Full wwPDB X-ray Structure Validation Report ⓘ

Jul 18, 2022 – 04:05 pm BST

PDB ID	:	7BJQ
Title	:	Crystal structure of RecJCdc45 from Methanothermobacter thermoautotrophicus in complex with ssDNA
Authors	:	De March, M.; Onesti, S.
Deposited on	:	2021-01-14
Resolution	:	2.70 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:

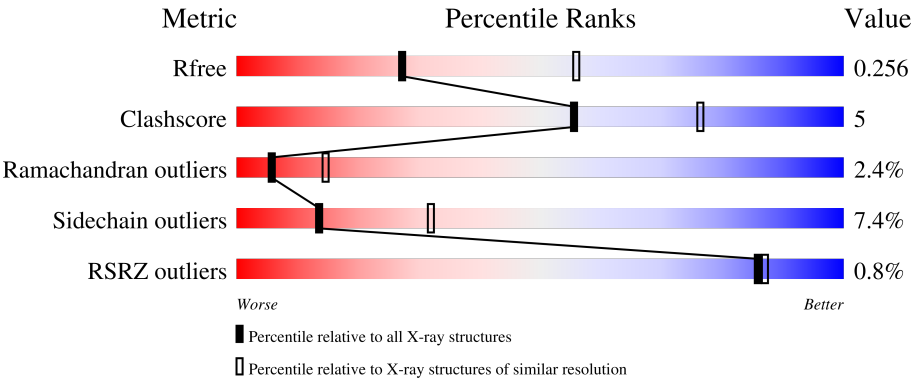
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	464	% 81% 13%
1	B	464	% 79% 14%
2	D	6	83% 17%
2	E	6	50% 50%
2	F	6	50% 50%

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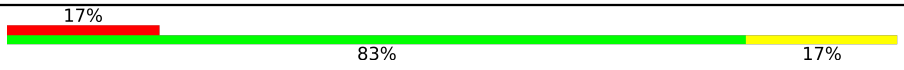
Mol	Chain	Length	Quality of chain
2	G	6	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7031 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 Conserved protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	0	0	0
			3266	2055	570	628	13			
1	B	445	Total	C	N	O	S	0	0	0
			3230	2036	566	616	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	458	ALA	-	expression tag	UNP O27473
A	459	GLU	-	expression tag	UNP O27473
A	460	ASN	-	expression tag	UNP O27473
A	461	LEU	-	expression tag	UNP O27473
A	462	TYR	-	expression tag	UNP O27473
A	463	PHE	-	expression tag	UNP O27473
A	464	GLN	-	expression tag	UNP O27473
B	458	ALA	-	expression tag	UNP O27473
B	459	GLU	-	expression tag	UNP O27473
B	460	ASN	-	expression tag	UNP O27473
B	461	LEU	-	expression tag	UNP O27473
B	462	TYR	-	expression tag	UNP O27473
B	463	PHE	-	expression tag	UNP O27473
B	464	GLN	-	expression tag	UNP O27473

- Molecule 2 is a DNA chain called DNA (5'-D(*5P*'P*-P*CP*AP*TP*GP*GP*CP*-P*3P*')-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			
2	E	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			
2	G	6	Total	C	N	O	P	0	0	0
			123	58	23	36	6			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		

- Molecule 4 is water.

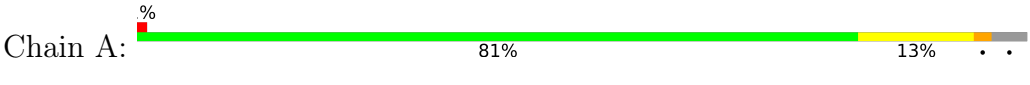
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	14	Total	O	0	0
			14	14		
4	D	1	Total	O	0	0
			1	1		

