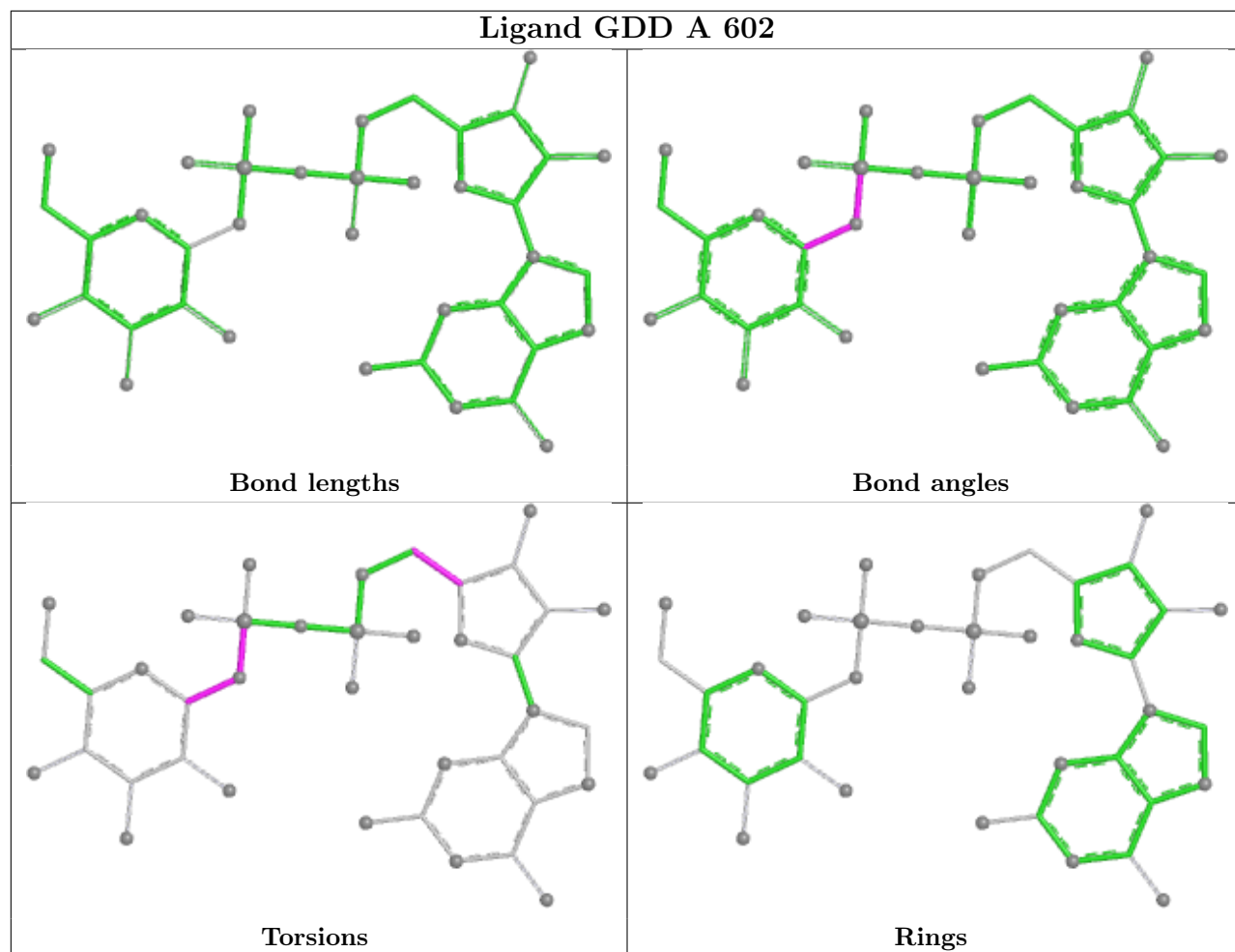
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	GDD	1	0
4	D	605	GOL	1	0

