



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 9, 2025 – 01:40 am BST

PDB ID : 9H6J / pdb_00009h6j
Title : Human B4GALNT1 Apo Structure
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Deposited on : 2024-10-24
Resolution : 2.96 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

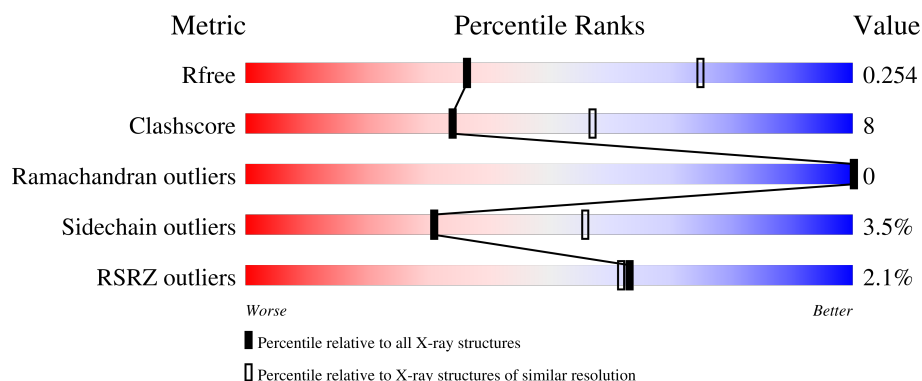
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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}	164625	1044 (2.98-2.94)
Clashscore	180529	1097 (2.98-2.94)
Ramachandran outliers	177936	1049 (2.98-2.94)
Sidechain outliers	177891	1049 (2.98-2.94)
RSRZ outliers	164620	1044 (2.98-2.94)

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	499	 2% 69% 17% •• 11%
1	B	499	 2% 73% 16% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ACY	A	604	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7067 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 Beta-1,4 N-acetylgalactosaminyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3498	2216	624	649	9			
1	B	450	Total	C	N	O	S	0	0	0
			3517	2227	628	653	9			

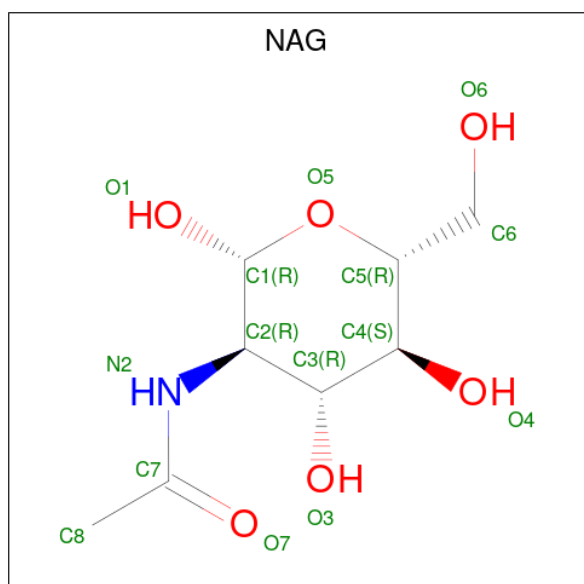
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	HIS	-	expression tag	UNP Q00973
A	36	HIS	-	expression tag	UNP Q00973
A	37	HIS	-	expression tag	UNP Q00973
A	38	HIS	-	expression tag	UNP Q00973
A	39	HIS	-	expression tag	UNP Q00973
A	40	HIS	-	expression tag	UNP Q00973
A	41	HIS	-	expression tag	UNP Q00973
A	42	HIS	-	expression tag	UNP Q00973
A	43	HIS	-	expression tag	UNP Q00973
A	44	HIS	-	expression tag	UNP Q00973
A	45	GLY	-	expression tag	UNP Q00973
A	46	THR	-	expression tag	UNP Q00973
B	35	HIS	-	expression tag	UNP Q00973
B	36	HIS	-	expression tag	UNP Q00973
B	37	HIS	-	expression tag	UNP Q00973
B	38	HIS	-	expression tag	UNP Q00973
B	39	HIS	-	expression tag	UNP Q00973
B	40	HIS	-	expression tag	UNP Q00973
B	41	HIS	-	expression tag	UNP Q00973
B	42	HIS	-	expression tag	UNP Q00973
B	43	HIS	-	expression tag	UNP Q00973
B	44	HIS	-	expression tag	UNP Q00973
B	45	GLY	-	expression tag	UNP Q00973
B	46	THR	-	expression tag	UNP Q00973

