



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 01:17 AM UTC

PDB ID : 9M3A / pdb_00009m3a
Title : Crystal structure of the DgpB2/C2 complex from W974-1 in substrate free form
Authors : Ma, W.
Deposited on : 2025-03-01
Resolution : 2.23 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

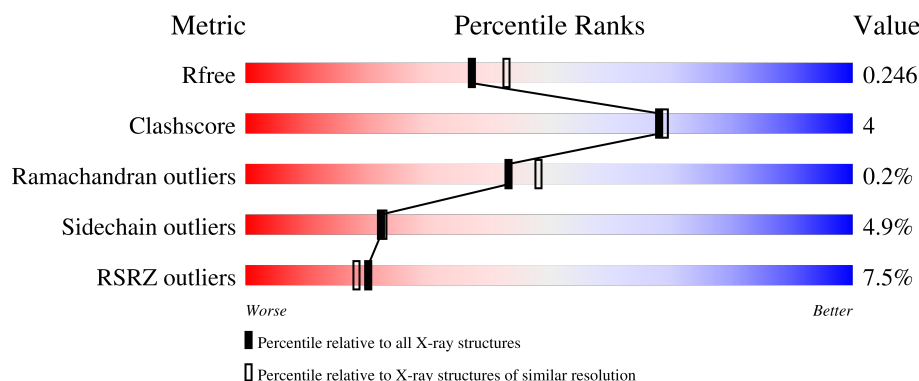
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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.



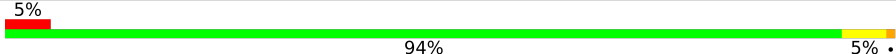


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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	325	<div> <div>5%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	C	325	<div> <div>13%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
1	F	325	<div> <div>6%</div> <div>86%</div> <div>14%</div> <div>.</div> </div>
1	H	325	<div> <div>12%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
2	B	147	<div> <div>4%</div> <div>88%</div> <div>7%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	147	 5% 94% 5% •
2	G	147	 2% 82% 14% ••
2	I	147	 3% 88% 11% •

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15790 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 Xylose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2585	1656	415	495	19			
1	C	324	Total	C	N	O	S	0	0	0
			2578	1651	414	495	18			
1	F	324	Total	C	N	O	S	0	0	0
			2584	1657	414	495	18			
1	H	325	Total	C	N	O	S	0	0	0
			2582	1656	411	496	19			

- Molecule 2 is a protein called DUF6379 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1155	739	198	210	8			
2	D	147	Total	C	N	O	S	0	0	0
			1179	756	201	213	9			
2	G	144	Total	C	N	O	S	0	0	0
			1155	739	198	210	8			
2	I	145	Total	C	N	O	S	0	0	0
			1166	748	199	211	8			

- 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	F	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

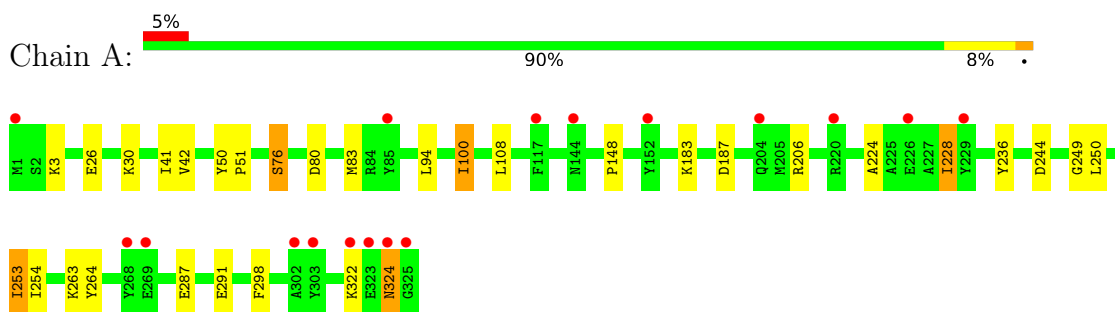
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	128	Total 128	O 128	0	0
4	B	76	Total 76	O 76	0	0
4	C	112	Total 112	O 112	0	0
4	D	87	Total 87	O 87	0	0
4	F	127	Total 127	O 127	0	0
4	G	83	Total 83	O 83	0	0
4	H	113	Total 113	O 113	0	0
4	I	77	Total 77	O 77	0	0

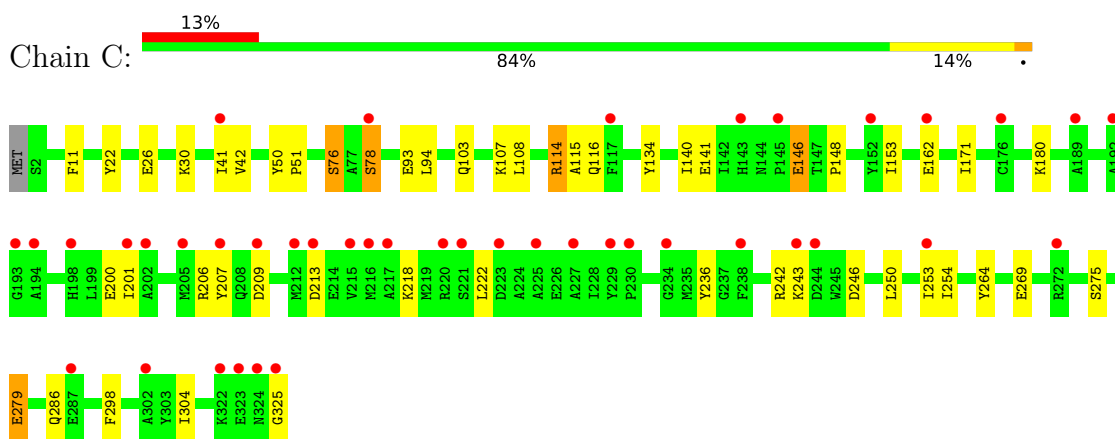
3 Residue-property plots [i](#)

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.

