



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:41 AM UTC

PDB ID : 8SNF / pdb_00008snf
Title : Crystal structure of metformin hydrolase (MfmAB) from *Pseudomonas mendocina* sp. MET-2 with Ni²⁺ bound
Authors : Tassoulas, L.J.; Rankin, J.A.; Elias, M.H.; Wackett, L.P.
Deposited on : 2023-04-27
Resolution : 2.30 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

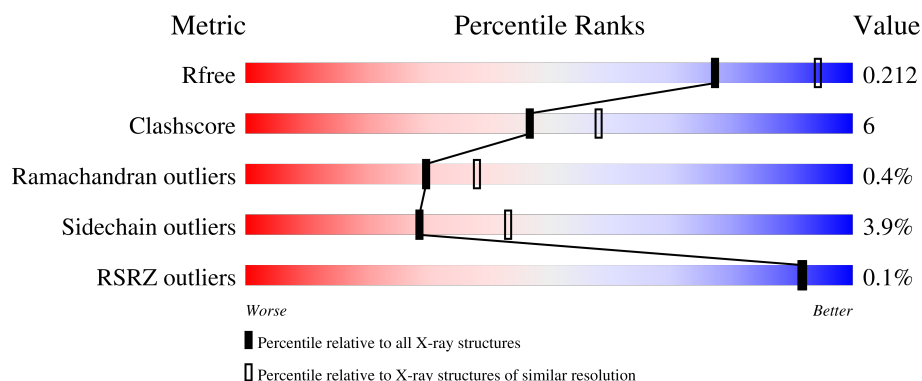
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

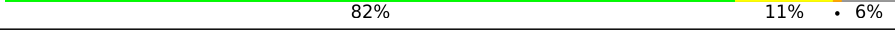
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	348	 79% 13% .. 6%
1	B	348	 81% 11% • 6%
1	C	348	 79% 12% .. 6%
1	E	348	 82% 11% • 6%
2	D	364	 79% 14% .. 5%

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Mol	Chain	Length	Quality of chain
2	F	364	81% 13% •• 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15792 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 metformin hydrolase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2507	1579	439	470	19			
1	B	326	Total	C	N	O	S	0	0	0
			2507	1579	439	470	19			
1	C	326	Total	C	N	O	S	0	0	0
			2507	1579	439	470	19			
1	E	326	Total	C	N	O	S	0	0	0
			2507	1579	439	470	19			

- Molecule 2 is a protein called metformin hydrolase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	347	Total	C	N	O	S	0	0	0
			2715	1711	476	505	23			
2	F	347	Total	C	N	O	S	0	0	0
			2715	1711	476	505	23			

- Molecule 3 is NICKEL (II) ION (CCD ID: NI) (formula: Ni) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Ni	0	0
			2	2		
3	F	2	Total	Ni	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total	O	0	0
			55	55		

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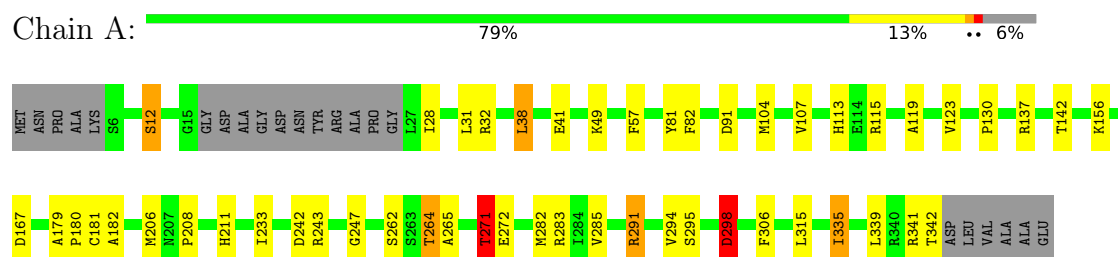
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	27	Total 27	O 27	0	0
4	C	24	Total 24	O 24	0	0
4	D	91	Total 91	O 91	0	0
4	E	57	Total 57	O 57	0	0
4	F	76	Total 76	O 76	0	0

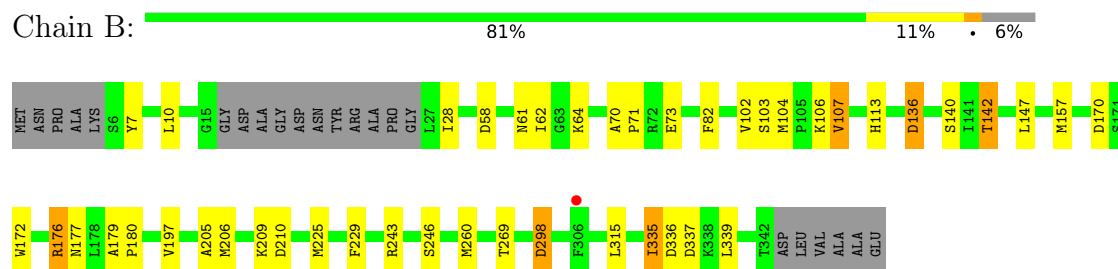
3 Residue-property plots

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.