- 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		0	0
			1	1			
2	B	1	Total	Mn		0	0
			1	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

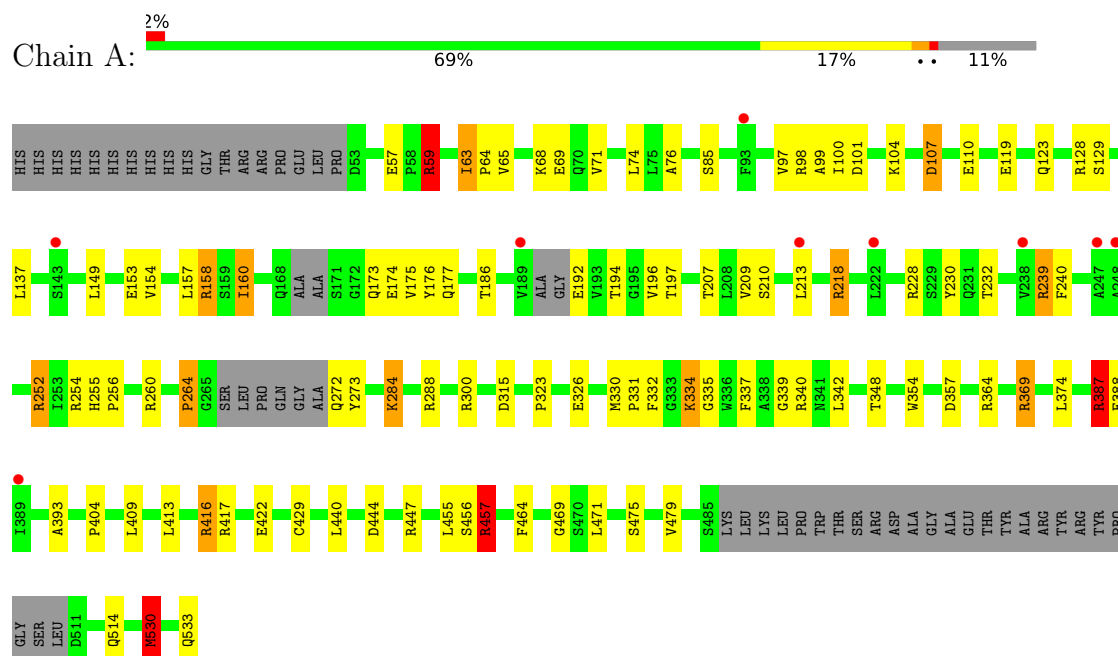
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total	O	0	0
			7	7		
5	B	7	Total	O	0	0
			7	7		

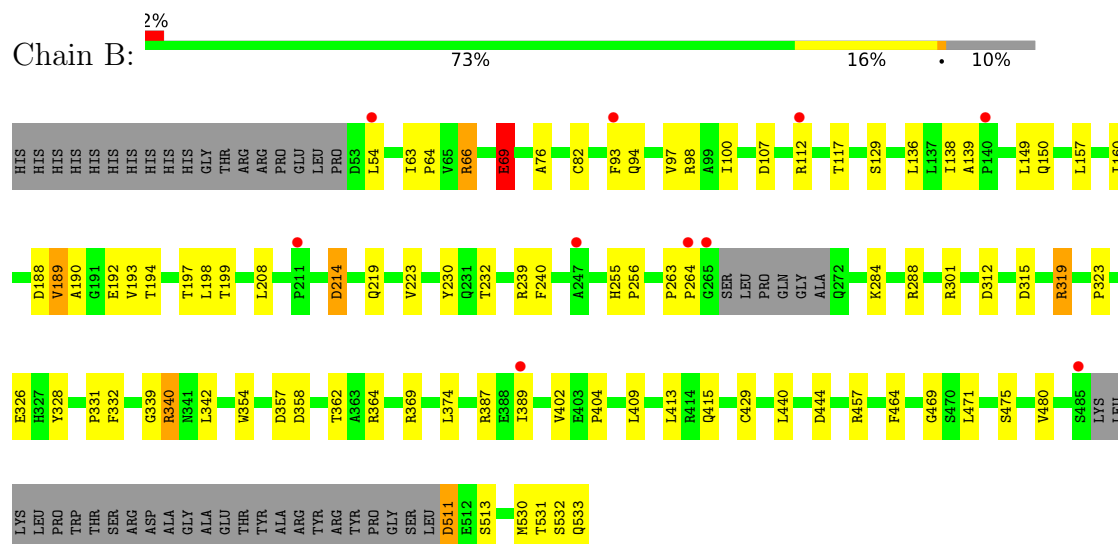
3 Residue-property plots [i](#)