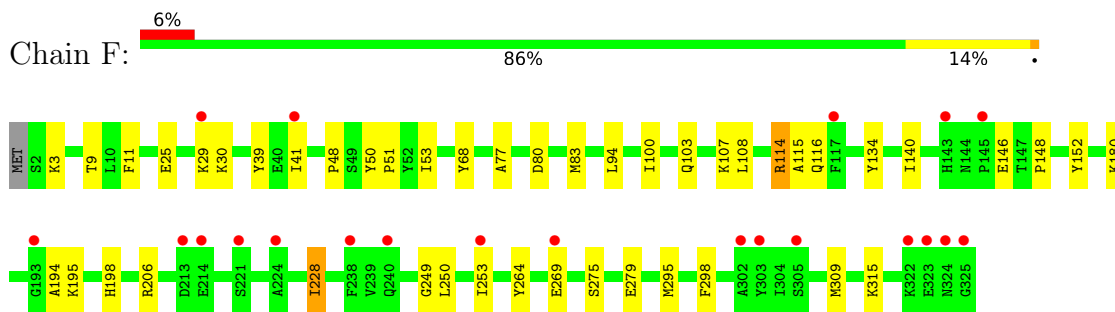
- Molecule 1: Xylose isomerase



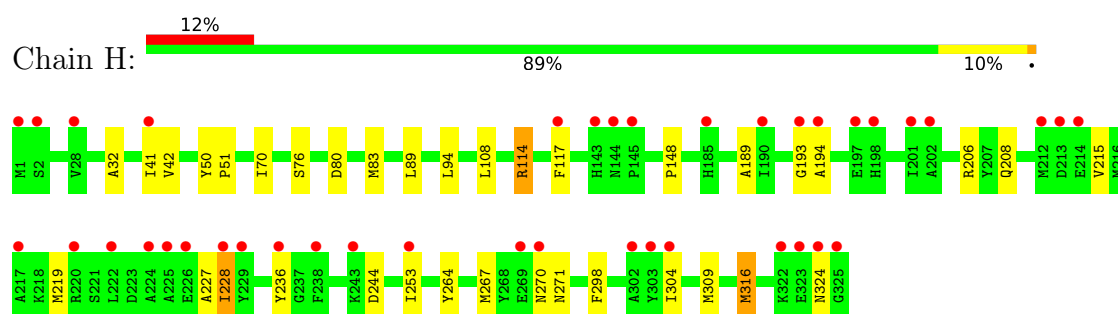
- Molecule 1: Xylose isomerase



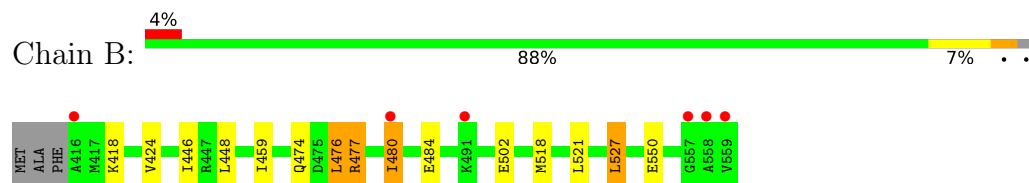
- Molecule 1: Xylose isomerase



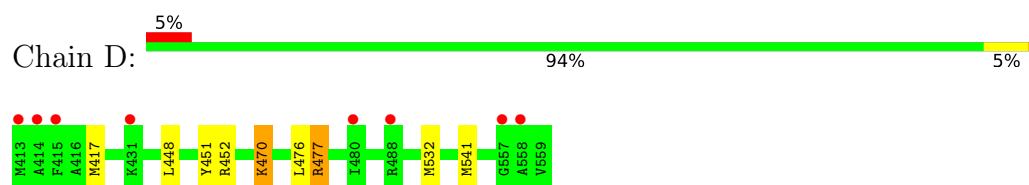
- Molecule 1: Xylose isomerase



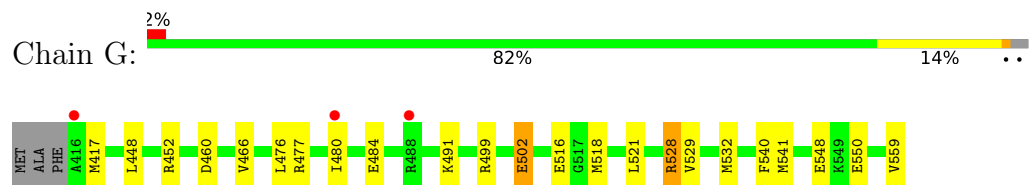
- Molecule 2: DUF6379 domain-containing protein



