



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:51 PM UTC

PDB ID : 7XRF / pdb_00007xrf
Title : Crystal structure of DgpB/C complex
Authors : Ma, M.; He, P.
Deposited on : 2022-05-10
Resolution : 2.14 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

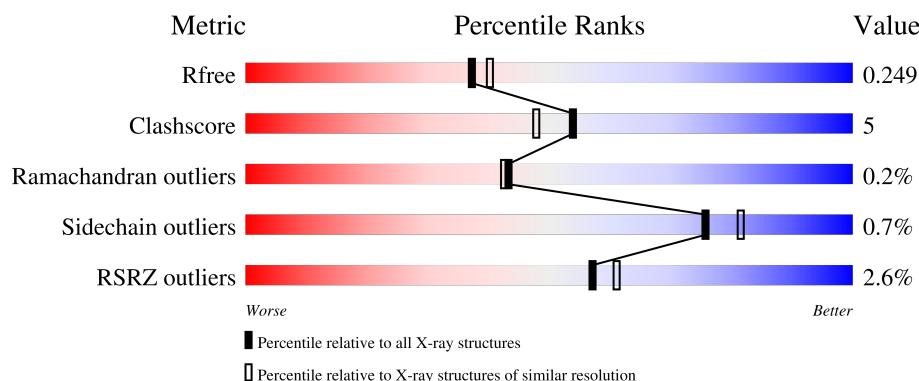
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	324	2% 83% 15% .
1	C	324	2% 85% 14% .
1	E	324	2% 90% 9%
1	G	324	7% 80% 14% . 6%
2	B	142	0% 89% 9% .

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Mol	Chain	Length	Quality of chain
2	D	142	 91%7% •
2	F	142	 89%8% •
2	H	142	 90%8% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14639 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 AP_endonuc_2 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2546	1615	421	483	27			
1	C	323	Total	C	N	O	S	0	0	0
			2550	1617	421	485	27			
1	E	323	Total	C	N	O	S	0	0	0
			2539	1611	420	481	27			
1	G	305	Total	C	N	O	S	0	0	0
			2318	1465	387	443	23			

- Molecule 2 is a protein called DgpB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1111	714	179	214	4			
2	D	139	Total	C	N	O	S	0	0	0
			1111	714	179	214	4			
2	F	139	Total	C	N	O	S	0	0	0
			1111	714	179	214	4			
2	H	139	Total	C	N	O	S	0	0	0
			1111	714	179	214	4			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		

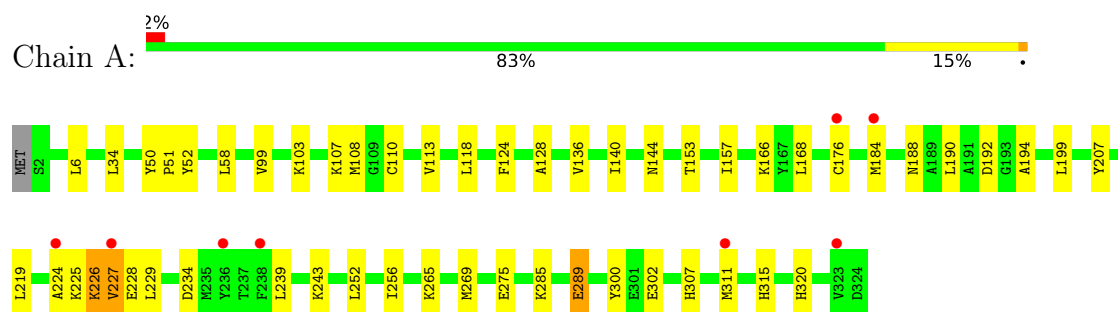
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total 24	O 24	0	0
4	B	27	Total 27	O 27	0	0
4	C	42	Total 42	O 42	0	0
4	D	27	Total 27	O 27	0	0
4	E	33	Total 33	O 33	0	0
4	F	32	Total 32	O 32	0	0
4	G	30	Total 30	O 30	0	0
4	H	23	Total 23	O 23	0	0

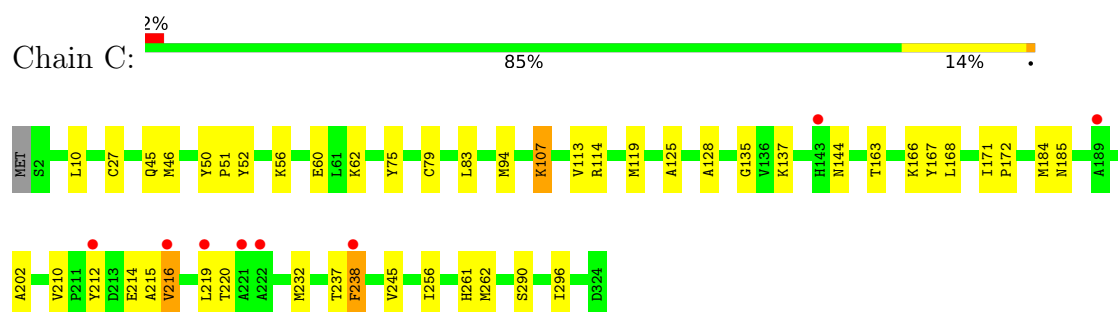
3 Residue-property plots [i](#)

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.