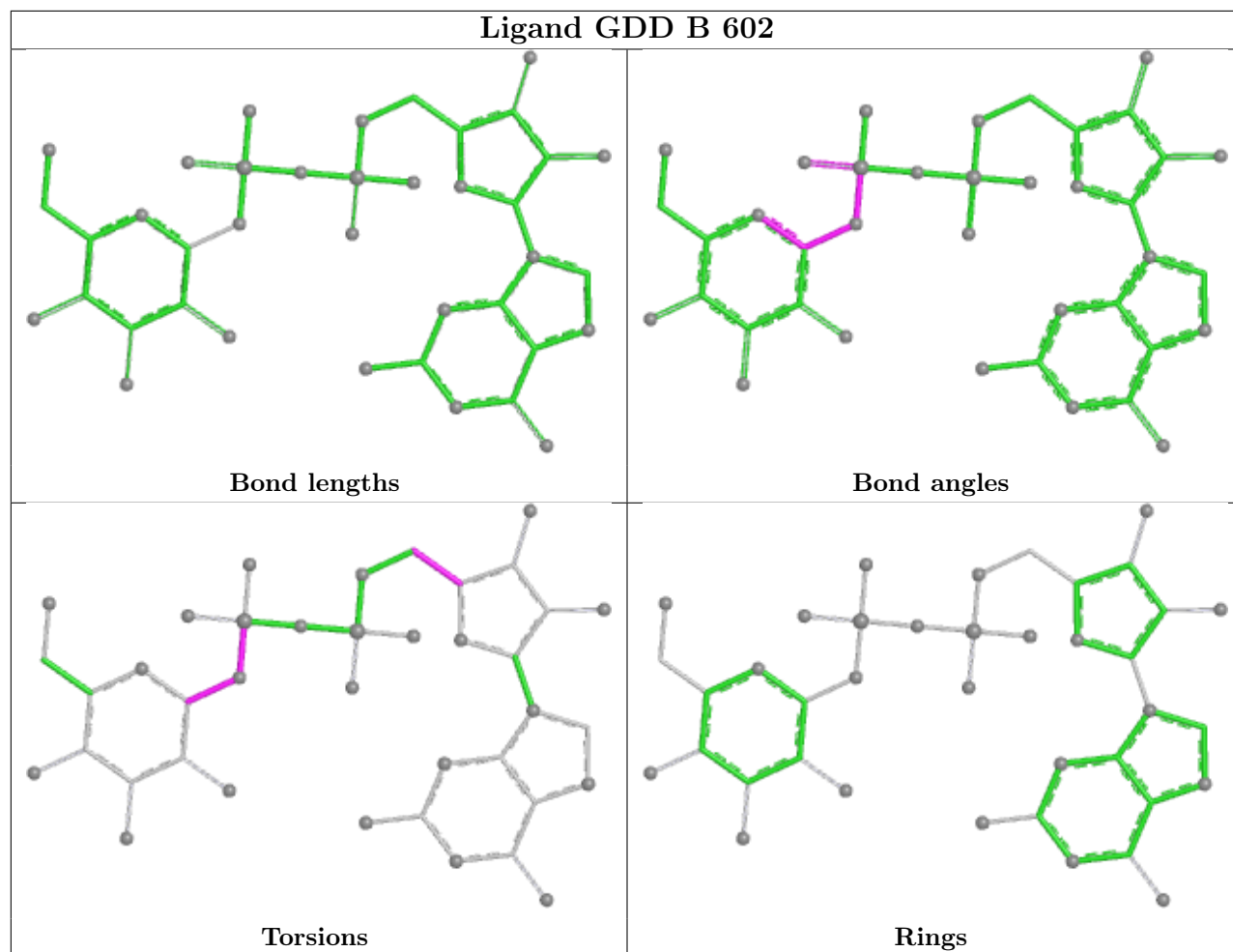
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	507/548 (92%)	0.25	5 (0%) 79 72	46, 73, 109, 138	0
1	B	514/548 (93%)	0.22	8 (1%) 70 61	49, 71, 109, 158	0
1	C	511/548 (93%)	0.22	10 (1%) 65 56	50, 74, 114, 158	0
1	D	509/548 (92%)	0.27	10 (1%) 65 56	48, 74, 114, 174	0
All	All	2041/2192 (93%)	0.24	33 (1%) 70 61	46, 73, 112, 174	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	50	VAL	4.7
1	A	518	ILE	4.4
1	B	518	ILE	4.4
1	C	5	TRP	4.0
1	D	518	ILE	3.6
1	B	5	TRP	3.5
1	B	50	VAL	3.2
1	B	296	GLU	2.9
1	C	518	ILE	2.9
1	B	212	SER	2.9
1	A	4	CYS	2.8
1	D	4	CYS	2.8
1	D	47	LEU	2.8
1	D	22	VAL	2.6
1	C	338	PHE	2.5
1	A	76	THR	2.5
1	D	386	LEU	2.4
1	D	499	PHE	2.4
1	C	296	GLU	2.2
1	B	58	LEU	2.2
1	B	52	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	394	SER	2.2
1	D	107	PHE	2.2
1	B	108	LEU	2.2
1	C	106	GLN	2.2
1	A	107	PHE	2.1
1	C	119	LEU	2.1
1	A	25	ILE	2.1
1	D	92	VAL	2.0
1	D	13	PRO	2.0
1	C	210	LYS	2.0
1	C	55	ILE	2.0
1	C	390	VAL	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 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(Å ²)	Q<0.9
5	NA	C	608	1/1	0.50	0.23	96,96,96,96	0
5	NA	B	607	1/1	0.66	0.17	90,90,90,90	0
4	GOL	D	605	6/6	0.76	0.16	99,99,102,102	0
4	GOL	B	606	6/6	0.77	0.22	97,99,100,101	0
4	GOL	D	603	6/6	0.78	0.27	86,86,87,90	0
4	GOL	A	607	6/6	0.79	0.19	90,92,93,93	0
4	GOL	C	603	6/6	0.81	0.21	81,88,91,91	0
4	GOL	A	605	6/6	0.82	0.12	85,87,89,90	0
4	GOL	C	605	6/6	0.83	0.15	100,105,106,111	0
4	GOL	D	606	6/6	0.84	0.19	88,91,92,93	0
4	GOL	A	603	6/6	0.84	0.14	69,72,72,72	0

