



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 03:30 PM BST

PDB ID : 6LE9
Title : The Human Telomeric Nucleosome Displays Distinct Structural and Dynamic Properties
Authors : Soman, A.; Liew, C.W.; Teo, H.L.; Berezhnoy, N.; Korolev, N.; Rhodes, D.; Nordenskiöld, L.
Deposited on : 2019-11-24
Resolution : 2.60 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 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	:	2.13.1
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)	:	2.13.1

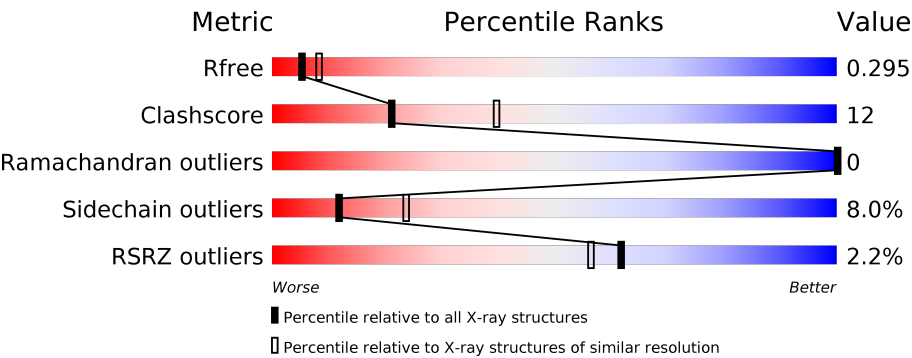
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	96	<div><div></div><div>72%24%..</div></div>
1	E	96	<div>2%</div> <div><div></div><div>75%24%.</div></div>
2	B	87	<div><div></div><div>76%23%. </div></div>
2	F	87	<div>%</div> <div><div></div><div>64%23%.. 10%</div></div>
3	C	105	<div>%</div> <div><div></div><div>77%18%.. </div></div>
3	G	105	<div>4%</div> <div><div></div><div>77%19%. </div></div>

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Mol	Chain	Length	Quality of chain
4	D	95	<div><div><div></div><div></div><div></div></div><div>2%79%18%</div><div></div></div>
4	H	95	<div><div><div></div><div></div><div></div></div><div>%81%16%</div><div></div></div>
5	I	145	<div><div><div></div><div></div><div></div></div><div>3%60%40%</div><div></div></div>
6	J	145	<div><div><div></div><div></div><div></div></div><div>6%56%44%</div><div></div></div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11925 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 Histone H3.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	95	Total	C	N	O	S	0	0	0
			784	494	151	135	4			
1	E	96	Total	C	N	O	S	0	0	0
			790	497	152	137	4			

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	87	Total	C	N	O	S	0	0	0
			703	442	142	118	1			
2	F	78	Total	C	N	O	S	0	0	0
			619	391	120	107	1			

- Molecule 3 is a protein called Histone H2A type 1-B/E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	103	Total	C	N	O	0	0	0
			796	502	155	139			
3	G	105	Total	C	N	O	0	0	0
			810	511	158	141			

- Molecule 4 is a protein called Histone H2B type 1-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	95	Total	C	N	O	S	0	0	0
			745	467	136	140	2			
4	H	94	Total	C	N	O	S	0	0	0
			735	461	134	138	2			

- Molecule 5 is a DNA chain called Human Telomeric DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	145	Total	C	N	O	P	0	0	0
			2878	1380	510	844	144			

- Molecule 6 is a DNA chain called Human Telomeric DNA (145-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	145	Total	C	N	O	P	0	0	0
			3061	1449	576	892	144			

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Mn	0	0
			1	1		
7	A	1	Total	Mn	0	0
			1	1		
7	J	2	Total	Mn	0	0
			2	2		

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: Histone H3.1

Chain A: 



- Molecule 1: Histone H3.1

Chain E: 



- Molecule 2: Histone H4

Chain B: 




- Molecule 2: Histone H4

Chain F: 

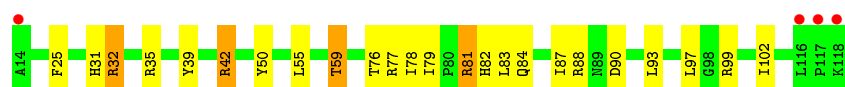
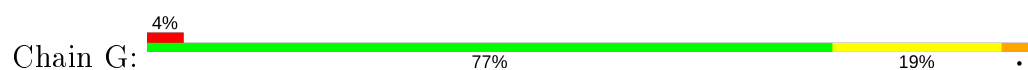


- Molecule 3: Histone H2A type 1-B/E

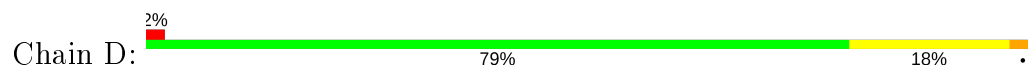
Chain C: 



