



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:02 pm BST

PDB ID : 5W4U
Title : Pol II elongation complex with an N6-methyladenine-containing template
Authors : Wang, W.; Wang, D.
Deposited on : 2017-06-13
Resolution : 3.60 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

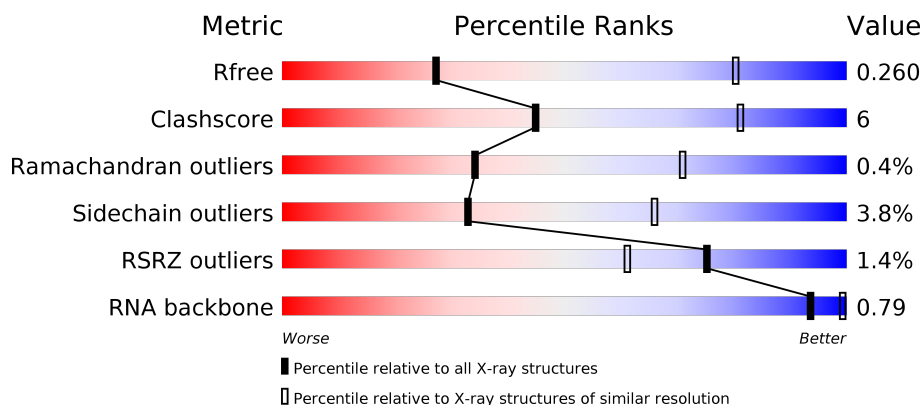
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

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	1733	<div> <div>8%</div> <div>63% 15% • 21%</div> </div>
2	B	1224	<div> <div>70% 18% • 11%</div> </div>
3	C	318	<div> <div>68% 14% • 16%</div> </div>
4	E	215	<div> <div>8%</div> <div>87% 12% •</div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<p>%</p> <p>43% 10% 46%</p>
6	H	146	<p>6%</p> <p>69% 18% 11%</p>
7	I	122	<p>80% 14% 6%</p>
8	J	70	<p>76% 16% 7%</p>
9	K	120	<p>76% 18% 5%</p>
10	L	70	<p>6%</p> <p>51% 11% 37%</p>
11	T	29	<p>3%</p> <p>72% 28%</p>
12	N	14	<p>14%</p> <p>43% 57%</p>
13	R	9	<p>44% 56%</p>

2 Entry composition [i](#)

There are 15 unique types of molecules in this entry. The entry contains 28821 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1371	Total	C	N	O	S	0	0	0
			10787	6806	1886	2034	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1089	Total	C	N	O	S	0	0	0
			8657	5485	1517	1601	54			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	213	Total	C	N	O	S	0	0	0
			1744	1107	308	318	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	130	Total	C	N	O	S	0	0	0
			1043	660	173	206	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	115	Total	C	N	O	S	0	0	0
			935	575	170	180	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called 29mer template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	29	Total	C	N	O	P	0	0	0
			588	283	107	170	28			

- Molecule 12 is a DNA chain called 14mer non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 13 is a RNA chain called 9mer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			198	89	42	59	8			

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total 1	Zn 1	0	0
14	B	1	Total 1	Zn 1	0	0
14	I	2	Total 2	Zn 2	0	0
14	C	1	Total 1	Zn 1	0	0
14	A	2	Total 2	Zn 2	0	0
14	L	1	Total 1	Zn 1	0	0

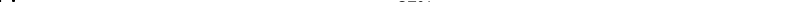
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total 1	Mg 1	0	0

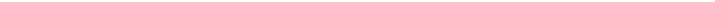
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

- [illegible]

[illegible]

- Chain E: 

Category	Item	Value	Color
Left Column	V142	100	Blue
	H146	100	Blue
	L165	100	Blue
	R169	100	Blue
	L170	100	Blue
	I178	100	Blue
	I198	100	Blue
	K201	100	Blue
	R212	100	Blue
	K215	100	Blue
Right Column	ASP	100	Blue
	Q3	100	Blue
	E4	100	Blue
	R7	100	Blue
	I8	100	Blue
	R19	100	Blue
	L12	100	Blue
	K20	100	Blue
	E34	100	Blue
	R52	100	Blue
	M58	100	Blue
	T65	100	Blue
	I69	100	Blue
	W79	100	Blue
	F82	100	Blue
	C83	100	Blue
	D84	100	Blue
	P85	100	Blue
	P86	100	Blue
	M93	100	Blue
K94	100	Blue	
T95	100	Blue	
F96	100	Blue	
U97	100	Blue	
I98	100	Blue	
H99	100	Blue	
I100	100	Blue	
Q101	100	Blue	
E102	100	Blue	
F105	100	Blue	
Q106	100	Blue	
I109	100	Blue	
F110	100	Blue	
V111	100	Blue	
L123	100	Blue	
S126	100	Blue	
I127	100	Blue	
I132	100	Blue	
F135	100	Blue	
L140	100	Blue	
W141	100	Blue	

- Chain F:  %

HIS	GLU	GLN	ILE	ARG	LYS	THR	LEU	LEU	GLU	K72	K76	R79	T81	T82	P83	Y84	Y88	I93	R97	Q100	V107	F108	V109	I130	P131	I134	P139	W146	L155																		
Met	Ser	Asp	Tyr	GLU	GLU	PHE	ASN	ASP	GLY	ASN	GLU	ASN	PHE	ASP	VAL	GLU	HIS	PHE	SER	ASP	GLU	GLU	LYS	PRO	GLN	PHE	LYS	ASP	ALA	ASN	GLY	LYS	THR	THR	ILE	VAL	THR	GLY	GLY	ASN	GLY	PRO	GLU	ASP	PHE	GLN	GLN


- Chain H: 

A horizontal bar chart showing the distribution of amino acid types across 1000 random sequences. The chart is divided into two main sections: 'Amino acid types' on the left and 'Amino acid types' on the right. The left section lists amino acids from N134 to R146, and the right section lists amino acids from MET to Y129. Each bar is color-coded by type: MET, SER, and H3 are grey; F6, D8, and I19 are yellow; E14 and G18 are green; E27 and V44 are yellow; P48 and I59 are green; L63 and ASN are green; LEU, GLU, ASP, THR, PRO, ALA, ASN, ASP, SER, and SER are grey; T76, R77, W79, R80, P81, P82, Q83, R84, G85, and D86 are green; L89, A90, D91, D92, and Y93 are yellow; R123 and R124 are green; Y129 is yellow; ARG and ASN are grey; I132 and H132 are yellow; and H132 is green. The chart shows that the distribution of amino acid types is highly variable across the 1000 random sequences.

- Chain I: 80% 14% • 6%


[illegible]

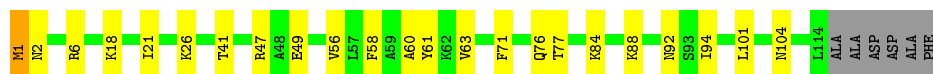
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Chain J:  76% 16% 7%



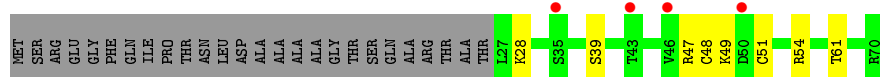
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:  76% 18% 5%



- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:  6% 51% 11% 37%




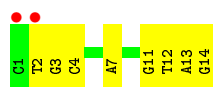
- Molecule 11: 29mer template DNA

Chain T:  3% 72% 28%



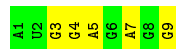
- Molecule 12: 14mer non-template DNA

Chain N:  14% 43% 57%



- Molecule 13: 9mer RNA

Chain R:  44% 56%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.21Å 221.99Å 192.70Å 90.00° 100.58° 90.00°	Depositor
Resolution (Å)	81.02 – 3.60 95.77 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.4 (81.02-3.60) 89.4 (95.77-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.227 , 0.259 0.229 , 0.260	Depositor DCC
R_{free} test set	3546 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	28821	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 6MA