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: Beta-1,4 N-acetylgalactosaminyltransferase 1



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.46Å 136.49Å 87.43Å 90.00° 96.08° 90.00°	Depositor
Resolution (Å)	86.94 – 2.96 86.94 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.2 (86.94-2.96) 99.2 (86.94-2.96)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, R_{free}	0.202 , 0.254 0.202 , 0.254	Depositor DCC
R_{free} test set	1456 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	95.0	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 93.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: ACY, NAG, 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	0.59	0/3573	1.29	27/4855 (0.6%)
1	B	0.61	0/3594	1.31	20/4887 (0.4%)
All	All	0.60	0/7167	1.30	47/9742 (0.5%)

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	9
1	B	0	2
All	All	0	11

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	107	ASP	CB-CA-C	-9.13	92.61	109.51
1	B	240	PHE	CA-CB-CG	7.86	121.66	113.80
1	B	149	LEU	N-CA-CB	-7.73	98.59	110.42
1	B	107	ASP	CA-CB-CG	7.65	120.25	112.60
1	A	387	ARG	CG-CD-NE	-7.54	95.41	112.00
1	A	256	PRO	CB-CA-C	7.40	118.12	111.17
1	A	369	ARG	CB-CA-C	7.15	123.00	110.85
1	B	471	LEU	N-CA-CB	-7.11	99.41	110.57
1	B	256	PRO	CB-CA-C	6.93	117.69	111.17
1	B	369	ARG	CB-CA-C	6.63	122.84	110.70
1	A	107	ASP	CB-CA-C	6.56	119.92	109.62
1	A	240	PHE	CA-CB-CG	6.50	120.31	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	GLN	CB-CA-C	-6.44	97.60	110.42
1	B	232	THR	CA-CB-OG1	-6.33	100.10	109.60
1	A	471	LEU	N-CA-CB	-6.15	100.35	110.68
1	A	284	LYS	CB-CG-CD	5.99	125.07	111.30
1	B	312	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	358	ASP	CA-CB-CG	5.95	118.55	112.60
1	B	464	PHE	CA-CB-CG	-5.88	107.92	113.80
1	B	94	GLN	N-CA-CB	-5.88	101.22	110.69
1	A	416	ARG	CB-CG-CD	5.85	124.76	111.30
1	A	422	GLU	CB-CG-CD	5.72	122.33	112.60
1	A	252	ARG	CA-CB-CG	5.71	125.52	114.10
1	A	348	THR	CA-CB-OG1	-5.59	101.22	109.60
1	A	110	GLU	N-CA-CB	-5.56	101.95	110.12
1	B	340	ARG	CD-NE-CZ	5.52	132.13	124.40
1	B	457	ARG	CB-CG-CD	5.49	123.93	111.30
1	A	530	MET	CG-SD-CE	5.45	112.88	100.90
1	A	59	ARG	NE-CZ-NH1	-5.42	116.08	121.50
1	A	260	ARG	CB-CA-C	-5.40	103.78	112.09
1	A	68	LYS	N-CA-CB	5.38	118.36	110.35
1	A	457	ARG	CB-CA-C	5.34	120.13	111.26
1	B	93	PHE	CB-CA-C	5.33	118.99	110.09
1	B	69	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	214	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	194	THR	CA-CB-OG1	-5.12	101.92	109.60
1	B	323	PRO	CB-CA-C	5.11	118.06	111.46
1	A	232	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	199	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	417	ARG	CB-CG-CD	5.09	123.00	111.30
1	A	252	ARG	CB-CA-C	5.08	118.11	109.84
1	A	514	GLN	CB-CA-C	5.04	118.86	110.90
1	A	369	ARG	N-CA-CB	-5.03	102.72	110.16
1	A	464	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	479	VAL	N-CA-CB	5.02	117.08	111.21
1	A	98	ARG	CB-CA-C	5.02	118.95	109.37
1	A	323	PRO	CB-CA-C	5.01	117.92	111.46