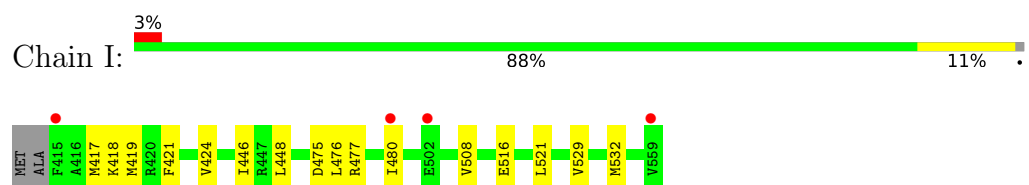
- Molecule 2: DUF6379 domain-containing protein



- Molecule 2: DUF6379 domain-containing protein



- Molecule 2: DUF6379 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.34Å 131.81Å 155.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.81 – 2.23 81.81 – 2.23	Depositor EDS
% Data completeness (in resolution range)	95.4 (81.81-2.23) 95.4 (81.81-2.23)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.211 , 0.247 0.211 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15790	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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	0.10	0/2649	0.29	0/3581
1	C	0.10	0/2642	0.29	0/3573
1	F	0.10	0/2649	0.29	0/3582
1	H	0.10	0/2647	0.30	0/3581
2	B	0.10	0/1180	0.30	0/1586
2	D	0.10	0/1205	0.28	0/1619
2	G	0.09	0/1180	0.29	0/1586
2	I	0.10	0/1192	0.28	0/1602
All	All	0.10	0/15344	0.29	0/20710

There are no bond length outliers.

There are no bond angle outliers.

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	2585	0	2508	16	0
1	C	2578	0	2496	24	0
1	F	2584	0	2503	26	0
1	H	2582	0	2493	14	0
2	B	1155	0	1142	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1179	0	1165	6	0
2	G	1155	0	1142	10	0
2	I	1166	0	1151	8	0
3	A	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
4	A	128	0	0	0	0
4	B	76	0	0	0	0
4	C	112	0	0	1	0
4	D	87	0	0	0	0
4	F	127	0	0	0	0
4	G	83	0	0	0	0
4	H	113	0	0	0	0
4	I	77	0	0	0	0
All	All	15790	0	14600	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 4.