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	0.21	0/10979	0.37	0/14843
2	B	0.21	0/8824	0.37	0/11898
3	C	0.20	0/2133	0.37	0/2891
4	E	0.21	0/1780	0.36	0/2395
5	F	0.20	0/691	0.38	0/933
6	H	0.21	0/1060	0.39	1/1434 (0.1%)
7	I	0.21	0/953	0.35	0/1284
8	J	0.21	0/541	0.35	0/727
9	K	0.21	0/937	0.35	0/1265
10	L	0.20	0/353	0.35	0/468
11	T	0.47	0/580	0.85	0/884
12	N	0.44	0/317	0.91	0/488
13	R	0.13	0/223	0.59	0/348
All	All	0.22	0/29371	0.40	1/39858 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	H	89	LEU	CA-CB-CG	5.36	127.64	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10787	0	10874	157	0
2	B	8657	0	8693	137	0
3	C	2095	0	2051	31	0
4	E	1744	0	1772	15	0
5	F	679	0	701	10	0
6	H	1043	0	1015	14	0
7	I	935	0	887	12	0
8	J	532	0	542	9	0
9	K	919	0	929	14	0
10	L	351	0	375	5	0
11	T	588	0	333	7	0
12	N	284	0	161	5	0
13	R	198	0	99	3	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	28821	0	28432	368	0

