Full wwPDB X-ray Structure Validation Report ⓘ

Dec 27, 2023 – 12:10 AM JST

PDB ID	:	8X6Z
Title	:	1-naphthylamine GS from Pseudomonas sp. JS3066
Authors	:	Zhou, N.Y.; Zhang, S.T.
Deposited on	:	2023-11-22
Resolution	:	2.95 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:

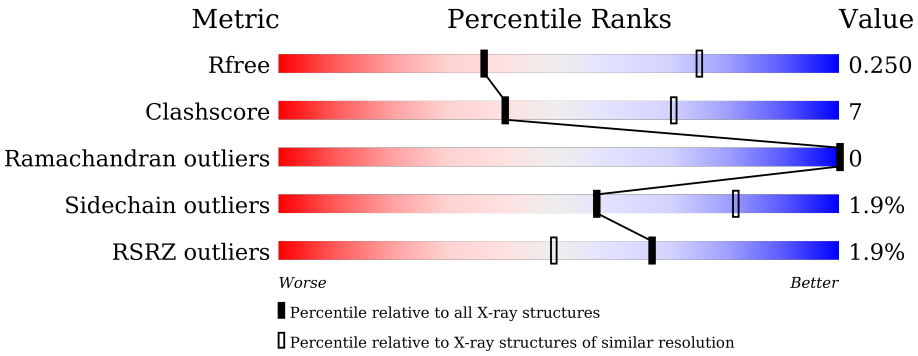
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 <=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	510	2% 78% 16% 5%
1	B	510	2% 84% 12% 5%
1	C	510	2% 77% 18% 5%
1	D	510	% 74% 20% • 5%
1	E	510	3% 73% 21% • 5%
1	F	510	% 79% 16% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23407 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 Glutamine synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3771	2403	634	716	18			
1	B	487	Total	C	N	O	S	0	0	0
			3801	2421	640	722	18			
1	C	484	Total	C	N	O	S	0	0	0
			3782	2412	637	715	18			
1	D	482	Total	C	N	O	S	0	0	0
			3767	2403	635	711	18			
1	E	483	Total	C	N	O	S	0	0	0
			3761	2397	635	711	18			
1	F	485	Total	C	N	O	S	0	0	0
			3786	2413	637	718	18			

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

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

- Molecule 3 is water.

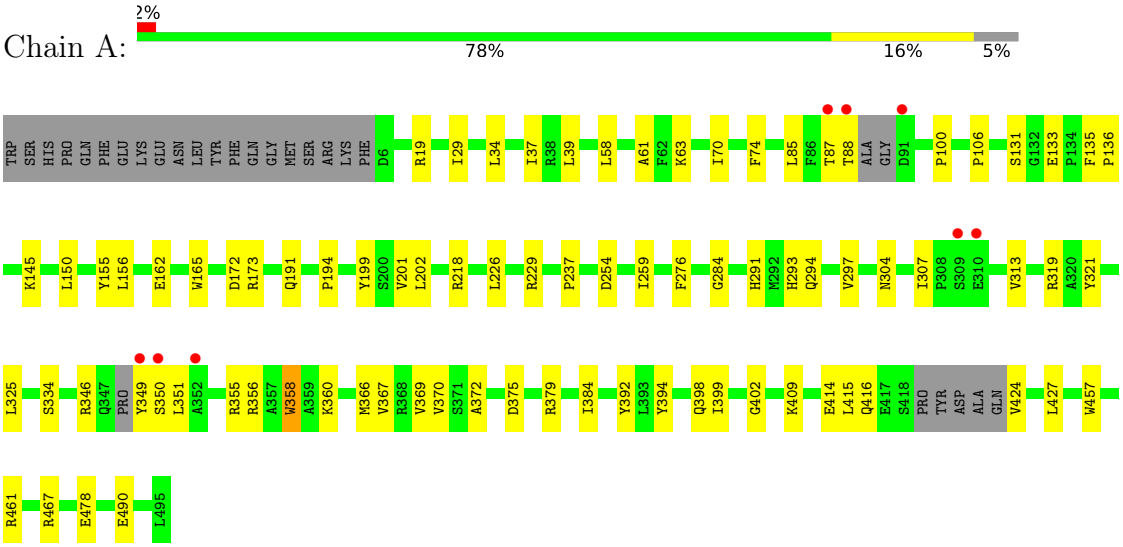
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	143	Total O 143 143	0	0
3	B	113	Total O 113 113	0	0
3	C	129	Total O 129 129	0	0
3	D	126	Total O 126 126	0	0
3	E	112	Total O 112 112	0	0
3	F	106	Total O 106 106	0	0

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.

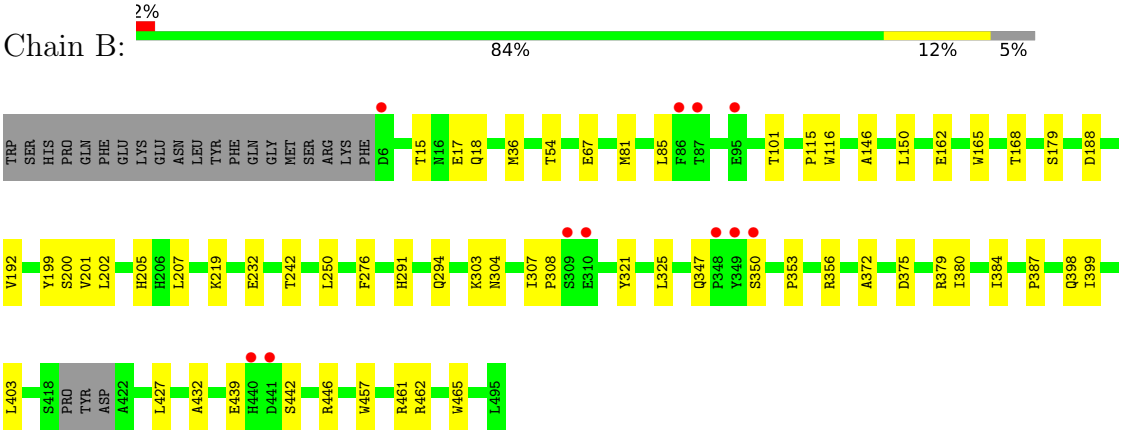
• Molecule 1: Glutamine synthetase

Chain A:



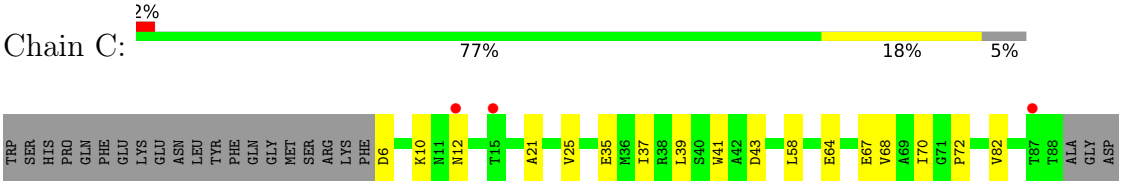
• Molecule 1: Glutamine synthetase

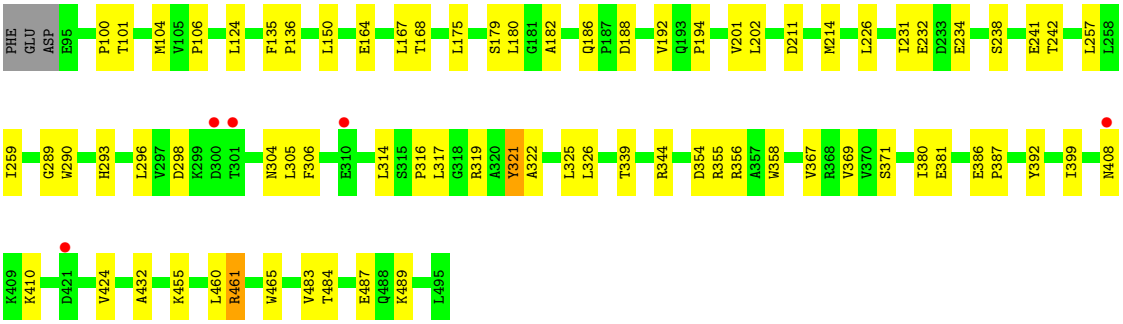
Chain B:



• Molecule 1: Glutamine synthetase

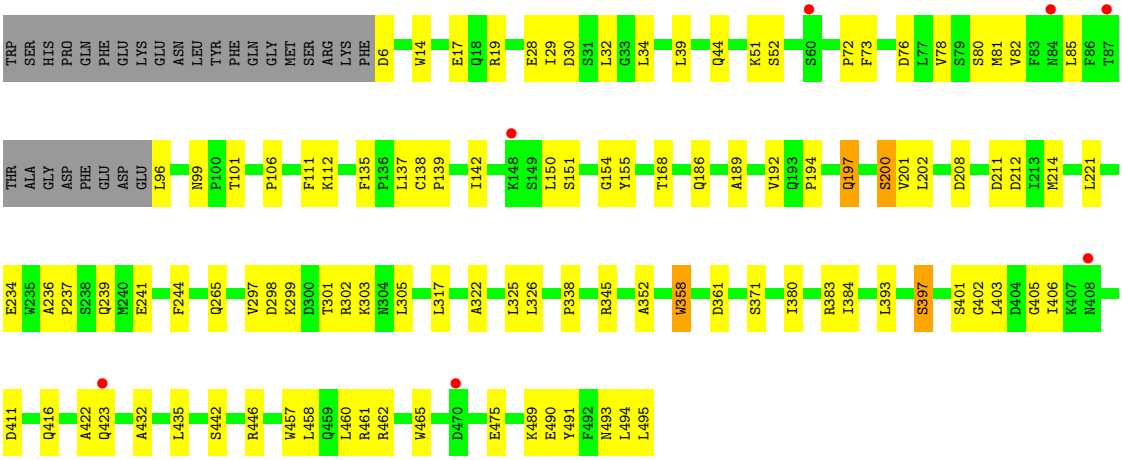
Chain C:





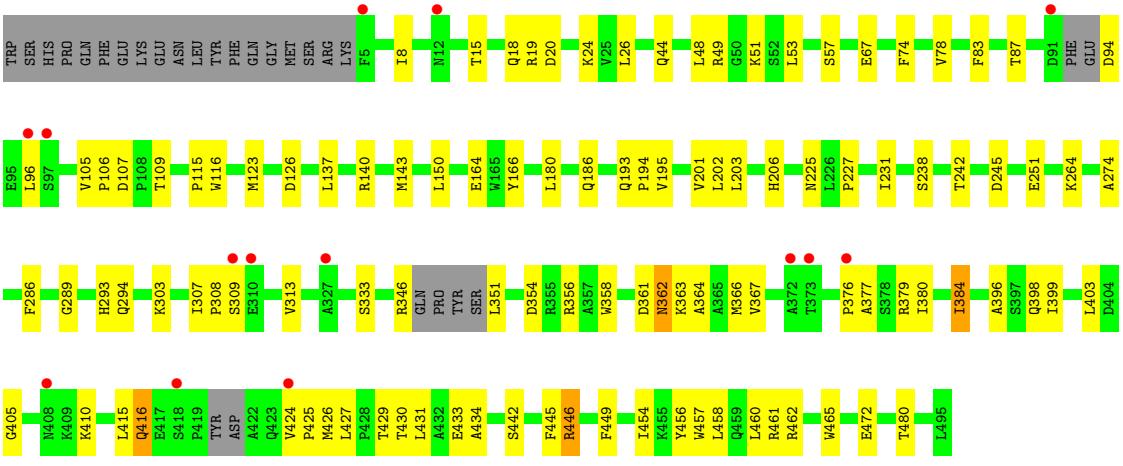
• Molecule 1: Glutamine synthetase

Chain D:



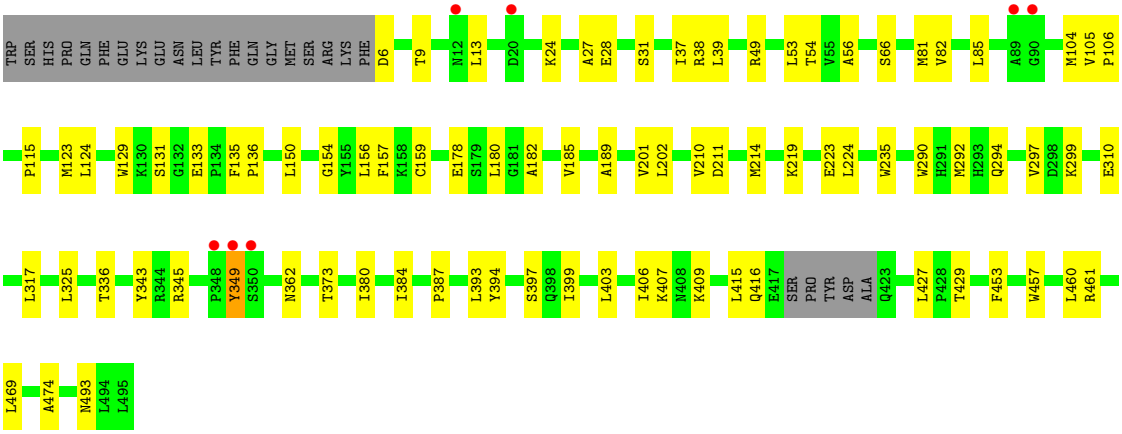
• Molecule 1: Glutamine synthetase

Chain E:



• Molecule 1: Glutamine synthetase

Chain F:


TRP SER HIS PRO GLN PHE GLU LYS GLU ASN LEU TYR PHE GLN GLY MET SER ARG LYS PHE D6 T9 N12 L13 D20 K24 A27 E28 S31 I37 R38 L39 R49 L53 T54 V55 A56 S66 M81 V82 L85 A89 G90 M104 V105 P106
P115 M123 L124 W129 K130 S131 G132 E133 P134 F135 P136 L150 G154 Y155 L156 F157 K158 C159 E178 S179 L180 G181 A182 V185 A189 V201 L202 V210 D211 M214 K219 E223 L224 W235 W290 H291 M292 H293 Q294 V297 D298 K299 E310
L317 L325 T336 Y343 R344 R345 P348 Y349 S350 N362 T373 I380 I384 P387 L393 Y394 S397 Q398 I399 L403 I406 K407 N408 K409 L415 Q416 E417 SER PRO TYR ASP ALA Q423 L427 P428 T429 F453 W457 L460 R461
L469 A474 N493 L494 L495

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	121.64Å 140.14Å 218.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.95 19.98 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-2.95) 99.9 (19.98-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.93Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.224 , 0.247 0.227 , 0.250	Depositor DCC
R_{free} test set	3911 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.872	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23407	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0331e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.50	0/3859	0.66	0/5229
1	B	0.50	0/3892	0.69	1/5278 (0.0%)
1	C	0.50	0/3874	0.70	0/5257
1	D	0.50	0/3859	0.66	0/5235
1	E	0.46	0/3849	0.67	0/5217
1	F	0.49	0/3877	0.67	0/5258
All	All	0.49	0/23210	0.67	1/31474 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	TYR	CB-CA-C	5.69	121.78	110.40

There are no chirality outliers.

There are no planarity outliers.

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	3771	0	3704	53	0
1	B	3801	0	3734	40	0
1	C	3782	0	3723	60	0
1	D	3767	0	3710	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	3761	0	3700	63	0
1	F	3786	0	3718	61	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	143	0	0	4	0
3	B	113	0	0	2	0
3	C	129	0	0	0	0
3	D	126	0	0	3	0
3	E	112	0	0	1	0
3	F	106	0	0	2	0
All	All	23407	0	22289	323	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 7.