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	ARG	Sidechain
1	A	158	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	218	ARG	Sidechain
1	A	264	PRO	Peptide
1	A	369	ARG	Sidechain
1	A	387	ARG	Sidechain
1	A	416	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	59	ARG	Sidechain
1	B	112	ARG	Sidechain
1	B	387	ARG	Sidechain

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	3498	0	3474	76	1
1	B	3517	0	3494	52	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	8	0	6	6	0
5	A	7	0	0	1	0
5	B	7	0	0	0	0
All	All	7067	0	7000	106	1

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 8.

All (106) 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:A:177:GLN:NE2	1:A:209:VAL:CG2	2.27	0.98
1:A:177:GLN:CD	1:A:209:VAL:HG22	1.89	0.96
1:B:511:ASP:OD2	1:B:513:SER:OG	1.85	0.94
1:A:413:LEU:HD23	1:A:530:MET:HE2	1.52	0.91
1:A:284:LYS:HD2	1:A:339:GLY:HA3	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ARG:HG2	1:B:63:ILE:HG21	1.55	0.88
1:A:177:GLN:NE2	1:A:209:VAL:HG22	1.91	0.83
1:A:177:GLN:NE2	1:A:209:VAL:HG21	1.99	0.78
1:A:174:GLU:O	1:A:175:VAL:HG23	1.83	0.78
1:B:413:LEU:HD23	1:B:530:MET:HE2	1.67	0.77
1:A:264:PRO:HG3	1:B:117:THR:HG21	1.67	0.76
1:A:340:ARG:HD3	1:A:354:TRP:CZ2	2.22	0.74
1:A:192:GLU:O	1:B:66:ARG:NH2	2.23	0.72
1:A:239:ARG:HH11	1:A:239:ARG:CG	2.02	0.72
1:B:340:ARG:HD3	1:B:354:TRP:CZ2	2.24	0.72
1:A:444:ASP:OD2	4:A:604:ACY:CH3	2.37	0.71
1:B:136:LEU:HD11	1:B:138:ILE:HD11	1.71	0.71
1:A:239:ARG:HH11	1:A:239:ARG:HG2	1.54	0.71
1:A:413:LEU:HD23	1:A:530:MET:CE	2.22	0.70
1:A:177:GLN:CD	1:A:209:VAL:CG2	2.64	0.69
1:A:177:GLN:CG	1:A:209:VAL:HG22	2.22	0.68
1:A:158:ARG:NH1	1:B:402:VAL:O	2.26	0.67
1:A:149:LEU:HD12	1:B:139:ALA:HB2	1.76	0.67
1:A:255:HIS:CD2	1:B:469:GLY:HA2	2.30	0.67
1:A:196:VAL:HG13	1:A:210:SER:HB2	1.78	0.65
1:A:272:GLN:HG3	1:A:273:TYR:H	1.62	0.65
1:A:315:ASP:HB3	1:A:332:PHE:CD2	2.32	0.64
1:B:315:ASP:HB3	1:B:332:PHE:CD2	2.34	0.62
1:A:97:VAL:HG22	1:A:533:GLN:HG2	1.83	0.61
1:A:444:ASP:HA	4:A:604:ACY:H3	1.82	0.61
1:A:177:GLN:HG3	1:A:209:VAL:HG22	1.82	0.60
1:A:444:ASP:OD2	4:A:604:ACY:H2	2.01	0.60
1:A:447:ARG:HE	4:A:604:ACY:H1	1.67	0.59
1:B:97:VAL:HG22	1:B:533:GLN:HG2	1.83	0.59
1:A:364:ARG:HG2	1:A:364:ARG:HH11	1.68	0.59
1:A:177:GLN:HE21	1:A:207:THR:HG21	1.68	0.58
1:B:301:ARG:HG2	1:B:301:ARG:NH1	2.18	0.58
1:A:447:ARG:HE	4:A:604:ACY:CH3	2.19	0.56
1:B:284:LYS:HD3	1:B:339:GLY:HA3	1.88	0.56
1:B:301:ARG:HG2	1:B:301:ARG:HH11	1.71	0.54
1:A:272:GLN:HG3	1:A:273:TYR:N	2.22	0.53
1:B:342:LEU:C	1:B:342:LEU:HD23	2.32	0.53
1:B:76:ALA:HB1	1:B:404:PRO:HG3	1.91	0.53
1:A:76:ALA:HB1	1:A:404:PRO:HG3	1.90	0.52
1:A:330:MET:HE2	1:A:334:LYS:HB3	1.92	0.52
1:A:255:HIS:CD2	1:B:469:GLY:CA	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ARG:HG2	1:A:239:ARG:NH1	2.24	0.52
1:B:189:VAL:HG21	1:B:198:LEU:HD13	1.92	0.52
1:A:177:GLN:HE21	1:A:207:THR:CG2	2.23	0.51
1:B:415:GLN:NE2	1:B:532:SER:HA	2.25	0.51
1:A:65:VAL:HG22	1:B:193:VAL:HG22	1.93	0.51
4:A:603:ACY:CH3	1:B:444:ASP:OD1	2.59	0.50