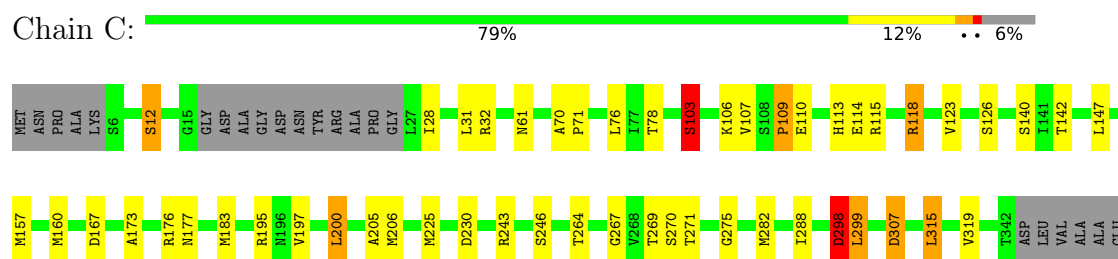
• Molecule 1: metformin hydrolase subunit B



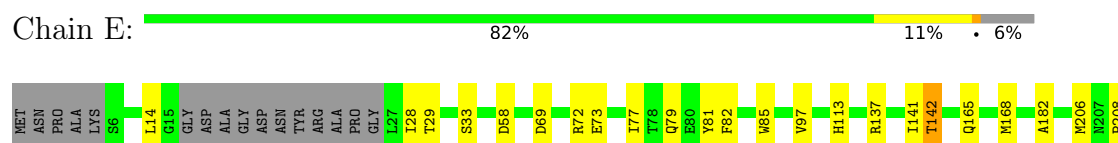
• Molecule 1: metformin hydrolase subunit B



• Molecule 1: metformin hydrolase subunit B



• Molecule 1: metformin hydrolase subunit B





• Molecule 2: metformin hydrolase subunit A

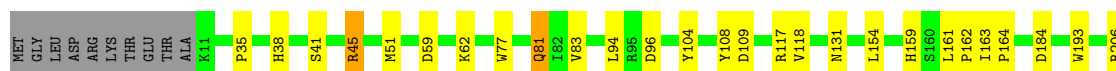
Chain D: 79% 14% 5%



GLN

• Molecule 2: metformin hydrolase subunit A

Chain F: 81% 13% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.40Å 96.40Å 96.70Å 115.50° 106.20° 101.10°	Depositor
Resolution (Å)	19.86 – 2.30 19.86 – 2.30	Depositor EDS
% Data completeness (in resolution range)	91.6 (19.86-2.30) 91.6 (19.86-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.172 , 0.219 0.171 , 0.212	Depositor DCC
R_{free} test set	5056 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	15792	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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:
NI

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	0.63	0/2558	1.06	4/3459 (0.1%)
1	B	0.56	0/2558	0.92	1/3459 (0.0%)
1	C	0.57	0/2558	0.96	2/3459 (0.1%)
1	E	0.62	0/2558	1.03	2/3459 (0.1%)
2	D	0.60	0/2787	1.07	8/3777 (0.2%)
2	F	0.60	0/2787	1.02	4/3777 (0.1%)
All	All	0.60	0/15806	1.01	21/21390 (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	A	0	5
1	E	0	3
2	D	0	2
2	F	0	4
All	All	0	14

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	318	ASP	CA-CB-CG	8.18	120.78	112.60
2	D	158	ASP	CB-CA-C	-7.90	94.70	110.42
1	E	298	ASP	CA-CB-CG	7.76	120.36	112.60
2	D	336	THR	N-CA-CB	-6.85	100.02	110.16
1	A	271	THR	CB-CA-C	-6.56	96.24	109.68
2	D	336	THR	CB-CA-C	6.50	121.90	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	318	ASP	CA-CB-CG	6.34	118.94	112.60
2	D	318	ASP	CB-CA-C	6.28	121.37	109.37
1	E	227	ASP	CA-CB-CG	6.21	118.81	112.60
2	F	336	THR	CB-CA-C	6.18	122.99	110.38
1	C	298	ASP	CA-CB-CG	5.74	118.34	112.60
2	F	184	ASP	CA-CB-CG	5.70	118.30	112.60
2	D	328	PRO	N-CA-C	5.63	121.16	113.84
2	D	191	PRO	N-CA-C	-5.36	106.08	113.53
2	F	318	ASP	CB-CA-C	5.34	119.86	109.33
1	A	298	ASP	CA-CB-CG	5.33	117.92	112.60
1	A	264	THR	CB-CA-C	-5.32	99.50	109.72
2	D	328	PRO	CB-CA-C	-5.22	104.44	111.85
1	B	136	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	307	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	167	ASP	CA-CB-CG	5.08	117.68	112.60

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	137	ARG	Sidechain
1	A	243	ARG	Sidechain
1	A	291	ARG	Sidechain
1	A	32	ARG	Sidechain
2	D	224	ARG	Sidechain
2	D	45	ARG	Sidechain
1	E	137	ARG	Sidechain
1	E	341	ARG	Sidechain
1	E	58	ASP	Peptide
2	F	117	ARG	Sidechain
2	F	206	ARG	Sidechain
2	F	347	ARG	Sidechain
2	F	45	ARG	Sidechain