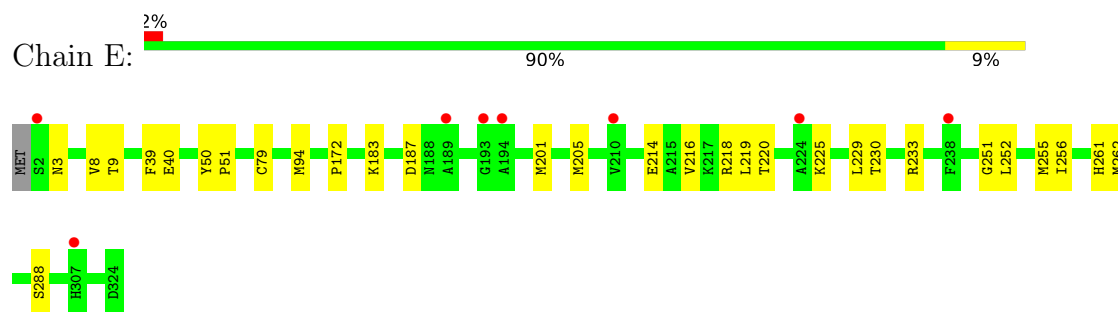
- Molecule 1: AP_endonuc_2 domain-containing protein



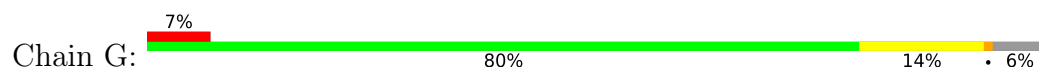
- Molecule 1: AP_endonuc_2 domain-containing protein

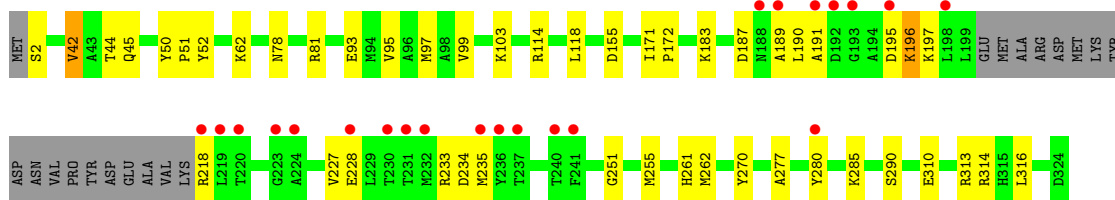


- Molecule 1: AP_endonuc_2 domain-containing protein

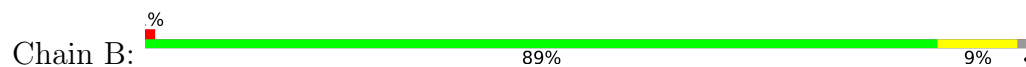


- Molecule 1: AP_endonuc_2 domain-containing protein





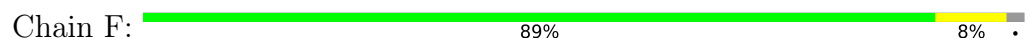
● Molecule 2: DgpB



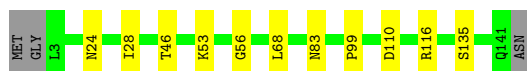
● Molecule 2: DgpB



● Molecule 2: DgpB



● Molecule 2: DgpB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.08Å 159.70Å 176.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 2.14 19.84 – 2.14	Depositor EDS
% Data completeness (in resolution range)	96.0 (19.84-2.14) 94.7 (19.84-2.14)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.91 (at 2.13Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.206 , 0.251 0.207 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14639	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% 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	0.39	0/2602	0.55	0/3512
1	C	0.61	0/2606	0.65	4/3517 (0.1%)
1	E	0.38	0/2595	0.52	1/3504 (0.0%)
1	G	0.50	0/2368	0.76	9/3202 (0.3%)
2	B	0.30	0/1137	0.44	0/1543
2	D	0.31	0/1137	0.46	0/1543
2	F	0.36	0/1137	0.49	0/1543
2	H	0.31	0/1137	0.46	0/1543
All	All	0.44	0/14719	0.58	14/19907 (0.1%)

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	C	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	THR	CB-CA-C	-7.64	99.64	110.34
1	G	227	VAL	CA-C-N	6.73	134.39	121.54
1	G	227	VAL	C-N-CA	6.73	134.39	121.54
1	E	3	ASN	CB-CA-C	5.89	119.56	110.14
1	G	234	ASP	N-CA-C	-5.67	105.00	112.72
1	G	196	LYS	N-CA-C	-5.65	104.51	111.75
1	C	237	THR	CA-C-N	5.56	132.15	121.54
1	C	237	THR	C-N-CA	5.56	132.15	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	190	LEU	CA-C-N	5.17	131.41	121.54
1	G	190	LEU	C-N-CA	5.17	131.41	121.54
1	G	277	ALA	CA-C-N	-5.05	117.87	123.43
1	G	277	ALA	C-N-CA	-5.05	117.87	123.43
1	G	189	ALA	CA-C-O	-5.05	116.12	122.63
1	C	238	PHE	N-CA-CB	5.01	118.96	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	144	ASN	Peptide

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	2546	0	2467	41	0
1	C	2550	0	2471	31	0
1	E	2539	0	2454	16	0
1	G	2318	0	2153	26	0
2	B	1111	0	1072	7	0
2	D	1111	0	1072	8	0
2	F	1111	0	1072	7	0
2	H	1111	0	1072	7	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	24	0	0	0	0
4	B	27	0	0	0	0
4	C	42	0	0	1	0
4	D	27	0	0	0	0
4	E	33	0	0	1	0
4	F	32	0	0	0	0
4	G	30	0	0	5	0
4	H	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14639	0	13833	137	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 5.