All (323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:THR:HG22	1:B:17:GLU:H	1.30	0.94
1:A:321:TYR:O	1:A:325:LEU:HD13	1.77	0.84
1:C:164:GLU:HG2	1:C:241:GLU:HG3	1.63	0.78
1:A:201:VAL:HG22	1:A:202:LEU:HG	1.66	0.77
1:C:408:ASN:OD1	1:C:408:ASN:O	2.04	0.75
1:A:366:MET:HG3	1:A:367:VAL:HG23	1.69	0.72
1:D:194:PRO:HG2	1:F:180:LEU:HD11	1.72	0.72
1:E:429:THR:HG23	1:E:430:THR:HG23	1.74	0.70
1:E:458:LEU:O	1:E:462:ARG:HG3	1.90	0.69
1:E:346:ARG:HD3	1:E:480:THR:HA	1.74	0.69
1:E:106:PRO:HB2	1:E:123:MET:HE1	1.74	0.68
1:E:442:SER:HB3	1:E:446:ARG:HE	1.58	0.68
1:D:416:GLN:HG2	1:D:422:ALA:HB2	1.75	0.68
1:B:304:ASN:O	1:B:307:ILE:HG13	1.94	0.68
1:A:372:ALA:HB3	1:A:375:ASP:HB2	1.76	0.67
1:D:322:ALA:HB2	1:D:380:ILE:HD11	1.76	0.66
1:E:354:ASP:OD2	1:E:426:MET:HE1	1.96	0.66
1:E:363:LYS:H	1:E:363:LYS:HD2	1.61	0.66
1:A:150:LEU:HD22	1:A:399:ILE:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LYS:HE3	1:A:369:VAL:HG13	1.79	0.65
1:A:87:THR:HG22	1:A:88:THR:HG23	1.77	0.65
1:C:367:VAL:HG13	1:C:380:ILE:HG23	1.79	0.65
1:E:8:ILE:HD12	1:E:105:VAL:HG13	1.80	0.64
1:A:191:GLN:NE2	3:A:602:HOH:O	2.27	0.64
1:F:82:VAL:HG21	1:F:460:LEU:HD12	1.79	0.64
1:F:201:VAL:HG22	1:F:202:LEU:HG	1.80	0.64
1:C:37:ILE:HD13	1:C:58:LEU:HD22	1.80	0.63
1:F:317:LEU:HD11	1:F:406:ILE:HD13	1.81	0.63
1:A:70:ILE:HG12	1:A:100:PRO:HD2	1.82	0.62
1:B:201:VAL:HG22	1:B:202:LEU:HG	1.82	0.62
1:F:310:GLU:HG2	1:F:373:THR:HG21	1.82	0.61
1:F:28:GLU:HA	1:F:31:SER:HB3	1.81	0.61
1:C:201:VAL:HG22	1:C:202:LEU:HG	1.83	0.61
1:C:82:VAL:HG21	1:C:460:LEU:HD12	1.82	0.60
1:D:150:LEU:HG	1:D:155:TYR:HB2	1.84	0.60
1:B:356:ARG:HG2	1:B:427:LEU:HG	1.84	0.60
1:D:442:SER:HB3	1:D:446:ARG:HE	1.66	0.60
1:F:129:TRP:HD1	1:F:133:GLU:HG2	1.66	0.60
1:B:179:SER:HB3	1:B:188:ASP:HB2	1.84	0.60
1:B:372:ALA:HB3	1:B:375:ASP:HB2	1.84	0.60
1:D:393:LEU:O	1:D:397:SER:HB2	2.02	0.60
1:F:106:PRO:HB3	1:F:123:MET:HE1	1.83	0.59
1:C:316:PRO:HA	1:C:319:ARG:HG2	1.83	0.59
1:F:135:PHE:CD1	1:F:136:PRO:HD2	2.37	0.59
1:E:362:ASN:HD22	1:E:363:LYS:N	2.00	0.59
1:C:290:TRP:HB2	1:C:387:PRO:HA	1.84	0.59
1:F:159:CYS:SG	1:F:292:MET:SD	3.00	0.59
1:F:182:ALA:H	1:F:185:VAL:HB	1.68	0.59
1:B:353:PRO:HB2	1:B:384:ILE:HG22	1.85	0.59
1:E:107:ASP:OD1	1:E:109:THR:OG1	2.21	0.59
1:C:298:ASP:HB2	1:C:305:LEU:HD11	1.85	0.59
1:C:135:PHE:CD1	1:C:136:PRO:HD2	2.38	0.58
1:D:150:LEU:HD12	1:D:403:LEU:HD22	1.85	0.58
1:D:201:VAL:HG22	1:D:202:LEU:HG	1.86	0.58
1:C:179:SER:HB3	1:C:188:ASP:HB2	1.86	0.57
1:A:467:ARG:NH2	1:A:490:GLU:OE1	2.28	0.57
1:D:458:LEU:O	1:D:462:ARG:HG3	2.05	0.57
1:D:155:TYR:CE1	1:D:317:LEU:HD21	2.40	0.56
1:A:131:SER:OG	1:A:133:GLU:HG3	2.05	0.56
1:F:460:LEU:HD23	1:F:461:ARG:HD2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:457:TRP:O	1:F:461:ARG:HG2	2.06	0.56
1:D:432:ALA:HB2	1:D:465:TRP:CE2	2.41	0.55
1:A:29:ILE:HG23	1:A:34:LEU:HB2	1.88	0.55
1:D:297:VAL:HG13	1:D:302:ARG:HA	1.87	0.55
1:D:234:GLU:HG2	1:D:241:GLU:HB2	1.89	0.55
1:D:197:GLN:HA	1:D:237:PRO:HB3	1.88	0.55
1:A:199:TYR:CE2	1:C:182:ALA:HA	2.42	0.55
1:C:369:VAL:HG12	1:C:371:SER:HB3	1.89	0.55
1:E:429:THR:HG22	1:E:433:GLU:CD	2.28	0.54
1:F:39:LEU:HD21	1:F:123:MET:HE2	1.89	0.54
1:F:131:SER:OG	1:F:133:GLU:OE1	2.20	0.54
1:E:362:ASN:ND2	1:E:364:ALA:H	2.06	0.54
1:A:457:TRP:O	1:A:461:ARG:HG2	2.07	0.54
1:D:221:LEU:HD13	1:D:244:PHE:HZ	1.72	0.54
1:E:143:MET:HE2	1:E:396:ALA:HB2	1.88	0.54
1:F:219:LYS:O	1:F:223:GLU:HG3	2.08	0.54
1:C:6:ASP:HA	1:C:64:GLU:OE2	2.07	0.54
1:D:17:GLU:N	1:D:17:GLU:OE1	2.39	0.54
1:A:356:ARG:HG3	1:A:427:LEU:HG	1.90	0.54
1:E:201:VAL:HG22	1:E:202:LEU:HG	1.90	0.54
1:E:429:THR:HG22	1:E:433:GLU:OE1	2.08	0.54
1:A:321:TYR:O	1:A:325:LEU:CD1	2.55	0.53
1:B:432:ALA:HB2	1:B:465:TRP:CE2	2.44	0.53
1:F:13:LEU:HD13	1:F:105:VAL:HG21	1.90	0.53
1:C:355:ARG:HB3	1:C:424:VAL:HG13	1.89	0.53
1:D:200:SER:HB3	1:F:49:ARG:HH12	1.73	0.53
1:F:453:PHE:N	3:F:602:HOH:O	2.33	0.53
1:C:305:LEU:HB3	1:C:317:LEU:HD13	1.91	0.53
1:E:264:LYS:HE2	1:E:274:ALA:O	2.09	0.53
1:E:251:GLU:OE1	1:E:251:GLU:N	2.41	0.53
1:E:457:TRP:O	1:E:461:ARG:HG2	2.08	0.53
1:A:370:VAL:HG23	1:A:370:VAL:O	2.08	0.53
1:E:354:ASP:O	1:E:426:MET:HE3	2.08	0.52
1:F:415:LEU:HD12	1:F:415:LEU:H	1.73	0.52
1:C:168:THR:HB	1:C:192:VAL:HB	1.92	0.52
1:E:20:ASP:O	1:E:24:LYS:HG2	2.10	0.52
1:E:231:ILE:HG12	1:E:242:THR:HG22	1.92	0.52
1:C:231:ILE:HG12	1:C:242:THR:HG22	1.90	0.52
1:D:44:GLN:OE1	1:D:73:PHE:HA	2.09	0.52
1:C:186:GLN:OE1	1:C:489:LYS:HB2	2.09	0.52
1:C:232:GLU:OE2	1:E:51:LYS:HD3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:PRO:HB3	1:F:123:MET:CE	2.40	0.51
1:B:442:SER:HB2	1:B:446:ARG:HE	1.75	0.51
1:D:402:GLY:O	1:D:405:GLY:N	2.44	0.51
1:D:211:ASP:HA	1:D:214:MET:HB2	1.93	0.51
1:C:70:ILE:HG12	1:C:100:PRO:HD2	1.91	0.51
1:D:298:ASP:HB3	1:D:301:THR:HB	1.93	0.51
1:D:101:THR:HG22	3:D:680:HOH:O	2.10	0.51
1:E:20:ASP:OD2	1:E:24:LYS:NZ	2.44	0.51
1:E:303:LYS:HE2	1:E:307:ILE:HD12	1.91	0.51
1:B:457:TRP:O	1:B:461:ARG:HG2	2.11	0.51
1:E:294:GLN:OE1	1:E:398:GLN:HB3	2.10	0.51
1:B:165:TRP:HE1	1:B:242:THR:HG23	1.76	0.51
1:D:154:GLY:C	1:D:299:LYS:HG2	2.31	0.51
1:D:186:GLN:HB3	1:D:489:LYS:O	2.12	0.51
1:F:154:GLY:HA2	1:F:299:LYS:HD3	1.93	0.51
1:B:201:VAL:HG13	1:D:72:PRO:HG3	1.93	0.50
1:D:305:LEU:HB3	1:D:317:LEU:HD23	1.92	0.50
1:A:360:LYS:HG3	1:A:415:LEU:HD13	1.94	0.50
1:B:294:GLN:OE1	1:B:398:GLN:HB3	2.12	0.50
1:C:82:VAL:HG11	1:C:460:LEU:HA	1.92	0.50
1:D:139:PRO:HA	1:D:142:ILE:HD12	1.93	0.50
1:A:199:TYR:OH	1:A:284:GLY:O	2.27	0.50
1:B:325:LEU:HD12	1:B:380:ILE:HD12	1.93	0.50
1:D:82:VAL:HG11	1:D:460:LEU:HA	1.94	0.50
1:E:15:THR:HG23	1:E:18:GLN:OE1	2.12	0.50
1:E:195:VAL:HG22	1:E:238:SER:HB2	1.94	0.50
1:E:51:LYS:NZ	1:E:67:GLU:O	2.40	0.50
1:F:211:ASP:HA	1:F:214:MET:HB2	1.92	0.50
1:D:78:VAL:HG11	1:D:186:GLN:HG2	1.94	0.50
1:E:74:PHE:CD1	1:E:83:PHE:CD1	3.00	0.50
1:E:377:ALA:O	1:E:379:ARG:HD3	2.12	0.50
1:D:135:PHE:CE2	1:D:137:LEU:HB2	2.47	0.49
1:F:189:ALA:HA	1:F:493:ASN:HD21	1.77	0.49
1:D:403:LEU:HA	1:D:406:ILE:HD13	1.95	0.49
1:C:68:VAL:HG11	1:C:104:MET:HG3	1.94	0.49
1:E:166:TYR:OH	1:E:286:PHE:N	2.45	0.49
1:E:445:PHE:O	1:E:449:PHE:HB2	2.13	0.49
1:E:193:GLN:HG2	1:E:194:PRO:HD2	1.94	0.49
1:E:356:ARG:HE	1:E:425:PRO:HB2	1.77	0.48
1:C:296:LEU:HB2	1:C:306:PHE:CE1	2.48	0.48
1:C:39:LEU:HD21	1:C:106:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:LEU:HD22	3:F:639:HOH:O	2.14	0.48
1:A:162:GLU:HB2	1:A:291:HIS:HB2	1.96	0.48
1:B:219:LYS:NZ	3:B:603:HOH:O	2.37	0.48
1:A:313:VAL:HG11	1:A:415:LEU:HD21	1.95	0.48
1:D:39:LEU:HD21	1:D:106:PRO:HG3	1.94	0.48
1:E:115:PRO:HD2	1:E:116:TRP:CE3	2.48	0.48
1:F:39:LEU:HD12	1:F:53:LEU:HD12	1.95	0.48
1:D:154:GLY:HA2	1:D:299:LYS:HD3	1.96	0.48
1:F:115:PRO:HD3	1:F:224:LEU:HD21	1.94	0.48
1:B:321:TYR:CE1	1:B:380:ILE:HD11	2.49	0.47
1:C:194:PRO:HG2	1:E:180:LEU:HD11	1.95	0.47
1:C:432:ALA:HB2	1:C:465:TRP:CE2	2.49	0.47
1:D:14:TRP:HE3	1:D:19:ARG:HE	1.62	0.47
1:F:6:ASP:HB3	1:F:9:THR:OG1	2.14	0.47
1:A:254:ASP:OD1	1:A:392:TYR:OH	2.25	0.47
1:C:226:LEU:HD13	1:C:259:ILE:HG12	1.96	0.47
1:D:326:LEU:HD11	1:D:358:TRP:HB3	1.95	0.47
1:E:293:HIS:HA	1:E:380:ILE:O	2.15	0.47
1:E:361:ASP:O	1:E:363:LYS:NZ	2.40	0.47
1:E:446:ARG:HG3	1:E:454:ILE:HD11	1.97	0.47
1:A:355:ARG:HG2	1:A:424:VAL:HG22	1.97	0.47
1:A:39:LEU:HD21	1:A:106:PRO:HG3	1.96	0.47
1:B:115:PRO:HD2	1:B:116:TRP:CE3	2.51	0.47
1:D:325:LEU:HD23	1:D:401:SER:HB2	1.96	0.47
1:F:81:MET:SD	1:F:85:LEU:HB2	2.55	0.47
1:C:322:ALA:O	1:C:326:LEU:HD22	2.15	0.46
1:F:336:THR:HG22	1:F:394:TYR:CD1	2.50	0.46