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	2507	0	2475	25	0
1	B	2507	0	2475	33	0
1	C	2507	0	2475	36	0
1	E	2507	0	2475	28	0
2	D	2715	0	2600	38	0
2	F	2715	0	2600	35	0
3	D	2	0	0	0	0
3	F	2	0	0	0	0
4	A	55	0	0	0	0
4	B	27	0	0	0	0
4	C	24	0	0	1	0
4	D	91	0	0	1	0
4	E	57	0	0	1	0
4	F	76	0	0	0	0
All	All	15792	0	15100	174	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (174) 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)
2:D:94:LEU:HD23	2:D:336:THR:CG2	2.04	0.88
2:F:94:LEU:HD23	2:F:336:THR:HG23	1.59	0.84
1:B:113:HIS:ND1	1:B:142:THR:HG21	1.95	0.81
1:A:81:TYR:HA	1:B:206:MET:HE1	1.61	0.80
2:D:94:LEU:HD23	2:D:336:THR:HG23	1.64	0.80
2:D:81:GLN:HB2	2:D:158:ASP:OD1	1.84	0.77
1:A:208:PRO:HG2	1:A:211:HIS:CD2	2.26	0.71
2:F:221:MET:CE	2:F:261:ILE:HG12	2.21	0.70
2:F:45:ARG:HD3	2:F:96:ASP:OD2	1.90	0.70
1:C:206:MET:HE1	1:E:81:TYR:HA	1.72	0.70
1:B:260:MET:HG3	1:B:315:LEU:HD21	1.73	0.70
2:F:59:ASP:OD2	2:F:62:LYS:HG2	1.92	0.69
1:C:197:VAL:O	1:C:243:ARG:NH2	2.23	0.69
2:D:257:CYS:O	2:D:261:ILE:HD13	1.92	0.69
1:C:113:HIS:ND1	1:C:142:THR:HG21	2.09	0.68
2:D:158:ASP:HB3	2:D:160:SER:H	1.59	0.67
1:C:173:ALA:HA	1:E:14:LEU:O	1.95	0.67
2:F:221:MET:HE2	2:F:261:ILE:HG12	1.76	0.67
2:F:333:ALA:O	2:F:336:THR:HG22	1.96	0.66
1:C:114:GLU:O	1:C:118:ARG:HD3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:NH1	4:C:401:HOH:O	2.28	0.66
2:D:60:ARG:NH1	2:D:147:GLU:HG2	2.12	0.64
1:B:113:HIS:ND1	1:B:142:THR:CG2	2.61	0.63
1:A:81:TYR:HA	1:B:206:MET:CE	2.29	0.61
2:F:356:LYS:O	2:F:357:GLN:C	2.43	0.61
1:C:147:LEU:HD23	1:C:157:MET:HE3	1.82	0.61
2:F:222:GLY:HA2	2:F:249:MET:HE1	1.83	0.60
1:B:7:TYR:HB3	1:B:10:LEU:HD12	1.84	0.60
2:D:45:ARG:HD3	2:D:96:ASP:OD1	2.03	0.58
2:F:279:ASP:HB3	2:F:289:ASN:OD1	2.04	0.57
1:E:208:PRO:HG2	1:E:211:HIS:CD2	2.39	0.57
1:A:298:ASP:OD1	1:A:298:ASP:C	2.47	0.56
1:B:260:MET:HG3	1:B:315:LEU:CD2	2.35	0.56
1:B:170:ASP:OD1	1:B:176:ARG:NH2	2.38	0.56
1:E:141:ILE:HD11	1:E:182:ALA:HA	1.86	0.56
1:A:91:ASP:HB2	1:A:335:ILE:HD11	1.88	0.56
1:B:298:ASP:C	1:B:298:ASP:OD1	2.48	0.56
2:D:29:ASN:ND2	4:D:504:HOH:O	2.37	0.56
1:C:123:VAL:O	1:C:126:SER:OG	2.24	0.55
1:C:205:ALA:O	1:E:82:PHE:HB2	2.07	0.55
2:F:104:TYR:OH	2:F:109:ASP:OD1	2.24	0.55
2:F:159:HIS:CG	2:F:320:VAL:HG21	2.42	0.54
1:A:341:ARG:O	1:A:342:THR:C	2.49	0.54
1:B:70:ALA:N	1:B:71:PRO:CD	2.71	0.54
2:F:51:MET:HG2	2:F:51:MET:O	2.06	0.54
2:F:45:ARG:CD	2:F:96:ASP:OD2	2.57	0.53
1:B:61:ASN:HD21	1:B:269:THR:HG21	1.73	0.52
1:A:12:SER:OG	1:B:210:ASP:OD2	2.26	0.52
2:D:113:LEU:HA	2:D:118:VAL:HG13	1.91	0.52
1:E:314:ARG:HB2	1:E:314:ARG:NH1	2.25	0.52
1:B:28:ILE:HD11	1:E:28:ILE:HG12	1.90	0.52
2:D:51:MET:O	2:D:51:MET:HG2	2.10	0.52
2:F:161:LEU:N	2:F:162:PRO:HD2	2.25	0.51
2:F:221:MET:HE1	2:F:261:ILE:HG12	1.90	0.51
2:D:76:PRO:O	2:D:77:TRP:C	2.53	0.51
1:C:267:GLY:HA3	1:C:307:ASP:HB2	1.91	0.51
1:C:282:MET:HE1	1:C:319:VAL:HG22	1.92	0.51
1:A:306:PHE:O	2:D:329:SER:HB3	2.11	0.50
1:A:156:LYS:HE3	1:A:247:GLY:O	2.11	0.50
2:F:94:LEU:HD23	2:F:336:THR:CG2	2.36	0.50
1:A:28:ILE:HG12	1:C:28:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:MET:CE	1:E:81:TYR:HA	2.40	0.49
2:D:35:PRO:HB2	2:D:38:HIS:O	2.13	0.49
2:D:254:LEU:HD23	2:D:304:GLN:NE2	2.28	0.49
1:B:106:LYS:O	1:B:107:VAL:C	2.55	0.49
1:C:140:SER:OG	1:C:298:ASP:OD1	2.28	0.49
1:A:271:THR:HG21	2:D:331:ILE:HG22	1.95	0.49
1:B:179:ALA:HB3	1:B:180:PRO:HD3	1.95	0.49
1:C:264:THR:HG22	1:C:315:LEU:HD13	1.94	0.48
2:F:246:MET:HG2	2:F:295:TYR:O	2.13	0.48
1:B:225:MET:HE2	1:B:229:PHE:CE1	2.48	0.48
2:F:221:MET:HG3	2:F:249:MET:HE2	1.95	0.48
1:A:38:LEU:HD21	1:A:119:ALA:HA	1.94	0.48
1:C:70:ALA:N	1:C:71:PRO:CD	2.77	0.48
2:D:94:LEU:HD23	2:D:336:THR:HG22	1.93	0.48
2:F:35:PRO:HB2	2:F:38:HIS:O	2.13	0.48
1:C:31:LEU:HD12	1:C:78:THR:HB	1.95	0.48
2:F:77:TRP:CZ2	2:F:131:ASN:HA	2.49	0.48
1:B:140:SER:OG	1:B:298:ASP:OD2	2.26	0.48
2:D:333:ALA:O	2:D:336:THR:HG22	2.13	0.48
2:F:271:SER:HA	2:F:315:ASP:OD1	2.14	0.48
2:D:246:MET:HG2	2:D:295:TYR:O	2.15	0.47
2:D:356:LYS:O	2:D:357:GLN:C	2.57	0.47
2:F:343:TYR:CD2	2:F:343:TYR:C	2.93	0.47
2:D:154:LEU:O	2:D:318:ASP:HA	2.15	0.47
1:A:242:ASP:OD1	1:A:291:ARG:NH2	2.47	0.47
1:C:206:MET:HA	1:C:206:MET:HE2	1.96	0.46