All (137) 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:285:LYS:HD2	1:A:289:GLU:OE1	1.70	0.90
1:E:79:CYS:SG	1:E:94:MET:HE2	2.18	0.84
1:A:194:ALA:HA	1:A:227:VAL:HG21	1.64	0.79
1:A:285:LYS:O	1:A:289:GLU:HB2	1.83	0.77
1:A:307:HIS:HB2	1:A:311:MET:HE2	1.69	0.73
1:C:172:PRO:HG2	1:C:262:MET:HG2	1.72	0.71
1:G:62:LYS:NZ	4:G:503:HOH:O	2.24	0.70
1:C:212:TYR:O	1:C:216:VAL:HG22	1.92	0.68
1:A:307:HIS:HB2	1:A:311:MET:CE	2.24	0.67
1:C:79:CYS:SG	1:C:94:MET:HE3	2.36	0.66
1:E:201:MET:HE2	1:E:219:LEU:HD12	1.77	0.66
1:E:288:SER:OG	4:E:501:HOH:O	2.15	0.65
1:G:2:SER:N	4:G:504:HOH:O	2.31	0.63
1:C:10:LEU:HD22	1:C:27:CYS:HB3	1.82	0.61
1:C:56:LYS:O	1:C:60:GLU:HG3	2.00	0.60
1:A:269:MET:HE3	1:A:315:HIS:ND1	2.16	0.60
1:C:51:PRO:HG2	1:C:52:TYR:CE2	2.36	0.60
2:F:6:ARG:NH1	2:F:133:CYS:O	2.29	0.58
1:G:42:VAL:HG13	1:G:45:GLN:HB3	1.85	0.57
1:G:251:GLY:O	1:G:255:MET:HG3	2.04	0.57
1:E:50:TYR:CG	1:E:51:PRO:HA	2.39	0.57
1:A:194:ALA:CA	1:A:227:VAL:HG21	2.34	0.57
1:C:262:MET:HB2	1:C:296:ILE:HG12	1.87	0.57
1:C:94:MET:HE2	1:C:119:MET:HA	1.87	0.56
1:C:256:ILE:HG21	1:C:290:SER:HB2	1.88	0.56
1:A:51:PRO:HG2	1:A:52:TYR:CE2	2.42	0.55
1:A:229:LEU:H	1:A:229:LEU:HD12	1.72	0.55
1:A:190:LEU:HD21	1:A:199:LEU:HD12	1.89	0.54
1:A:194:ALA:HA	1:A:227:VAL:CG2	2.37	0.54
1:A:225:LYS:O	1:A:229:LEU:HD12	2.08	0.53
1:C:94:MET:CE	1:C:119:MET:HA	2.39	0.53
1:E:225:LYS:O	1:E:229:LEU:HD12	2.08	0.53
1:A:50:TYR:CG	1:A:51:PRO:HA	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:310:GLU:OE2	1:G:313:ARG:NH1	2.41	0.52
1:A:207:TYR:CD1	1:A:243:LYS:HB2	2.44	0.52
1:A:252:LEU:O	1:A:256:ILE:HG12	2.10	0.52
2:F:18:LEU:HD11	2:F:102:LEU:HD12	1.91	0.52
1:C:50:TYR:CG	1:C:51:PRO:HA	2.45	0.52
1:C:202:ALA:HA	1:C:232:MET:HE2	1.92	0.51
1:A:124:PHE:CD1	1:A:140:ILE:HD11	2.45	0.51
1:C:172:PRO:HD2	1:C:261:HIS:O	2.11	0.51
1:G:2:SER:HB2	1:G:290:SER:O	2.10	0.51
2:B:53:LYS:HE2	2:B:56:GLY:HA2	1.91	0.51
1:A:307:HIS:CB	1:A:311:MET:HE2	2.40	0.51
2:D:12:VAL:O	2:D:34:VAL:HA	2.11	0.51
1:A:190:LEU:HD23	1:A:194:ALA:HB3	1.93	0.50
1:A:234:ASP:HB3	1:A:239:LEU:HD12	1.92	0.50
1:A:269:MET:HE2	1:A:275:GLU:HG2	1.93	0.50
1:C:216:VAL:O	1:C:220:THR:HG23	2.11	0.50
1:G:99:VAL:HG12	1:G:103:LYS:HE3	1.94	0.50
2:F:6:ARG:HD2	2:F:131:ASP:O	2.12	0.49
1:A:153:THR:O	1:A:157:ILE:HG13	2.11	0.49
1:G:196:LYS:O	1:G:218:ARG:CB	2.60	0.49
2:D:83:ASN:OD1	2:H:83:ASN:ND2	2.46	0.49
1:A:128:ALA:HB2	1:A:168:LEU:HD11	1.94	0.49
1:G:50:TYR:CG	1:G:51:PRO:HA	2.48	0.48
1:C:114:ARG:HG2	1:C:171:ILE:HD12	1.95	0.48
1:E:172:PRO:HG2	1:E:262:MET:HG2	1.96	0.47
1:G:51:PRO:HG2	1:G:52:TYR:CE2	2.50	0.47
1:C:125:ALA:HB1	1:C:163:THR:HG21	1.96	0.47
1:C:128:ALA:HB2	1:C:168:LEU:HD11	1.96	0.47
1:A:225:LYS:HD2	1:A:226:LYS:NZ	2.30	0.47
1:A:113:VAL:HG23	1:A:136:VAL:HG11	1.97	0.47
1:A:285:LYS:HD2	1:A:289:GLU:CD	2.37	0.46
1:C:107:LYS:HB3	1:C:107:LYS:HE3	1.58	0.46
2:H:46:THR:HA	2:H:116:ARG:NH1	2.30	0.46
1:E:214:GLU:OE2	1:E:218:ARG:NH1	2.47	0.46
1:G:114:ARG:HG2	1:G:171:ILE:HD12	1.97	0.46
1:C:214:GLU:C	1:C:216:VAL:N	2.74	0.46
1:C:210:VAL:HG23	1:C:215:ALA:HB2	1.97	0.46
1:C:137:LYS:HG2	1:C:167:TYR:HA	1.99	0.45
1:A:6:LEU:HD12	1:A:320:HIS:CE1	2.52	0.45
2:B:46:THR:HA	2:B:116:ARG:NH1	2.32	0.45
1:G:78:ASN:OD1	4:G:501:HOH:O	2.21	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG12	1:A:103:LYS:HE3	1.98	0.45