1:A:342:LEU:C	1:A:342:LEU:HD23	2.36	0.50
1:A:335:GLY:HA3	5:A:706:HOH:O	2.12	0.49
1:B:340:ARG:CD	1:B:354:TRP:CZ2	2.96	0.48
1:B:288:ARG:NH2	1:B:357:ASP:OD1	2.46	0.48
1:A:340:ARG:CD	1:A:354:TRP:CZ2	2.94	0.48
1:A:194:THR:OG1	1:B:64:PRO:HG2	2.12	0.48
1:A:288:ARG:NH2	1:A:357:ASP:OD1	2.47	0.48
1:A:100:ILE:N	1:A:100:ILE:HD12	2.29	0.47
1:A:174:GLU:O	1:A:175:VAL:CG2	2.59	0.47
1:A:334:LYS:HG3	1:B:328:TYR:OH	2.15	0.47
1:A:334:LYS:HE2	1:B:326:GLU:OE2	2.14	0.47
1:A:63:ILE:HD11	1:B:214:ASP:HB3	1.96	0.46
1:A:337:PHE:HB2	1:A:455:LEU:O	2.15	0.46
1:A:101:ASP:OD1	1:A:104:LYS:HG3	2.16	0.46
1:A:137:LEU:HB2	1:B:150:GLN:HG2	1.98	0.46
1:A:469:GLY:CA	1:B:255:HIS:CD2	2.99	0.46
1:B:189:VAL:HG13	1:B:223:VAL:HG22	1.98	0.46
1:A:218:ARG:HG2	1:B:63:ILE:CG2	2.35	0.45
1:A:469:GLY:HA2	1:B:255:HIS:CD2	2.52	0.45
1:A:228:ARG:HD3	1:A:228:ARG:HA	1.64	0.45
1:A:63:ILE:CD1	1:B:214:ASP:HB3	2.46	0.45
1:A:457:ARG:HA	1:A:457:ARG:HD3	1.76	0.45
1:A:99:ALA:C	1:A:100:ILE:HD12	2.42	0.44
1:B:263:PRO:HA	1:B:264:PRO:HD3	1.91	0.44
1:A:157:LEU:HD11	1:A:230:TYR:HB2	1.99	0.44
1:A:326:GLU:HB3	1:B:331:PRO:HG2	1.99	0.44
1:A:374:LEU:HD12	1:A:440:LEU:HD23	1.99	0.44
1:A:154:VAL:HB	1:A:160:ILE:HG12	2.00	0.43
1:A:342:LEU:HG	1:B:342:LEU:HG	2.01	0.43
1:B:82:CYS:HB3	1:B:531:THR:HG23	2.01	0.42
1:A:334:LYS:HE2	1:B:328:TYR:OH	2.19	0.42
1:B:69:GLU:H	1:B:69:GLU:HG2	1.59	0.42
1:B:364:ARG:HH21	1:B:364:ARG:HG3	1.83	0.42
1:B:208:LEU:HD23	1:B:219:GLN:CG	2.50	0.42
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:VAL:HG11	1:B:190:ALA:H	1.85	0.42
1:B:319:ARG:HA	1:B:319:ARG:HD3	1.49	0.42
1:A:186:THR:HG23	1:A:228:ARG:HG3	2.01	0.41
1:B:362:THR:OG1	1:B:364:ARG:HB2	2.19	0.41
1:A:176:TYR:CE2	1:A:213:LEU:HB2	2.55	0.41
1:B:429:CYS:HA	1:B:475:SER:O	2.20	0.41
1:B:100:ILE:HD13	1:B:100:ILE:HA	1.84	0.41
1:B:157:LEU:HD11	1:B:230:TYR:HB2	2.02	0.41
1:B:239:ARG:NH1	1:B:239:ARG:HG3	2.34	0.41
1:A:429:CYS:HA	1:A:475:SER:O	2.20	0.41
1:B:364:ARG:HB3	1:B:480:VAL:HB	2.03	0.41
1:A:300:ARG:HH11	1:A:300:ARG:HD3	1.71	0.41
1:A:63:ILE:HA	1:A:64:PRO:HD3	1.87	0.41
1:A:153:GLU:HG3	1:A:252:ARG:HG2	2.02	0.41
1:A:119:GLU:O	1:A:123:GLN:HG2	2.21	0.41
1:A:331:PRO:HD2	1:B:328:TYR:CE1	2.56	0.41
1:A:252:ARG:HD3	1:A:254:ARG:NH1	2.36	0.40
1:A:387:ARG:HA	1:A:393:ALA:HA	2.02	0.40
1:B:374:LEU:HD12	1:B:440:LEU:HD23	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:SER:O	1:B:98:ARG:NH2[2_546]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	436/499 (87%)	424 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	444/499 (89%)	427 (96%)	17 (4%)	0	100	100
All	All	880/998 (88%)	851 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	382/423 (90%)	368 (96%)	14 (4%)	29	54
1	B	382/423 (90%)	369 (97%)	13 (3%)	32	57
All	All	764/846 (90%)	737 (96%)	27 (4%)	31	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	GLU
1	A	59	ARG
1	A	63	ILE
1	A	69	GLU
1	A	107	ASP
1	A	129	SER
1	A	160	ILE
1	A	197	THR
1	A	239	ARG
1	A	334	LYS
1	A	388	GLU
1	A	409	LEU
1	A	456	SER
1	A	530	MET
1	B	54	LEU
1	B	66	ARG
1	B	69	GLU
1	B	129	SER