1:C:225:MET:HE3	1:C:275:GLY:HA2	1.98	0.46
2:D:204:ALA:HB3	2:D:205:PRO:HD3	1.97	0.46
1:E:141:ILE:CG1	1:E:182:ALA:HA	2.46	0.46
1:A:206:MET:O	1:A:206:MET:HG3	2.16	0.46
1:B:337:ASP:OD1	1:B:337:ASP:C	2.59	0.45
2:F:310:GLY:O	2:F:347:ARG:HA	2.15	0.45
2:D:221:MET:SD	2:D:261:ILE:HD11	2.56	0.45
1:B:64:LYS:N	1:B:64:LYS:HD2	2.32	0.45
1:A:113:HIS:ND1	1:A:142:THR:OG1	2.44	0.45
1:C:12:SER:HB3	2:F:193:TRP:CE3	2.51	0.45
1:C:167:ASP:O	1:C:183:MET:HB2	2.16	0.45
2:D:279:ASP:HB3	2:D:289:ASN:OD1	2.16	0.45
1:C:12:SER:OG	2:F:231:ASP:OD2	2.34	0.45
1:C:61:ASN:HD21	1:C:269:THR:HG21	1.82	0.45
2:D:319:ILE:HD12	2:D:339:MET:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ASP:C	1:C:298:ASP:OD2	2.60	0.45
2:D:257:CYS:O	2:D:261:ILE:CD1	2.63	0.45
1:E:33:SER:HB3	1:E:97:VAL:HA	1.98	0.45
1:E:69:ASP:HB3	1:E:72:ARG:NH2	2.32	0.45
1:B:62:ILE:CD1	1:B:172:TRP:CE2	3.00	0.45
1:B:197:VAL:O	1:B:243:ARG:NH2	2.48	0.45
1:A:272:GLU:OE1	2:D:101:TYR:OH	2.33	0.44
1:A:283:ARG:HH22	1:B:229:PHE:HB3	1.82	0.44
2:D:81:GLN:HG3	2:D:83:VAL:H	1.82	0.44
1:E:315:LEU:O	1:E:315:LEU:HG	2.17	0.44
1:C:12:SER:HB3	2:F:193:TRP:CZ3	2.52	0.44
2:D:45:ARG:HD3	2:D:96:ASP:CG	2.41	0.44
1:E:113:HIS:ND1	1:E:142:THR:CG2	2.80	0.44
1:C:200:LEU:N	1:C:200:LEU:CD2	2.80	0.44
2:D:189:ALA:HA	2:D:205:PRO:CD	2.48	0.44
2:D:59:ASP:OD2	2:D:62:LYS:HG2	2.18	0.44
1:E:77:ILE:HG21	1:E:314:ARG:HA	1.99	0.44
1:A:181:CYS:O	1:A:182:ALA:C	2.60	0.44
1:B:336:ASP:OD2	1:B:339:LEU:HD13	2.17	0.44
1:C:264:THR:CG2	1:C:315:LEU:HD13	2.47	0.43
1:E:29:THR:O	1:E:79:GLN:NE2	2.51	0.43
1:E:277:GLU:HG3	2:F:300:ARG:NH2	2.33	0.43
2:F:45:ARG:HD3	2:F:96:ASP:CG	2.43	0.43
1:B:147:LEU:HD23	1:B:157:MET:HE3	2.00	0.43
2:D:70:ILE:HD13	2:D:151:LYS:HB2	2.00	0.43
1:E:298:ASP:OD1	1:E:298:ASP:C	2.62	0.43
1:C:206:MET:HE3	1:E:81:TYR:CD1	2.53	0.43
1:C:109:PRO:C	1:C:110:GLU:HG2	2.44	0.43
2:D:101:TYR:CD2	2:D:337:VAL:HG11	2.54	0.43
1:E:242:ASP:O	1:E:246:SER:HB2	2.19	0.43
1:B:102:VAL:HG12	1:B:104:MET:CE	2.49	0.42
1:B:209:LYS:O	1:B:209:LYS:HD3	2.18	0.42
1:C:205:ALA:HB2	1:E:85:TRP:CE2	2.54	0.42
2:D:159:HIS:CG	2:D:320:VAL:HG21	2.54	0.42
1:A:82:PHE:HB2	1:B:205:ALA:O	2.18	0.42
1:E:168:MET:HB2	1:E:211:HIS:HB3	2.02	0.42
1:B:10:LEU:HD11	1:B:335:ILE:HD13	2.01	0.42
2:D:161:LEU:N	2:D:162:PRO:HD2	2.34	0.42
1:E:234:TYR:N	1:E:235:PRO:CD	2.82	0.42
1:A:123:VAL:HG11	1:A:130:PRO:HB3	2.01	0.42
1:C:103:SER:O	1:C:115:ARG:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:ARG:CD	2:D:96:ASP:OD1	2.68	0.42
2:D:111:ASP:OD2	2:D:114:SER:OG	2.26	0.42
2:F:163:ILE:HB	2:F:164:PRO:HD3	2.01	0.42
2:F:81:GLN:HG3	2:F:83:VAL:H	1.83	0.42
1:B:206:MET:HA	1:B:206:MET:HE2	2.02	0.42
1:E:73:GLU:HG3	4:E:418:HOH:O	2.19	0.42
1:E:141:ILE:CD1	1:E:182:ALA:HA	2.50	0.42
1:C:315:LEU:O	1:C:319:VAL:HG23	2.20	0.42
1:A:57:PHE:HB2	1:A:104:MET:HE1	2.02	0.41
2:F:108:TYR:HE1	2:F:307:ARG:HD3	1.86	0.41
1:A:49:LYS:HA	1:A:49:LYS:HD2	1.88	0.41
1:A:265:ALA:O	1:A:271:THR:HG23	2.20	0.41
1:C:113:HIS:ND1	1:C:142:THR:CG2	2.82	0.41
1:B:62:ILE:HD13	1:B:172:TRP:CE2	2.55	0.41
1:A:262:SER:HA	1:A:271:THR:HG22	2.03	0.41
1:B:10:LEU:HD11	1:B:335:ILE:CD1	2.51	0.41
1:B:62:ILE:CD1	1:B:172:TRP:CZ2	3.03	0.41
1:E:165:GLN:OE1	1:E:206:MET:HE2	2.21	0.41
2:F:246:MET:HA	2:F:249:MET:HE3	2.03	0.41
1:C:299:LEU:N	1:C:299:LEU:HD23	2.36	0.41
2:D:262:PHE:O	2:D:266:LYS:HG3	2.20	0.41
1:E:113:HIS:ND1	1:E:142:THR:HG21	2.36	0.41
2:F:159:HIS:NE2	2:F:275:THR:OG1	2.51	0.41
1:B:82:PHE:CZ	2:D:229:PRO:HG3	2.56	0.41
1:C:160:MET:HE1	1:C:288:ILE:HG12	2.03	0.41
2:F:154:LEU:O	2:F:318:ASP:HA	2.20	0.41
2:F:163:ILE:HB	2:F:164:PRO:CD	2.52	0.40
1:E:336:ASP:OD1	1:E:338:LYS:HD3	2.21	0.40
1:C:28:ILE:HD13	1:C:76:LEU:HD21	2.03	0.40
1:A:179:ALA:N	1:A:180:PRO:HD2	2.36	0.40
1:E:245:TRP:CH2	1:E:288:ILE:HG23	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/348 (92%)	311 (97%)	10 (3%)	1 (0%)	36	46
1	B	322/348 (92%)	311 (97%)	10 (3%)	1 (0%)	36	46
1	C	322/348 (92%)	307 (95%)	12 (4%)	3 (1%)	14	17
1	E	322/348 (92%)	311 (97%)	10 (3%)	1 (0%)	36	46
2	D	345/364 (95%)	323 (94%)	21 (6%)	1 (0%)	36	46
2	F	345/364 (95%)	323 (94%)	22 (6%)	0	100	100
All	All	1978/2120 (93%)	1886 (95%)	85 (4%)	7 (0%)	30	38