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

All (368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.65	0.79
1:A:1239:ARG:HH22	1:A:1241:ARG:HH21	1.31	0.78
1:A:42:ASP:HB3	1:A:46:THR:H	1.47	0.78
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.69	0.72
8:J:5:VAL:HG22	8:J:6:ARG:HG3	1.72	0.72
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.71	0.72
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.57	0.70
3:C:48:SER:HB3	3:C:158:VAL:HB	1.75	0.69
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.74	0.69
2:B:287:ARG:NH1	2:B:324:ILE:O	2.27	0.68
7:I:92:ARG:HB3	7:I:95:THR:HG23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.76	0.67
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.77	0.66
1:A:35:ILE:HG13	1:A:241:VAL:HG21	1.77	0.66
3:C:41:ILE:HB	3:C:172:PRO:HG3	1.77	0.66
2:B:1129:ARG:NH1	11:T:21:DC:OP1	2.29	0.66
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.78	0.66
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.29	0.66
10:L:48:CYS:SG	10:L:49:LYS:N	2.70	0.65
3:C:6:PRO:HB2	9:K:101:LEU:HD23	1.77	0.65
1:A:666:ILE:HG23	2:B:1026:LEU:HB2	1.78	0.64
7:I:101:PHE:HE1	7:I:112:SER:HB3	1.61	0.64
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.79	0.64
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.29	0.64
1:A:338:GLY:HA2	2:B:1129:ARG:HH21	1.61	0.63
1:A:40:THR:HB	1:A:41:MET:HA	1.80	0.63
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.63	0.63
2:B:642:ASP:HB3	2:B:649:LYS:HG2	1.81	0.62
4:E:178:ILE:HB	4:E:212:ARG:HD3	1.81	0.62
1:A:601:LYS:HB2	1:A:603:ASN:HD22	1.64	0.62
2:B:468:GLU:HA	2:B:470:LYS:H	1.63	0.62
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.28	0.62
2:B:857:ARG:NH2	11:T:25:DC:OP1	2.32	0.62
2:B:487:THR:OG1	2:B:777:ALA:O	2.17	0.62
1:A:67:CYS:H	1:A:71:GLN:HA	1.63	0.62
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.32	0.62
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	1.81	0.62
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.82	0.61
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.33	0.61
2:B:1174:LYS:HB2	2:B:1179:GLN:HB2	1.83	0.60
1:A:49:LYS:HB2	1:A:56:PRO:HD3	1.83	0.60
2:B:60:GLN:NE2	2:B:64:CYS:SG	2.74	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.82	0.60
1:A:1281:ARG:HG2	1:A:1309:ASP:HB2	1.84	0.60
1:A:760:GLN:HG2	1:A:765:VAL:HA	1.83	0.60
2:B:400:HIS:NE2	2:B:699:GLU:OE1	2.32	0.59
5:F:82:THR:HG22	5:F:84:TYR:H	1.67	0.59
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.84	0.59
4:E:4:GLU:OE1	4:E:7:ARG:NH2	2.35	0.59
2:B:810:GLU:OE1	2:B:815:ARG:NH2	2.35	0.59
1:A:134:ARG:NH1	1:A:220:THR:O	2.35	0.59
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:ARG:NH1	2:B:321:GLY:O	2.36	0.59
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.85	0.59
1:A:993:LEU:HD22	1:A:1046:LEU:HG	1.84	0.58
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.68	0.58
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.85	0.58
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.68	0.58
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.68	0.58
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.85	0.58
6:H:129:TYR:O	6:H:132:LEU:N	2.36	0.58
2:B:63:ILE:O	2:B:67:SER:OG	2.18	0.58
2:B:118:ARG:NH2	2:B:194:GLU:OE1	2.33	0.58
1:A:365:GLY:HA3	1:A:469:ARG:HB2	1.85	0.58
8:J:14:VAL:HB	8:J:50:ILE:HD11	1.86	0.57
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.38	0.57
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.85	0.57
1:A:562:THR:O	1:A:576:GLN:NE2	2.38	0.57
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.86	0.57
2:B:995:ARG:NH1	2:B:997:GLU:OE1	2.37	0.57
3:C:46:ILE:HB	3:C:68:GLY:HA2	1.86	0.57
3:C:46:ILE:HD13	3:C:159:ALA:HB2	1.87	0.57
1:A:1155:ASP:OD2	1:A:1241:ARG:NH2	2.38	0.57
1:A:378:GLU:OE2	1:A:384:ASN:ND2	2.37	0.57
2:B:165:VAL:HG21	2:B:448:ILE:HD12	1.87	0.57
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.86	0.56
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.85	0.56
3:C:69:LEU:HD12	8:J:6:ARG:HD3	1.88	0.56
2:B:902:GLY:HA3	10:L:61:THR:HG22	1.85	0.56
6:H:137:GLN:HG3	6:H:139:ASN:H	1.71	0.56
2:B:357:GLN:NE2	2:B:371:GLU:OE1	2.38	0.56
9:K:88:LYS:O	9:K:92:ASN:ND2	2.35	0.55
2:B:496:ARG:NH2	2:B:540:SER:O	2.33	0.55
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.39	0.55
2:B:916:THR:HG23	2:B:935:ARG:HB2	1.89	0.55
7:I:32:CYS:SG	7:I:33:SER:N	2.80	0.55
5:F:76:LYS:O	5:F:79:ARG:NH1	2.37	0.55
1:A:1120:LEU:HD21	1:A:1131:ALA:HB2	1.89	0.55
3:C:163:ILE:HG22	3:C:165:LYS:H	1.72	0.55
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.89	0.54
12:N:3:DG:H2"	12:N:4:DC:H5"	1.88	0.54
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.89	0.54
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.89	0.54
1:A:1325:THR:OG1	4:E:146:HIS:O	2.26	0.54
1:A:881:GLN:NE2	1:A:958:VAL:O	2.36	0.53
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.53
6:H:89:LEU:HD13	6:H:89:LEU:H	1.74	0.53
2:B:301:ILE:HG13	2:B:379:GLY:HA2	1.90	0.53
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.89	0.53
1:A:1438:THR:HA	5:F:88:TYR:HB3	1.91	0.53
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	1.90	0.53
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.91	0.53
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.90	0.53
1:A:636:GLU:OE1	1:A:966:ASN:ND2	2.41	0.53
1:A:4:GLN:NE2	1:A:76:GLU:OE1	2.41	0.53
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.74	0.53
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.90	0.53
1:A:997:LEU:O	1:A:1011:GLN:NE2	2.42	0.53
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.90	0.52
1:A:39:GLU:HB3	1:A:41:MET:HB2	1.90	0.52
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.92	0.52
1:A:826:ASP:O	1:A:830:LYS:HB2	2.09	0.52
1:A:1116:LEU:HD23	1:A:1311:VAL:HA	1.91	0.52
1:A:34:LYS:H	1:A:34:LYS:HD3	1.75	0.52
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.92	0.52
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.91	0.51
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.91	0.51
3:C:11:ARG:NH2	3:C:19:ASP:OD1	2.44	0.51
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.91	0.51
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.92	0.51
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.93	0.51
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.91	0.51
6:H:6:PHE:HB3	6:H:59:ILE:HB	1.93	0.51
1:A:1276:VAL:HG11	1:A:1316:VAL:HG22	1.93	0.51
1:A:1281:ARG:NE	1:A:1309:ASP:OD2	2.43	0.51
1:A:302:THR:OG1	1:A:306:ASN:OD1	2.28	0.51
1:A:840:ARG:NH2	1:A:1106:ASN:OD1	2.41	0.51
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.43	0.51
3:C:99:LEU:HB3	3:C:120:ILE:HD13	1.93	0.51
11:T:7:6MA:H61	12:N:7:DA:N6	2.09	0.51
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.93	0.51
3:C:46:ILE:HD12	3:C:157:CYS:HB3	1.91	0.51
1:A:1423:GLY:O	1:A:1427:ASN:ND2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HB3	1:A:289:ILE:HG22	1.91	0.50
8:J:10:CYS:SG	8:J:11:GLY:N	2.84	0.50
2:B:1097:HIS:HB3	2:B:1102:LYS:HZ1	1.76	0.50
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.76	0.50
8:J:64:ASN:N	8:J:65:PRO:HD2	2.27	0.50
1:A:396:PRO:HG3	1:A:416:ARG:HB3	1.93	0.50
1:A:475:THR:OG1	1:A:480:ALA:O	2.29	0.50
2:B:103:ASN:OD1	2:B:169:ARG:NH2	2.38	0.50
2:B:294:ASP:HB2	7:I:12:ASN:HA	1.93	0.50
3:C:54:ASN:ND2	3:C:60:ASP:OD1	2.36	0.50
2:B:193:LYS:HE2	8:J:65:PRO:HG3	1.94	0.50
1:A:1364:ASN:OD1	1:A:1366:ARG:NH1	2.45	0.50
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.45	0.50
2:B:468:GLU:HG3	2:B:469:GLN:HA	1.93	0.50
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.94	0.50
2:B:680:THR:O	2:B:683:SER:OG	2.25	0.50
1:A:1424:VAL:HG22	1:A:1436:ILE:HG21	1.94	0.49
6:H:91:ASP:OD1	6:H:92:ASP:N	2.45	0.49
6:H:8:ASP:OD1	6:H:9:ILE:N	2.44	0.49
1:A:446:ARG:HB2	1:A:487:MET:HG2	1.94	0.49
1:A:707:GLY:O	1:A:1281:ARG:NH1	2.42	0.49
11:T:7:6MA:H2'	11:T:8:DT:H5'	1.95	0.49
3:C:75:MET:O	3:C:246:ARG:NH2	2.46	0.49
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.94	0.49
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.94	0.49
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.94	0.49
1:A:42:ASP:H	1:A:43:GLU:HA	1.78	0.48
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.95	0.48
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.94	0.48
7:I:14:LEU:HD13	7:I:27:PHE:HB3	1.95	0.48
1:A:38:PRO:HA	1:A:270:LEU:HD13	1.95	0.48
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.94	0.48
5:F:107:VAL:HG12	5:F:109:VAL:H	1.78	0.48
2:B:776:GLN:NE2	13:R:7:A:O3'	2.46	0.48
2:B:1001:PHE:HE2	3:C:178:PHE:HB3	1.79	0.48
10:L:28:LYS:HA	10:L:39:SER:HA	1.96	0.48
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.96	0.48
10:L:47:ARG:HG2	10:L:54:ARG:HG2	1.95	0.48
1:A:453:MET:HB3	1:A:477:PRO:HB2	1.96	0.48
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.95	0.48
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:487:THR:HG22	2:B:489:SER:H	1.79	0.48
1:A:1187:GLN:HG3	1:A:1188:GLN:HG3	1.96	0.48
1:A:1286:LYS:HE2	1:A:1302:PRO:HB2	1.95	0.48
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.95	0.48
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.95	0.47
9:K:1:MET:SD	9:K:2:ASN:ND2	2.86	0.47
9:K:63:VAL:HG22	9:K:71:PHE:HB3	1.95	0.47
1:A:1064:VAL:HA	1:A:1067:LEU:HB3	1.96	0.47
2:B:761:HIS:HB2	2:B:1024:ALA:HB2	1.96	0.47