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Mol	Chain	Res	Type
1	B	160	ILE
1	B	188	ASP
1	B	189	VAL
1	B	192	GLU
1	B	197	THR
1	B	319	ARG
1	B	389	ILE
1	B	409	LEU
1	B	511	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	GLN
1	A	177	GLN
1	A	245	HIS
1	A	255	HIS
1	A	518	HIS
1	B	173	GLN
1	B	255	HIS
1	B	346	GLN
1	B	415	GLN

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	ACY	A	603	-	3,3,3	1.14	0	3,3,3	0.82	0
3	NAG	B	602	1	14,14,15	0.42	0	17,19,21	1.08	1 (5%)
3	NAG	A	602	1	14,14,15	0.41	0	17,19,21	1.29	2 (11%)
4	ACY	A	604	-	3,3,3	0.67	0	3,3,3	1.14	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
3	NAG	B	602	1	-	3/6/23/26	0/1/1/1
3	NAG	A	602	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	NAG	C2-N2-C7	2.61	126.62	122.90
3	A	602	NAG	O5-C5-C6	2.58	111.25	107.20
3	B	602	NAG	C3-C4-C5	-2.09	106.50	110.24

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	NAG	C8-C7-N2-C2
3	A	602	NAG	O5-C5-C6-O6
3	A	602	NAG	C4-C5-C6-O6
3	B	602	NAG	O7-C7-N2-C2
3	B	602	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	ACY	1	0
4	A	604	ACY	5	0

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 [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	446/499 (89%)	-0.21	9 (2%) 64 63	65, 115, 205, 259	0
1	B	450/499 (90%)	-0.27	10 (2%) 62 60	62, 108, 175, 222	0
All	All	896/998 (89%)	-0.24	19 (2%) 63 62	62, 111, 193, 259	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	PRO	3.5
1	B	140	PRO	3.4
1	B	54	LEU	2.9
1	A	189	VAL	2.9
1	A	93	PHE	2.8
1	A	213	LEU	2.6
1	B	389	ILE	2.6
1	A	222	LEU	2.5
1	A	389	ILE	2.5
1	A	247	ALA	2.3
1	B	93	PHE	2.3
1	B	211	PRO	2.2
1	A	238	VAL	2.2
1	A	248	ALA	2.2
1	A	143	SER	2.2
1	B	265	GLY	2.1
1	B	247	ALA	2.1
1	B	112	ARG	2.1
1	B	485	SER	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](#)