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	103	SER
1	B	107	VAL
1	C	107	VAL
1	E	233	ILE
2	D	83	VAL
1	A	233	ILE
1	C	109	PRO

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	265/279 (95%)	250 (94%)	15 (6%)	18	27
1	B	265/279 (95%)	255 (96%)	10 (4%)	29	44
1	C	265/279 (95%)	250 (94%)	15 (6%)	18	27
1	E	265/279 (95%)	258 (97%)	7 (3%)	40	59
2	D	287/302 (95%)	279 (97%)	8 (3%)	38	56
2	F	287/302 (95%)	279 (97%)	8 (3%)	38	56
All	All	1634/1720 (95%)	1571 (96%)	63 (4%)	28	43

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	31	LEU
1	A	38	LEU
1	A	41	GLU
1	A	107	VAL
1	A	264	THR
1	A	271	THR
1	A	282	MET
1	A	285	VAL
1	A	294	VAL
1	A	295	SER
1	A	298	ASP
1	A	315	LEU
1	A	335	ILE
1	A	339	LEU
1	B	58	ASP
1	B	73	GLU
1	B	103	SER
1	B	136	ASP
1	B	142	THR
1	B	176	ARG
1	B	177	ASN
1	B	246	SER
1	B	298	ASP
1	B	335	ILE
1	C	12	SER
1	C	32	ARG
1	C	103	SER
1	C	106	LYS
1	C	118	ARG
1	C	177	ASN
1	C	195	ARG
1	C	200	LEU
1	C	230	ASP
1	C	246	SER
1	C	270	SER
1	C	271	THR
1	C	298	ASP
1	C	299	LEU
1	C	315	LEU
2	D	41	SER
2	D	81	GLN