1:G:50:TYR:CD1	1:G:51:PRO:HA	2.52	0.45
1:C:83:LEU:HD11	2:D:43:PHE:CD1	2.52	0.44
1:C:245:VAL:O	1:C:245:VAL:HG23	2.15	0.44
2:F:53:LYS:HB3	2:F:110:ASP:HB2	2.00	0.44
2:H:68:LEU:HD12	2:H:68:LEU:HA	1.81	0.44
1:A:184:MET:O	1:A:188:ASN:ND2	2.39	0.44
1:E:183:LYS:NZ	1:E:187:ASP:OD2	2.50	0.44
1:A:300:TYR:CZ	1:A:302:GLU:HB2	2.53	0.44
1:C:75:TYR:HB3	1:C:113:VAL:HG22	1.99	0.44
1:A:58:LEU:HD22	1:A:107:LYS:HG2	1.98	0.44
1:A:225:LYS:O	1:A:229:LEU:CD1	2.66	0.44
1:A:307:HIS:CB	1:A:311:MET:CE	2.96	0.44
2:B:3:LEU:HD12	2:B:4:ALA:H	1.82	0.44
1:G:233:ARG:C	1:G:235:MET:H	2.26	0.44
1:E:8:VAL:O	1:E:39:PHE:HA	2.18	0.43
2:F:28:ILE:HA	2:F:99:PRO:HA	2.00	0.43
2:B:12:VAL:O	2:B:34:VAL:HA	2.18	0.43
1:C:219:LEU:HD13	1:C:232:MET:HE1	2.00	0.43
1:A:108:MET:HE2	1:A:110:CYS:SG	2.59	0.43
2:B:123:SER:OG	2:B:126:GLU:HG2	2.19	0.43
1:G:195:ASP:C	1:G:197:LYS:N	2.75	0.43
2:H:53:LYS:HE3	2:H:56:GLY:HA2	1.99	0.43
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.88	0.43
1:A:124:PHE:CG	1:A:140:ILE:HD11	2.53	0.43
1:C:62:LYS:HA	1:C:62:LYS:HD2	1.68	0.43
1:E:205:MET:SD	1:E:218:ARG:HD2	2.58	0.43
2:H:110:ASP:OD1	2:H:135:SER:HB3	2.19	0.43
2:D:71:LYS:HD3	1:G:52:TYR:CD2	2.54	0.43
1:E:9:THR:HB	1:E:40:GLU:HB3	2.00	0.42
1:G:172:PRO:HG2	1:G:262:MET:HG2	2.00	0.42
1:G:316:LEU:HD23	1:G:316:LEU:HA	1.89	0.42
1:A:265:LYS:HE3	1:A:265:LYS:HB2	1.90	0.42
2:F:67:CYS:HB2	2:F:93:THR:HB	2.01	0.42
1:G:270:TYR:O	1:G:314:ARG:HD3	2.20	0.42
1:G:93:GLU:O	1:G:97:MET:HG3	2.18	0.42
1:A:144:ASN:OD1	1:A:176:CYS:HA	2.19	0.42
1:A:166:LYS:N	1:A:166:LYS:HD2	2.35	0.42
1:G:155:ASP:OD1	4:G:502:HOH:O	2.21	0.42
1:E:172:PRO:HD2	1:E:261:HIS:O	2.20	0.42
1:C:185:ASN:ND2	4:C:501:HOH:O	2.13	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:LEU:O	1:E:256:ILE:HG12	2.19	0.41
2:H:28:ILE:HA	2:H:99:PRO:HA	2.02	0.41
2:B:83:ASN:HB3	2:F:83:ASN:HD21	1.83	0.41
1:E:230:THR:HA	1:E:233:ARG:HB2	2.02	0.41
1:G:44:THR:HG23	4:G:501:HOH:O	2.21	0.41
1:C:45:GLN:HG2	1:C:46:MET:HG3	2.03	0.41
1:C:166:LYS:HD3	1:C:166:LYS:HA	1.79	0.41
1:E:251:GLY:O	1:E:255:MET:HB2	2.20	0.41
1:G:95:VAL:O	1:G:99:VAL:HG23	2.20	0.41
1:A:219:LEU:HG	1:A:224:ALA:HB2	2.03	0.41
1:A:225:LYS:N	1:A:228:GLU:OE1	2.53	0.41
2:B:39:TYR:HH	2:B:119:TYR:HH	1.57	0.41
1:G:81:ARG:NH1	1:G:118:LEU:HD22	2.36	0.41
1:G:172:PRO:HD2	1:G:261:HIS:O	2.21	0.41
2:D:71:LYS:HD3	1:G:52:TYR:CE2	2.55	0.41
1:C:135:GLY:HA3	2:H:24:ASN:ND2	2.36	0.40
2:D:67:CYS:HA	2:D:71:LYS:O	2.21	0.40
1:E:216:VAL:O	1:E:220:THR:OG1	2.30	0.40
1:C:184:MET:HA	1:C:184:MET:HE2	2.04	0.40
2:D:17:SER:HB2	2:D:33:ASP:H	1.85	0.40
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.92	0.40
2:D:46:THR:HA	2:D:116:ARG:NH1	2.36	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	321/324 (99%)	305 (95%)	16 (5%)	0	100	100
1	C	321/324 (99%)	304 (95%)	16 (5%)	1 (0%)	36	33
1	E	321/324 (99%)	310 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	301/324 (93%)	275 (91%)	23 (8%)	3 (1%)	12	7
2	B	137/142 (96%)	134 (98%)	3 (2%)	0	100	100
2	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
2	F	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
2	H	137/142 (96%)	132 (96%)	5 (4%)	0	100	100
All	All	1812/1864 (97%)	1730 (96%)	78 (4%)	4 (0%)	43	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	238	PHE
1	G	228	GLU
1	G	187	ASP
1	G	191	ALA