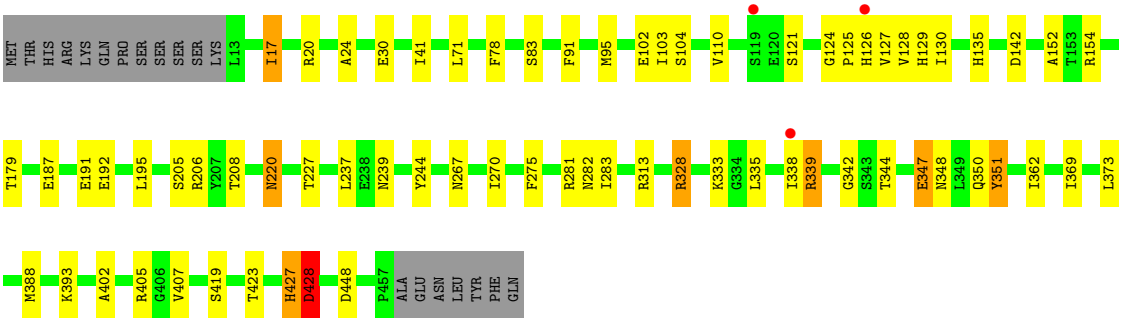
3 Residue-property plots (i)

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: Conserved protein

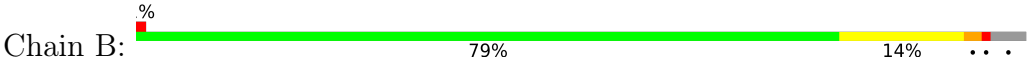
Chain A:

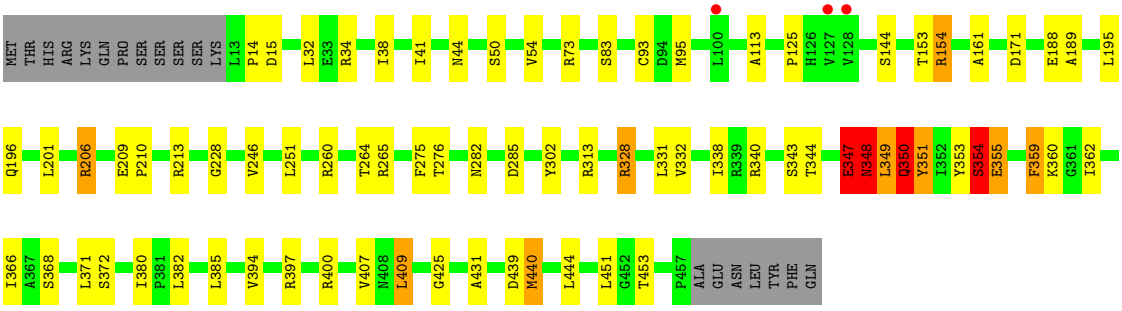




• Molecule 1: Conserved protein

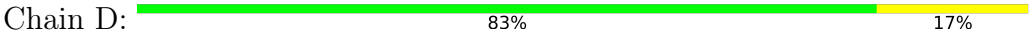
Chain B:





• Molecule 2: DNA (5'-D(*5P*'P*-P*CP*AP*TP*GP*GP*CP*-P*3P*')-3')

Chain D:



• Molecule 2: DNA (5'-D(*5P*'P*-P*CP*AP*TP*GP*GP*CP*-P*3P*')-3')

Chain E:

• Molecule 2: DNA (5'-D(*5P*'P*-P*CP*AP*TP*GP*GP*CP*-P*3P*')-3')

Chain F:

• Molecule 2: DNA (5'-D(*5P*'P*-P*CP*AP*TP*GP*GP*CP*-P*3P*')-3')

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	63.08Å 69.50Å 72.21Å 86.12° 69.26° 69.53°	Depositor
Resolution (Å)	67.38 – 2.70 67.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (67.38-2.70) 97.7 (67.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.196 , 0.258 0.199 , 0.256	Depositor DCC
R_{free} test set	1462 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	57.7	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7031	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.59	0/3323	0.83	7/4510 (0.2%)
1	B	0.61	0/3287	0.88	7/4466 (0.2%)
2	D	0.40	0/137	0.82	0/209
2	E	0.53	0/137	1.00	0/209
2	F	0.50	0/137	0.91	1/209 (0.5%)
2	G	0.34	0/137	0.68	0/209
All	All	0.59	0/7158	0.85	15/9812 (0.2%)