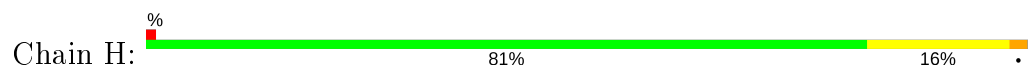
- Molecule 3: Histone H2A type 1-B/E



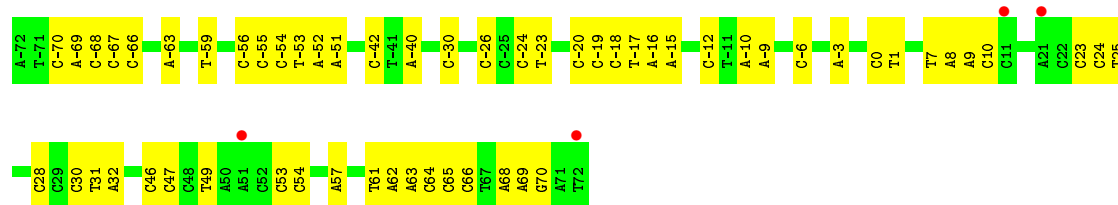
- Molecule 4: Histone H2B type 1-K



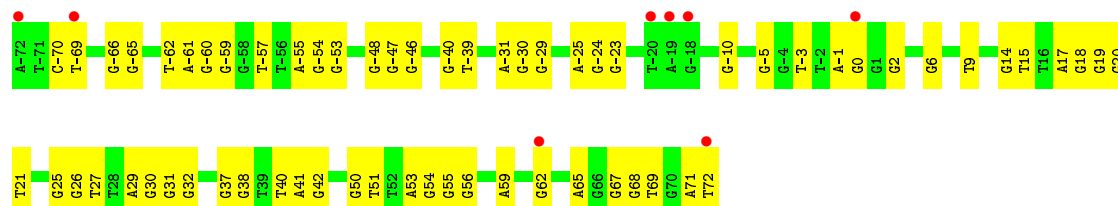
- Molecule 4: Histone H2B type 1-K



- Molecule 5: Human Telomeric DNA (145-MER)



- Molecule 6: Human Telomeric DNA (145-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.45Å 109.39Å 176.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.60 48.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	51.8 (49.00-2.60) 51.8 (48.65-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.238 , 0.281 0.256 , 0.295	Depositor DCC
R_{free} test set	1622 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11925	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/794	0.63	0/1064
1	E	0.42	0/800	0.57	0/1071
2	B	0.48	0/711	0.72	2/948 (0.2%)
2	F	0.39	0/626	0.64	1/837 (0.1%)
3	C	0.39	0/806	0.55	0/1089
3	G	0.46	0/820	0.58	0/1107
4	D	0.43	0/756	0.59	1/1014 (0.1%)
4	H	0.47	0/746	0.57	0/1003
5	I	0.71	0/3217	0.84	0/4934
6	J	0.66	0/3445	0.84	0/5345
All	All	0.58	0/12721	0.75	4/18412 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	95	ARG	N-CA-C	-7.13	91.75	111.00
2	B	95	ARG	N-CA-C	-6.59	93.20	111.00
4	D	101	GLY	N-CA-C	6.21	128.63	113.10
2	B	95	ARG	C-N-CA	5.53	135.53	121.70

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	784	0	824	26	0
1	E	790	0	829	23	0
2	B	703	0	755	23	0
2	F	619	0	659	27	0
3	C	796	0	848	14	0
3	G	810	0	866	18	0
4	D	745	0	769	11	0
4	H	735	0	756	18	0
5	I	2878	0	1622	104	0
6	J	3061	0	1646	117	0
7	A	1	0	0	0	0
7	I	1	0	0	0	0
7	J	2	0	0	0	0
All	All	11925	0	9574	255	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 12.