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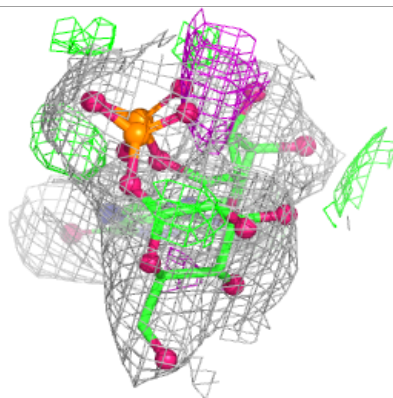
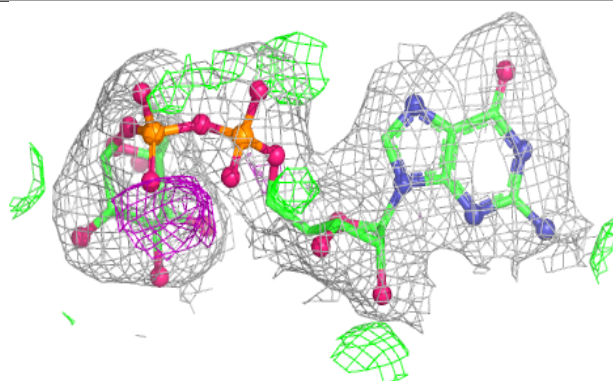
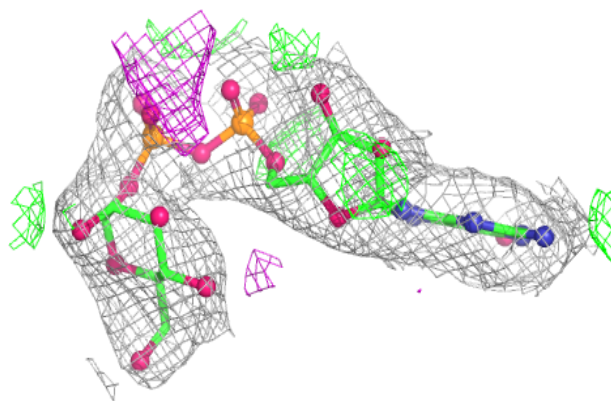
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	606	6/6	0.84	0.20	91,95,98,101	0
5	NA	D	607	1/1	0.84	0.16	80,80,80,80	0
4	GOL	C	606	6/6	0.85	0.18	95,96,97,98	0
4	GOL	B	605	6/6	0.86	0.14	87,92,95,96	0
5	NA	A	608	1/1	0.87	0.23	74,74,74,74	0
4	GOL	B	603	6/6	0.89	0.16	81,84,85,91	0
4	GOL	C	604	6/6	0.90	0.14	78,82,84,88	0
4	GOL	A	604	6/6	0.90	0.16	75,81,82,86	0
5	NA	C	607	1/1	0.91	0.20	70,70,70,70	0
4	GOL	B	604	6/6	0.92	0.14	79,81,83,84	0
4	GOL	D	604	6/6	0.95	0.10	75,77,78,78	0
3	GDD	A	602	39/39	0.95	0.07	49,57,61,64	0
3	GDD	C	602	39/39	0.96	0.06	56,59,62,63	0
3	GDD	D	602	39/39	0.96	0.07	48,54,60,61	0
3	GDD	B	602	39/39	0.96	0.07	50,54,58,60	0
2	MN	A	601	1/1	0.99	0.09	64,64,64,64	0
2	MN	D	601	1/1	1.00	0.09	63,63,63,63	0
2	MN	B	601	1/1	1.00	0.06	61,61,61,61	0
2	MN	C	601	1/1	1.00	0.09	64,64,64,64	0