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	270/277 (98%)	266 (98%)	4 (2%)	57	63
1	C	271/277 (98%)	269 (99%)	2 (1%)	76	81
1	E	268/277 (97%)	268 (100%)	0	100	100
1	G	231/277 (83%)	227 (98%)	4 (2%)	53	58
2	B	123/125 (98%)	123 (100%)	0	100	100
2	D	123/125 (98%)	123 (100%)	0	100	100
2	F	123/125 (98%)	123 (100%)	0	100	100
2	H	123/125 (98%)	123 (100%)	0	100	100
All	All	1532/1608 (95%)	1522 (99%)	10 (1%)	76	81

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	ASP
1	A	226	LYS
1	A	227	VAL
1	A	289	GLU
1	C	107	LYS
1	C	216	VAL
1	G	42	VAL
1	G	183	LYS
1	G	280	TYR
1	G	285	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	C	3	ASN
1	C	185	ASN
1	C	267	HIS
2	D	8	ASN
2	D	31	GLN
2	D	139	ASN
1	E	185	ASN
1	G	106	HIS
1	G	261	HIS
2	H	31	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	323/324 (99%)	0.22	8 (2%) 58 62	44, 60, 90, 104	0
1	C	323/324 (99%)	0.30	8 (2%) 58 62	46, 60, 90, 103	0
1	E	323/324 (99%)	0.36	8 (2%) 58 62	48, 62, 88, 101	0
1	G	305/324 (94%)	0.40	22 (7%) 21 25	44, 61, 100, 113	0
2	B	139/142 (97%)	-0.12	1 (0%) 84 86	43, 52, 65, 82	0
2	D	139/142 (97%)	-0.08	0 100 100	42, 50, 63, 75	0
2	F	139/142 (97%)	0.06	0 100 100	43, 55, 70, 81	0
2	H	139/142 (97%)	-0.04	0 100 100	44, 54, 68, 83	0
All	All	1830/1864 (98%)	0.21	47 (2%) 57 61	42, 58, 89, 113	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	198	LEU	4.2
1	G	189	ALA	3.5
1	G	188	ASN	3.5
1	A	311	MET	3.3
1	G	232	MET	3.3
1	G	240	THR	3.2
1	G	193	GLY	3.1
1	C	238	PHE	3.1
1	A	224	ALA	3.0
1	G	236	TYR	2.9
1	G	230	THR	2.9
1	G	192	ASP	2.8
1	G	231	THR	2.8
1	E	194	ALA	2.8
1	G	219	LEU	2.8
1	C	222	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	212	TYR	2.7
1	G	228	GLU	2.6
1	G	218	ARG	2.6
1	A	238	PHE	2.5
1	G	235	MET	2.4
1	E	224	ALA	2.4
1	G	195	ASP	2.4
1	C	189	ALA	2.3
1	C	221	ALA	2.3
1	C	219	LEU	2.3
1	G	191	ALA	2.3
1	C	216	VAL	2.3
1	E	2	SER	2.2
1	G	224	ALA	2.2
1	E	238	PHE	2.2
1	E	210	VAL	2.2
1	E	193	GLY	2.2
1	E	189	ALA	2.2
1	G	280	TYR	2.1
1	A	227	VAL	2.1
1	A	323	VAL	2.1
1	G	237	THR	2.1
1	C	143	HIS	2.1
1	G	223	GLY	2.1
1	G	241	PHE	2.1
2	B	24	ASN	2.1
1	E	307	HIS	2.1
1	A	184	MET	2.0
1	A	176	CYS	2.0
1	G	220	THR	2.0
1	A	236	TYR	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