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	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	328	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	350	GLN	N-CA-C	-5.96	94.92	111.00
1	A	339	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	206	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	427	HIS	C-N-CA	5.77	136.12	121.70
1	A	338	ILE	C-N-CA	5.74	136.05	121.70
1	B	347	GLU	CA-C-N	5.69	129.72	117.20
1	B	347	GLU	C-N-CA	5.54	135.56	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	338	ILE	CA-C-N	5.51	129.31	117.20
1	B	328	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	206	ARG	CB-CA-C	-5.24	99.93	110.40
1	A	428	ASP	N-CA-C	-5.22	96.90	111.00
1	B	409	LEU	CA-CB-CG	5.06	126.94	115.30
2	F	1	DC	C5'-C4'-C3'	5.04	123.17	114.10
1	A	427	HIS	CA-C-N	5.02	128.25	117.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	LYS	Peptide
1	B	347	GLU	Peptide
1	B	354	SER	Peptide

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	3266	0	3124	27	0
1	B	3230	0	3057	39	0
2	D	123	0	68	1	0
2	E	123	0	68	2	0
2	F	123	0	68	1	0
2	G	123	0	68	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	24	0	0	0	0
4	B	14	0	0	0	0
4	D	1	0	0	0	0
All	All	7031	0	6453	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) 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:439:ASP:HA	1:B:440:MET:CB	2.08	0.83
1:A:427:HIS:HB3	1:A:428:ASP:HB3	1.66	0.78
1:B:397:ARG:NH2	2:E:2:DA:OP2	2.20	0.75
1:B:338:ILE:HD11	1:B:366:ILE:CG2	2.16	0.74
1:B:344:THR:CB	1:B:350:GLN:OE1	2.37	0.73
1:B:201:LEU:O	1:B:206:ARG:NH2	2.22	0.73
1:A:427:HIS:CB	1:A:428:ASP:HB3	2.18	0.72
1:A:344:THR:O	1:A:350:GLN:O	2.08	0.71
1:B:338:ILE:CD1	1:B:366:ILE:CG2	2.78	0.60
1:A:102:GLU:OE1	1:A:102:GLU:N	2.34	0.60
1:A:41:ILE:HG22	1:A:95:MET:CE	2.32	0.59
1:A:227:THR:HB	1:A:373:LEU:HD21	1.85	0.58
1:B:41:ILE:HG22	1:B:95:MET:HE3	1.85	0.58
1:A:104:SER:O	1:A:126:HIS:CE1	2.56	0.58
1:B:439:ASP:CA	1:B:440:MET:CB	2.82	0.58
1:B:210:PRO:HG2	1:B:213:ARG:HG3	1.87	0.56
1:B:348:ASN:N	1:B:348:ASN:OD1	2.39	0.55
1:A:103:ILE:CG2	1:A:110:VAL:HG11	2.38	0.54
1:B:260:ARG:O	1:B:264:THR:OG1	2.23	0.53
1:B:50:SER:O	1:B:54:VAL:HG23	2.08	0.53
1:A:281:ARG:O	1:A:282:ASN:HB2	2.09	0.53
1:B:385:LEU:CD2	1:B:394:VAL:HG22	2.38	0.53
1:B:161:ALA:HB1	1:B:189:ALA:HB2	1.90	0.52
1:A:205:SER:OG	1:A:328:ARG:NH2	2.41	0.52
1:A:335:LEU:HD11	1:A:369:ILE:HG21	1.93	0.51
1:B:32:LEU:CD1	1:B:38:ILE:HD11	2.41	0.51
1:B:347:GLU:N	1:B:348:ASN:O	2.44	0.51
1:B:338:ILE:HD11	1:B:366:ILE:HG21	1.91	0.51
1:B:353:TYR:O	1:B:354:SER:CB	2.58	0.51
1:A:17:ILE:HD12	1:A:135:HIS:CD2	2.46	0.50
1:A:427:HIS:HB3	1:A:428:ASP:CB	2.38	0.49
1:A:20:ARG:HD3	1:A:129:HIS:O	2.11	0.49
1:B:425:GLY:O	1:B:431:ALA:HB1	2.12	0.49
1:B:32:LEU:HD12	1:B:38:ILE:HD11	1.94	0.48
1:A:283:ILE:HD12	1:A:283:ILE:N	2.29	0.48
1:B:350:GLN:HA	1:B:351:TYR:HB3	1.96	0.47
1:B:195:LEU:HD11	1:B:275:PHE:HB3	1.97	0.46
1:B:354:SER:HA	1:B:355:GLU:CB	2.45	0.46
1:A:41:ILE:N	1:A:41:ILE:HD12	2.31	0.45
1:A:195:LEU:HD11	1:A:275:PHE:HB3	1.99	0.45
1:A:237:LEU:HD13	1:A:244:TYR:HA	1.97	0.45
1:A:267:ASN:O	1:A:270:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:GLU:HB2	1:A:448:ASP:OD2	2.16	0.45
1:B:41:ILE:HG22	1:B:95:MET:CE	2.46	0.45
1:B:44:ASN:HB2	1:B:302:TYR:CE1	2.53	0.45
1:B:359:PHE:CD1	1:B:359:PHE:N	2.83	0.45
1:B:154:ARG:NH2	1:B:188:GLU:OE1	2.50	0.44
1:B:349:LEU:O	1:B:350:GLN:HG2	2.18	0.44
1:B:275:PHE:O	1:B:285:ASP:HB2	2.17	0.44
1:B:328:ARG:O	1:B:332:VAL:HG23	2.19	0.43
1:A:388:MET:SD	1:A:393:LYS:HB2	2.59	0.42
1:B:349:LEU:O	1:B:380:ILE:CG2	2.67	0.42
1:A:402:ALA:O	1:A:407:VAL:HB	2.19	0.42
2:D:1:DC:C6	2:G:6:DC:H2'	2.55	0.42
1:A:124:GLY:HA3	1:A:127:VAL:HB	2.01	0.42
1:B:331:LEU:HD23	1:B:362:ILE:HD12	2.01	0.42
1:A:130:ILE:HD12	1:A:152:ALA:HB2	2.00	0.42
1:A:220:ASN:C	1:A:220:ASN:HD22	2.23	0.41
1:B:350:GLN:O	1:B:382:LEU:HA	2.21	0.41
1:B:93:CYS:HA	1:B:113:ALA:O	2.21	0.41
2:E:4:DG:H2"	2:E:5:DG:C8	2.56	0.41
1:A:71:LEU:HD11	1:A:78:PHE:CE1	2.56	0.41
1:B:161:ALA:CB	1:B:189:ALA:HB2	2.51	0.41
1:B:228:GLY:O	1:B:332:VAL:HG13	2.20	0.41
1:B:354:SER:CA	1:B:355:GLU:CB	2.99	0.41
1:A:24:ALA:HB2	1:A:128:VAL:HG11	2.03	0.41
1:B:338:ILE:HD12	1:B:366:ILE:HG23	2.03	0.41
2:F:3:DT:H2"	2:F:4:DG:C8	2.56	0.40
1:B:338:ILE:CD1	1:B:366:ILE:HG23	2.50	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	443/464 (96%)	407 (92%)	29 (6%)	7 (2%)	9 24
1	B	443/464 (96%)	405 (91%)	24 (5%)	14 (3%)	4 9
All	All	886/928 (96%)	812 (92%)	53 (6%)	21 (2%)	6 15