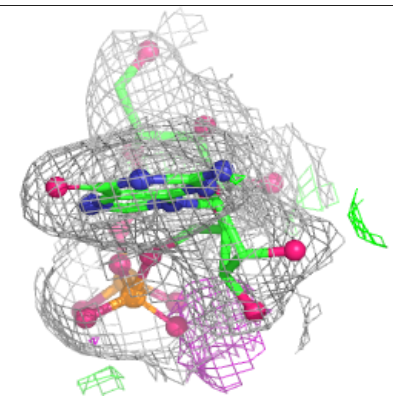
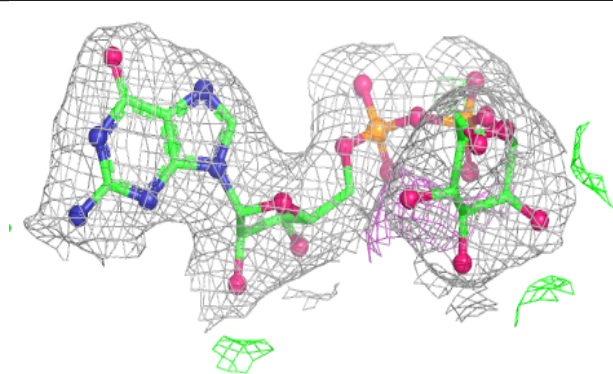
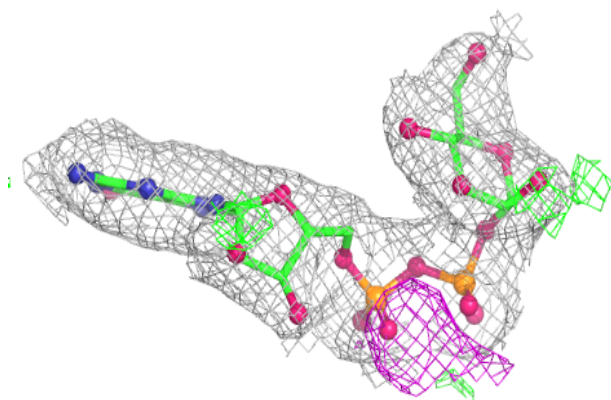
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDD A 602:

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

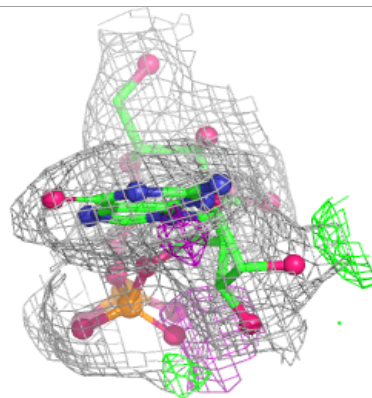
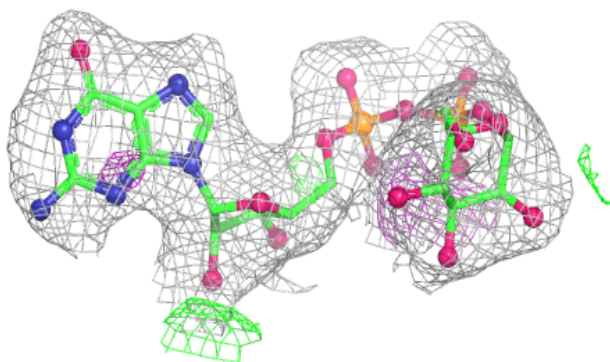
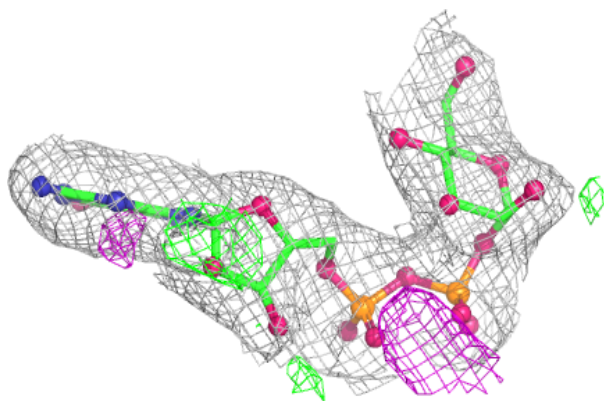
**Electron density around GDD C 602:**