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:C:114:ARG:HD3	1:C:141:GLU:HB2	1.67	0.74
1:H:194:ALA:HB1	1:H:228:ILE:HD12	1.74	0.68
2:B:459:ILE:HG12	2:B:527:LEU:HD22	1.80	0.64
1:F:9:THR:HG22	1:F:11:PHE:H	1.65	0.61
1:H:267:MET:HE1	1:H:316:MET:HE3	1.84	0.60
2:B:477:ARG:HG3	2:B:484:GLU:HB3	1.85	0.59
1:H:83:MET:HE3	1:H:89:LEU:HD11	1.84	0.58
2:D:417:MET:HG3	2:D:541:MET:HE3	1.85	0.57
1:F:29:LYS:HG2	1:F:68:TYR:CZ	2.40	0.56
1:H:80:ASP:HB2	1:H:83:MET:HE2	1.87	0.56
1:H:76:SER:HA	1:H:114:ARG:HB3	1.89	0.55
1:C:78:SER:O	1:C:116:GLN:HG3	2.07	0.55
1:F:25:GLU:O	1:F:29:LYS:HG3	2.06	0.55
1:F:148:PRO:HB3	1:F:253:ILE:HG12	1.88	0.54
1:F:77:ALA:O	1:F:114:ARG:NH1	2.41	0.53
1:A:80:ASP:HB2	1:A:83:MET:HE2	1.90	0.53
1:C:206:ARG:HD3	1:C:236:TYR:CZ	2.44	0.53
2:I:529:VAL:HG11	2:I:532:MET:HE3	1.90	0.53
1:C:250:LEU:O	1:C:254:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:PRO:HB3	1:H:253:ILE:HD13	1.92	0.52
1:F:180:LYS:HB2	1:F:275:SER:HA	1.92	0.52
1:H:189:ALA:HA	1:H:227:ALA:HB1	1.93	0.51
1:C:206:ARG:HH21	1:C:236:TYR:HA	1.76	0.51
1:A:148:PRO:HB3	1:A:253:ILE:HG12	1.92	0.51
1:F:80:ASP:HB2	1:F:83:MET:HE2	1.93	0.51
1:F:279:GLU:H	1:F:279:GLU:CD	2.18	0.51
2:G:477:ARG:HG2	2:G:484:GLU:HB3	1.93	0.50
1:C:114:ARG:HG2	1:C:171:ILE:HD12	1.92	0.50
1:C:146:GLU:HG3	1:C:153:ILE:HG12	1.94	0.50
2:G:528:ARG:HG3	2:G:540:PHE:HB2	1.92	0.50
1:F:194:ALA:HB1	1:F:228:ILE:HG12	1.93	0.50
1:A:42:VAL:HA	1:A:76:SER:HB3	1.94	0.50
2:B:480:ILE:HG12	2:B:502:GLU:OE2	2.12	0.50
1:F:146:GLU:OE2	1:F:152:TYR:HB3	2.12	0.49
1:F:39:TYR:HA	1:F:295:MET:HE1	1.95	0.49
1:A:264:TYR:CZ	1:A:298:PHE:HB2	2.48	0.48
1:H:206:ARG:HD3	1:H:236:TYR:CZ	2.49	0.48
2:B:476:LEU:O	2:B:477:ARG:HD3	2.14	0.48
1:C:218:LYS:HZ3	1:C:222:LEU:HD11	1.78	0.47
1:A:50:TYR:CD1	1:A:51:PRO:HA	2.49	0.47
1:H:264:TYR:CZ	1:H:298:PHE:HB2	2.49	0.47
1:A:80:ASP:HB3	1:A:83:MET:HB3	1.95	0.47
1:C:218:LYS:NZ	1:C:222:LEU:HD11	2.29	0.47
1:F:195:LYS:HD2	1:F:198:HIS:CE1	2.50	0.47
1:F:100:ILE:HD11	2:I:477:ARG:NH1	2.29	0.47
2:G:460:ASP:OD1	2:G:528:ARG:NH1	2.46	0.47
2:D:470:LYS:HB2	2:D:470:LYS:NZ	2.31	0.46
2:D:477:ARG:HD3	2:D:477:ARG:HA	1.62	0.46
1:C:26:GLU:O	1:C:30:LYS:HG2	2.16	0.46
1:A:183:LYS:HE3	1:A:187:ASP:OD2	2.15	0.46
1:H:32:ALA:HB2	1:H:70:ILE:HD13	1.98	0.46
1:C:115:ALA:HB3	1:C:140:ILE:HD13	1.98	0.46
1:A:100:ILE:HD11	2:D:477:ARG:CZ	2.45	0.46
2:G:499:ARG:HB2	2:G:502:GLU:HB2	1.98	0.45
1:C:11:PHE:HE1	2:D:451:TYR:CD1	2.33	0.45
1:F:50:TYR:CD1	1:F:51:PRO:HA	2.51	0.45
1:F:115:ALA:HB3	1:F:140:ILE:HD13	1.98	0.45
2:I:475:ASP:O	2:I:508:VAL:HA	2.16	0.45
1:C:264:TYR:CZ	1:C:298:PHE:HB2	2.50	0.45
1:C:103:GLN:HG2	1:C:134:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:TYR:CD1	1:C:51:PRO:HA	2.52	0.45
1:F:250:LEU:HD12	1:F:253:ILE:HD11	1.99	0.45
1:A:206:ARG:HD3	1:A:236:TYR:CZ	2.52	0.45
1:A:250:LEU:O	1:A:254:ILE:HG13	2.17	0.45
1:C:286:GLN:NE2	1:C:325:GLY:HA3	2.32	0.44
1:H:264:TYR:HE2	1:H:309:MET:HG2	1.82	0.44
1:H:42:VAL:HA	1:H:76:SER:HB3	2.00	0.44
1:C:42:VAL:HA	1:C:76:SER:HB3	2.00	0.44
1:F:103:GLN:HG2	1:F:134:TYR:CZ	2.51	0.44
2:D:417:MET:HE1	2:D:532:MET:HE1	1.99	0.44
1:F:48:PRO:O	2:G:499:ARG:HD3	2.18	0.44
2:I:417:MET:HE3	2:I:417:MET:HB2	1.88	0.44
1:C:201:ILE:HG22	4:C:495:HOH:O	2.18	0.44
2:I:419:MET:HE2	2:I:421:PHE:HZ	1.83	0.44
1:F:100:ILE:HD11	2:I:477:ARG:CZ	2.48	0.43
2:G:518:MET:HE3	2:G:550:GLU:HG2	1.99	0.43
1:H:50:TYR:CD1	1:H:51:PRO:HA	2.53	0.43
1:A:224:ALA:HB1	1:A:228:ILE:HD13	2.00	0.43
1:A:322:LYS:HE3	1:A:322:LYS:HB2	1.83	0.43
1:F:29:LYS:HG2	1:F:68:TYR:CE2	2.53	0.43
1:F:249:GLY:O	1:F:253:ILE:HG13	2.19	0.43
2:I:424:VAL:O	2:I:446:ILE:HA	2.19	0.43
1:C:180:LYS:HB2	1:C:275:SER:HA	2.00	0.43
1:F:315:LYS:HB3	1:F:315:LYS:NZ	2.34	0.43
1:F:53:ILE:HB	1:F:107:LYS:HD3	2.01	0.42
1:C:148:PRO:HB3	1:C:253:ILE:HD13	2.00	0.42
1:C:148:PRO:HG2	1:C:246:ASP:OD2	2.19	0.42
2:I:418:LYS:HE2	2:I:418:LYS:HB3	1.87	0.42
2:G:466:VAL:HG22	2:G:521:LEU:HD12	2.01	0.42
1:C:279:GLU:CD	1:C:279:GLU:H	2.27	0.42
1:F:269:GLU:H	1:F:269:GLU:CD	2.28	0.42
2:G:529:VAL:HG11	2:G:532:MET:HE3	2.01	0.42
1:C:207:TYR:HD1	1:C:243:LYS:HD3	1.84	0.42
1:F:264:TYR:CZ	1:F:298:PHE:HB2	2.55	0.41
2:G:417:MET:HE3	2:G:541:MET:HG2	2.02	0.41
2:G:417:MET:HE3	2:G:417:MET:HB2	1.98	0.41
2:B:424:VAL:O	2:B:446:ILE:HA	2.20	0.41
1:A:249:GLY:O	1:A:253:ILE:HG13	2.20	0.41
1:A:263:LYS:HE2	1:A:263:LYS:HB2	1.88	0.41
1:A:30:LYS:HD3	1:A:30:LYS:HA	1.86	0.41
1:F:30:LYS:HA	1:F:30:LYS:HD3	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:215:VAL:O	1:H:219:MET:HG2	2.21	0.41
2:B:518:MET:HE3	2:B:550:GLU:HG2	2.04	0.40
1:A:3:LYS:HB2	1:A:291:GLU:HG3	2.02	0.40
1:C:22:TYR:CZ	1:C:30:LYS:HG3	2.56	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	323/325 (99%)	317 (98%)	5 (2%)	1 (0%)	36	38
1	C	322/325 (99%)	311 (97%)	11 (3%)	0	100	100
1	F	322/325 (99%)	317 (98%)	5 (2%)	0	100	100
1	H	323/325 (99%)	307 (95%)	14 (4%)	2 (1%)	21	20
2	B	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
2	D	145/147 (99%)	143 (99%)	2 (1%)	0	100	100
2	G	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
2	I	143/147 (97%)	140 (98%)	3 (2%)	0	100	100
All	All	1862/1888 (99%)	1812 (97%)	47 (2%)	3 (0%)	43	48