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Mol	Chain	Res	Type
2	D	118	VAL
2	D	158	ASP
2	D	255	GLU
2	D	261	ILE
2	D	318	ASP
2	D	336	THR
1	E	142	THR
1	E	246	SER
1	E	264	THR
1	E	282	MET
1	E	298	ASP
1	E	315	LEU
1	E	335	ILE
2	F	41	SER
2	F	81	GLN
2	F	118	VAL
2	F	255	GLU
2	F	318	ASP
2	F	319	ILE
2	F	336	THR
2	F	356	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	35	HIS
1	B	61	ASN
1	B	161	HIS
1	B	177	ASN
1	C	177	ASN
2	D	304	GLN
2	D	357	GLN
1	E	89	ASN
1	E	161	HIS
2	F	217	ASN
2	F	338	ASN

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 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 [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	326/348 (93%)	-0.45	0 100 100	54, 72, 103, 150	0
1	B	326/348 (93%)	-0.36	1 (0%) 90 90	62, 82, 115, 181	0
1	C	326/348 (93%)	-0.33	0 100 100	63, 84, 117, 174	0
1	E	326/348 (93%)	-0.49	0 100 100	53, 70, 101, 139	0
2	D	347/364 (95%)	-0.43	0 100 100	54, 70, 95, 149	0
2	F	347/364 (95%)	-0.42	1 (0%) 90 90	55, 72, 100, 140	0
All	All	1998/2120 (94%)	-0.41	2 (0%) 92 91	53, 75, 108, 181	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	227	LEU	2.6
1	B	306	PHE	2.5

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

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

6.3 Carbohydrates [i](#)

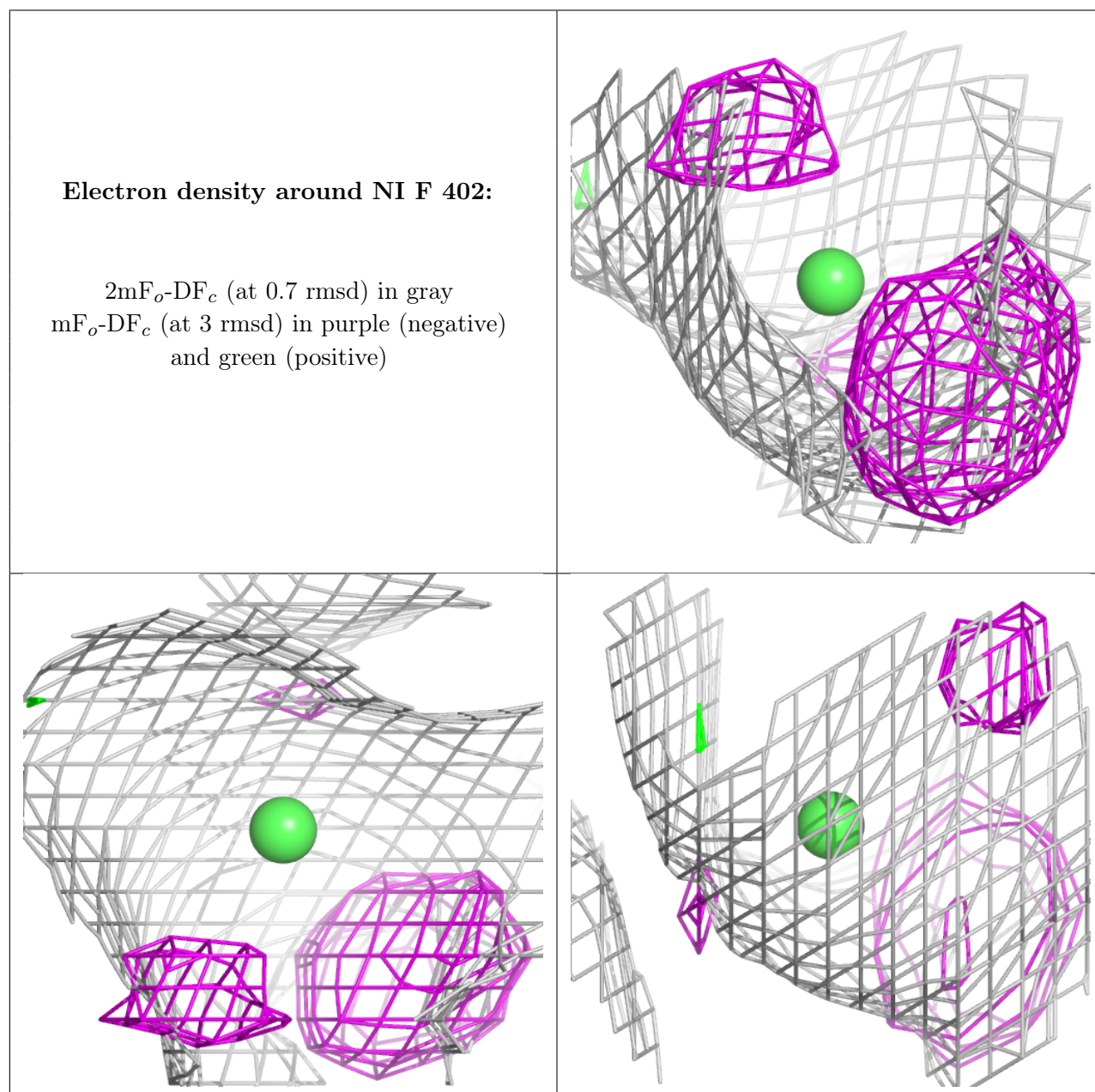
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