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ARG
1	A	351	TYR
1	A	405	ARG
1	A	428	ASP
1	B	14	PRO
1	B	343	SER
1	B	348	ASN
1	B	350	GLN
1	B	351	TYR
1	B	354	SER
1	B	355	GLU
1	B	440	MET
1	B	360	LYS
1	A	121	SER
1	B	15	ASP
1	B	125	PRO
1	B	347	GLU
1	B	453	THR
1	B	407	VAL
1	A	125	PRO
1	A	342	GLY

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	323/379 (85%)	302 (94%)	21 (6%)	17 38
1	B	311/379 (82%)	285 (92%)	26 (8%)	11 25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	634/758 (84%)	587 (93%)	47 (7%)	13 32

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

Mol	Chain	Res	Type
1	A	17	ILE
1	A	30	GLU
1	A	83	SER
1	A	91	PHE
1	A	142	ASP
1	A	154	ARG
1	A	179	THR
1	A	187	GLU
1	A	191	GLU
1	A	192	GLU
1	A	206	ARG
1	A	208	THR
1	A	220	ASN
1	A	239	ASN
1	A	313	ARG
1	A	347	GLU
1	A	348	ASN
1	A	351	TYR
1	A	362	ILE
1	A	419	SER
1	A	423	THR
1	B	34	ARG
1	B	73	ARG
1	B	83	SER
1	B	144	SER
1	B	153	THR
1	B	154	ARG
1	B	171	ASP
1	B	196	GLN
1	B	209	GLU
1	B	246	VAL
1	B	251	LEU
1	B	265	ARG
1	B	276	THR
1	B	282	ASN
1	B	313	ARG
1	B	340	ARG