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	270	ASN
1	A	324	ASN
1	H	193	GLY

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	274/275 (100%)	263 (96%)	11 (4%)	28	32
1	C	273/275 (99%)	256 (94%)	17 (6%)	16	15
1	F	274/275 (100%)	265 (97%)	9 (3%)	33	39
1	H	273/275 (99%)	261 (96%)	12 (4%)	25	27
2	B	122/124 (98%)	114 (93%)	8 (7%)	15	13
2	D	124/124 (100%)	119 (96%)	5 (4%)	28	32
2	G	122/124 (98%)	112 (92%)	10 (8%)	10	7
2	I	123/124 (99%)	118 (96%)	5 (4%)	27	30
All	All	1585/1596 (99%)	1508 (95%)	77 (5%)	22	23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLU
1	A	41	ILE
1	A	76	SER
1	A	94	LEU
1	A	100	ILE
1	A	108	LEU
1	A	228	ILE
1	A	244	ASP
1	A	253	ILE
1	A	287	GLU
1	A	324	ASN
2	B	418	LYS
2	B	448	LEU
2	B	474	GLN
2	B	476	LEU
2	B	477	ARG
2	B	480	ILE
2	B	521	LEU
2	B	527	LEU

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Mol	Chain	Res	Type
1	C	41	ILE
1	C	76	SER
1	C	78	SER
1	C	93	GLU
1	C	94	LEU
1	C	107	LYS
1	C	108	LEU
1	C	114	ARG
1	C	146	GLU
1	C	162	GLU
1	C	200	GLU
1	C	209	ASP
1	C	213	ASP
1	C	242	ARG
1	C	269	GLU
1	C	279	GLU
1	C	304	ILE
2	D	448	LEU
2	D	452	ARG
2	D	470	LYS
2	D	476	LEU
2	D	477	ARG
1	F	3	LYS
1	F	41	ILE
1	F	94	LEU
1	F	108	LEU
1	F	114	ARG
1	F	116	GLN
1	F	206	ARG
1	F	228	ILE
1	F	309	MET
2	G	448	LEU
2	G	452	ARG
2	G	476	LEU
2	G	480	ILE
2	G	491	LYS
2	G	502	GLU
2	G	516	GLU
2	G	528	ARG
2	G	548	GLU
2	G	559	VAL
1	H	41	ILE

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Mol	Chain	Res	Type
1	H	94	LEU
1	H	108	LEU
1	H	114	ARG
1	H	117	PHE
1	H	208	GLN
1	H	228	ILE
1	H	244	ASP
1	H	271	ASN
1	H	304	ILE
1	H	316	MET
1	H	324	ASN
2	I	448	LEU
2	I	476	LEU
2	I	480	ILE
2	I	516	GLU
2	I	521	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	106	HIS
1	A	116	GLN
1	A	154	GLN
1	C	79	ASN
1	C	286	GLN
2	D	433	ASN
2	D	443	GLN
1	F	103	GLN
1	H	103	GLN
1	H	116	GLN
1	H	144	ASN
1	H	265	HIS
1	H	271	ASN
2	I	524	HIS