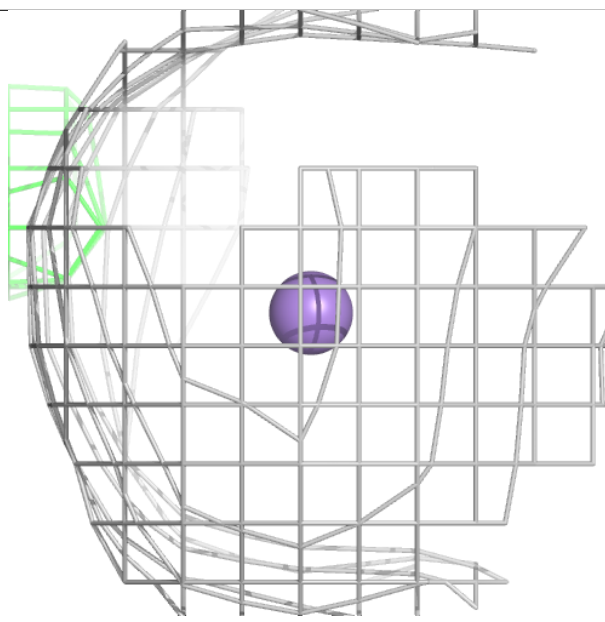
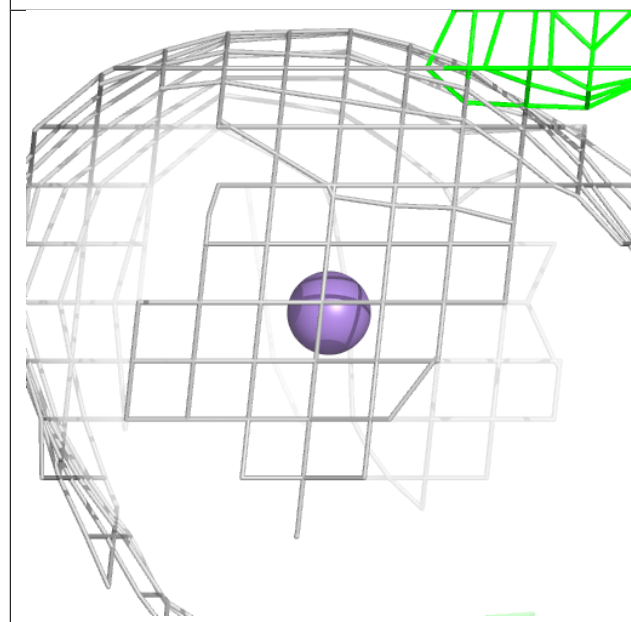
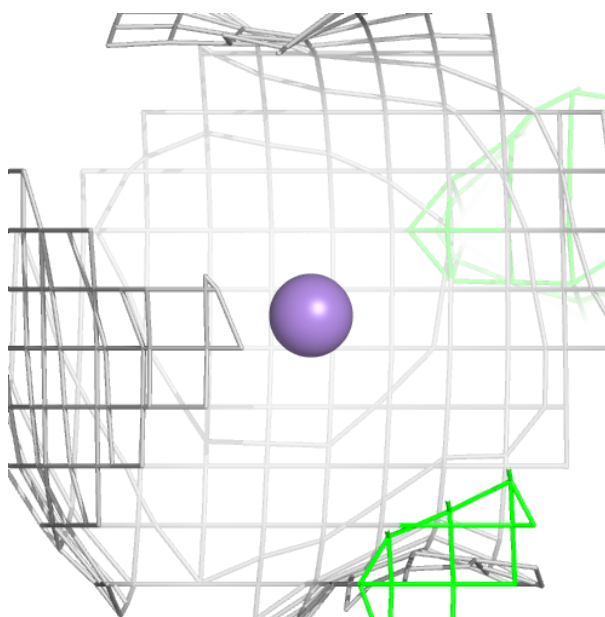
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NAG	A	602	14/15	0.80	0.12	118,146,161,162	0
3	NAG	B	602	14/15	0.81	0.14	118,139,164,181	0
2	MN	A	601	1/1	0.87	0.09	160,160,160,160	0
2	MN	B	601	1/1	0.87	0.14	149,149,149,149	0
4	ACY	A	603	4/4	0.89	0.21	63,88,91,96	0
4	ACY	A	604	4/4	0.96	0.15	62,78,81,83	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.