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Mol	Chain	Res	Type
1	B	348	ASN
1	B	349	LEU
1	B	359	PHE
1	B	368	SER
1	B	371	LEU
1	B	372	SER
1	B	400	ARG
1	B	409	LEU
1	B	444	LEU
1	B	451	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	182	ASN
1	A	220	ASN
1	A	239	ASN
1	A	390	GLN
1	A	445	GLN
1	B	36	ASN
1	B	182	ASN
1	B	282	ASN

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 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

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	445/464 (95%)	-0.26	3 (0%) 87 89	36, 62, 95, 134	0
1	B	445/464 (95%)	-0.23	3 (0%) 87 89	36, 60, 90, 120	0
2	D	6/6 (100%)	-0.93	0 100 100	69, 80, 92, 101	0
2	E	6/6 (100%)	-0.29	0 100 100	65, 89, 104, 114	0
2	F	6/6 (100%)	-0.80	0 100 100	70, 78, 87, 117	0
2	G	6/6 (100%)	0.24	1 (16%) 1 1	107, 123, 157, 158	0
All	All	914/952 (96%)	-0.25	7 (0%) 86 87	36, 62, 94, 158	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	VAL	3.4
2	G	1	DC	3.1
1	A	119	SER	2.7
1	A	126	HIS	2.3
1	A	338	ILE	2.3
1	B	128	VAL	2.2
1	B	100	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

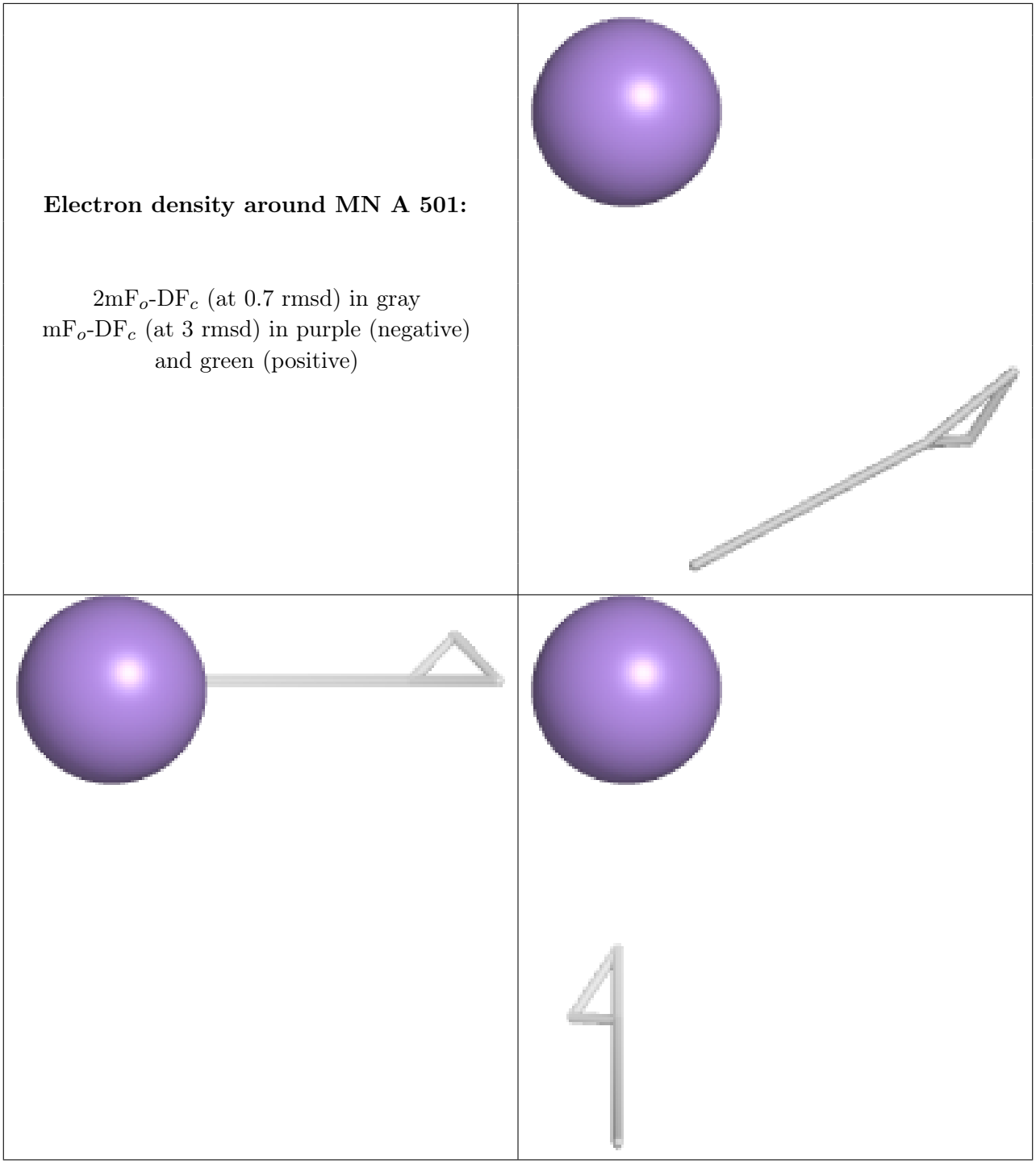
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	MN	A	501	1/1	0.94	0.08	101,101,101,101	0
3	MN	A	502	1/1	0.98	0.08	98,98,98,98	0
3	MN	B	501	1/1	0.98	0.08	84,84,84,84	0
3	MN	B	502	1/1	0.99	0.07	89,89,89,89	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