1:B:146:ALA:HB1	1:B:399:ILE:HG21	1.98	0.46
1:E:143:MET:HE1	1:E:396:ALA:N	2.30	0.46
1:A:218:ARG:NH1	1:C:35:GLU:OE1	2.48	0.46
1:B:115:PRO:HD2	1:B:116:TRP:CZ3	2.51	0.46
1:C:326:LEU:O	1:C:356:ARG:NE	2.47	0.46
1:C:354:ASP:OD1	1:C:355:ARG:HG3	2.16	0.46
1:B:384:ILE:HD11	3:B:639:HOH:O	2.15	0.46
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.80	0.46
1:C:321:TYR:HE1	1:C:325:LEU:HD21	1.81	0.46
1:F:157:PHE:CG	1:F:399:ILE:HD11	2.51	0.46
1:F:469:LEU:HD21	1:F:474:ALA:HA	1.98	0.46
1:C:41:TRP:HH2	1:C:72:PRO:HG2	1.82	0.45
1:A:409:LYS:HD3	1:A:409:LYS:HA	1.59	0.45
1:C:460:LEU:HD23	1:C:461:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:TYR:HB3	1:F:429:THR:O	2.16	0.45
1:C:314:LEU:HG	1:C:369:VAL:HG13	1.98	0.45
1:F:82:VAL:HG11	1:F:460:LEU:HA	1.98	0.45
1:F:384:ILE:HG21	1:F:427:LEU:HD13	1.98	0.45
1:F:66:SER:HB3	1:F:104:MET:HE2	1.98	0.45
1:C:211:ASP:HA	1:C:214:MET:HB2	1.99	0.45
1:E:431:LEU:HB3	1:E:465:TRP:CE3	2.52	0.45
1:A:294:GLN:OE1	1:A:398:GLN:HB3	2.16	0.45
1:A:478:GLU:HA	1:A:478:GLU:OE1	2.17	0.45
1:D:435:LEU:HD13	1:D:462:ARG:HG2	1.99	0.45
1:D:200:SER:CB	1:F:49:ARG:HH12	2.30	0.45
1:F:54:THR:HG22	1:F:56:ALA:H	1.82	0.45
1:A:346:ARG:HH22	1:A:351:LEU:CD2	2.30	0.44
1:B:81:MET:SD	1:B:85:LEU:HD12	2.57	0.44
1:D:85:LEU:HG	1:D:99:ASN:HB2	1.99	0.44
1:F:54:THR:HG22	1:F:56:ALA:N	2.32	0.44
1:E:307:ILE:HA	1:E:308:PRO:HD3	1.84	0.44
1:E:366:MET:HG2	1:E:367:VAL:HG23	1.99	0.44
1:C:10:LYS:HB3	1:C:10:LYS:HE3	1.60	0.44
1:D:96:LEU:N	3:D:607:HOH:O	2.49	0.44
1:D:189:ALA:HA	1:D:493:ASN:OD1	2.18	0.44
1:F:154:GLY:O	1:F:299:LYS:HG2	2.17	0.44
1:E:78:VAL:HG11	1:E:186:GLN:HG2	2.00	0.44
1:F:469:LEU:HD23	1:F:469:LEU:HA	1.73	0.44
1:A:165:TRP:HB3	1:A:276:PHE:CD1	2.53	0.44
1:C:67:GLU:HG3	1:C:101:THR:HB	2.00	0.44
1:C:68:VAL:CG1	1:C:104:MET:HG3	2.47	0.44
1:A:145:LYS:NZ	3:A:610:HOH:O	2.50	0.44
1:C:293:HIS:CD2	1:C:381:GLU:HG3	2.52	0.44
1:F:178:GLU:CD	1:F:178:GLU:H	2.20	0.44
1:F:235:TRP:HH2	1:F:349:TYR:HB3	1.83	0.44
1:F:325:LEU:HA	1:F:325:LEU:HD23	1.75	0.44
1:F:409:LYS:HA	1:F:409:LYS:HD2	1.66	0.44
1:A:293:HIS:CE1	1:A:379:ARG:HH21	2.36	0.43
1:F:294:GLN:HB2	1:F:380:ILE:HD11	2.00	0.43
1:B:205:HIS:CD2	1:D:265:GLN:HE21	2.35	0.43
1:F:210:VAL:O	1:F:214:MET:HB2	2.18	0.43
1:A:74:PHE:HB2	1:A:85:LEU:HD21	2.00	0.43
1:A:319:ARG:NH1	1:A:358:TRP:HZ3	2.16	0.43
1:E:416:GLN:HE21	1:E:424:VAL:HG21	1.83	0.43
1:E:126:ASP:OD1	1:E:140:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLU:CD	1:B:462:ARG:HH21	2.22	0.43
1:C:150:LEU:HD22	1:C:399:ILE:HG23	2.00	0.43
1:C:21:ALA:O	1:C:25:VAL:HG23	2.18	0.43
1:D:111:PHE:O	1:D:112:LYS:HG2	2.18	0.43
1:A:155:TYR:O	1:A:156:LEU:HD23	2.19	0.43
1:B:307:ILE:HA	1:B:308:PRO:HD3	1.83	0.43
1:D:28:GLU:HG3	1:D:32:LEU:HD22	1.99	0.43
1:D:236:ALA:HB3	1:D:239:GLN:HB2	2.01	0.43
1:B:17:GLU:OE1	1:B:17:GLU:HA	2.19	0.43
1:C:234:GLU:HG2	1:C:241:GLU:HB2	2.00	0.43
1:A:194:PRO:HD2	1:C:175:LEU:O	2.19	0.43
1:E:313:VAL:HG11	1:E:415:LEU:HD21	2.00	0.43
1:F:393:LEU:O	1:F:397:SER:HB3	2.19	0.43
1:A:321:TYR:CD1	1:A:402:GLY:HA3	2.54	0.42
1:B:276:PHE:HB3	1:B:387:PRO:HB2	2.00	0.42
1:E:164:GLU:HB2	1:E:289:GLY:H	1.84	0.42
1:F:182:ALA:N	1:F:185:VAL:HB	2.34	0.42
1:B:294:GLN:O	1:B:379:ARG:HB2	2.19	0.42
1:D:82:VAL:HG21	1:D:460:LEU:HD12	2.01	0.42
1:E:384:ILE:HD13	1:E:427:LEU:HD13	2.01	0.42
1:F:124:LEU:HA	1:F:124:LEU:HD23	1.78	0.42
1:F:150:LEU:HD12	1:F:150:LEU:HA	1.86	0.42
1:A:304:ASN:HB3	1:A:307:ILE:HD11	2.00	0.42
1:B:15:THR:N	1:B:18:GLN:OE1	2.49	0.42
1:D:345:ARG:HG2	1:D:352:ALA:HB1	2.01	0.42
1:F:345:ARG:H	1:F:345:ARG:HG2	1.61	0.42
1:E:137:LEU:HD22	1:E:456:TYR:CD2	2.54	0.42
1:A:349:TYR:N	3:A:612:HOH:O	2.51	0.42
1:B:150:LEU:HD23	1:B:150:LEU:HA	1.86	0.42
1:C:150:LEU:HD12	1:C:150:LEU:HA	1.87	0.42
1:A:37:ILE:HD13	1:A:58:LEU:HD22	2.01	0.42
1:A:156:LEU:HB2	1:A:297:VAL:HG22	2.01	0.42
1:D:457:TRP:CE2	1:D:461:ARG:HG3	2.54	0.42
1:E:307:ILE:HD11	1:E:376:PRO:HA	2.00	0.42
1:E:454:ILE:HA	1:E:457:TRP:HB3	2.02	0.42
1:B:150:LEU:HD23	1:B:403:LEU:HD22	2.02	0.42
1:C:257:LEU:HD22	1:C:392:TYR:CE2	2.55	0.42
1:A:370:VAL:HG21	1:A:379:ARG:CZ	2.49	0.42
1:B:15:THR:HG22	1:B:17:GLU:N	2.14	0.42
1:B:162:GLU:HB2	1:B:291:HIS:HB2	2.02	0.42
1:C:344:ARG:HD2	1:C:483:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:HB3	1:E:57:SER:HB2	2.01	0.42
1:E:150:LEU:HD13	1:E:399:ILE:HG23	2.02	0.42
1:F:362:ASN:ND2	1:F:416:GLN:OE1	2.53	0.42
1:A:226:LEU:HD13	1:A:259:ILE:HG13	2.02	0.41
1:B:207:LEU:HD13	1:D:52:SER:HB2	2.02	0.41
1:D:345:ARG:NH2	1:D:383:ARG:O	2.49	0.41
1:D:406:ILE:HD12	1:D:406:ILE:H	1.85	0.41
1:B:146:ALA:HB1	1:B:399:ILE:CG2	2.50	0.41
1:B:232:GLU:HG2	1:D:51:LYS:HG2	2.02	0.41
1:C:293:HIS:NE2	1:C:381:GLU:OE2	2.53	0.41
1:D:138:CYS:HB3	3:D:622:HOH:O	2.19	0.41
1:E:405:GLY:HA2	1:E:410:LYS:HG3	2.01	0.41
1:C:484:THR:OG1	1:C:487:GLU:HG3	2.20	0.41
1:D:491:TYR:O	1:D:495:LEU:HB2	2.20	0.41
1:E:203:LEU:HD23	1:E:206:HIS:CD2	2.55	0.41
1:D:490:GLU:HG2	1:D:491:TYR:CE1	2.55	0.41
1:A:416:GLN:HE22	1:A:424:VAL:HG11	1.86	0.41
1:A:135:PHE:CD1	1:A:136:PRO:HD2	2.55	0.41
1:B:168:THR:HB	1:B:192:VAL:HB	2.02	0.41
1:E:403:LEU:HD12	1:E:403:LEU:HA	1.85	0.41
1:F:290:TRP:CD1	1:F:290:TRP:C	2.94	0.41
1:A:384:ILE:HG21	3:A:671:HOH:O	2.20	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.82	0.41
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.82	0.41
1:C:167:LEU:O	1:C:238:SER:HB3	2.21	0.41
1:D:29:ILE:HG23	1:D:34:LEU:HB2	2.02	0.41
1:D:168:THR:HB	1:D:192:VAL:HB	2.03	0.41
1:D:301:THR:HG22	1:D:303:LYS:HG2	2.03	0.41
1:D:338:PRO:O	1:D:461:ARG:NH2	2.44	0.41
1:E:44:GLN:HG3	1:E:460:LEU:HD21	2.03	0.41
1:F:24:LYS:HA	1:F:27:ALA:HB3	2.02	0.41
1:F:37:ILE:HD12	1:F:37:ILE:N	2.35	0.41
1:F:156:LEU:HB2	1:F:297:VAL:HG22	2.02	0.41
1:F:290:TRP:HB2	1:F:387:PRO:HA	2.03	0.41
1:A:61:ALA:C	1:A:63:LYS:H	2.25	0.41
1:B:67:GLU:HB3	1:B:101:THR:CG2	2.50	0.41
1:B:403:LEU:HD12	1:B:403:LEU:HA	1.82	0.41
1:C:314:LEU:HG	1:C:369:VAL:CG1	2.51	0.41
1:A:165:TRP:HB3	1:A:276:PHE:CE1	2.55	0.40
1:C:455:LYS:HE3	1:C:455:LYS:HB3	1.86	0.40
1:E:48:LEU:HD23	1:E:48:LEU:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:PRO:HB2	1:E:245:ASP:HB2	2.03	0.40
1:F:345:ARG:NH1	1:F:384:ILE:HG22	2.36	0.40
1:A:237:PRO:CB	1:C:180:LEU:HD13	2.52	0.40
1:A:321:TYR:CE1	1:A:402:GLY:HA3	2.57	0.40
1:B:36:MET:HE1	1:B:54:THR:HG22	2.03	0.40
1:C:289:GLY:HA2	1:C:387:PRO:HD3	2.04	0.40
1:C:314:LEU:HD23	1:C:314:LEU:HA	1.92	0.40
1:C:339:THR:OG1	1:C:386:GLU:OE1	2.29	0.40
1:D:208:ASP:HB2	1:F:38:ARG:HH12	1.86	0.40
1:D:494:LEU:HD23	1:D:494:LEU:HA	1.85	0.40
1:E:472:GLU:OE2	3:E:601:HOH:O	2.22	0.40
1:E:26:LEU:HD23	1:E:26:LEU:HA	1.84	0.40
1:A:172:ASP:OD1	1:A:173:ARG:N	2.54	0.40
1:C:304:ASN:OD1	1:C:306:PHE:HB2	2.22	0.40
1:E:333:SER:HB3	1:E:434:ALA:HB1	2.03	0.40
1:F:403:LEU:HG	1:F:407:LYS:HD3	2.03	0.40
1:A:237:PRO:HB2	1:C:180:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	474/510 (93%)	458 (97%)	16 (3%)	0	100	100
1	B	483/510 (95%)	459 (95%)	24 (5%)	0	100	100
1	C	480/510 (94%)	463 (96%)	17 (4%)	0	100	100
1	D	478/510 (94%)	459 (96%)	19 (4%)	0	100	100
1	E	475/510 (93%)	461 (97%)	14 (3%)	0	100	100
1	F	481/510 (94%)	466 (97%)	15 (3%)	0	100	100
All	All	2871/3060 (94%)	2766 (96%)	105 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/427 (94%)	397 (98%)	6 (2%)	65	85
1	B	405/427 (95%)	401 (99%)	4 (1%)	76	90
1	C	404/427 (95%)	398 (98%)	6 (2%)	65	85
1	D	402/427 (94%)	385 (96%)	17 (4%)	30	63
1	E	400/427 (94%)	387 (97%)	13 (3%)	38	70
1	F	403/427 (94%)	402 (100%)	1 (0%)	93	98
All	All	2417/2562 (94%)	2370 (98%)	47 (2%)	57	81