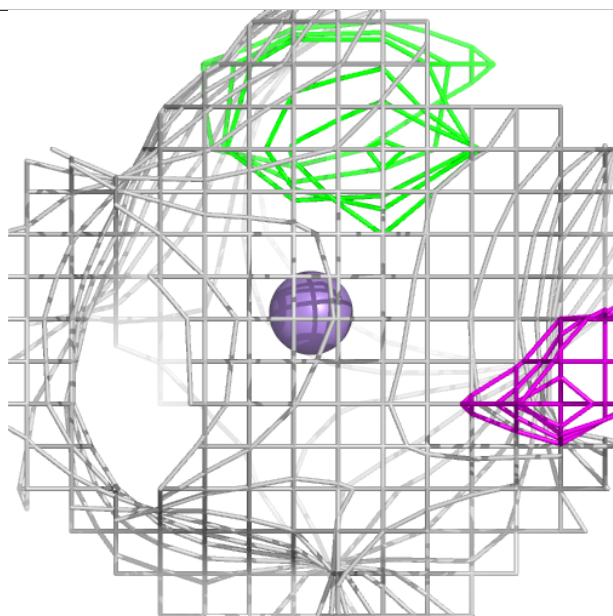
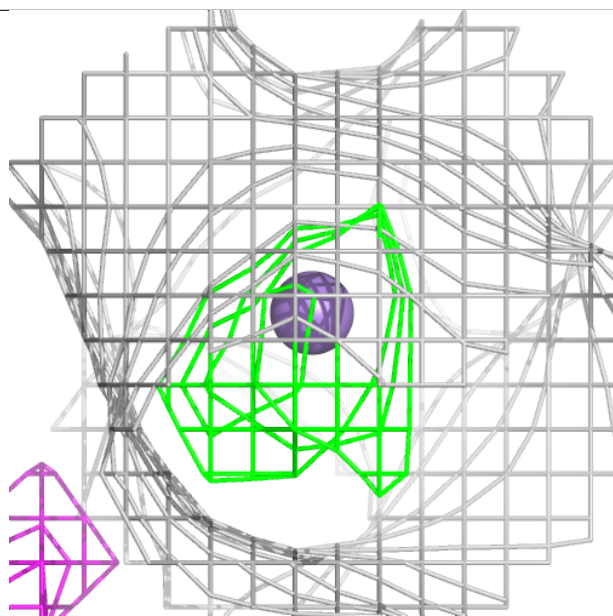
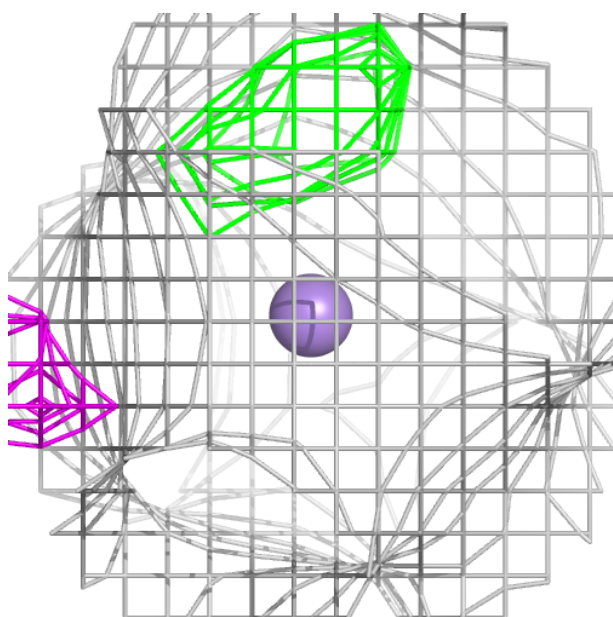
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MN	E	401	1/1	0.98	0.05	62,62,62,62	0
3	MN	A	401	1/1	0.99	0.03	53,53,53,53	0
3	MN	G	401	1/1	0.99	0.03	57,57,57,57	0
3	MN	C	401	1/1	1.00	0.03	54,54,54,54	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.