2:B:620:ARG:NH2	7:I:89:GLN:OE1	2.46	0.47
2:B:1082:MET:HA	3:C:189:THR:HA	1.97	0.47
1:A:208:LEU:HD23	1:A:235:ILE:HD13	1.97	0.47
2:B:95:ILE:HD11	2:B:128:LEU:HB3	1.96	0.47
2:B:759:PRO:HD2	2:B:1046:PRO:HA	1.95	0.47
1:A:35:ILE:HG23	1:A:52:GLY:HA3	1.97	0.47
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.96	0.47
9:K:58:PHE:HB3	9:K:76:GLN:HB3	1.95	0.47
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.50	0.47
1:A:419:LYS:HG3	1:A:420:ARG:HG3	1.96	0.47
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.97	0.47
11:T:19:6MA:H2"	11:T:20:DC:C6	2.49	0.47
1:A:226:GLU:HG3	1:A:227:VAL:HG13	1.97	0.47
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.96	0.47
2:B:843:GLN:HB2	2:B:993:THR:HB	1.96	0.47
2:B:394:ASP:H	7:I:91:ARG:HG3	1.80	0.47
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.96	0.46
1:A:701:LEU:HA	7:I:115:LYS:HE3	1.97	0.46
1:A:1373:ASP:HA	1:A:1376:THR:HG22	1.96	0.46
1:A:72:GLU:OE2	2:B:1176:ASN:ND2	2.47	0.46
1:A:962:ARG:O	1:A:966:ASN:HB2	2.15	0.46
2:B:987:LYS:H	2:B:987:LYS:HD3	1.79	0.46
1:A:107:CYS:SG	1:A:108:MET:N	2.89	0.46
1:A:1148:ILE:HD13	7:I:49:ILE:HD12	1.97	0.46
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.79	0.46
1:A:1227:ILE:HD12	1:A:1239:ARG:HH11	1.80	0.46
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.97	0.46
1:A:1279:ILE:HA	1:A:1310:GLY:HA3	1.97	0.46
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.96	0.46
3:C:77:ILE:HG12	3:C:129:ILE:HD11	1.96	0.46
1:A:206:GLU:O	1:A:210:ILE:HG12	2.16	0.46
1:A:854:ASN:HB2	1:A:1000:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1106:ARG:HH11	2:B:1126:GLY:HA2	1.81	0.46
4:E:79:TRP:HB2	4:E:105:PHE:HD2	1.80	0.46
4:E:12:LEU:HD21	4:E:58:MET:HE1	1.98	0.46
1:A:544:ASP:OD1	1:A:545:GLN:N	2.44	0.46
9:K:21:ILE:HD13	9:K:84:LYS:HE2	1.97	0.46
2:B:170:LEU:HD12	2:B:171:PRO:HD2	1.97	0.46
2:B:468:GLU:CG	2:B:469:GLN:HA	2.46	0.46
1:A:423:ASP:N	1:A:423:ASP:OD1	2.48	0.46
2:B:806:THR:HG22	2:B:808:ALA:H	1.81	0.46
3:C:6:PRO:HB3	3:C:25:VAL:HG13	1.97	0.45
1:A:1261:LYS:HB2	1:A:1261:LYS:HE3	1.84	0.45
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.31	0.45
1:A:663:SER:OG	1:A:664:THR:N	2.47	0.45
1:A:491:VAL:O	2:B:1150:ARG:NH2	2.49	0.45
6:H:83:GLN:HB3	6:H:86:ASP:HB3	1.98	0.45
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.97	0.45
1:A:783:THR:HG21	1:A:796:SER:O	2.16	0.45
11:T:26:DC:H42	13:R:3:G:H1	1.62	0.45
2:B:210:LYS:HE3	2:B:462:ALA:HA	1.99	0.45
4:E:20:LYS:NZ	4:E:34:GLU:O	2.45	0.45
1:A:68:GLN:HA	1:A:69:THR:HA	1.46	0.45
1:A:774:ARG:HG3	1:A:797:LYS:HZ2	1.82	0.45
1:A:1342:GLU:HG3	4:E:198:ILE:HG21	1.97	0.45
3:C:3:GLU:N	9:K:104:ASN:HD21	2.15	0.45
1:A:1064:VAL:HG23	1:A:1067:LEU:HD23	1.99	0.45
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.99	0.45
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.99	0.45
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.17	0.45
1:A:1163:ILE:HG22	1:A:1165:GLU:H	1.82	0.45
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.98	0.45
1:A:282:ASN:OD1	1:A:283:GLY:N	2.42	0.45
1:A:51:GLY:HA2	1:A:52:GLY:HA2	1.52	0.45
2:B:1013:ASN:OD1	2:B:1015:HIS:ND1	2.33	0.45
6:H:76:THR:OG1	6:H:77:ARG:N	2.50	0.45
2:B:307:ASP:OD1	2:B:392:ARG:NH1	2.44	0.44
1:A:901:LEU:HB2	1:A:926:GLN:HG2	2.00	0.44
1:A:977:LYS:HG3	1:A:978:PRO:HD2	1.99	0.44
1:A:12:ARG:HH11	2:B:1192:TYR:HE1	1.65	0.44
2:B:1067:ARG:NE	3:C:194:GLU:OE1	2.49	0.44
1:A:54:ASN:HD21	1:A:244:PRO:HB3	1.83	0.44
2:B:227:LYS:HG2	2:B:236:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:93:TYR:CD1	6:H:145:ARG:HB3	2.53	0.44
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.18	0.44
1:A:546:VAL:HG22	1:A:577:ILE:HG21	2.00	0.44
2:B:898:LEU:HD11	2:B:964:VAL:HG21	2.00	0.44
9:K:47:ARG:HD3	9:K:61:TYR:HD1	1.83	0.44
1:A:631:HIS:CE1	1:A:879:GLU:HG2	2.53	0.43
2:B:428:ILE:HD11	2:B:448:ILE:HG23	2.00	0.43
1:A:1261:LYS:O	1:A:1264:GLU:HG3	2.19	0.43
4:E:135:PHE:HB3	4:E:140:LEU:HD11	2.00	0.43
9:K:56:VAL:HG22	9:K:77:THR:HG22	2.00	0.43
1:A:1395:GLY:HA3	1:A:1426:GLU:OE2	2.18	0.43
1:A:1148:ILE:N	1:A:1196:GLU:O	2.51	0.43
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.00	0.43
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.54	0.43
1:A:834:THR:HG21	1:A:1077:THR:HA	1.99	0.43
2:B:274:PRO:HG2	2:B:359:GLU:HB3	2.01	0.43
2:B:899:ILE:HG21	2:B:949:VAL:HG21	2.00	0.43
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.46	0.43
1:A:531:ILE:HG21	1:A:622:VAL:HG11	2.01	0.43
2:B:796:LEU:HB3	2:B:799:PRO:HG3	2.01	0.43
2:B:726:ALA:HB1	2:B:1051:THR:HG21	2.01	0.42
2:B:916:THR:HA	2:B:917:PRO:HD3	1.86	0.42
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.91	0.42
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.94	0.42
2:B:1074:ASN:HB2	2:B:1081:LEU:HD21	2.01	0.42
2:B:166:PHE:HZ	2:B:169:ARG:HG3	1.84	0.42
2:B:28:GLU:OE1	2:B:807:ARG:NH1	2.49	0.42
2:B:778:MET:HE1	2:B:1094:ARG:NH1	2.30	0.42
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.02	0.42
2:B:468:GLU:HA	2:B:470:LYS:N	2.32	0.42
2:B:757:PRO:HG2	2:B:984:HIS:NE2	2.35	0.42
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.42
2:B:579:ARG:HA	2:B:589:VAL:HA	2.02	0.42
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.20	0.42
1:A:1371:LEU:O	1:A:1374:VAL:HG12	2.20	0.42
2:B:1175:LEU:C	2:B:1177:HIS:H	2.23	0.42
5:F:81:THR:OG1	5:F:146:TRP:NE1	2.50	0.42
7:I:10:CYS:HB3	7:I:12:ASN:HD22	1.84	0.42
12:N:13:DA:H2''	12:N:14:DG:H5'	2.00	0.42
1:A:679:ILE:HG23	1:A:729:ALA:HB1	2.01	0.42
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:89:LEU:HD22	6:H:90:ALA:N	2.34	0.42
1:A:607:ILE:HA	1:A:612:ILE:HA	2.01	0.42
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.92	0.42
3:C:98:VAL:HG22	3:C:158:VAL:HG22	2.01	0.42
1:A:55:ASP:HB2	1:A:56:PRO:HD2	2.02	0.42
1:A:666:ILE:H	1:A:666:ILE:HG13	1.56	0.42
2:B:199:MET:N	2:B:199:MET:SD	2.81	0.42
2:B:483:LEU:HD21	2:B:491:THR:HG23	2.01	0.42
1:A:131:SER:HB3	1:A:223:GLY:HA2	2.01	0.42
1:A:359:LEU:O	1:A:471:ASN:ND2	2.53	0.42
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.20	0.42
5:F:93:ILE:HD11	5:F:134:ILE:HD11	2.02	0.42
1:A:849:MET:HB3	1:A:1063:MET:SD	2.60	0.41
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.85	0.41
1:A:72:GLU:HG3	2:B:1175:LEU:HB2	2.02	0.41
1:A:22:PHE:HZ	1:A:30:ILE:HD12	1.85	0.41
1:A:42:ASP:N	1:A:43:GLU:HA	2.33	0.41
2:B:640:VAL:HG22	2:B:651:LEU:HD23	2.02	0.41
13:R:4:G:H2'	13:R:5:A:H8	1.84	0.41
1:A:901:LEU:HD22	1:A:919:ILE:HG23	2.02	0.41
2:B:30:SER:O	2:B:34:ILE:HG13	2.19	0.41
1:A:560:ILE:HB	6:H:79:TRP:H	1.84	0.41
2:B:975:GLN:N	2:B:978:ASP:OD2	2.51	0.41
8:J:23:ASN:O	8:J:27:GLU:HB3	2.20	0.41
12:N:11:DG:H2''	12:N:12:DT:C6	2.54	0.41
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.56	0.41
2:B:1037:LEU:HD23	8:J:44:TYR:HB3	2.02	0.41
2:B:258:LEU:HD13	2:B:269:ILE:HG12	2.03	0.41
2:B:952:VAL:HG22	2:B:966:VAL:HG13	2.03	0.41
1:A:848:ILE:HB	1:A:1065:GLY:HA3	2.03	0.41
2:B:904:ARG:HG2	2:B:948:ILE:HG12	2.03	0.41
6:H:81:PRO:HA	6:H:82:PRO:HD3	1.96	0.41
1:A:527:THR:O	1:A:653:VAL:HG11	2.21	0.41
2:B:463:THR:HG22	11:T:27:DA:H2''	2.01	0.41
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.03	0.41
2:B:629:ASP:OD1	2:B:630:ALA:N	2.54	0.41
2:B:830:TYR:HB3	2:B:831:SER:H	1.65	0.41
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.79	0.41
12:N:2:DT:H6	12:N:2:DT:H2'	1.70	0.41
1:A:1207:LEU:HD23	1:A:1274:ARG:HD2	2.02	0.41
2:B:600:LEU:HB3	2:B:615:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:TYR:HB3	5:F:81:THR:HG22	2.03	0.41
1:A:1157:ASP:HA	1:A:1158:PRO:HD3	1.91	0.41
1:A:306:ASN:HB2	1:A:324:SER:HB3	2.02	0.41
1:A:678:GLU:HA	1:A:681:GLU:HG2	2.03	0.41
1:A:878:ILE:HG12	1:A:957:PRO:HA	2.02	0.41
1:A:30:ILE:HG23	2:B:1170:THR:HG23	2.02	0.41
2:B:1135:ARG:HG3	2:B:1147:LEU:HD21	2.03	0.41
4:E:165:LEU:HD13	4:E:170:LEU:HB2	2.03	0.41
4:E:65:THR:O	4:E:69:ILE:HG12	2.21	0.41
1:A:1193:LEU:HD21	1:A:1264:GLU:HB3	2.03	0.41
1:A:798:GLY:HA2	1:A:815:PHE:CD2	2.56	0.41
2:B:30:SER:OG	2:B:743:ILE:O	2.33	0.41
2:B:861:ASP:OD1	2:B:862:GLN:N	2.54	0.41
10:L:48:CYS:HB3	10:L:51:CYS:HB3	2.02	0.41
1:A:1386:ARG:HB3	1:A:1403:GLU:HG3	2.02	0.40
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.36	0.40
2:B:120:ARG:HA	2:B:963:PHE:HZ	1.86	0.40
1:A:231:PRO:HA	1:A:234:MET:HG3	2.04	0.40
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.56	0.40
1:A:851:HIS:CG	5:F:139:PRO:HG3	2.56	0.40
2:B:846:ILE:HG23	2:B:974:PRO:HG2	2.04	0.40
1:A:244:PRO:HG2	1:A:245:PRO:HD3	2.02	0.40
2:B:806:THR:HB	2:B:809:MET:HG3	2.03	0.40
3:C:22:LEU:HD21	9:K:101:LEU:HD21	2.03	0.40
4:E:79:TRP:HB2	4:E:105:PHE:CD2	2.56	0.40
2:B:500:THR:HA	2:B:501:PRO:HD3	1.93	0.40
4:E:3:GLN:HB2	4:E:4:GLU:H	1.64	0.40
6:H:14:GLU:HB3	6:H:27:GLU:HB3	2.03	0.40
9:K:49:GLU:HG3	9:K:94:ILE:HG12	2.04	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	1357/1733 (78%)	1252 (92%)	103 (8%)	2 (0%)	51	83
2	B	1067/1224 (87%)	996 (93%)	66 (6%)	5 (0%)	29	68
3	C	264/318 (83%)	243 (92%)	19 (7%)	2 (1%)	19	59
4	E	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	29	68
5	F	82/155 (53%)	78 (95%)	4 (5%)	0	100	100
6	H	124/146 (85%)	109 (88%)	13 (10%)	2 (2%)	9	46
7	I	113/122 (93%)	98 (87%)	15 (13%)	0	100	100
8	J	63/70 (90%)	59 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	107 (96%)	4 (4%)	1 (1%)	17	57
10	L	42/70 (60%)	33 (79%)	9 (21%)	0	100	100
All	All	3435/4173 (82%)	3176 (92%)	246 (7%)	13 (0%)	34	71