All (255) 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:E:118:THR:HB	2:F:45:ARG:HB3	1.31	1.10
5:I:70:DG:H1	6:J:-70:DC:H42	1.01	0.98
5:I:-17:DT:H3	6:J:17:DA:N6	1.60	0.98
5:I:31:DT:H1'	5:I:32:DA:C8	2.00	0.95
4:H:92:GLN:HE21	4:H:96:ARG:HH12	1.10	0.95
1:A:118:THR:HB	2:B:45:ARG:HB3	1.45	0.95
5:I:-15:DA:H61	6:J:15:DT:H3	0.99	0.92
5:I:47:DC:N4	6:J:-47:DG:H1	1.66	0.92
5:I:-17:DT:H3	6:J:17:DA:H61	1.01	0.91
2:B:64:ASN:HD22	2:B:67:ARG:HH12	1.20	0.89
2:F:64:ASN:HD22	2:F:67:ARG:HH12	1.21	0.88
5:I:47:DC:H42	6:J:-47:DG:H1	0.89	0.87
1:E:118:THR:CB	2:F:45:ARG:HB3	2.03	0.87
3:G:55:LEU:O	3:G:59:THR:HG23	1.76	0.84
5:I:31:DT:H1'	5:I:32:DA:N7	1.92	0.84
5:I:-54:DC:N4	6:J:53:DA:N6	2.24	0.84
5:I:-66:DC:H42	6:J:65:DA:H61	1.23	0.83
1:E:118:THR:HB	2:F:45:ARG:CB	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB3	2:B:79:LYS:HZ3	1.44	0.82
3:G:42:ARG:HB2	4:H:85:THR:HG22	1.61	0.82
5:I:1:DT:H3	6:J:-1:DA:H61	1.28	0.82
1:A:65:LEU:HD23	6:J:17:DA:OP2	1.80	0.81
2:B:90:LEU:HB3	2:B:95:ARG:O	1.79	0.81
2:B:64:ASN:ND2	2:B:67:ARG:HH12	1.78	0.81
5:I:70:DG:N2	6:J:-70:DC:N3	2.29	0.81
5:I:61:DT:H1'	5:I:62:DA:C8	2.16	0.80
2:F:64:ASN:ND2	2:F:67:ARG:HH12	1.79	0.80
5:I:24:DC:N4	6:J:-25:DA:N6	2.29	0.80
5:I:46:DC:H42	6:J:-46:DG:H1	1.30	0.80
5:I:30:DC:H42	6:J:29:DA:N6	1.80	0.80
6:J:31:DG:H1'	6:J:32:DG:C8	2.17	0.80
2:B:64:ASN:HD22	2:B:67:ARG:NH1	1.78	0.80
2:F:64:ASN:HD22	2:F:67:ARG:NH1	1.79	0.79
2:F:90:LEU:HB3	2:F:95:ARG:O	1.82	0.79
5:I:-15:DA:N6	6:J:15:DT:H3	1.80	0.78
5:I:30:DC:N3	6:J:-30:DG:N2	2.32	0.77
5:I:24:DC:H42	6:J:-25:DA:N6	1.82	0.77
2:F:30:THR:HB	2:F:32:PRO:HD2	1.67	0.77
6:J:25:DG:H2''	6:J:26:DG:N7	2.01	0.76
5:I:-15:DA:N6	6:J:14:DG:N1	2.33	0.76
2:B:30:THR:HB	2:B:32:PRO:HD2	1.68	0.75
4:H:92:GLN:HE21	4:H:96:ARG:NH1	1.84	0.75
3:G:50:TYR:OH	4:H:92:GLN:HG3	1.86	0.75
5:I:30:DC:N4	6:J:-31:DA:H61	1.85	0.74
5:I:69:DA:H61	6:J:-69:DT:H3	1.37	0.73
4:H:45:VAL:HG12	4:H:46:HIS:ND1	2.02	0.73
5:I:-26:DC:N4	6:J:25:DG:N1	2.36	0.73
5:I:46:DC:N4	6:J:-46:DG:H1	1.85	0.73
3:C:38:ASN:HD22	4:H:79:HIS:CE1	2.07	0.72
1:A:81:ASP:HB3	2:B:79:LYS:NZ	2.05	0.72
5:I:-51:DA:H2	6:J:51:DT:H3	1.38	0.72
5:I:70:DG:H1	6:J:-70:DC:N4	1.83	0.72
1:E:118:THR:HG22	6:J:-3:DT:OP1	1.90	0.72
5:I:-30:DC:H42	6:J:29:DA:H61	1.38	0.72
5:I:0:DC:H42	6:J:0:DG:H1	1.35	0.71
1:E:63:ARG:HH11	1:E:63:ARG:H	1.39	0.71
5:I:-3:DA:N6	6:J:2:DG:N1	2.40	0.70
5:I:47:DC:N3	6:J:-47:DG:N2	2.33	0.70
5:I:-42:DC:H42	6:J:42:DG:H1	1.38	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:NH1	1:A:63:ARG:H	1.91	0.69
4:D:30:ARG:HA	6:J:50:DG:OP1	1.93	0.69
5:I:-67:DC:H42	6:J:67:DG:H1	1.41	0.68
6:J:-60:DG:H1'	6:J:-59:DG:C8	2.29	0.68
5:I:-53:DT:H1'	5:I:-52:DA:C8	2.28	0.68
1:A:118:THR:HG22	5:I:-3:DA:OP1	1.94	0.67
1:A:63:ARG:H	1:A:63:ARG:HH11	1.40	0.67
3:C:38:ASN:ND2	4:H:79:HIS:NE2	2.43	0.67
6:J:55:DG:H1'	6:J:56:DG:N7	2.08	0.67
1:E:42:ARG:NE	6:J:-5:DG:OP1	2.28	0.67
1:E:63:ARG:NH1	1:E:63:ARG:H	1.92	0.67
3:C:71:ARG:NH2	4:D:49:THR:OG1	2.29	0.66
6:J:31:DG:H1'	6:J:32:DG:H8	1.61	0.66
1:A:118:THR:CB	2:B:45:ARG:HB3	2.22	0.65
5:I:62:DA:H2	6:J:-62:DT:H3	1.42	0.65
5:I:-30:DC:N4	6:J:29:DA:H61	1.96	0.64
1:E:121:PRO:HB3	2:F:53:GLU:HG3	1.78	0.64
1:A:49:ARG:HD2	6:J:-66:DG:O3'	1.97	0.64
2:F:29:ILE:O	2:F:55:ARG:NH2	2.31	0.64
3:C:115:LEU:HD22	1:E:117:VAL:HG13	1.79	0.64
1:E:118:THR:CA	2:F:45:ARG:HB3	2.27	0.63
5:I:30:DC:N4	6:J:-31:DA:N6	2.47	0.62
3:G:83:LEU:O	3:G:87:ILE:HG12	2.00	0.61
3:C:83:LEU:O	3:C:87:ILE:HG12	2.00	0.61
5:I:-18:DC:N4	6:J:19:DG:H22	1.99	0.60
5:I:-16:DA:H2	6:J:17:DA:N1	2.00	0.60
2:B:61:PHE:HE2	2:B:95:ARG:HD3	1.67	0.59
1:E:68:GLN:HE21	1:E:72:ARG:HE	1.51	0.58
3:G:81:ARG:HD3	3:G:81:ARG:O	2.03	0.58
5:I:62:DA:N6	5:I:63:DA:N6	2.52	0.58
6:J:-24:DG:C2	6:J:-23:DG:C2	2.91	0.58
5:I:46:DC:N3	6:J:-46:DG:N2	2.50	0.57
6:J:-24:DG:H22	6:J:-23:DG:N2	2.01	0.57
5:I:-3:DA:N6	6:J:2:DG:H1	2.03	0.57
3:C:81:ARG:NH1	3:C:105:GLY:O	2.37	0.57
5:I:30:DC:N4	6:J:-30:DG:H1	2.02	0.57
5:I:57:DA:H61	6:J:-57:DT:H3	1.53	0.56
5:I:-66:DC:H42	6:J:65:DA:N6	2.00	0.56
1:A:99:TYR:HE1	1:A:131:ARG:HH12	1.53	0.56
6:J:-60:DG:H1'	6:J:-59:DG:H8	1.69	0.56
1:A:68:GLN:HE21	1:A:72:ARG:HE	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-20:DC:N4	5:I:-19:DC:N4	2.54	0.56
1:A:118:THR:HB	2:B:45:ARG:CB	2.28	0.55
1:E:99:TYR:HE1	1:E:131:ARG:HH12	1.55	0.55
5:I:-6:DC:H42	6:J:6:DG:H1	1.53	0.55
5:I:1:DT:H3	6:J:-1:DA:N6	2.02	0.55
5:I:-16:DA:C2	6:J:17:DA:N1	2.75	0.54
6:J:55:DG:H1'	6:J:56:DG:C8	2.42	0.54
5:I:54:DC:N4	6:J:-55:DA:N6	2.54	0.54
6:J:26:DG:H1'	6:J:27:DT:H5'	1.90	0.54
5:I:49:DT:N3	6:J:-48:DG:N2	2.55	0.54
6:J:-66:DG:N1	6:J:-65:DG:N2	2.55	0.54
5:I:-18:DC:C4	6:J:19:DG:N2	2.76	0.54
1:E:118:THR:HB	2:F:45:ARG:CG	2.37	0.54
5:I:7:DT:O2	5:I:8:DA:N7	2.40	0.54
5:I:-16:DA:H4'	5:I:-15:DA:H5'	1.90	0.53
6:J:-24:DG:N2	6:J:-23:DG:N2	2.55	0.53
2:B:68:ASP:OD2	2:B:93:GLN:NE2	2.41	0.53
3:G:31:HIS:CD2	3:G:35:ARG:HE	2.27	0.53
2:F:35:ARG:HG2	2:F:46:ILE:HD12	1.91	0.53
5:I:30:DC:H42	6:J:-30:DG:H1	1.56	0.53
3:C:39:TYR:HB3	4:D:75:SER:HB2	1.91	0.52
3:G:88:ARG:NH2	3:G:97:LEU:O	2.41	0.52
2:F:68:ASP:OD2	2:F:93:GLN:NE2	2.43	0.52
4:H:92:GLN:NE2	4:H:96:ARG:HH12	1.92	0.52
5:I:-26:DC:N4	6:J:25:DG:H1	2.06	0.52
5:I:69:DA:N6	6:J:-69:DT:H3	2.07	0.52
5:I:-54:DC:N4	6:J:53:DA:H61	2.06	0.52
3:G:102:ILE:HG23	4:H:58:ILE:HG12	1.91	0.52
6:J:20:DG:H2''	6:J:21:DT:H5''	1.91	0.52
5:I:-10:DA:C4	5:I:-9:DA:N7	2.78	0.51
6:J:-61:DA:C6	6:J:-60:DG:N2	2.79	0.51
3:C:102:ILE:HG23	4:D:58:ILE:HG12	1.93	0.51
5:I:66:DC:N3	6:J:-65:DG:N2	2.58	0.51
5:I:-15:DA:N6	6:J:14:DG:C6	2.79	0.51
1:A:72:ARG:HH22	5:I:-23:DT:P	2.33	0.51
2:B:75:HIS:O	4:D:89:ARG:NH1	2.42	0.51
5:I:-54:DC:H42	6:J:53:DA:N6	2.09	0.51
6:J:-66:DG:C2	6:J:-65:DG:N2	2.78	0.51