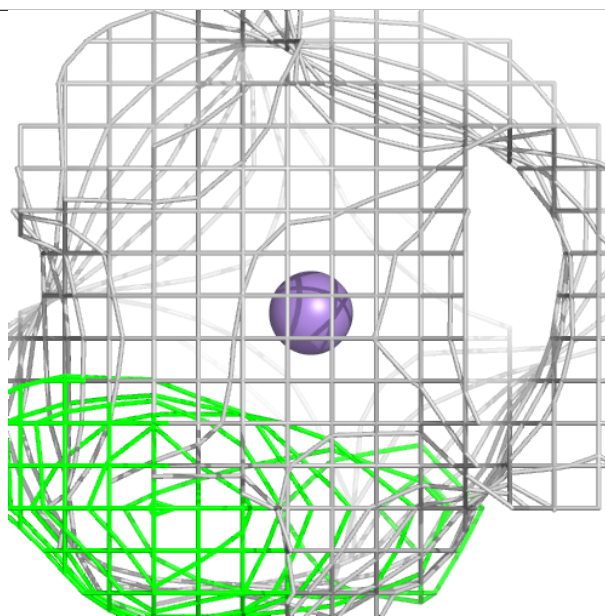
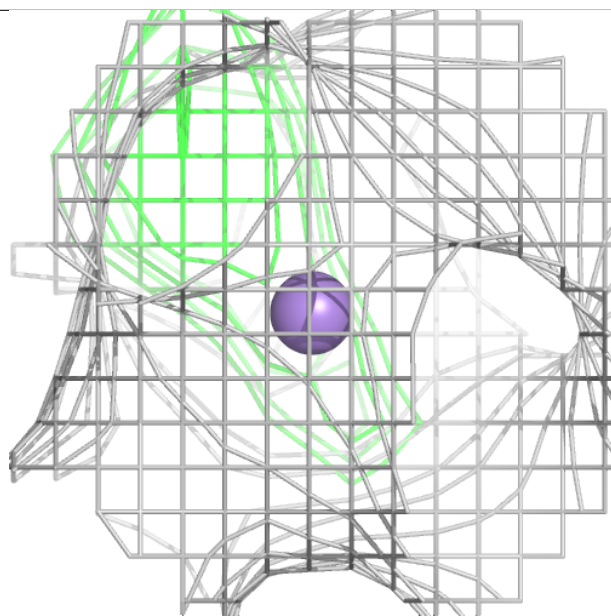
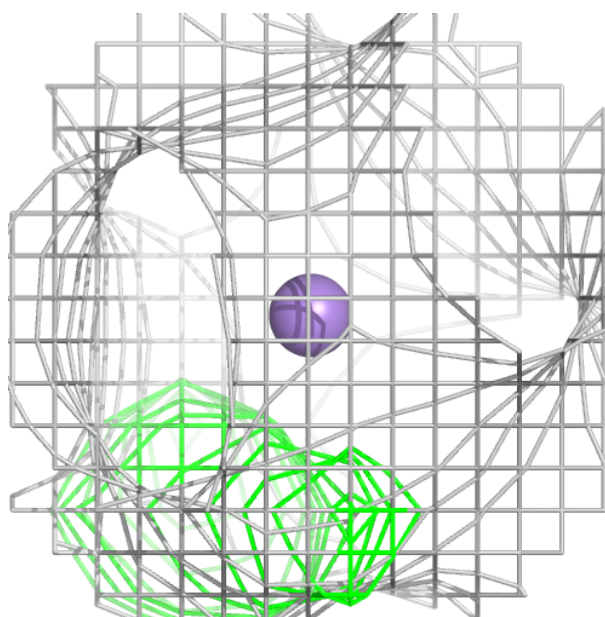
Electron density around MN E 401:

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



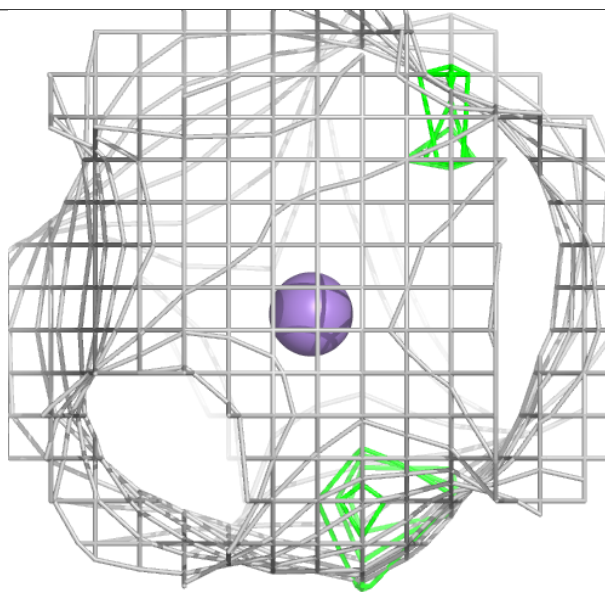
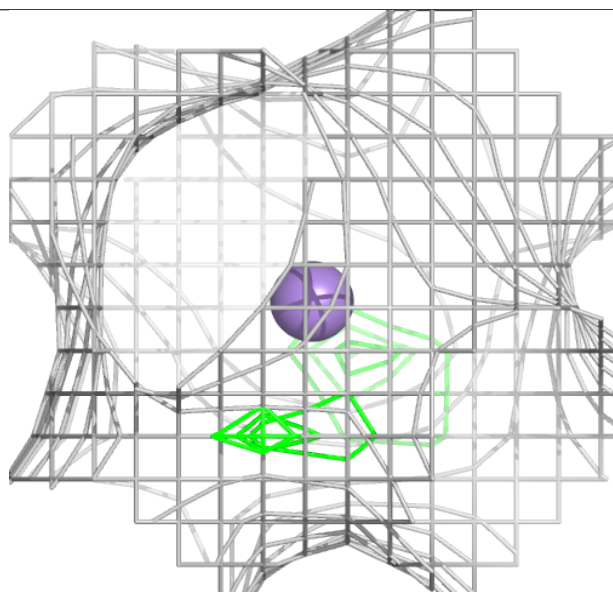
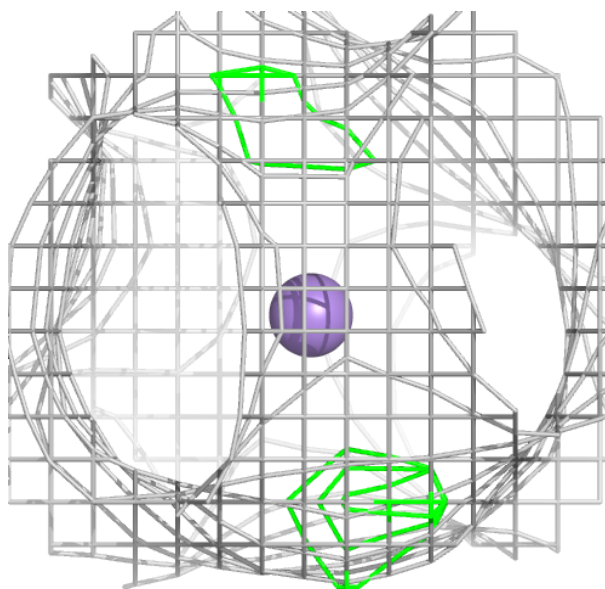
Electron density around MN A 401:

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



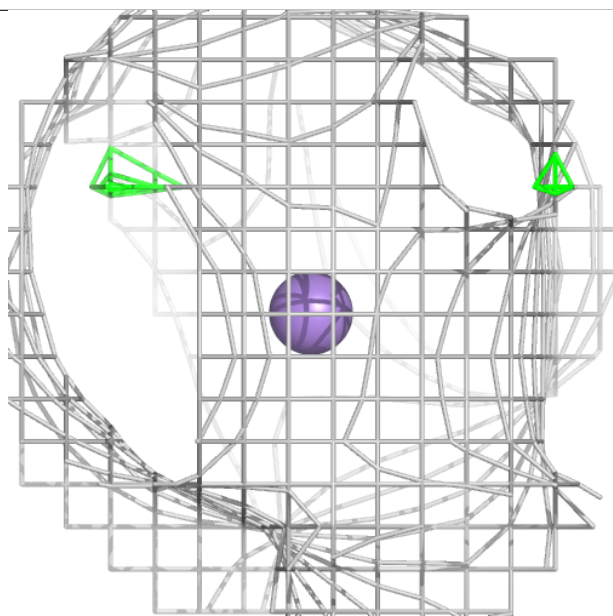
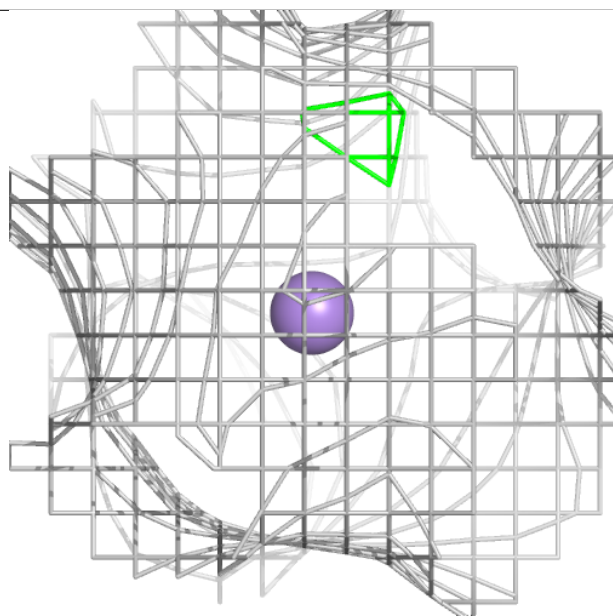
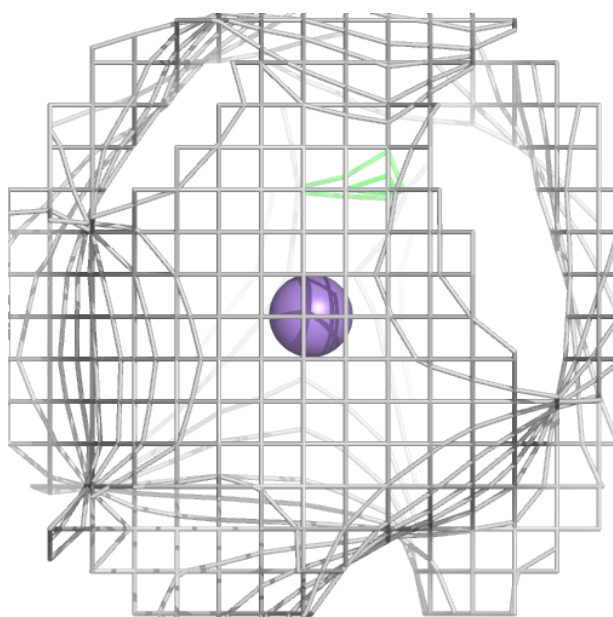
Electron density around MN G 401:

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



Electron density around MN C 401:

$2mF_o-DF_c$ (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.