5.3.3 RNA ⓘ

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 3 ligands modelled in this entry, 3 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 [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	325/325 (100%)	0.29	17 (5%) 33 31	19, 32, 54, 79	0
1	C	324/325 (99%)	0.73	42 (12%) 7 6	21, 40, 68, 88	0
1	F	324/325 (99%)	0.35	21 (6%) 25 23	18, 30, 55, 80	0
1	H	325/325 (100%)	0.59	40 (12%) 8 7	21, 33, 75, 94	0
2	B	144/147 (97%)	0.22	6 (4%) 40 39	20, 29, 45, 114	0
2	D	147/147 (100%)	0.21	8 (5%) 31 29	21, 30, 49, 96	0
2	G	144/147 (97%)	0.11	3 (2%) 63 65	21, 30, 44, 54	0
2	I	145/147 (98%)	0.01	4 (2%) 55 55	20, 28, 41, 73	0
All	All	1878/1888 (99%)	0.38	141 (7%) 20 18	18, 31, 64, 114	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	559	VAL	8.1
2	B	558	ALA	5.7
2	B	416	ALA	5.5
1	F	324	ASN	5.4
1	H	324	ASN	5.0
2	D	413	MET	4.9
1	F	323	GLU	4.9
2	I	415	PHE	4.9
1	A	117	PHE	4.8
1	A	325	GLY	4.8
1	A	1	MET	4.4
2	B	557	GLY	4.4
2	D	557	GLY	4.4
1	H	1	MET	4.3
1	H	325	GLY	4.3
1	H	2	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	224	ALA	4.1
2	B	480	ILE	4.0
1	F	322	LYS	4.0
1	C	238	PHE	4.0
1	C	324	ASN	4.0
1	F	325	GLY	3.9
1	H	323	GLU	3.9
1	H	238	PHE	3.9
2	D	558	ALA	3.9
1	C	117	PHE	3.8
1	F	303	TYR	3.8
1	H	269	GLU	3.8
1	C	213	ASP	3.7
1	C	325	GLY	3.6
1	A	303	TYR	3.5
1	F	238	PHE	3.5
2	D	415	PHE	3.5
1	C	192	ALA	3.5
1	H	117	PHE	3.5
2	B	491	LYS	3.4
1	H	145	PRO	3.4
1	H	214	GLU	3.3
1	A	324	ASN	3.3
1	C	244	ASP	3.3
1	H	193	GLY	3.3
1	A	302	ALA	3.2
1	C	302	ALA	3.2
1	C	205	MET	3.2
1	H	28	VAL	3.2
1	F	117	PHE	3.2
1	F	269	GLU	3.2
2	G	480	ILE	3.2
1	C	243	LYS	3.1
1	H	201	ILE	3.1
2	D	414	ALA	3.1
1	C	229	TYR	3.0
1	C	198	HIS	3.0
1	C	253	ILE	3.0
2	I	480	ILE	3.0
1	H	322	LYS	3.0
1	H	194	ALA	3.0
1	C	323	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	559	VAL	3.0
1	C	143	HIS	3.0
1	H	303	TYR	2.9
1	F	302	ALA	2.9
1	H	202	ALA	2.9
1	F	29	LYS	2.8
1	H	229	TYR	2.8
1	C	216	MET	2.8
1	C	201	ILE	2.8
1	C	230	PRO	2.8
1	A	323	GLU	2.8
1	F	240	GLN	2.7
1	C	220	ARG	2.7
1	A	269	GLU	2.7
1	H	225	ALA	2.7
1	A	220	ARG	2.7
1	H	217	ALA	2.6
2	D	431	LYS	2.6
1	C	234	GLY	2.6
1	F	143	HIS	2.6
1	C	194	ALA	2.6
1	C	227	ALA	2.6
1	C	152	TYR	2.6
2	D	480	ILE	2.6
1	H	143	HIS	2.6
1	F	214	GLU	2.6
1	H	41	ILE	2.6
1	H	220	ARG	2.6
1	A	152	TYR	2.6
2	G	488	ARG	2.5
1	A	144	ASN	2.5
1	H	270	ASN	2.5
1	H	197	GLU	2.5
1	C	215	VAL	2.4
1	H	228	ILE	2.4
1	C	225	ALA	2.4
1	C	207	TYR	2.4
1	C	209	ASP	2.4
2	G	416	ALA	2.4
1	C	212	MET	2.4
1	A	204	GLN	2.4
1	C	162	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	213	ASP	2.3
1	F	41	ILE	2.3
1	H	302	ALA	2.3
1	H	304	ILE	2.3
1	A	322	LYS	2.3
1	F	213	ASP	2.3
1	A	229	TYR	2.3
1	C	287	GLU	2.3
1	C	272	ARG	2.3
1	F	221	SER	2.3
1	F	305	SER	2.3
1	C	217	ALA	2.2
1	H	226	GLU	2.2
1	C	322	LYS	2.2
1	H	222	LEU	2.2
1	H	212	MET	2.2
1	A	268	TYR	2.2
2	D	488	ARG	2.2
2	I	502	GLU	2.2
1	C	176	CYS	2.2
1	H	198	HIS	2.1
1	C	189	ALA	2.1
1	C	202	ALA	2.1
1	H	253	ILE	2.1
1	C	145	PRO	2.1
1	H	185	HIS	2.1
1	C	78	SER	2.1
1	A	226	GLU	2.1
1	A	85	TYR	2.1
1	F	145	PRO	2.1
1	C	193	GLY	2.1
1	C	221	SER	2.1
1	C	41	ILE	2.1
1	F	253	ILE	2.1
1	H	236	TYR	2.1
1	F	193	GLY	2.1
1	C	223	ASP	2.0
1	H	243	LYS	2.0
1	F	224	ALA	2.0
1	H	144	ASN	2.0
1	H	190	ILE	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](#)