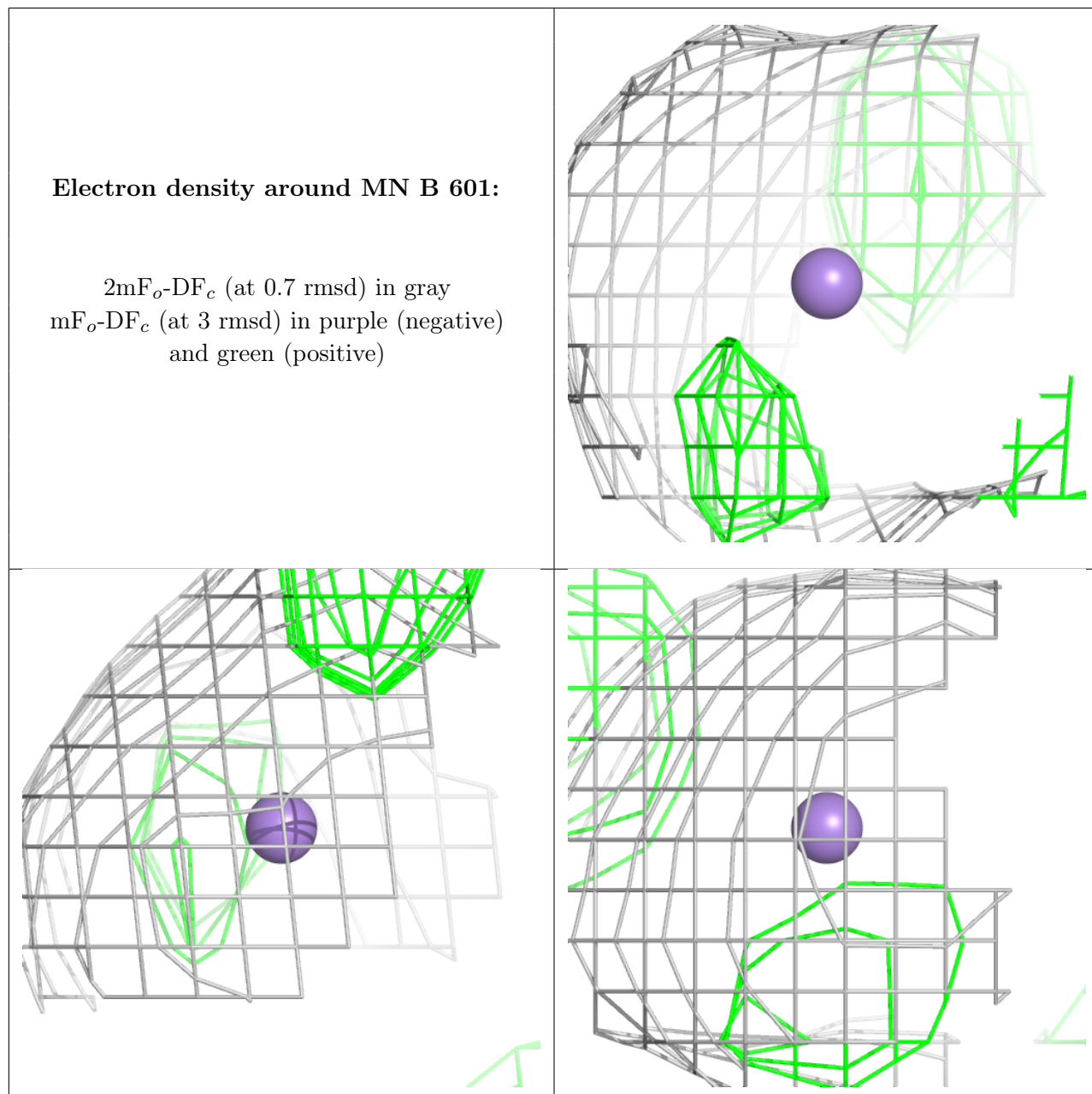
Electron density around MN A 601:

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



Electron density around MN 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.