3:G:32:ARG:HH22	4:H:32:GLU:CD	2.13	0.51
4:H:45:VAL:CG1	4:H:46:HIS:ND1	2.73	0.51
2:B:79:LYS:HD2	6:J:27:DT:OP1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:-26:DC:N4	6:J:25:DG:C6	2.79	0.50
4:D:46:HIS:HB3	4:D:49:THR:HB	1.93	0.50
6:J:30:DG:N7	6:J:31:DG:C6	2.79	0.50
5:I:64:DC:C4	5:I:65:DC:N4	2.80	0.49
2:F:79:LYS:N	5:I:28:DC:OP1	2.42	0.49
5:I:66:DC:H42	6:J:-66:DG:H1	1.59	0.49
6:J:53:DA:H2''	6:J:54:DG:N7	2.27	0.49
6:J:14:DG:H2''	6:J:15:DT:H5'	1.93	0.49
6:J:71:DA:C4	6:J:72:DT:C7	2.96	0.49
1:E:61:LEU:HD12	2:F:37:LEU:HD23	1.94	0.49
6:J:-24:DG:N2	6:J:-23:DG:C2	2.80	0.49
5:I:-59:DT:H3	6:J:59:DA:H61	1.59	0.49
5:I:-67:DC:N4	6:J:67:DG:H22	2.10	0.49
2:B:18:HIS:C	2:B:18:HIS:CD2	2.85	0.49
1:A:85:GLN:HG2	5:I:-24:DC:OP1	2.12	0.49
5:I:61:DT:H1'	5:I:62:DA:N7	2.28	0.48
1:E:61:LEU:HG	2:F:40:ARG:HH21	1.78	0.48
5:I:-40:DA:H2	6:J:40:DT:H3	1.62	0.48
5:I:-54:DC:N4	6:J:53:DA:C6	2.81	0.48
3:G:77:ARG:NE	6:J:-54:DG:H4'	2.28	0.48
5:I:30:DC:H42	6:J:-31:DA:N6	2.11	0.48
5:I:10:DC:H42	6:J:-10:DG:H1	1.62	0.48
4:D:41:VAL:HA	4:D:44:GLN:HE21	1.78	0.47
4:H:30:ARG:HD2	5:I:49:DT:O3'	2.14	0.47
1:E:118:THR:HA	2:F:45:ARG:HB3	1.95	0.47
2:F:35:ARG:HG3	2:F:51:TYR:HE1	1.78	0.47
2:B:75:HIS:CD2	4:D:93:THR:OG1	2.67	0.47
1:A:72:ARG:NH2	5:I:-23:DT:OP2	2.48	0.47
5:I:25:DT:H3	6:J:-25:DA:H61	1.62	0.47
5:I:-56:DC:H2''	5:I:-55:DC:C5	2.49	0.47
3:G:76:THR:HG21	5:I:57:DA:H5''	1.96	0.47
6:J:-54:DG:H2''	6:J:-53:DG:C8	2.49	0.47
1:A:52:ARG:O	1:A:56:LYS:HB2	2.15	0.47
1:A:58:THR:HG21	3:G:81:ARG:HG2	1.97	0.47
2:B:31:LYS:N	2:B:32:PRO:HD2	2.28	0.47
5:I:53:DC:H42	6:J:-53:DG:H1	1.62	0.47
1:A:81:ASP:CB	2:B:79:LYS:NZ	2.76	0.47
1:A:93:GLN:O	1:A:97:GLU:HG3	2.15	0.46
5:I:62:DA:C6	5:I:63:DA:N6	2.83	0.46
5:I:23:DC:H42	6:J:-24:DG:H1	1.63	0.46
5:I:7:DT:C2	5:I:8:DA:N7	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:-60:DG:C4	6:J:-59:DG:N7	2.84	0.46
5:I:66:DC:N4	6:J:-66:DG:H1	2.14	0.46
4:D:73:GLU:O	4:D:77:LEU:HD13	2.16	0.46
1:A:46:VAL:HB	6:J:9:DT:P	2.56	0.46
3:C:78:ILE:HA	3:C:82:HIS:ND1	2.31	0.46
5:I:-16:DA:H2	6:J:17:DA:C2	2.34	0.45
5:I:62:DA:C6	5:I:63:DA:C6	3.03	0.45
5:I:0:DC:N4	6:J:0:DG:H1	2.07	0.45
5:I:-19:DC:H2'	5:I:-18:DC:C6	2.52	0.45
5:I:-67:DC:H42	6:J:67:DG:H22	1.64	0.45
2:B:30:THR:HG22	5:I:-12:DC:OP1	2.16	0.45
6:J:-30:DG:C2	6:J:-29:DG:C2	3.05	0.45
6:J:40:DT:C7	6:J:41:DA:N7	2.79	0.45
6:J:40:DT:H71	6:J:41:DA:H62	1.82	0.45
6:J:37:DG:H2''	6:J:38:DG:C8	2.50	0.45
3:G:78:ILE:HA	3:G:82:HIS:ND1	2.32	0.45
1:E:72:ARG:HH22	6:J:-23:DG:P	2.39	0.44
5:I:-70:DC:N4	5:I:-69:DA:N6	2.66	0.44
1:E:93:GLN:O	1:E:97:GLU:HG3	2.17	0.44
3:G:79:ILE:HG12	3:G:82:HIS:CE1	2.53	0.44
5:I:-6:DC:N4	6:J:6:DG:H1	2.15	0.44
1:A:58:THR:CG2	3:G:81:ARG:HG2	2.47	0.44
4:H:46:HIS:HB3	4:H:49:THR:HB	2.00	0.44
3:G:39:TYR:HB3	4:H:75:SER:HB2	1.99	0.44
3:C:32:ARG:HH11	3:C:36:LYS:NZ	2.16	0.44
3:C:38:ASN:ND2	4:H:79:HIS:CE1	2.78	0.44
1:A:48:LEU:O	1:A:52:ARG:HG3	2.18	0.44
2:F:31:LYS:N	2:F:32:PRO:HD2	2.33	0.43
5:I:8:DA:H2''	5:I:9:DA:C8	2.53	0.43
4:D:35:SER:HA	4:D:56:MET:HE1	2.00	0.43
5:I:-68:DC:H2''	5:I:-67:DC:H5''	2.00	0.43
6:J:71:DA:C4	6:J:72:DT:H73	2.54	0.43
3:G:90:ASP:HB3	3:G:93:LEU:HB2	2.01	0.43
6:J:18:DG:H2''	6:J:19:DG:C8	2.53	0.43
5:I:-42:DC:N3	6:J:42:DG:N2	2.56	0.43
6:J:40:DT:C5	6:J:41:DA:N7	2.87	0.43
6:J:67:DG:C2	6:J:68:DG:C2	3.07	0.43
5:I:49:DT:H3	6:J:-48:DG:N2	2.16	0.43
3:G:25:PHE:CZ	3:G:59:THR:HG21	2.54	0.42
1:A:133:GLU:O	1:A:134:ARG:O	2.37	0.42
1:A:88:ALA:HA	2:B:83:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:62:DA:N1	5:I:63:DA:C6	2.87	0.42
6:J:30:DG:C8	6:J:31:DG:C5	3.07	0.42
3:C:79:ILE:HG12	3:C:82:HIS:CE1	2.53	0.42
5:I:68:DA:C4	5:I:69:DA:N7	2.88	0.42
6:J:31:DG:C4	6:J:32:DG:N7	2.88	0.42
1:A:72:ARG:O	1:A:76:GLN:HB2	2.20	0.42
2:F:75:HIS:CD2	4:H:93:THR:OG1	2.73	0.42
6:J:71:DA:C4	6:J:72:DT:H71	2.54	0.42
1:E:118:THR:HA	2:F:45:ARG:O	2.19	0.42
2:F:75:HIS:O	4:H:89:ARG:NH1	2.47	0.42
2:F:75:HIS:HB2	4:H:93:THR:HG21	2.00	0.42
2:F:30:THR:CB	2:F:32:PRO:HD2	2.44	0.42
1:E:129:ARG:HE	1:E:134:ARG:HG2	1.84	0.42
5:I:31:DT:H1'	5:I:32:DA:H8	1.72	0.41
6:J:-24:DG:N1	6:J:-23:DG:C2	2.88	0.41
2:F:35:ARG:HG2	2:F:46:ILE:CD1	2.49	0.41
2:B:61:PHE:CE2	2:B:95:ARG:HD3	2.52	0.41
1:E:62:ILE:HG21	1:E:67:PHE:HD1	1.85	0.41
1:A:126:LEU:HD22	1:E:113:HIS:CG	2.56	0.41
2:B:32:PRO:O	2:B:36:ARG:HG3	2.21	0.41
1:E:48:LEU:O	1:E:52:ARG:HG3	2.20	0.41
5:I:31:DT:C1'	5:I:32:DA:N7	2.75	0.41
5:I:31:DT:C2	5:I:32:DA:N7	2.88	0.41
5:I:-20:DC:C4	5:I:-19:DC:C4	3.08	0.41
3:C:84:GLN:NE2	3:C:88:ARG:HG3	2.35	0.40
3:C:50:TYR:CE2	4:D:92:GLN:HG2	2.55	0.40
2:F:32:PRO:O	2:F:36:ARG:HG3	2.20	0.40
6:J:-30:DG:N1	6:J:-29:DG:C2	2.89	0.40
5:I:-63:DA:N6	6:J:62:DG:N1	2.70	0.40
6:J:69:DT:H2'	6:J:69:DT:H6	1.73	0.40
2:B:30:THR:CB	2:B:32:PRO:HD2	2.46	0.40
6:J:-40:DG:C2	6:J:-39:DT:C2	3.09	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	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
1	E	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
2	B	85/87 (98%)	81 (95%)	4 (5%)	0	100	100
2	F	76/87 (87%)	74 (97%)	2 (3%)	0	100	100
3	C	101/105 (96%)	98 (97%)	3 (3%)	0	100	100
3	G	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
4	D	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
4	H	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
All	All	737/766 (96%)	709 (96%)	28 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	83/83 (100%)	76 (92%)	7 (8%)	11	21
1	E	83/83 (100%)	77 (93%)	6 (7%)	14	29
2	B	72/72 (100%)	66 (92%)	6 (8%)	11	22
2	F	63/72 (88%)	60 (95%)	3 (5%)	25	49
3	C	82/83 (99%)	74 (90%)	8 (10%)	8	15
3	G	83/83 (100%)	77 (93%)	6 (7%)	14	29
4	D	81/81 (100%)	73 (90%)	8 (10%)	8	15
4	H	80/81 (99%)	74 (92%)	6 (8%)	13	27
All	All	627/638 (98%)	577 (92%)	50 (8%)	12	24