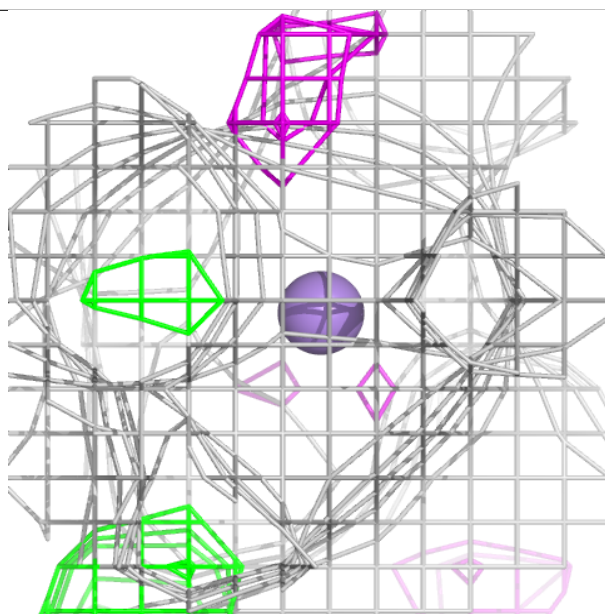
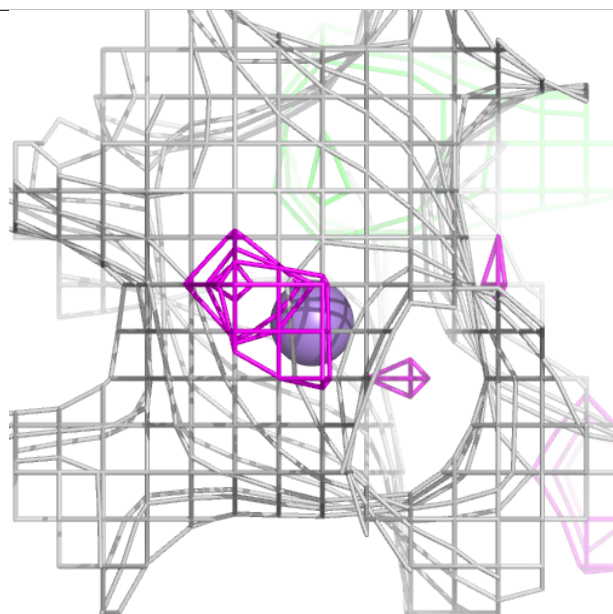
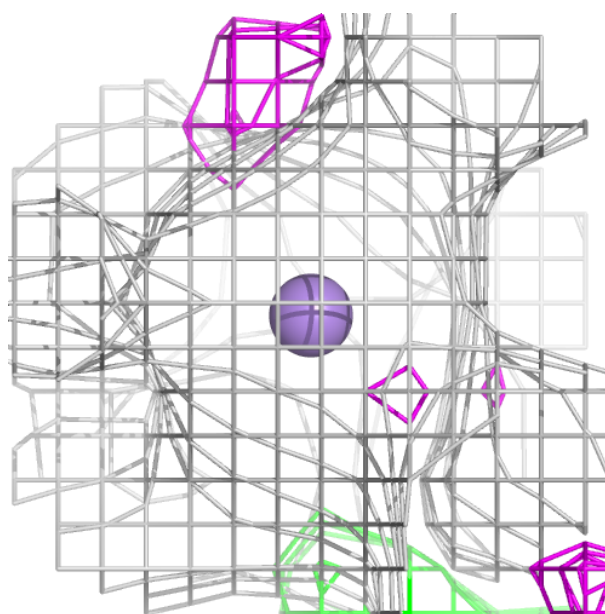
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MN	H	401	1/1	0.95	0.13	66,66,66,66	0
3	MN	F	401	1/1	0.97	0.20	48,48,48,48	0
3	MN	A	401	1/1	0.98	0.16	56,56,56,56	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.

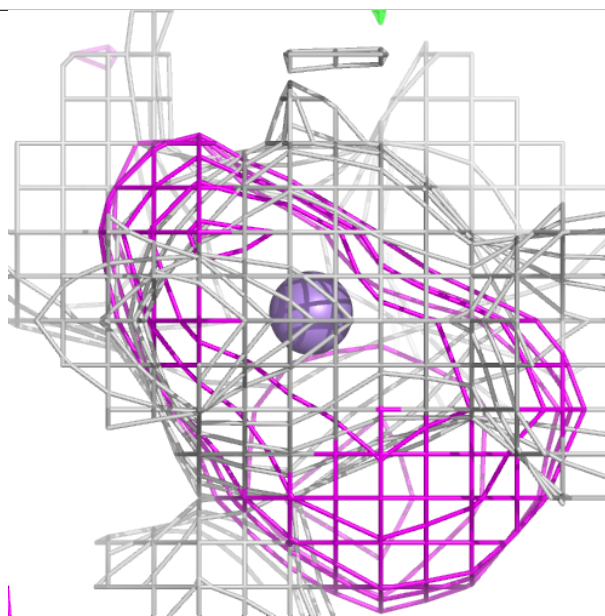
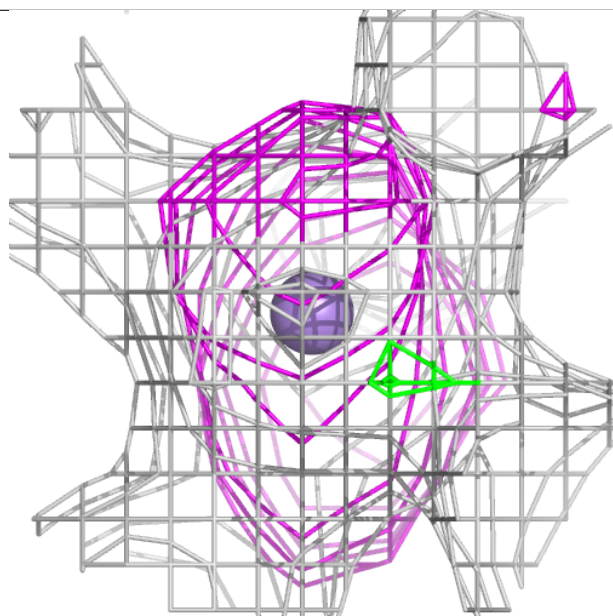
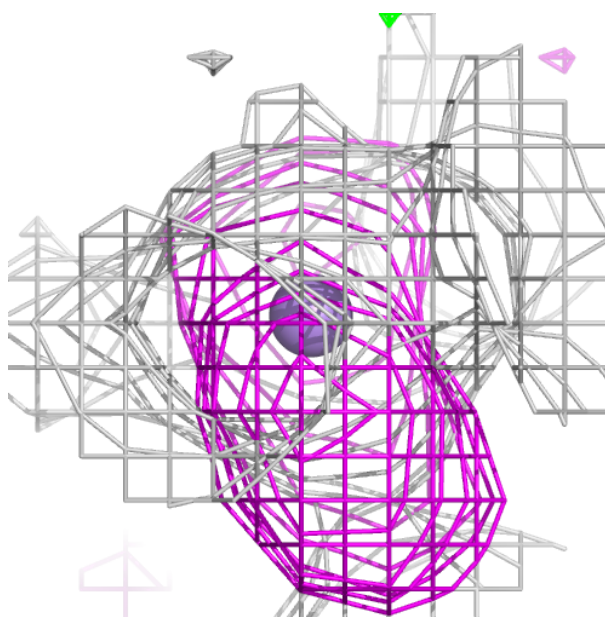
Electron density around MN H 401:

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



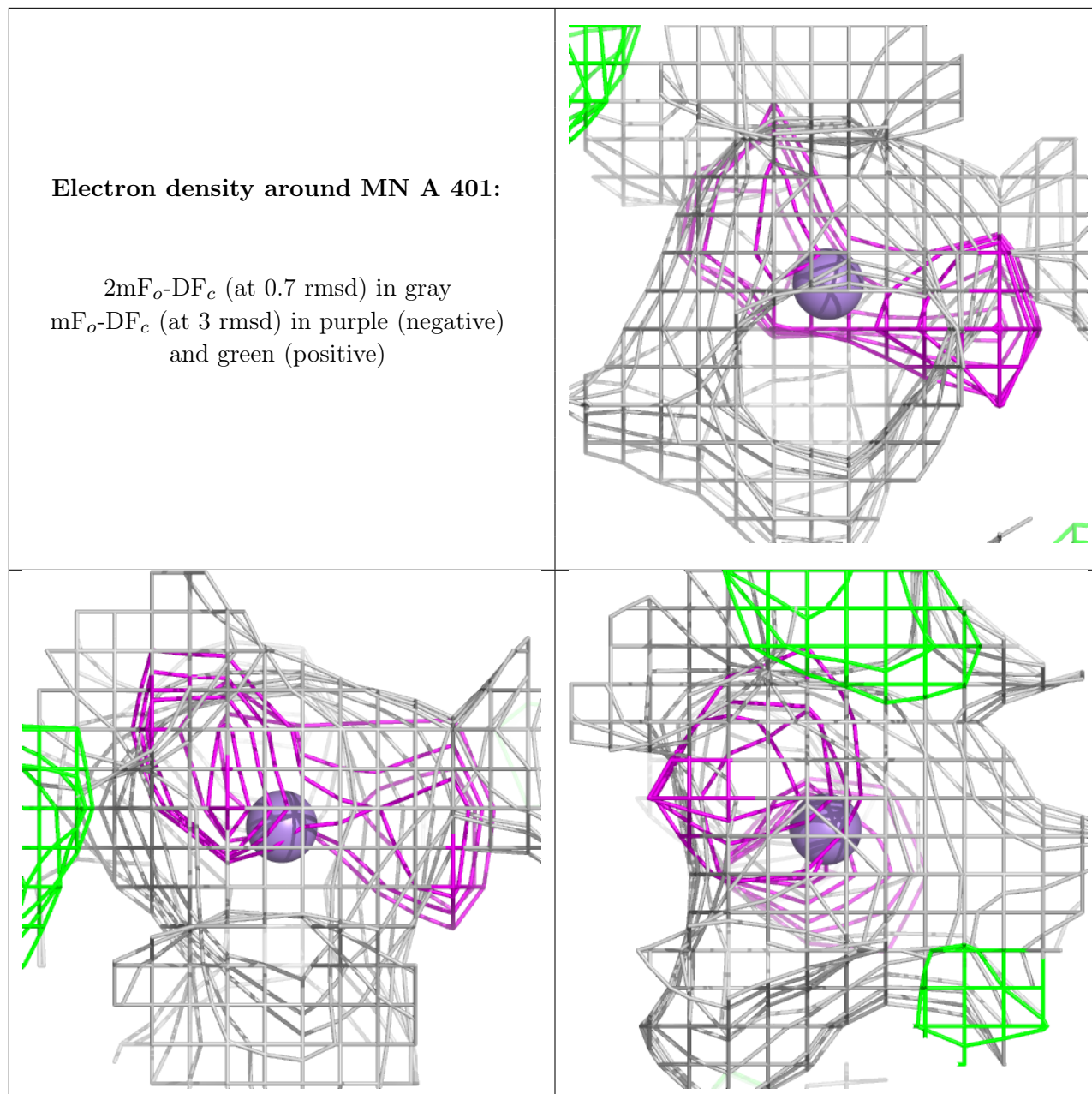
Electron density around MN F 401:

$2mF_o-DF_c$ (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)

**6.5 Other polymers** ⓘ

There are no such residues in this entry.