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1046	PRO
6	H	82	PRO
3	C	148	ARG
9	K	26	LYS
1	A	1156	PRO
2	B	974	PRO
4	E	86	PRO
2	B	367	LEU
2	B	1017	ILE
3	C	90	ASP
6	H	18	GLY
2	B	901	PRO
1	A	957	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1198/1520 (79%)	1141 (95%)	57 (5%)	25	60
2	B	944/1061 (89%)	908 (96%)	36 (4%)	33	66
3	C	234/274 (85%)	227 (97%)	7 (3%)	41	71
4	E	195/197 (99%)	189 (97%)	6 (3%)	40	71
5	F	74/137 (54%)	72 (97%)	2 (3%)	44	73
6	H	114/128 (89%)	110 (96%)	4 (4%)	36	68
7	I	109/116 (94%)	106 (97%)	3 (3%)	43	72
8	J	60/65 (92%)	59 (98%)	1 (2%)	60	82
9	K	99/102 (97%)	97 (98%)	2 (2%)	55	79
10	L	39/57 (68%)	39 (100%)	0	100	100
All	All	3066/3657 (84%)	2948 (96%)	118 (4%)	33	66

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	22	PHE
1	A	34	LYS
1	A	46	THR
1	A	69	THR
1	A	126	LEU
1	A	132	LYS
1	A	179	LEU
1	A	222	LEU
1	A	235	ILE
1	A	308	ILE
1	A	326	ARG
1	A	335	ARG
1	A	351	THR
1	A	434	ARG
1	A	441	PRO
1	A	443	LEU
1	A	444	PHE
1	A	451	HIS
1	A	470	LEU
1	A	532	ARG
1	A	612	ILE
1	A	618	GLU

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Mol	Chain	Res	Type
1	A	626	ASN
1	A	666	ILE
1	A	702	LEU
1	A	710	LEU
1	A	732	LEU
1	A	774	ARG
1	A	780	VAL
1	A	783	THR
1	A	826	ASP
1	A	830	LYS
1	A	885	THR
1	A	896	ARG
1	A	926	GLN
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1034	GLU
1	A	1035	TYR
1	A	1116	LEU
1	A	1172	LEU
1	A	1207	LEU
1	A	1230	GLU
1	A	1231	ASP
1	A	1262	LYS
1	A	1297	GLU
1	A	1300	LYS
1	A	1322	ILE
1	A	1333	ILE
1	A	1374	VAL
1	A	1377	THR
1	A	1400	CYS
1	A	1406	VAL
1	A	1407	GLU
2	B	46	GLN
2	B	109	THR
2	B	134	LYS
2	B	217	ARG
2	B	319	GLU
2	B	365	THR
2	B	393	LYS
2	B	483	LEU
2	B	549	THR

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Mol	Chain	Res	Type
2	B	552	MET
2	B	567	GLU
2	B	570	VAL
2	B	575	PRO
2	B	737	THR
2	B	751	VAL
2	B	791	THR
2	B	797	TYR
2	B	825	VAL
2	B	868	MET
2	B	916	THR
2	B	955	THR
2	B	983	ARG
2	B	987	LYS
2	B	997	GLU
2	B	999	MET
2	B	1028	GLU
2	B	1051	THR
2	B	1096	ARG
2	B	1099	VAL
2	B	1147	LEU
2	B	1158	PHE
2	B	1159	ARG
2	B	1176	ASN
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
3	C	22	LEU
3	C	25	VAL
3	C	77	ILE
3	C	99	LEU
3	C	137	LYS
3	C	222	LYS
3	C	240	VAL
4	E	3	GLN
4	E	98	ILE
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	169	ARG
5	F	72	LYS
5	F	97	ARG

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Mol	Chain	Res	Type
6	H	89	LEU
6	H	124	ARG
6	H	133	ASN
6	H	143	LEU
7	I	14	LEU
7	I	55	THR
7	I	111	THR
8	J	5	VAL
9	K	1	MET
9	K	18	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	325	GLN
2	B	762	ASN
2	B	984	HIS
2	B	1097	HIS
2	B	1176	ASN
2	B	1177	HIS
7	I	12	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	9	G