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	59	GLU
1	A	63	ARG
1	A	81	ASP
1	A	115	LYS
1	A	129	ARG
1	A	134	ARG
2	B	16	LYS
2	B	17	ARG
2	B	35	ARG
2	B	91	LYS
2	B	92	ARG
2	B	95	ARG
3	C	20	ARG
3	C	36	LYS
3	C	42	ARG
3	C	59	THR
3	C	71	ARG
3	C	81	ARG
3	C	95	LYS
3	C	99	ARG
4	D	28	ARG
4	D	37	TYR
4	D	39	TYR
4	D	68	GLU
4	D	89	ARG
4	D	92	GLN
4	D	93	THR
4	D	110	GLU
1	E	40	ARG
1	E	57	SER
1	E	59	GLU
1	E	63	ARG
1	E	81	ASP
1	E	86	SER
2	F	31	LYS
2	F	92	ARG
2	F	95	ARG
3	G	32	ARG
3	G	42	ARG
3	G	59	THR
3	G	81	ARG
3	G	84	GLN

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Mol	Chain	Res	Type
3	G	99	ARG
4	H	28	ARG
4	H	37	TYR
4	H	39	TYR
4	H	83	ARG
4	H	89	ARG
4	H	93	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
2	B	18	HIS
2	B	64	ASN
2	B	75	HIS
3	C	38	ASN
3	C	104	GLN
4	D	44	GLN
4	D	79	HIS
4	D	81	ASN
4	D	92	GLN
1	E	68	GLN
2	F	64	ASN
2	F	75	HIS
3	G	84	GLN
4	H	81	ASN
4	H	92	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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	95/96 (98%)	0.03	0 100 100	17, 39, 74, 96	0
1	E	96/96 (100%)	0.37	2 (2%) 63 58	42, 67, 103, 118	0
2	B	87/87 (100%)	-0.03	0 100 100	15, 33, 61, 86	0
2	F	78/87 (89%)	0.22	1 (1%) 77 73	32, 52, 82, 87	0
3	C	103/105 (98%)	0.14	1 (0%) 82 80	32, 58, 87, 94	0
3	G	105/105 (100%)	-0.05	4 (3%) 40 33	16, 35, 69, 99	0
4	D	95/95 (100%)	0.15	2 (2%) 63 58	25, 49, 87, 102	0
4	H	94/95 (98%)	-0.08	1 (1%) 80 78	14, 36, 66, 95	0
5	I	145/145 (100%)	0.35	4 (2%) 53 46	78, 142, 188, 200	0
6	J	145/145 (100%)	0.52	8 (5%) 25 19	85, 151, 194, 201	0
All	All	1043/1056 (98%)	0.19	23 (2%) 62 56	14, 58, 174, 201	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	14	ALA	5.6
3	G	116	LEU	3.9
5	I	72	DT	3.9
3	C	117	PRO	3.0
6	J	-72	DA	2.9
6	J	-19	DA	2.9
6	J	0	DG	2.9
4	D	28	ARG	2.9
6	J	72	DT	2.8
3	G	117	PRO	2.7
6	J	-20	DT	2.7
6	J	-18	DG	2.5
3	G	118	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	118	TYR	2.2
6	J	-69	DT	2.2
1	E	41	TYR	2.2
6	J	62	DG	2.1
5	I	21	DA	2.1
5	I	11	DC	2.1
4	D	39	TYR	2.1
2	F	94	GLY	2.1
5	I	51	DA	2.1
1	E	67	PHE	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](#)