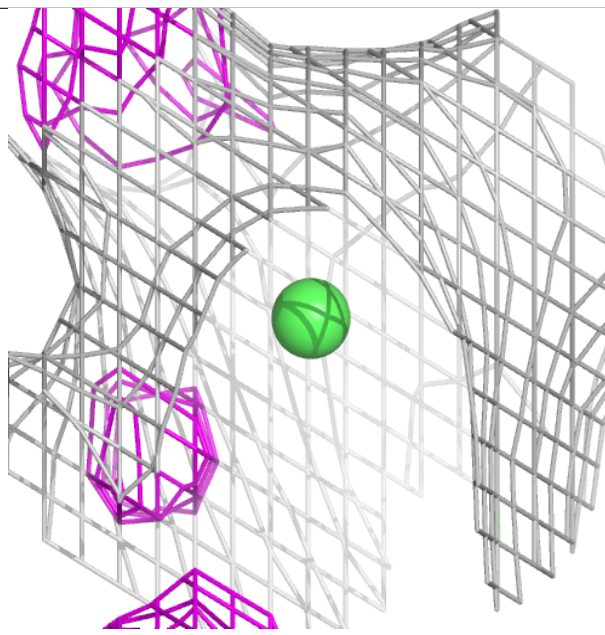
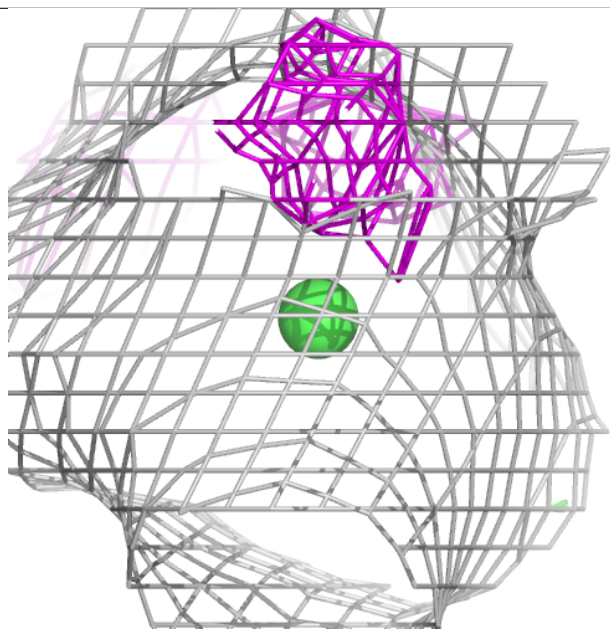
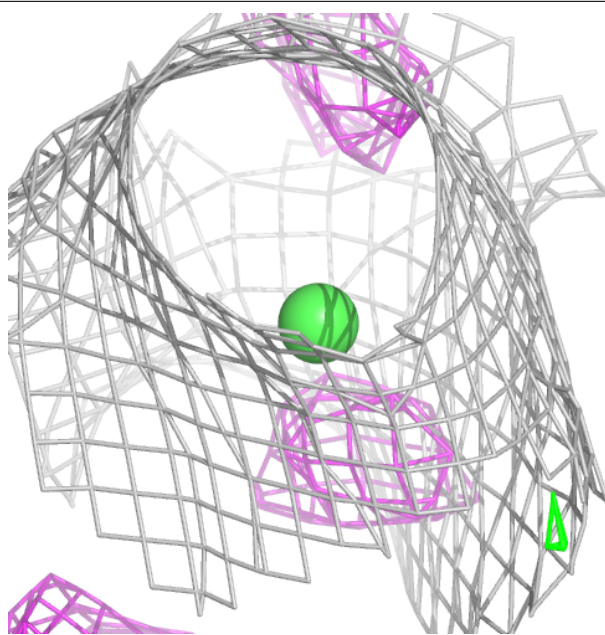
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NI	F	402	1/1	0.95	0.09	125,125,125,125	0
3	NI	F	401	1/1	0.98	0.06	95,95,95,95	0
3	NI	D	401	1/1	0.98	0.06	112,112,112,112	0
3	NI	D	402	1/1	0.99	0.04	87,87,87,87	0

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.



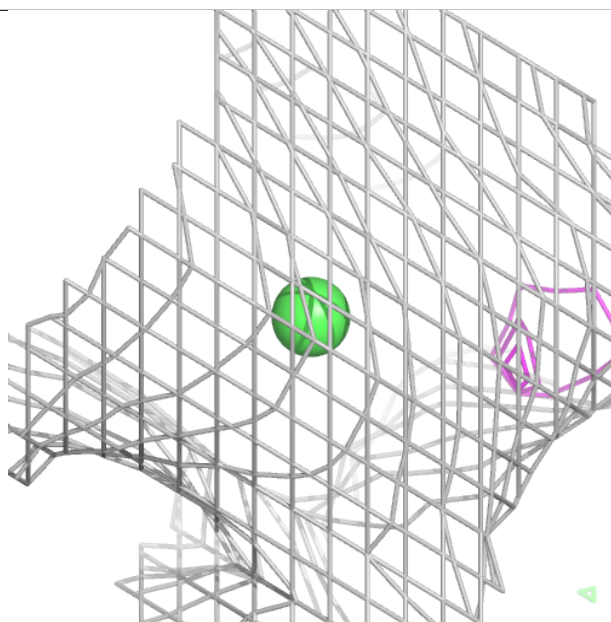
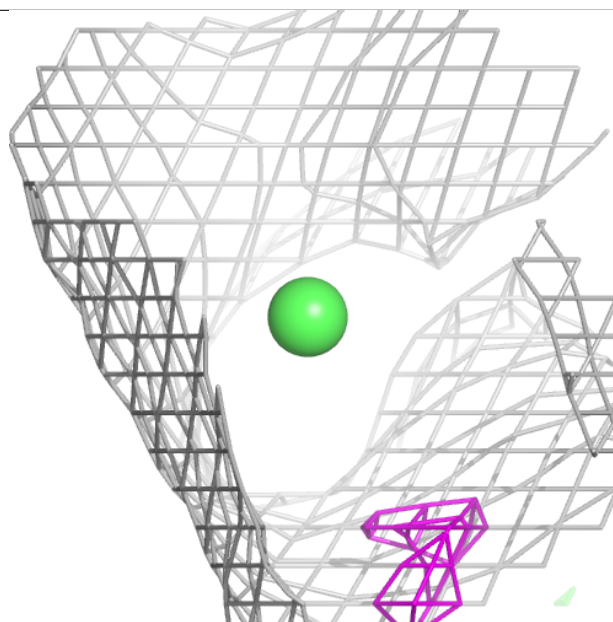
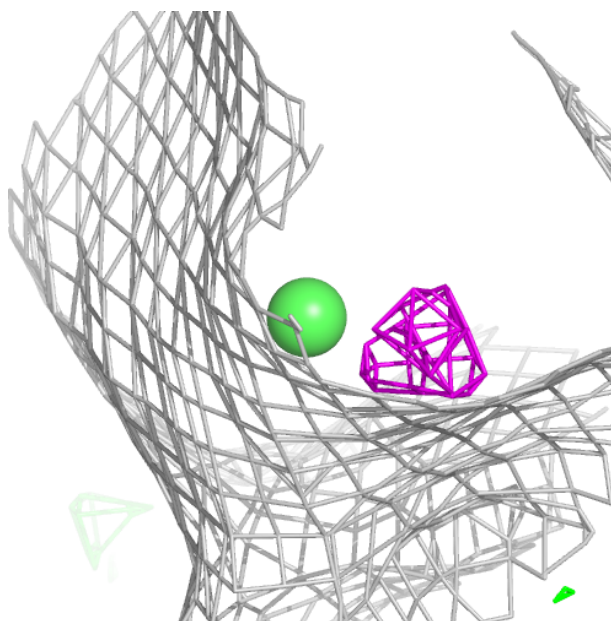
Electron density around NI F 401:

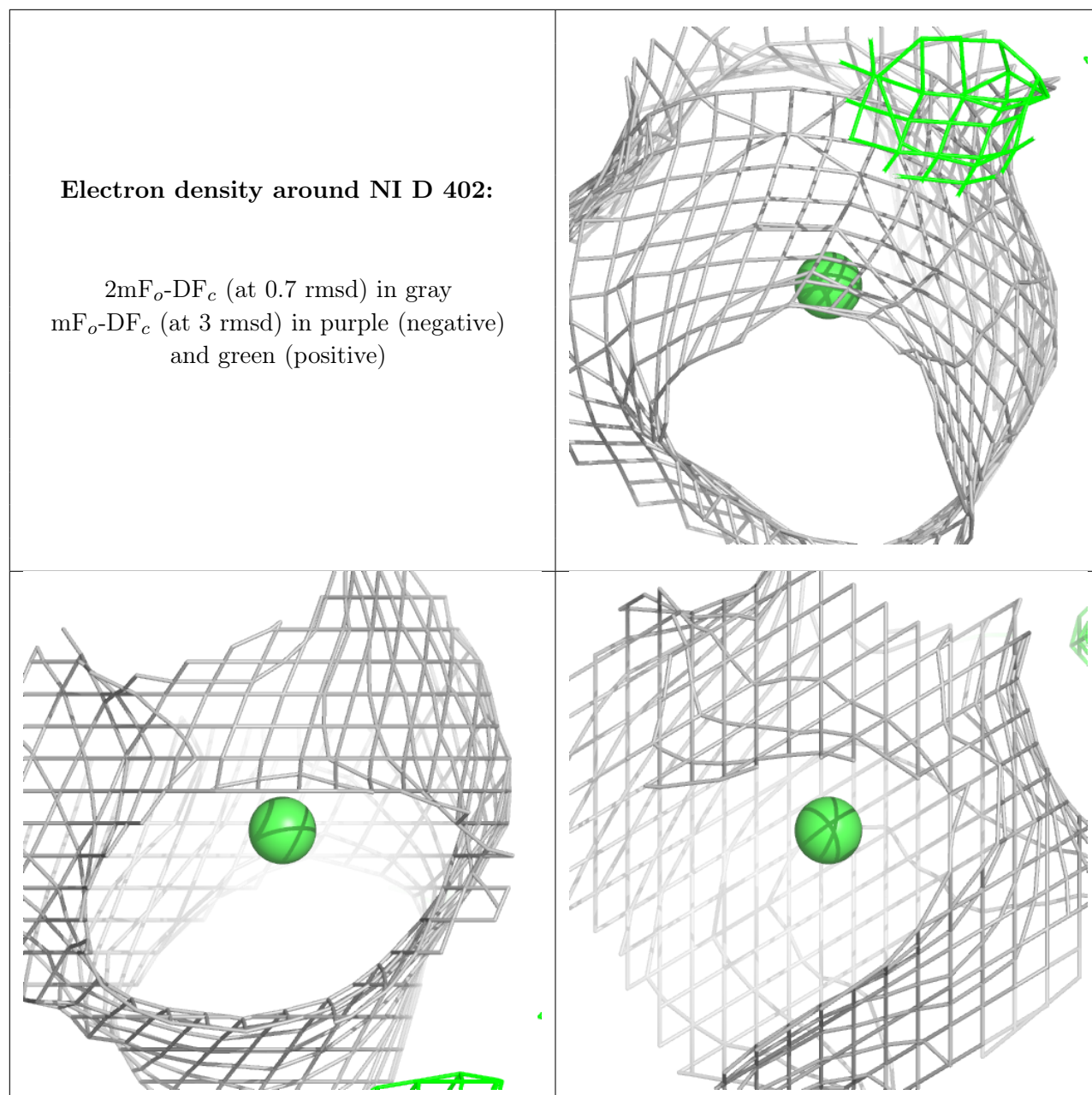
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NI D 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.