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

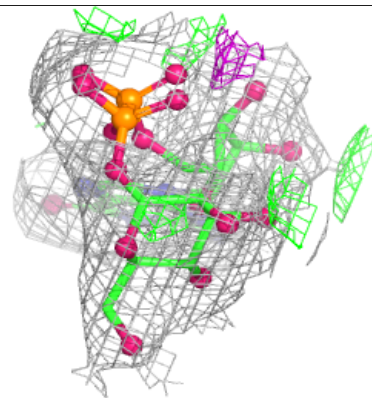
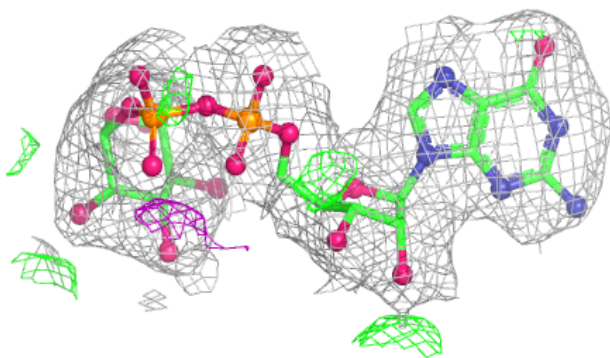
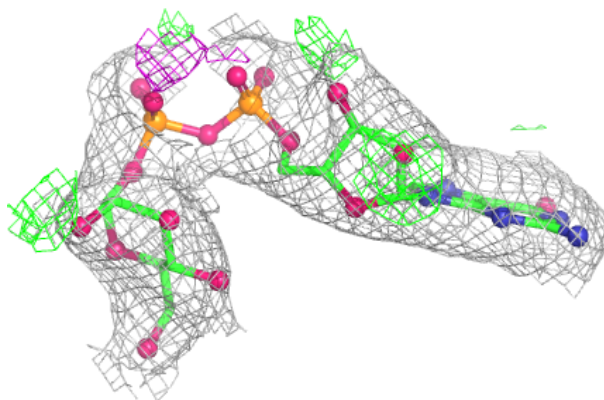


Electron density around GDD D 602:

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

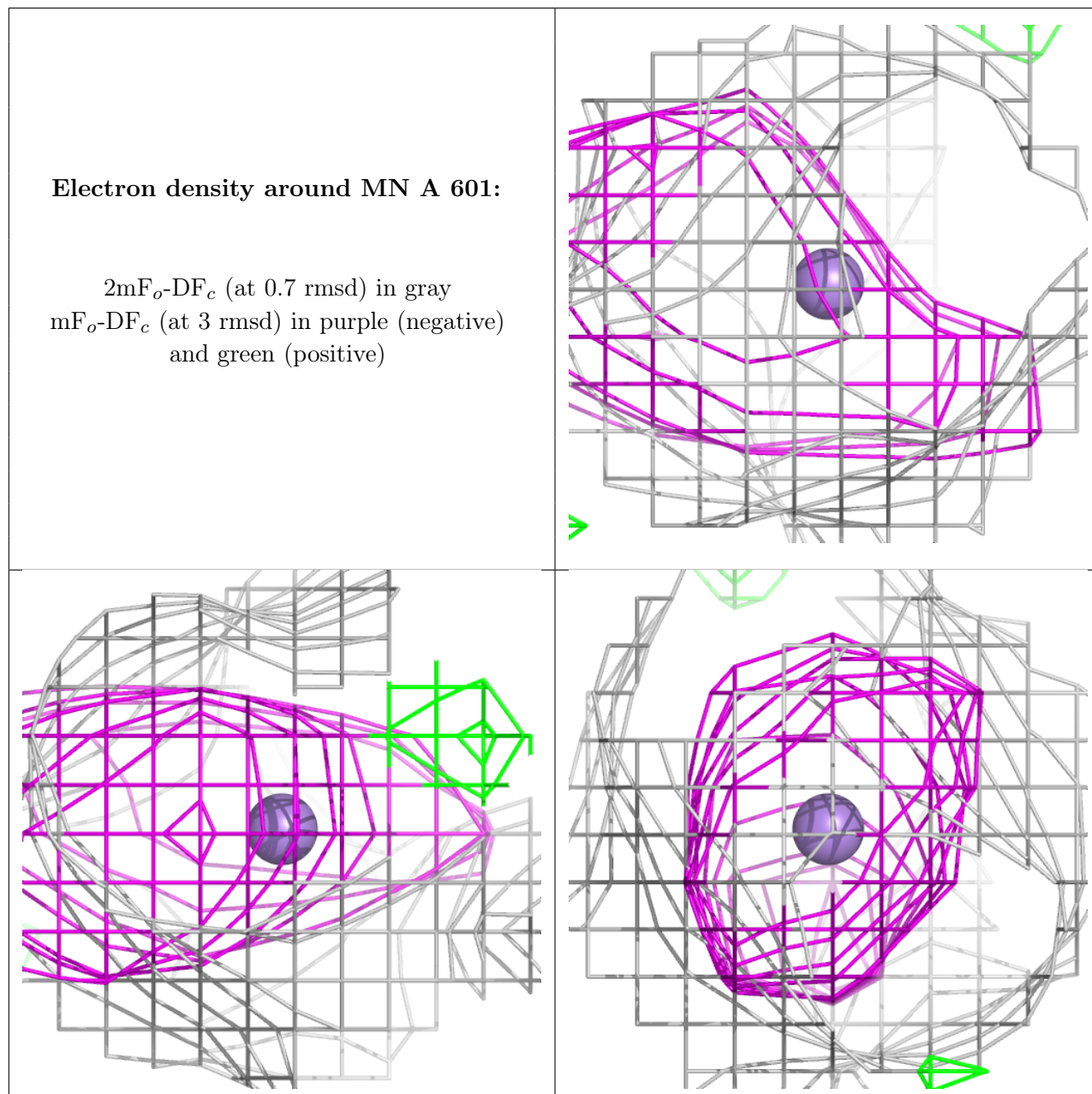
**Electron density around GDD B 602:**

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



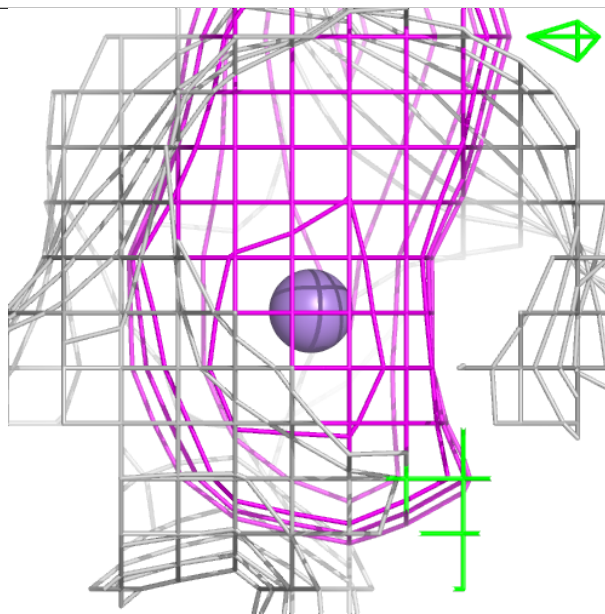
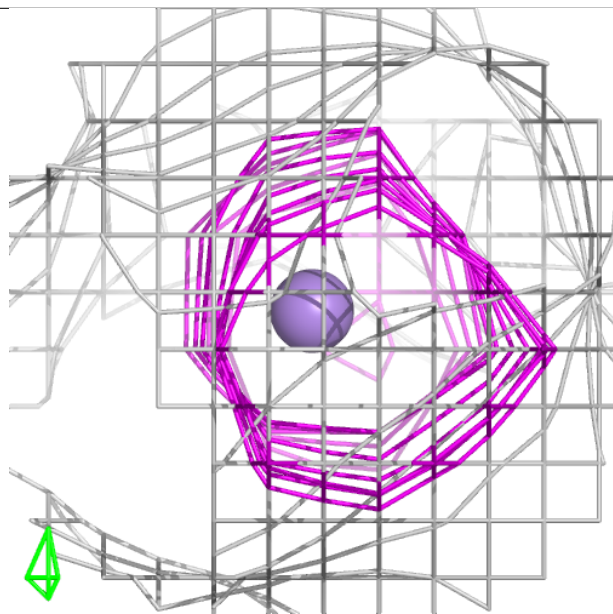
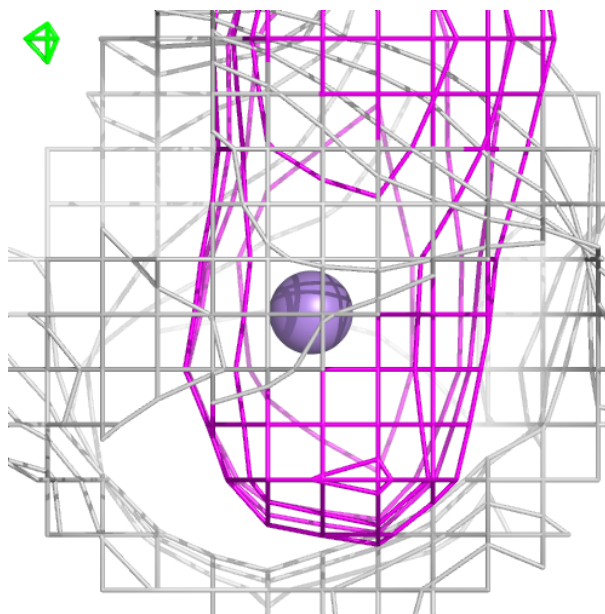
Electron density around MN A 601:

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



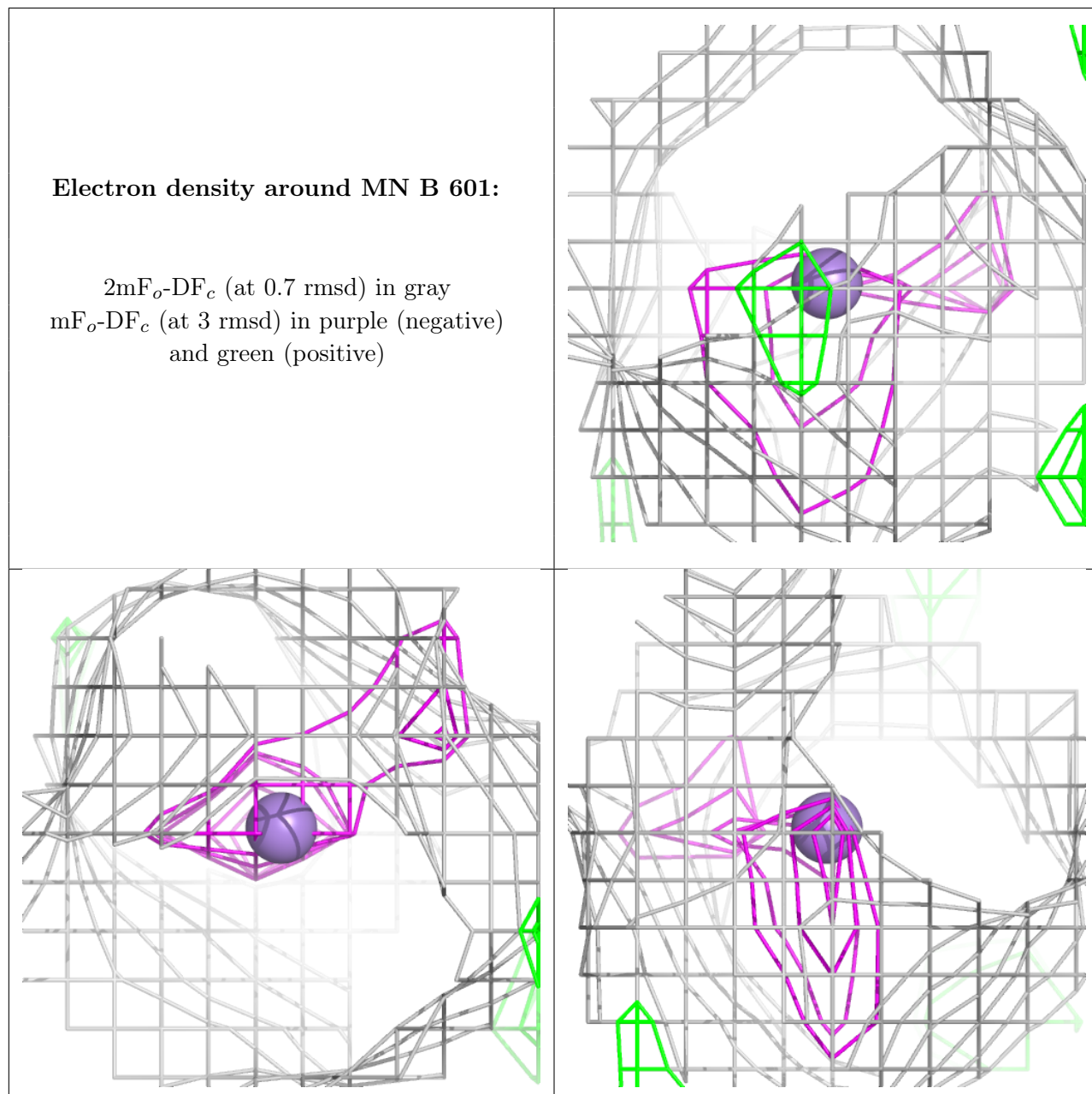
Electron density around MN D 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