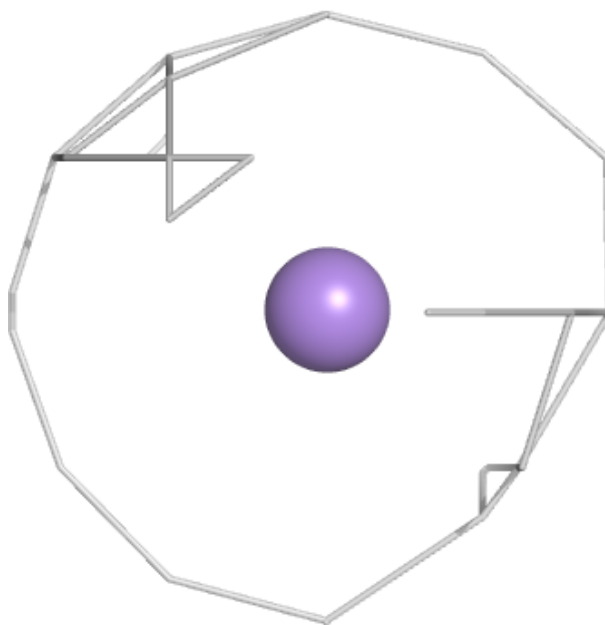
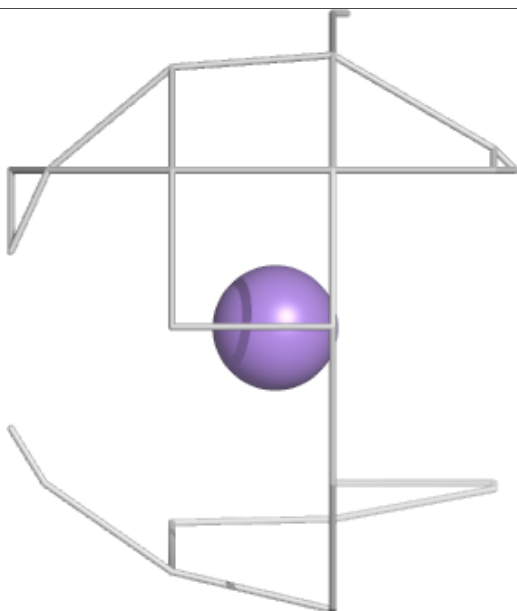
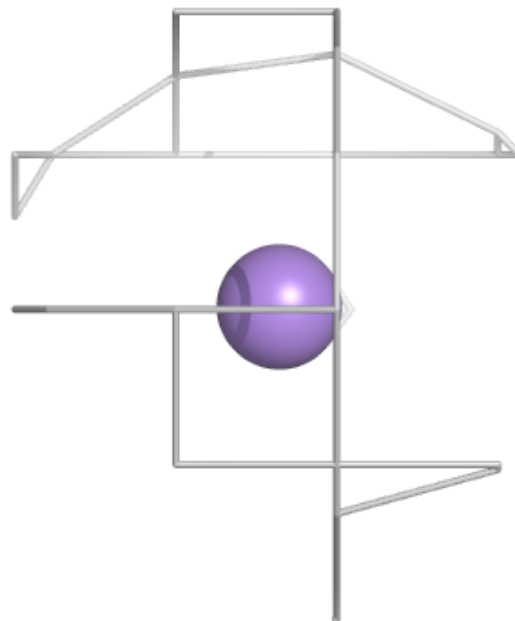
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MN	I	101	1/1	0.74	0.08	129,129,129,129	0
7	MN	J	101	1/1	0.76	0.13	140,140,140,140	0
7	MN	J	102	1/1	0.97	0.12	144,144,144,144	0
7	MN	A	201	1/1	0.99	0.21	42,42,42,42	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.