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	6MA	T	7	11,12	18,24,25	1.78	4 (22%)	15,34,37	1.22	1 (6%)
11	6MA	T	16	11	18,24,25	1.75	4 (22%)	15,34,37	1.42	2 (13%)
11	6MA	T	19	11	18,24,25	1.79	4 (22%)	15,34,37	1.44	4 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	6MA	T	7	11,12	-	5/5/23/24	0/3/3/3
11	6MA	T	16	11	-	1/5/23/24	0/3/3/3
11	6MA	T	19	11	-	2/5/23/24	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	16	6MA	C6-N6	4.41	1.42	1.35
11	T	7	6MA	C6-N6	4.38	1.42	1.35
11	T	19	6MA	C6-N6	4.28	1.42	1.35
11	T	19	6MA	C1'-N9	-3.61	1.38	1.49
11	T	7	6MA	C1'-N9	-3.44	1.39	1.49
11	T	16	6MA	C1'-N9	-3.37	1.39	1.49
11	T	7	6MA	C2-N3	2.56	1.36	1.32
11	T	19	6MA	C2-N3	2.52	1.36	1.32
11	T	16	6MA	C2-N3	2.50	1.36	1.32
11	T	16	6MA	C5-N7	2.07	1.47	1.39
11	T	19	6MA	C5-N7	2.06	1.47	1.39
11	T	7	6MA	C5-N7	2.06	1.47	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	19	6MA	C1-N6-C6	-3.70	119.69	122.87
11	T	16	6MA	C1-N6-C6	-3.47	119.88	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
11	T	7	6MA	C1-N6-C6	-3.20	120.12	122.87
11	T	16	6MA	C2'-C3'-C4'	2.47	107.91	102.76
11	T	19	6MA	C2'-C1'-N9	-2.27	109.03	114.27
11	T	19	6MA	C2-N1-C6	2.08	118.37	116.59
11	T	19	6MA	C2'-C3'-C4'	2.03	106.98	102.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	7	6MA	C3'-C4'-C5'-O5'
11	T	7	6MA	N1-C6-N6-C1
11	T	16	6MA	N1-C6-N6-C1
11	T	7	6MA	O4'-C4'-C5'-O5'
11	T	19	6MA	O4'-C4'-C5'-O5'
11	T	19	6MA	C3'-C4'-C5'-O5'
11	T	7	6MA	C4'-C5'-O5'-P
11	T	7	6MA	C5-C6-N6-C1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	7	6MA	2	0
11	T	19	6MA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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	1371/1733 (79%)	0.04	13 (0%) 84 73	17, 78, 165, 231	0
2	B	1089/1224 (88%)	-0.05	2 (0%) 95 91	18, 59, 129, 209	0
3	C	266/318 (83%)	0.08	0 100 100	29, 60, 112, 161	0
4	E	213/215 (99%)	0.53	18 (8%) 10 6	53, 120, 200, 234	0
5	F	84/155 (54%)	-0.01	1 (1%) 79 66	39, 76, 119, 161	0
6	H	130/146 (89%)	0.78	9 (6%) 16 10	68, 102, 171, 206	0
7	I	115/122 (94%)	0.16	0 100 100	37, 80, 130, 183	0
8	J	65/70 (92%)	-0.17	0 100 100	25, 45, 113, 145	0
9	K	114/120 (95%)	0.02	0 100 100	30, 63, 105, 124	0
10	L	44/70 (62%)	0.49	4 (9%) 9 5	49, 132, 197, 208	0
11	T	26/29 (89%)	0.45	1 (3%) 40 26	46, 241, 298, 321	0
12	N	14/14 (100%)	0.84	2 (14%) 2 2	209, 249, 297, 307	0
13	R	9/9 (100%)	0.17	0 100 100	37, 53, 102, 110	0
All	All	3540/4225 (83%)	0.08	50 (1%) 75 61	17, 73, 164, 321	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	H	84	ALA	4.9
4	E	93	MET	4.7
4	E	102	GLU	4.3
12	N	1	DC	4.0
1	A	286	HIS	3.6
2	B	643	ASP	3.5
4	E	126	SER	3.5
6	H	134	ASN	3.5
4	E	82	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
4	E	123	LEU	3.4
1	A	147	VAL	3.4
6	H	85	GLY	3.3
6	H	82	PRO	3.2
1	A	1173	HIS	3.1
10	L	46	VAL	3.1
4	E	83	CYS	3.1
10	L	50	ASP	3.0
4	E	96	PHE	3.0
4	E	9	ILE	2.9
4	E	109	ILE	2.9
1	A	49	LYS	2.9
4	E	95	THR	2.8
6	H	146	ARG	2.8
1	A	91	PHE	2.8
6	H	139	ASN	2.7
4	E	100	ILE	2.6
10	L	35	SER	2.5
1	A	140	THR	2.5
4	E	110	PHE	2.5
4	E	85	GLU	2.4
6	H	86	ASP	2.4
1	A	1156	PRO	2.4
1	A	69	THR	2.3
5	F	155	LEU	2.3
1	A	1258	HIS	2.2
4	E	132	ILE	2.2
4	E	98	ILE	2.2
11	T	11	DG	2.2
12	N	2	DT	2.2
6	H	136	LYS	2.1
2	B	1183	LYS	2.1
1	A	174	ILE	2.1
1	A	259	GLU	2.1
4	E	106	GLN	2.1
4	E	52	ARG	2.1
4	E	111	VAL	2.1
10	L	43	THR	2.1
6	H	123	MET	2.0
1	A	145	LYS	2.0
1	A	975	HIS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
11	6MA	T	16	22/23	0.67	0.29	178,189,201,211	0
11	6MA	T	7	22/23	0.73	0.28	244,245,251,255	0
11	6MA	T	19	22/23	0.94	0.21	64,84,103,110	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

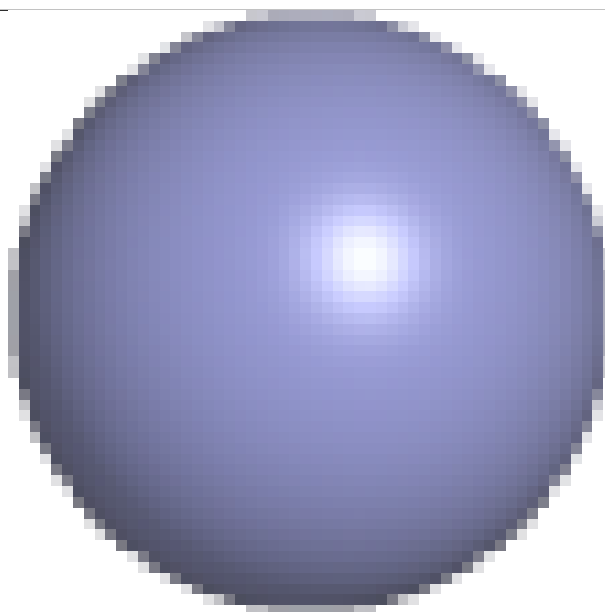
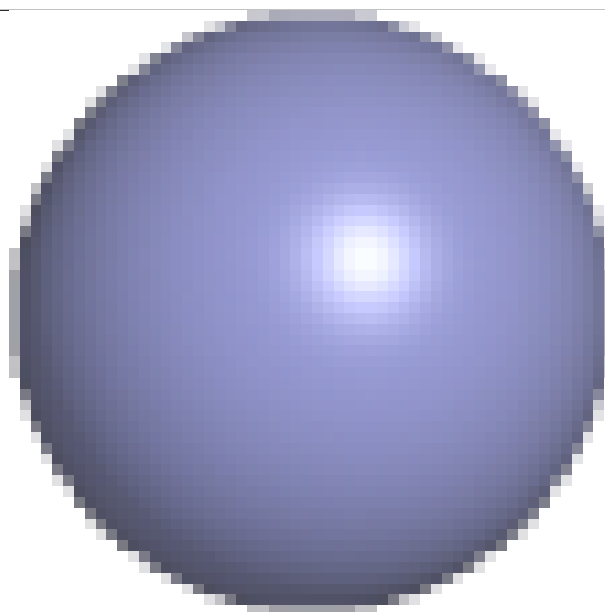
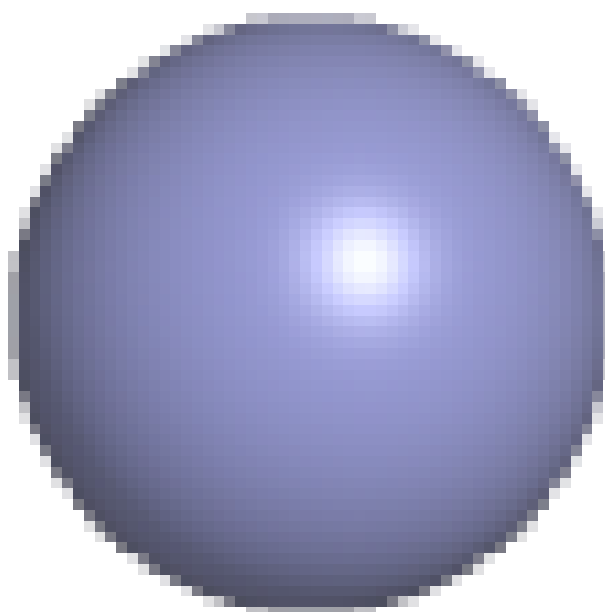
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	ZN	A	1801	1/1	0.76	0.06	198,198,198,198	0
14	ZN	L	101	1/1	0.88	0.06	129,129,129,129	0
14	ZN	A	1802	1/1	0.92	0.13	91,91,91,91	0
15	MG	A	1803	1/1	0.93	0.15	37,37,37,37	0
14	ZN	B	1301	1/1	0.96	0.10	117,117,117,117	0
14	ZN	I	201	1/1	0.98	0.10	71,71,71,71	0
14	ZN	C	401	1/1	0.98	0.16	52,52,52,52	0
14	ZN	J	101	1/1	0.99	0.11	32,32,32,32	0
14	ZN	I	202	1/1	0.99	0.14	50,50,50,50	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.