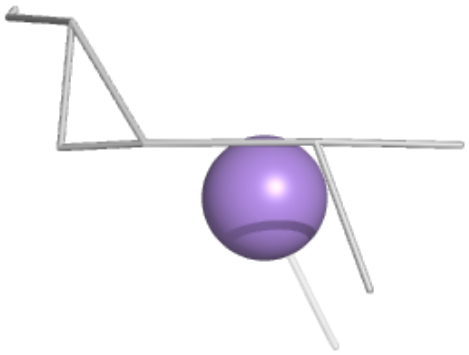
Electron density around MN A 501:

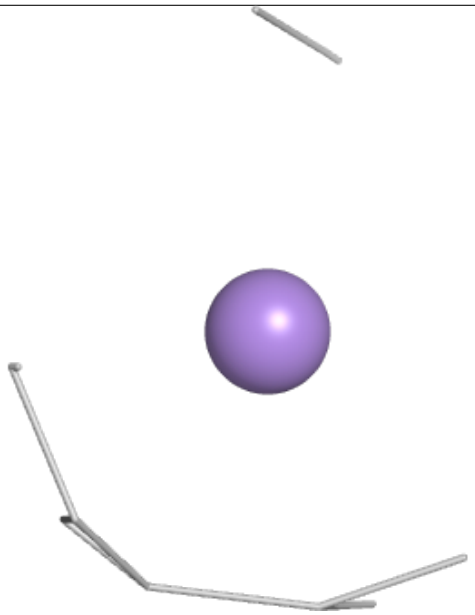
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

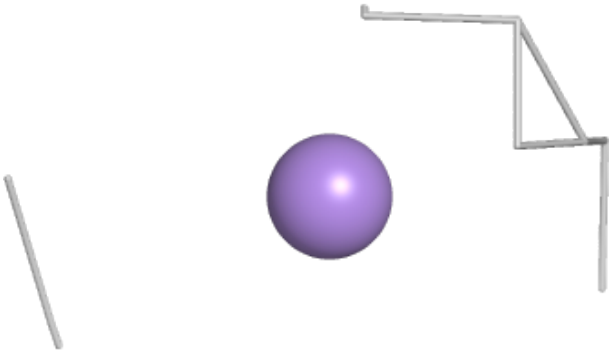


Electron density around MN A 502:

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

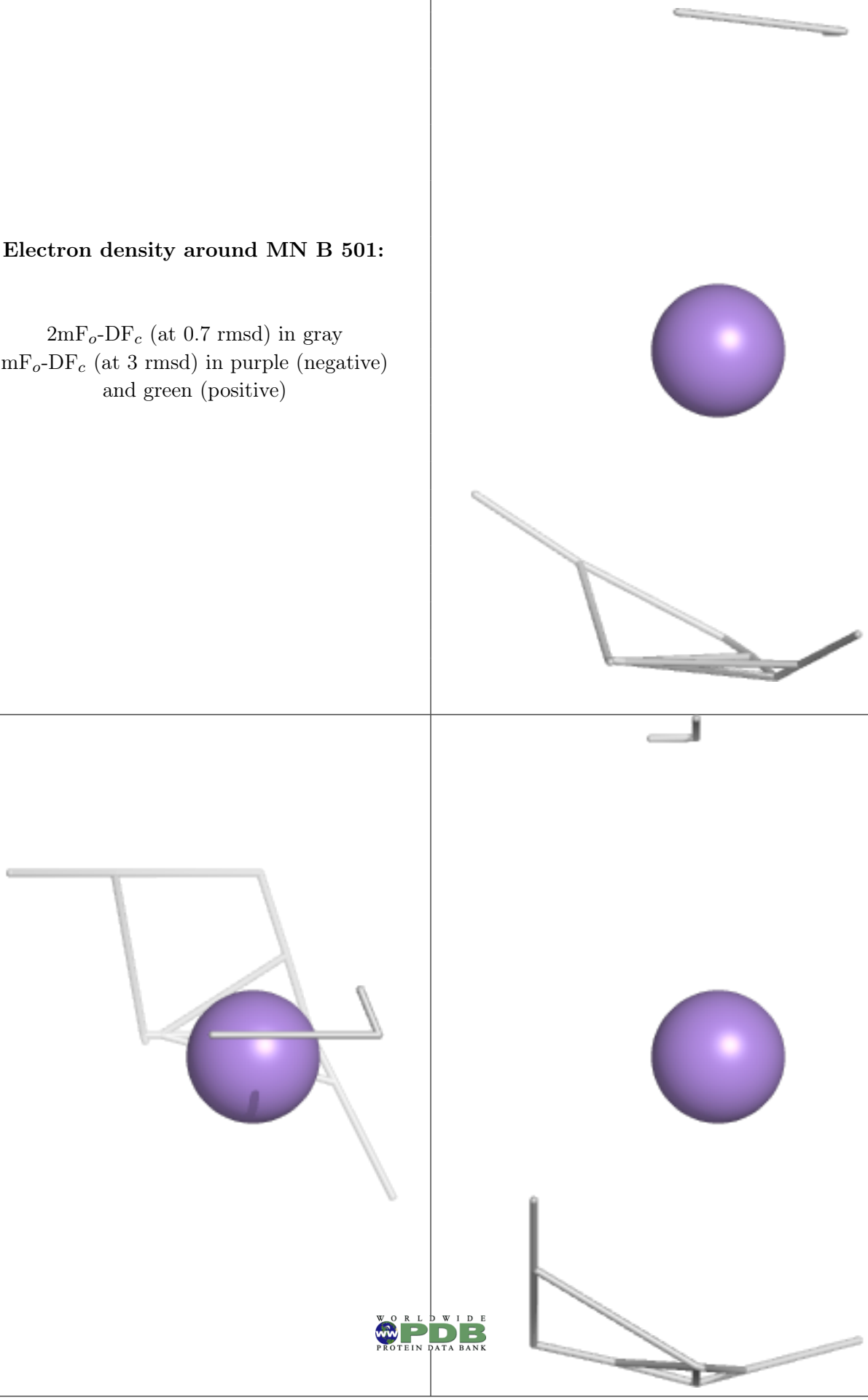






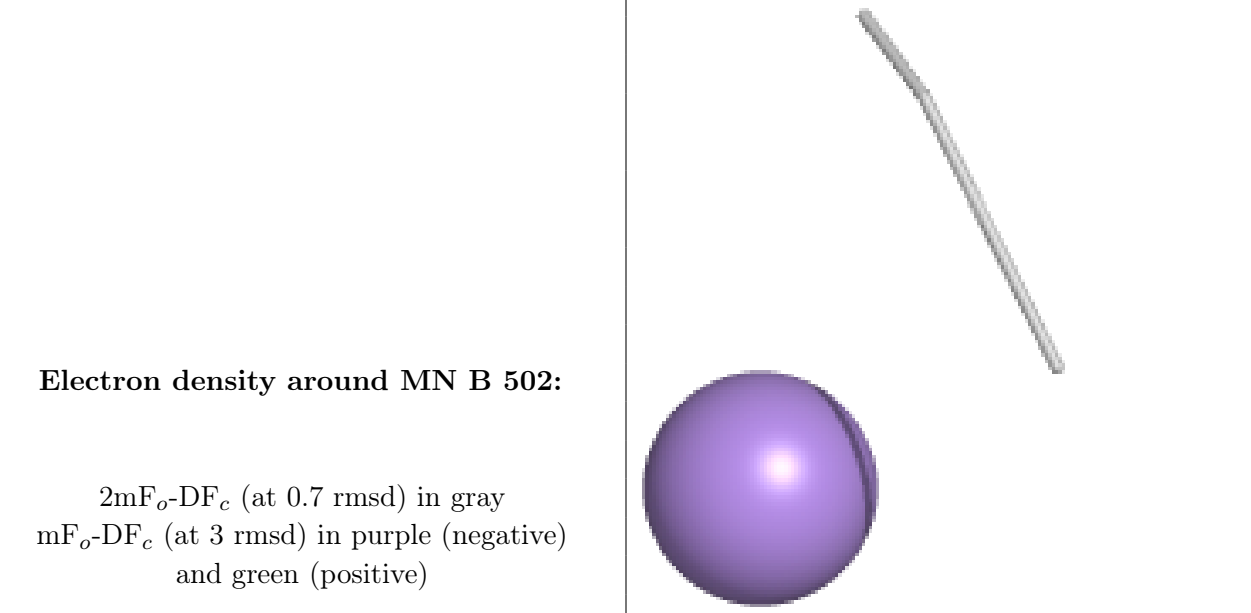
Electron density around MN B 501:

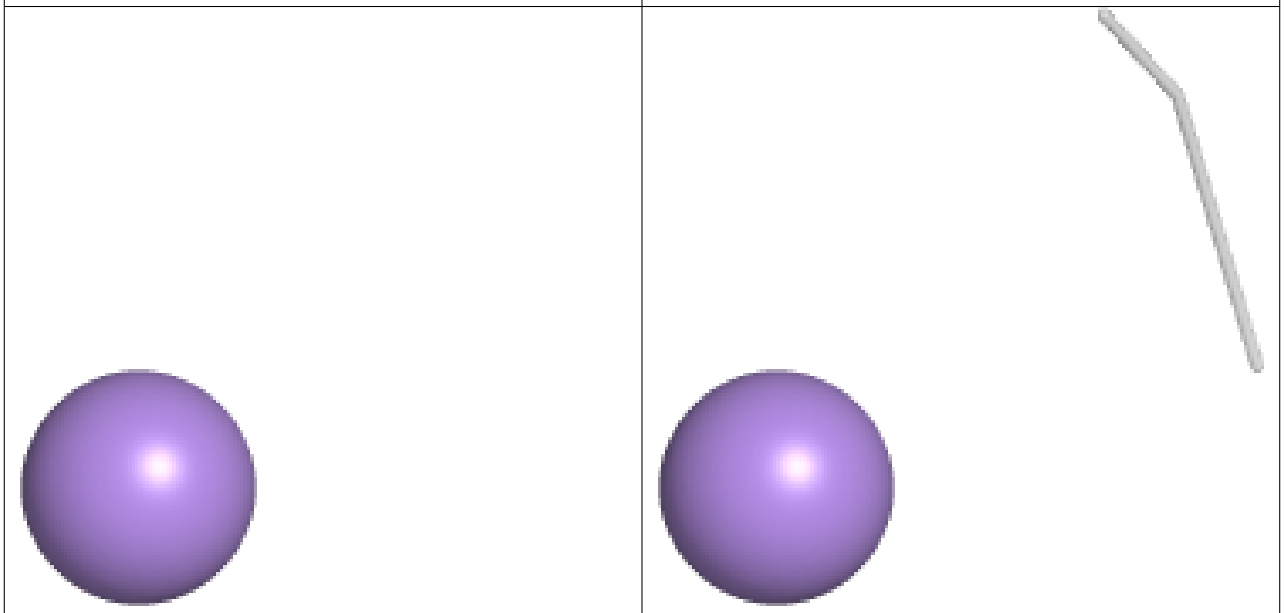
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around MN 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)





6.5 Other polymers (i)

There are no such residues in this entry.