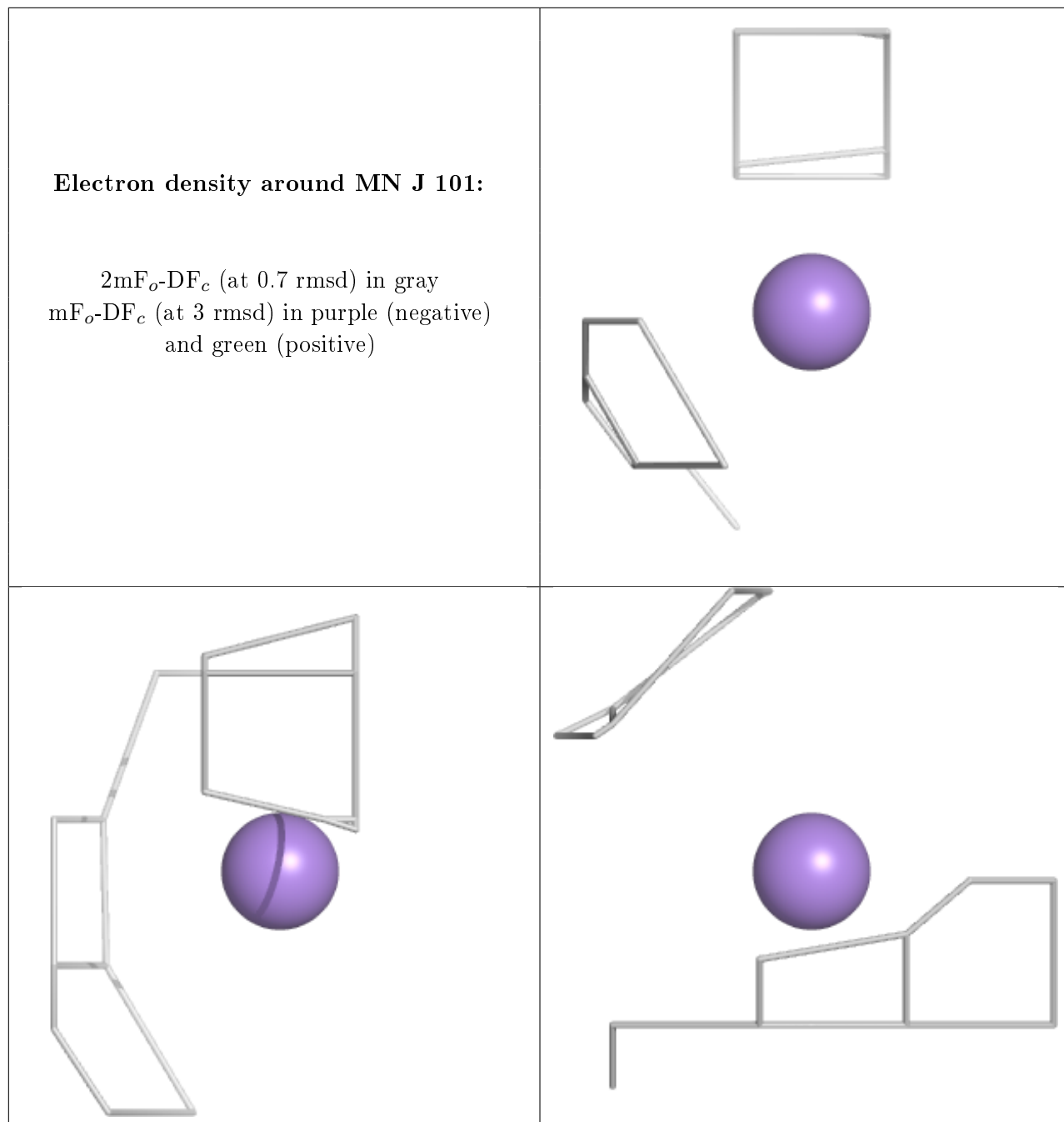
Electron density around MN I 101:

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



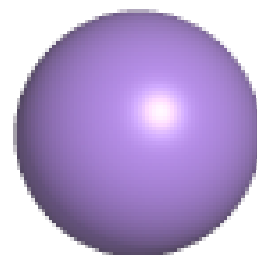
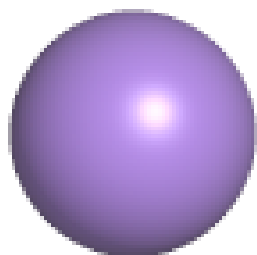
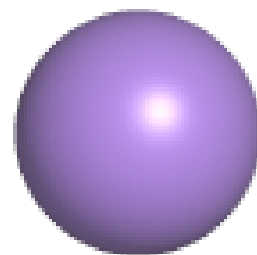
Electron density around MN J 101:

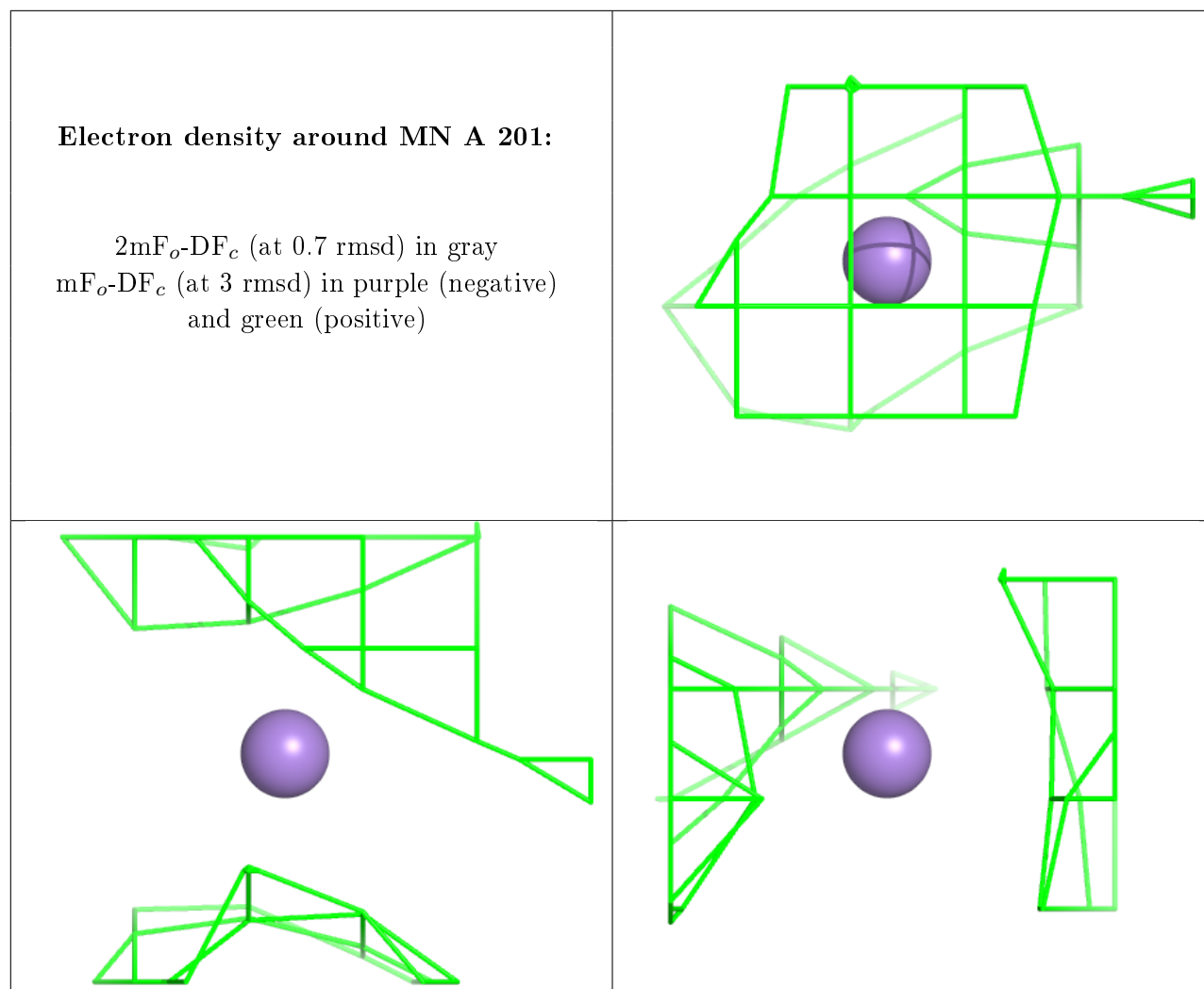
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN J 102:

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.