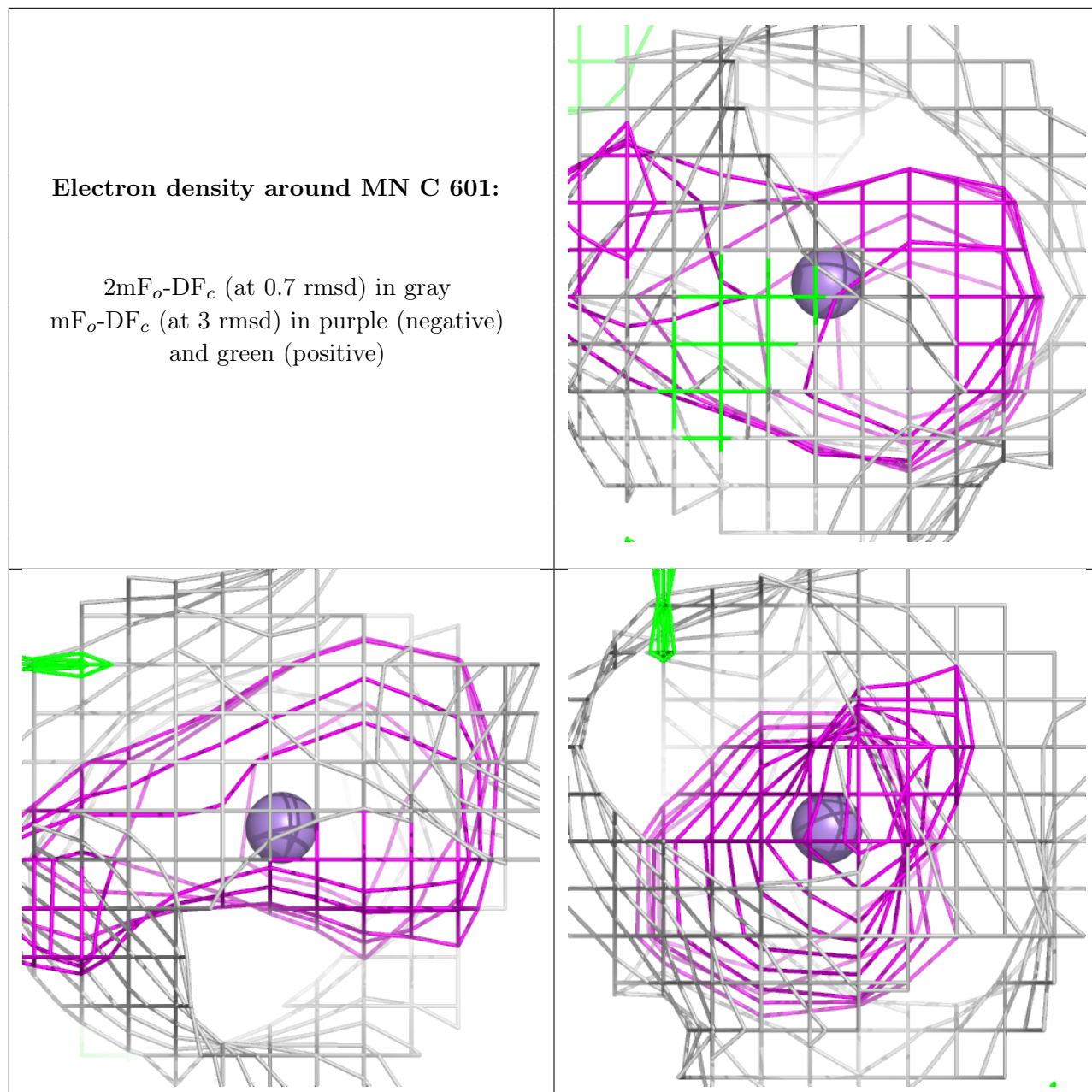
Electron density around MN B 601:

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



Electron density around MN 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)

**6.5 Other polymers** ⓘ

There are no such residues in this entry.