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	334	SER
1	A	350	SER
1	A	358	TRP
1	A	394	TYR
1	A	414	GLU
1	B	200	SER
1	B	303	LYS
1	B	347	GLN
1	B	350	SER
1	C	12	ASN
1	C	43	ASP
1	C	321	TYR
1	C	358	TRP
1	C	410	LYS
1	C	461	ARG
1	D	6	ASP
1	D	30	ASP
1	D	76	ASP

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Mol	Chain	Res	Type
1	D	80	SER
1	D	81	MET
1	D	151	SER
1	D	197	GLN
1	D	200	SER
1	D	212	ASP
1	D	358	TRP
1	D	361	ASP
1	D	371	SER
1	D	384	ILE
1	D	397	SER
1	D	411	ASP
1	D	423	GLN
1	D	475	GLU
1	E	19	ARG
1	E	49	ARG
1	E	87	THR
1	E	94	ASP
1	E	96	LEU
1	E	225	ASN
1	E	309	SER
1	E	351	LEU
1	E	358	TRP
1	E	362	ASN
1	E	384	ILE
1	E	416	GLN
1	E	446	ARG
1	F	349	TYR

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	416	GLN
1	B	191	GLN
1	B	205	HIS
1	C	191	GLN
1	C	408	ASN
1	D	205	HIS
1	E	11	ASN
1	E	362	ASN
1	F	191	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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, 95^{th} 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	482/510 (94%)	-0.23	8 (1%) 70 53	19, 36, 66, 87	0
1	B	487/510 (95%)	-0.15	11 (2%) 60 43	22, 37, 72, 102	0
1	C	484/510 (94%)	-0.11	8 (1%) 70 53	23, 39, 67, 90	0
1	D	482/510 (94%)	-0.11	7 (1%) 73 57	23, 40, 62, 77	0
1	E	483/510 (94%)	-0.02	14 (2%) 51 35	22, 43, 69, 96	0
1	F	485/510 (95%)	-0.09	7 (1%) 75 59	21, 40, 65, 87	0
All	All	2903/3060 (94%)	-0.12	55 (1%) 66 49	19, 39, 67, 102	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	TYR	4.7
1	E	91	ASP	4.6
1	E	5	PHE	4.1
1	B	348	PRO	4.0
1	D	423	GLN	3.9
1	F	350	SER	3.9
1	C	408	ASN	3.7
1	A	310	GLU	3.5
1	A	309	SER	3.4
1	E	12	ASN	3.2
1	F	348	PRO	3.1
1	C	87	THR	3.0
1	D	408	ASN	3.0
1	A	349	TYR	3.0
1	F	20	ASP	3.0
1	B	86	PHE	2.9
1	C	301	THR	2.9
1	E	424	VAL	2.8
1	E	372	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	89	ALA	2.7
1	B	95	GLU	2.7
1	E	408	ASN	2.7
1	E	309	SER	2.6
1	A	352	ALA	2.5
1	E	310	GLU	2.5
1	B	350	SER	2.4
1	F	349	TYR	2.4
1	F	90	GLY	2.4
1	F	12	ASN	2.4
1	E	376	PRO	2.4
1	C	12	ASN	2.4
1	D	148	LYS	2.3
1	C	15	THR	2.3
1	A	88	THR	2.3
1	E	327	ALA	2.3
1	C	310	GLU	2.3
1	C	300	ASP	2.2
1	B	309	SER	2.2
1	D	84	ASN	2.2
1	B	6	ASP	2.2
1	E	373	THR	2.2
1	B	310	GLU	2.2
1	D	470	ASP	2.2
1	B	87	THR	2.2
1	D	87	THR	2.2
1	B	441	ASP	2.1
1	B	440	HIS	2.1
1	A	87	THR	2.1
1	C	421	ASP	2.1
1	E	96	LEU	2.1
1	E	418	SER	2.0
1	A	91	ASP	2.0
1	D	60	SER	2.0
1	E	97	SER	2.0
1	A	350	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 monosaccharides in this entry.

6.4 Ligands (i)

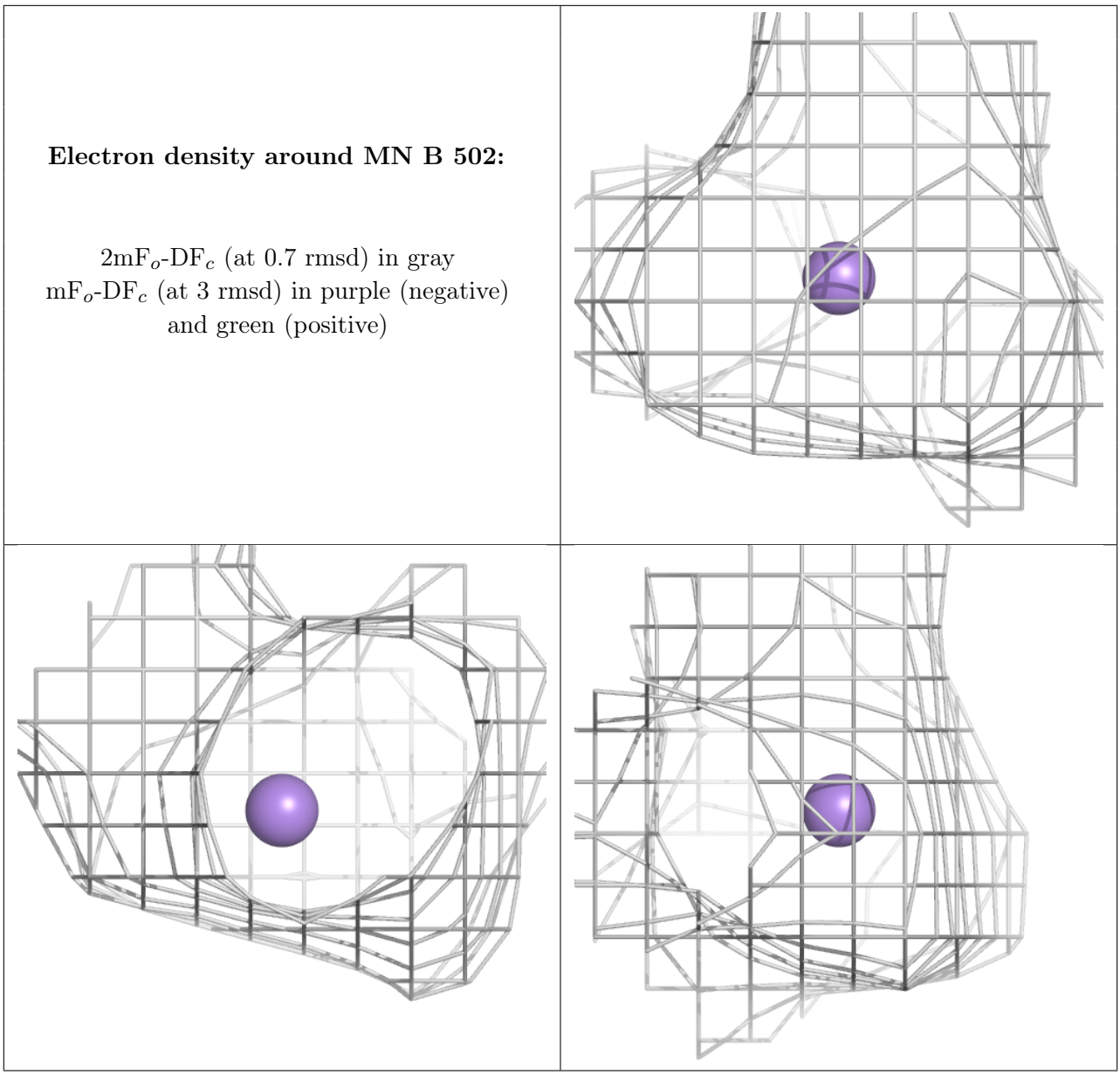
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	MN	B	502	1/1	0.53	0.16	95,95,95,95	0
2	MN	A	501	1/1	0.67	0.16	90,90,90,90	0
2	MN	C	501	1/1	0.71	0.12	104,104,104,104	0
2	MN	D	501	1/1	0.75	0.18	113,113,113,113	0
2	MN	E	501	1/1	0.81	0.12	85,85,85,85	0
2	MN	E	502	1/1	0.83	0.13	107,107,107,107	0
2	MN	B	501	1/1	0.91	0.08	64,64,64,64	0
2	MN	F	502	1/1	0.91	0.10	73,73,73,73	0
2	MN	A	502	1/1	0.94	0.06	74,74,74,74	0
2	MN	F	501	1/1	0.96	0.11	79,79,79,79	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.

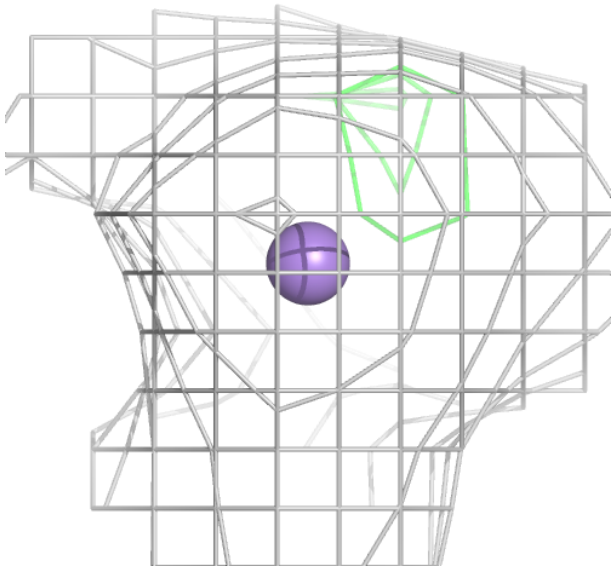
Electron density around MN B 502:

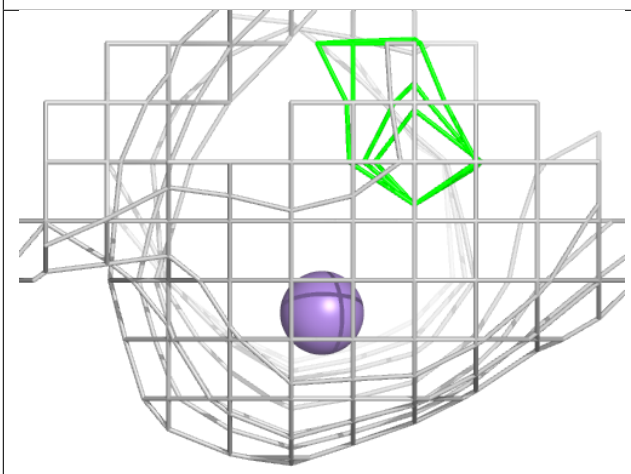
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

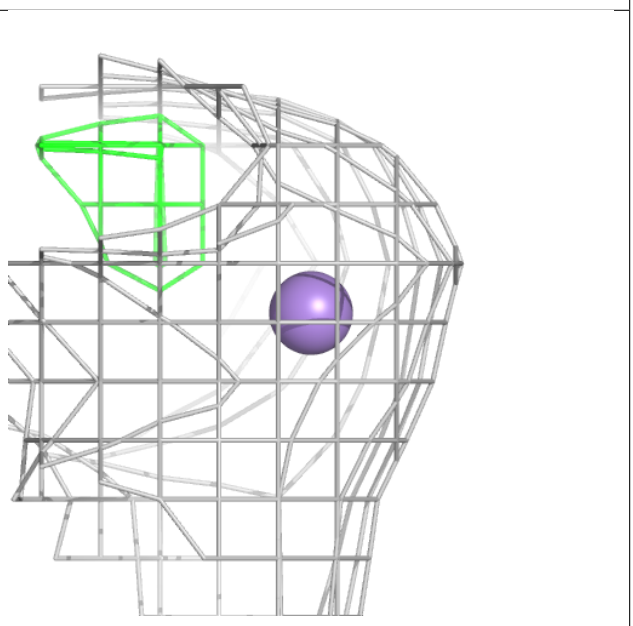


Electron density around MN A 501:

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

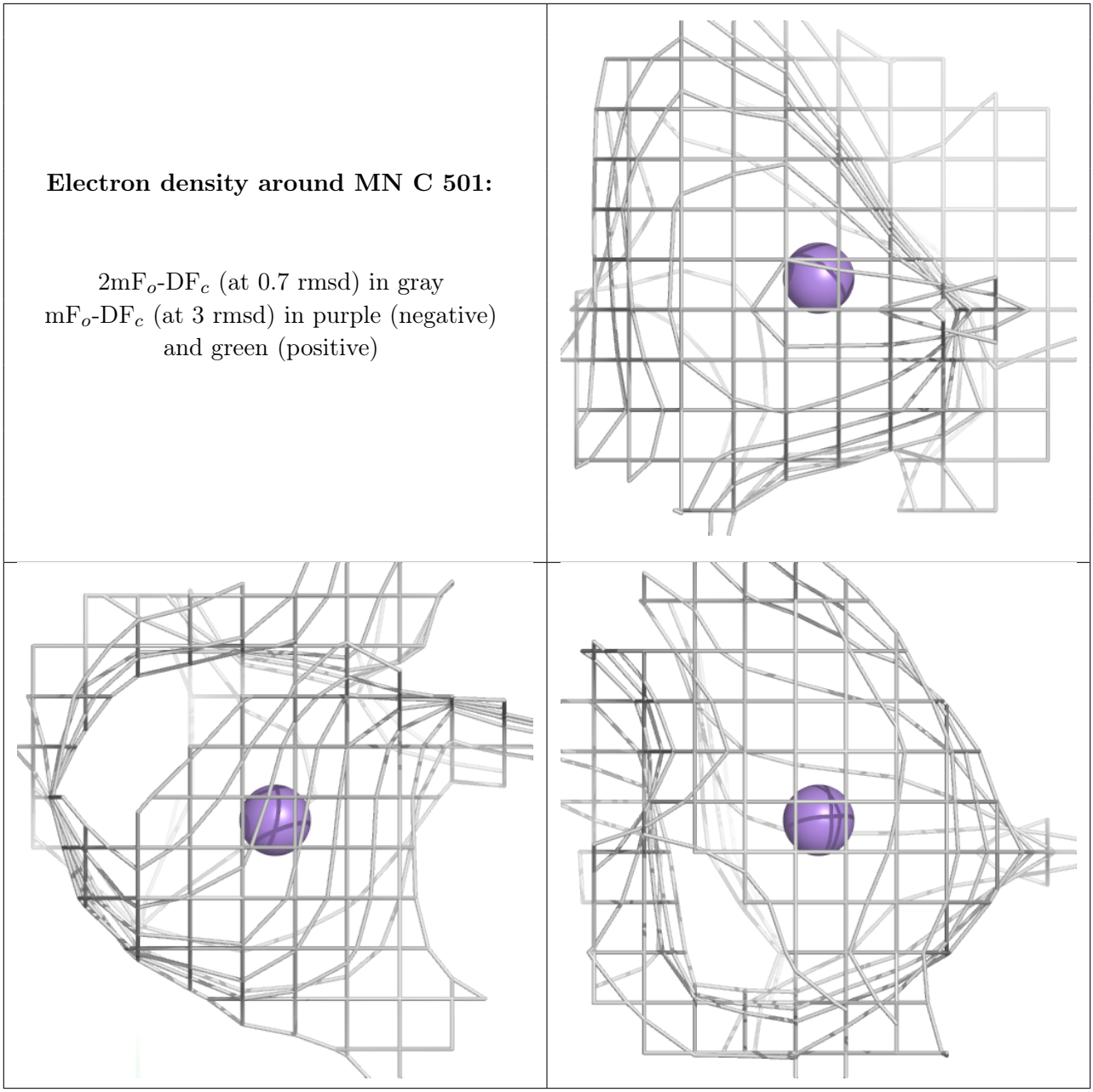






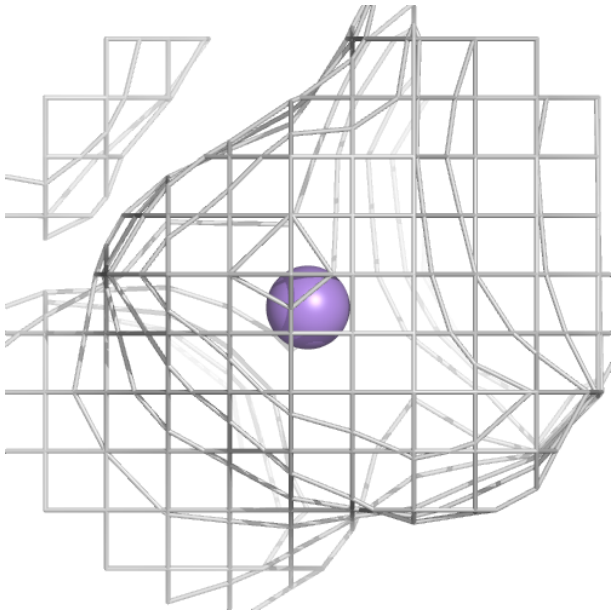
Electron density around MN C 501:

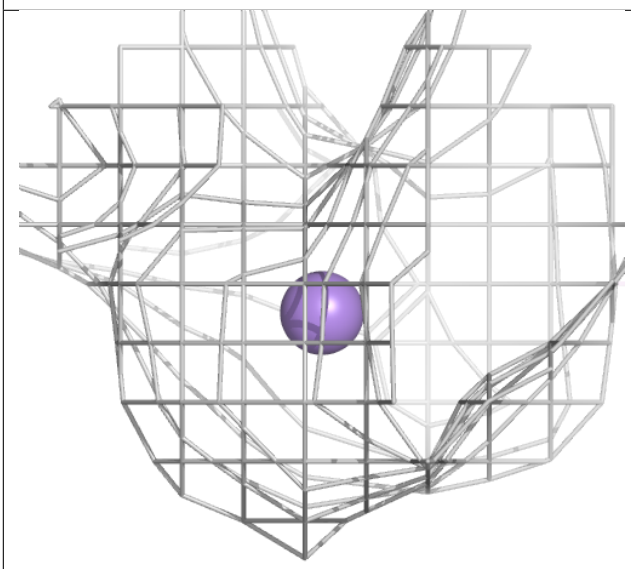
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

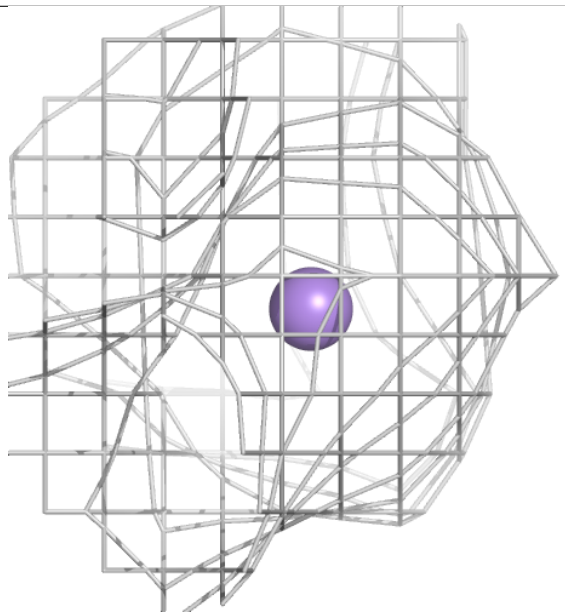


Electron density around MN D 501:

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

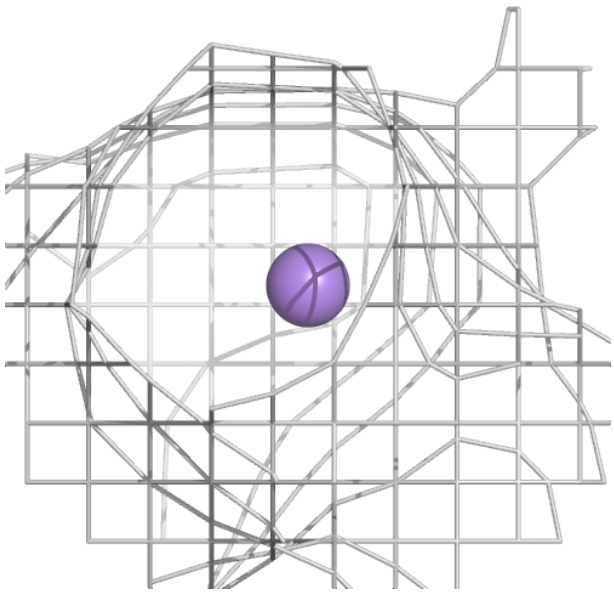


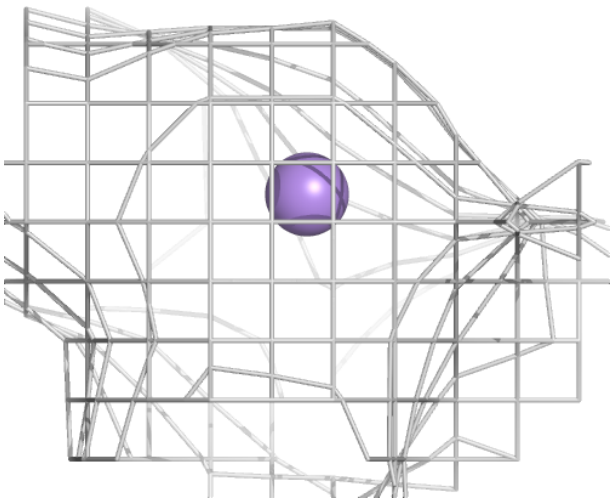


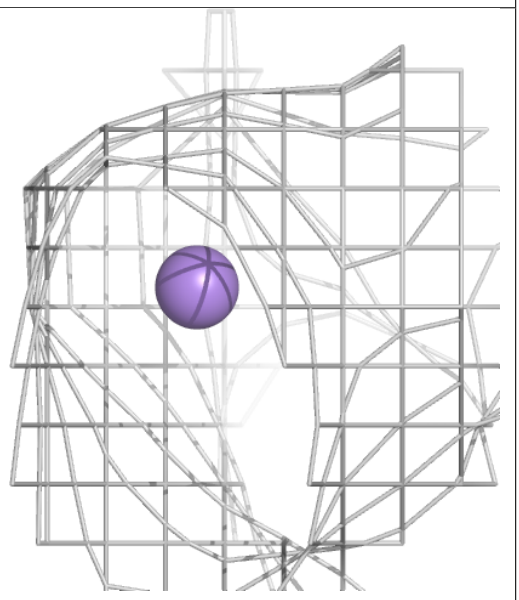


Electron density around MN E 501:

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

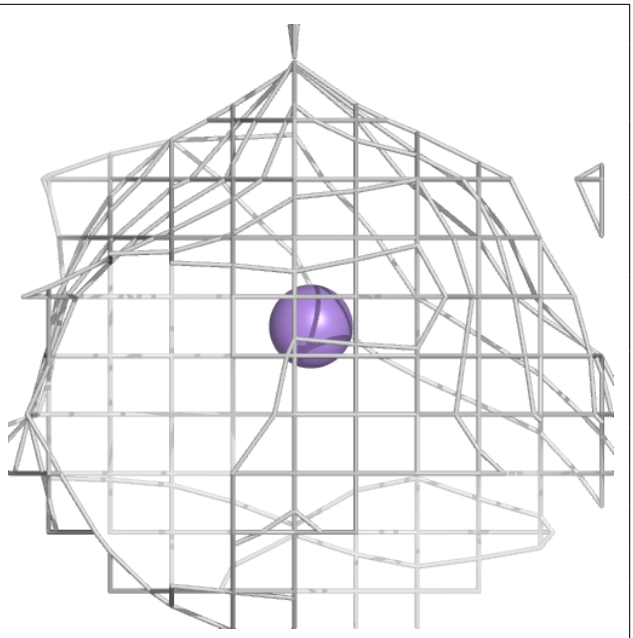


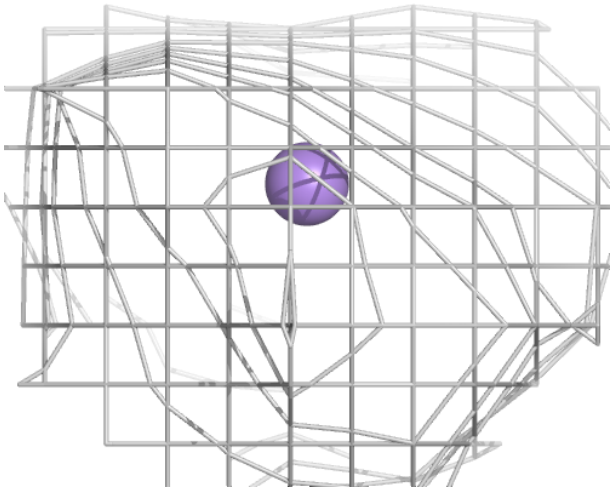


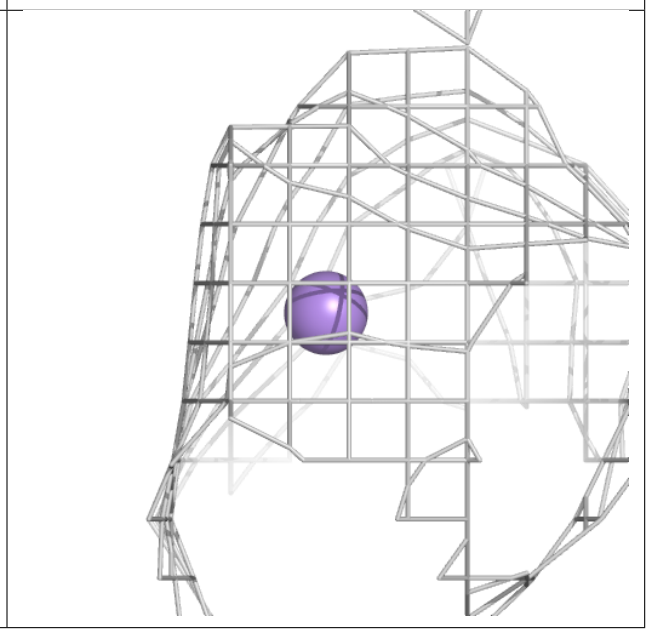


Electron density around MN E 502:

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

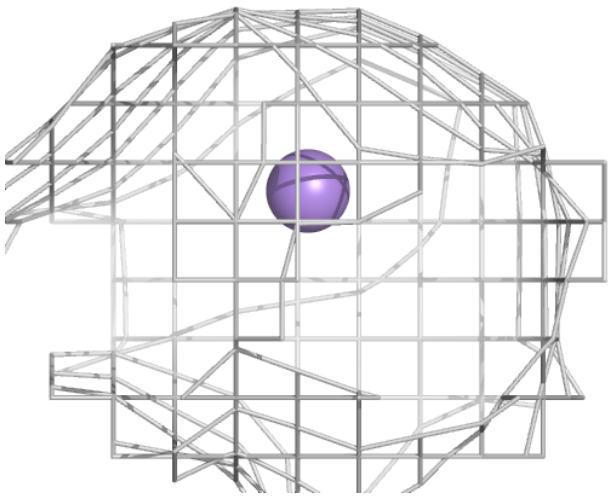


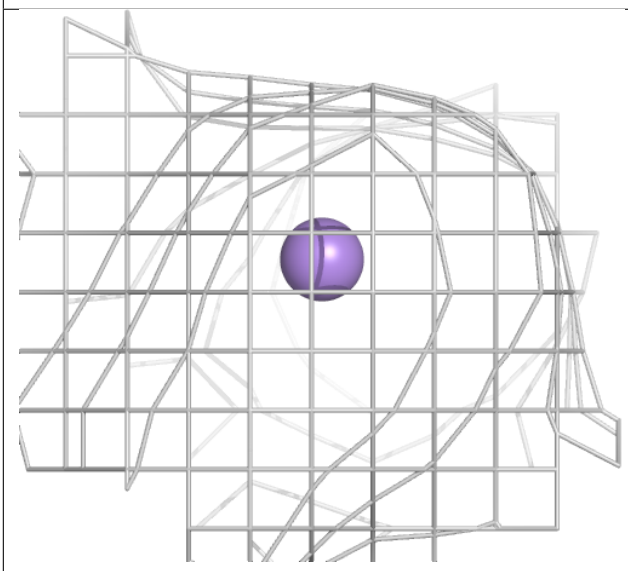


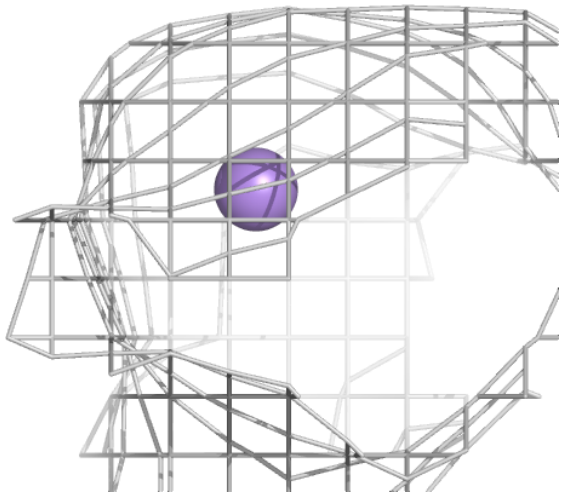


Electron density around MN B 501:

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

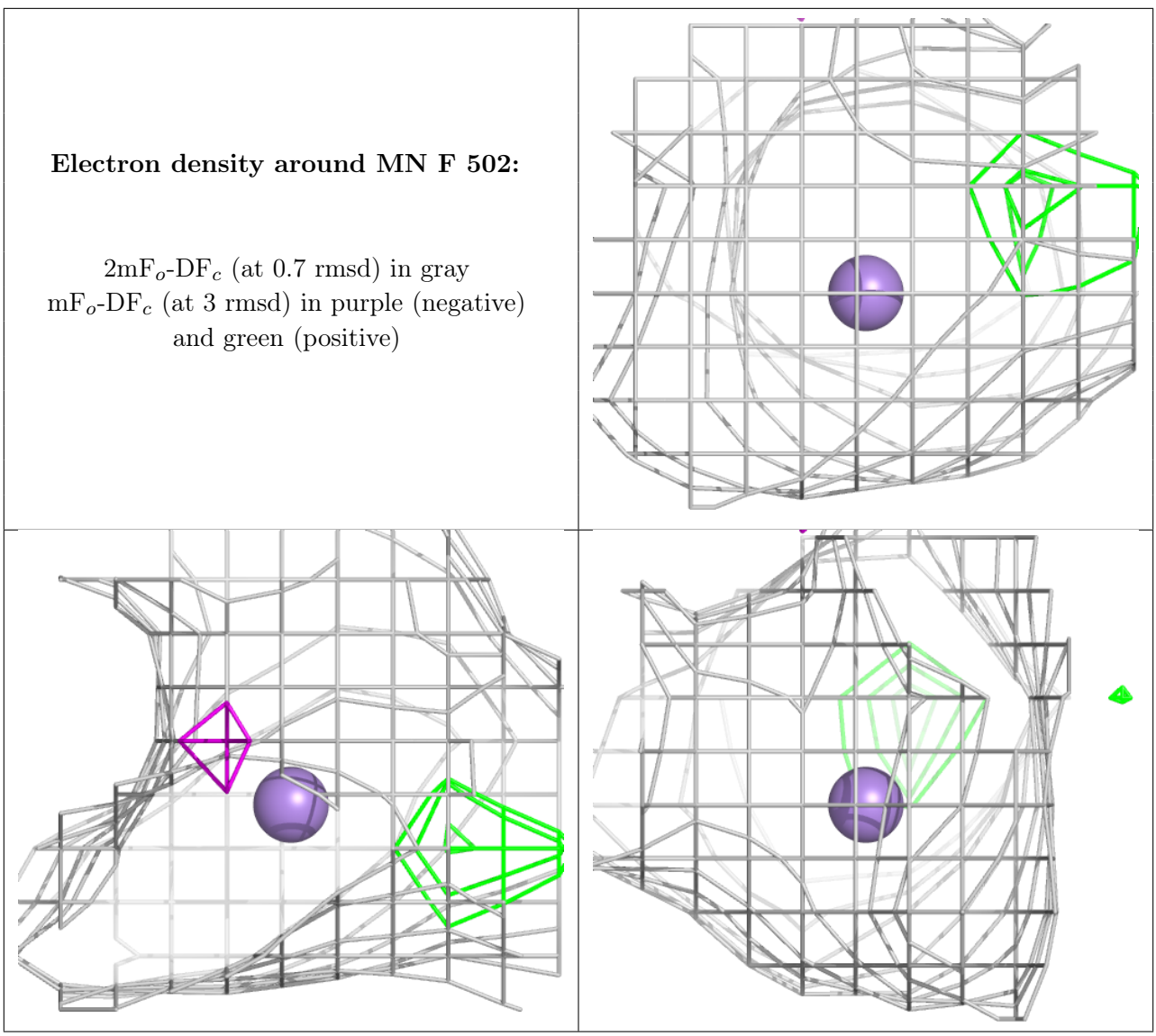






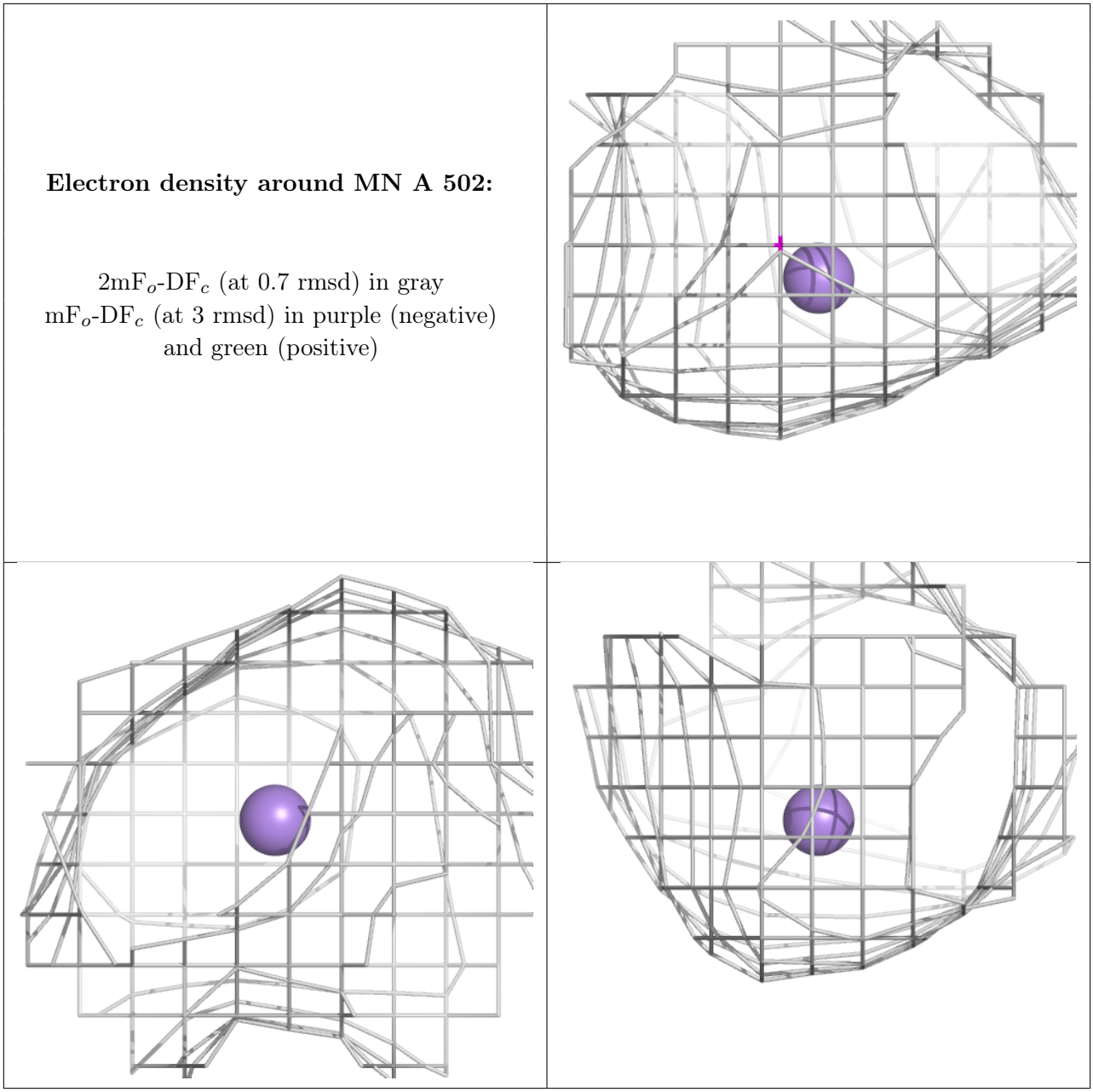
Electron density around MN F 502:

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



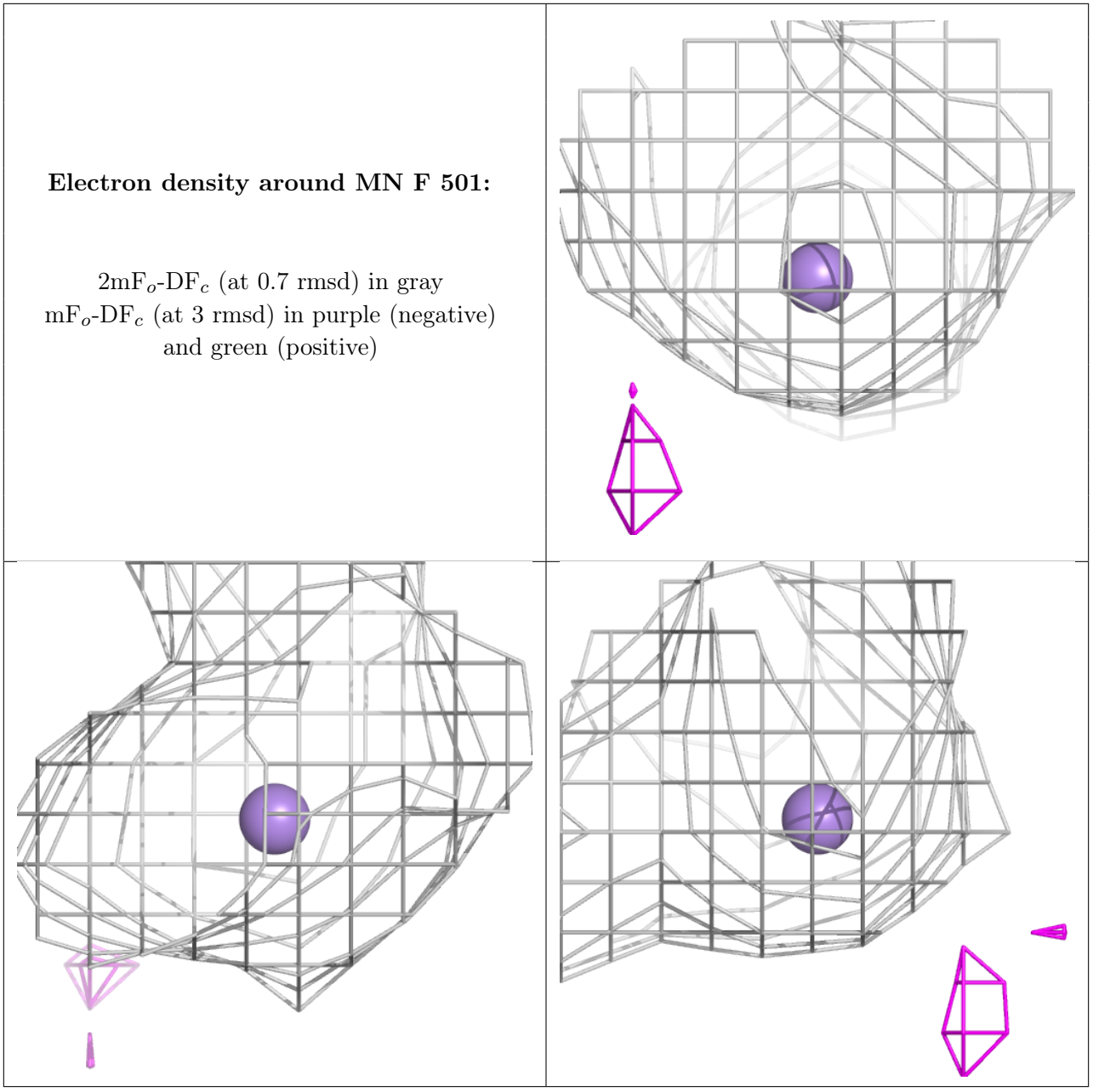
Electron density around MN A 502:

$2mF_o$-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 501:

$2mF_o$-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.