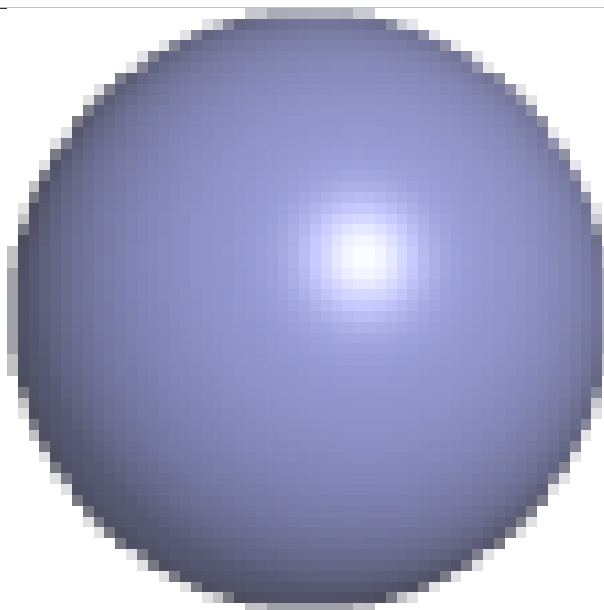
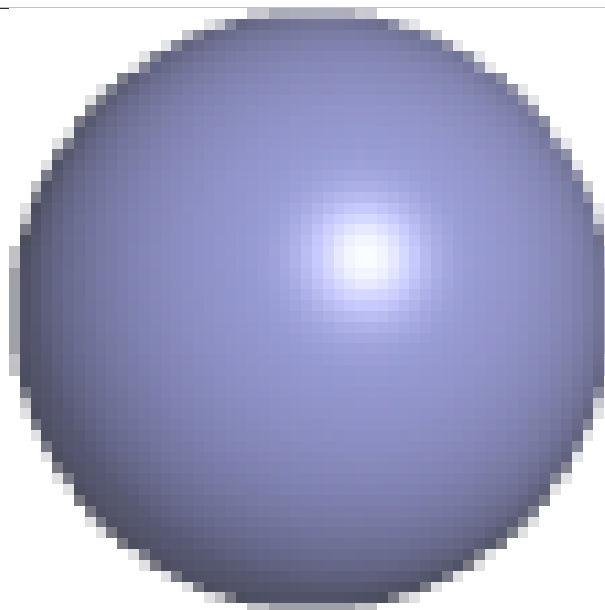
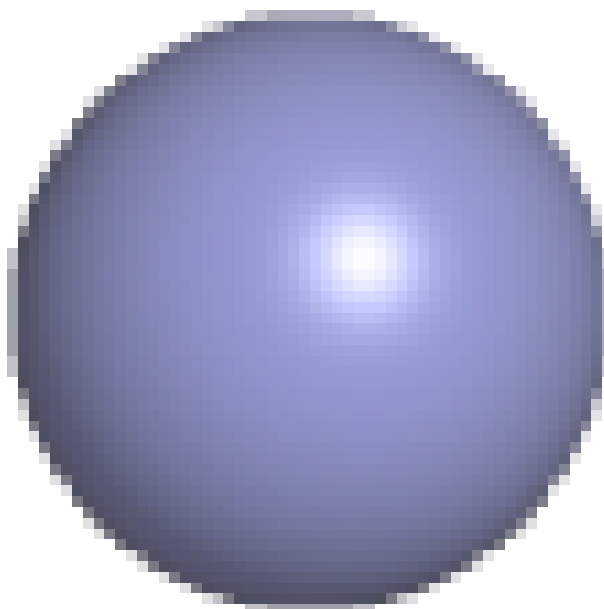
Electron density around ZN A 1801:

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



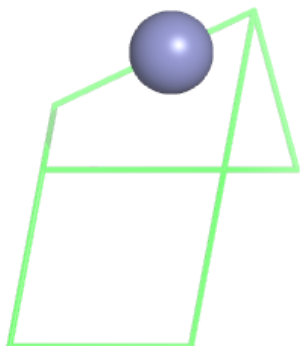
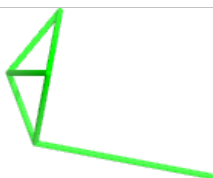
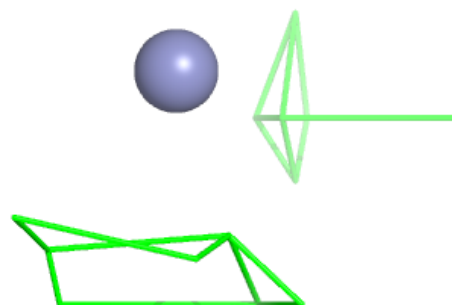
Electron density around ZN L 101:

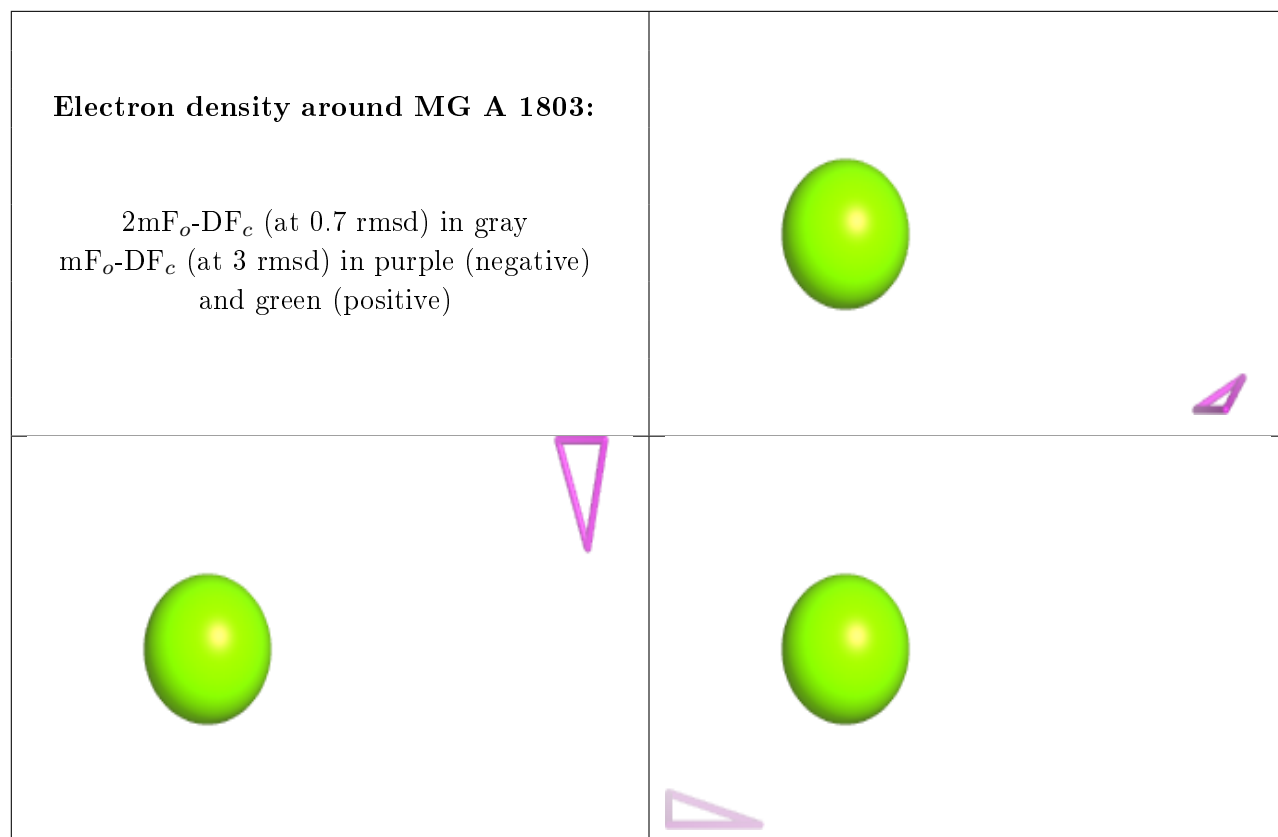
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 1802:

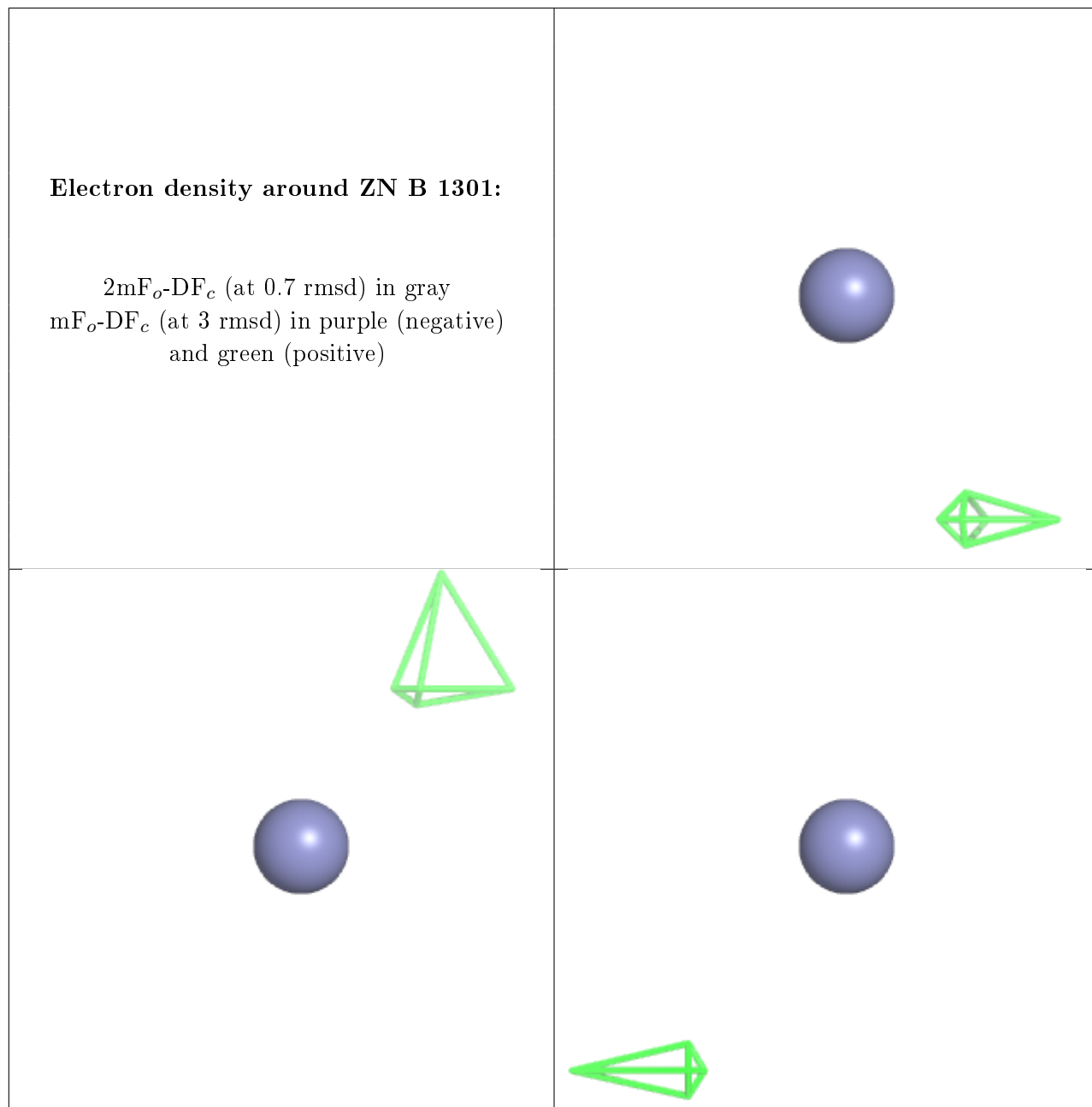
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

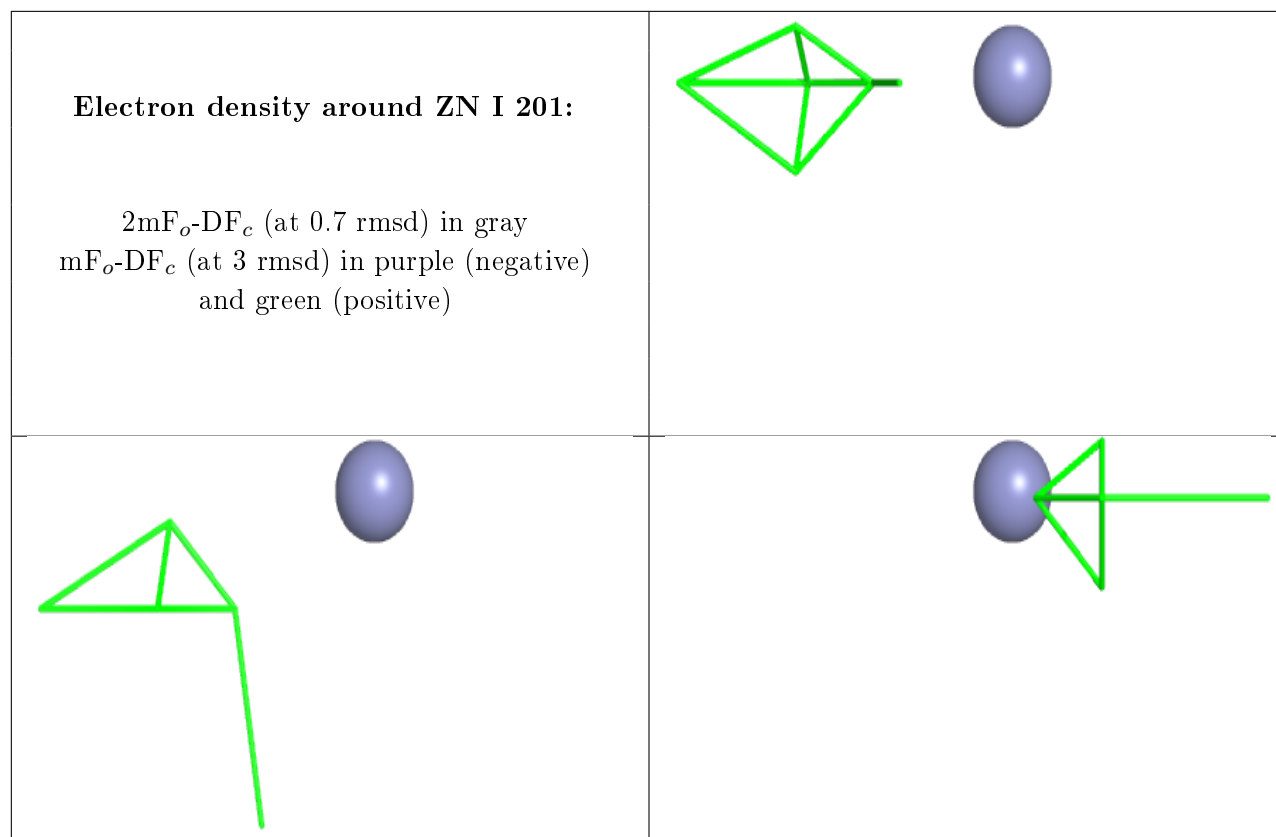




Electron density around ZN B 1301:

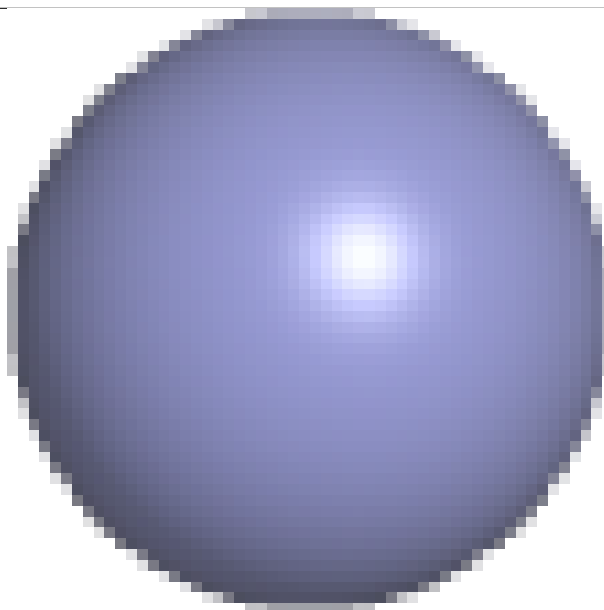
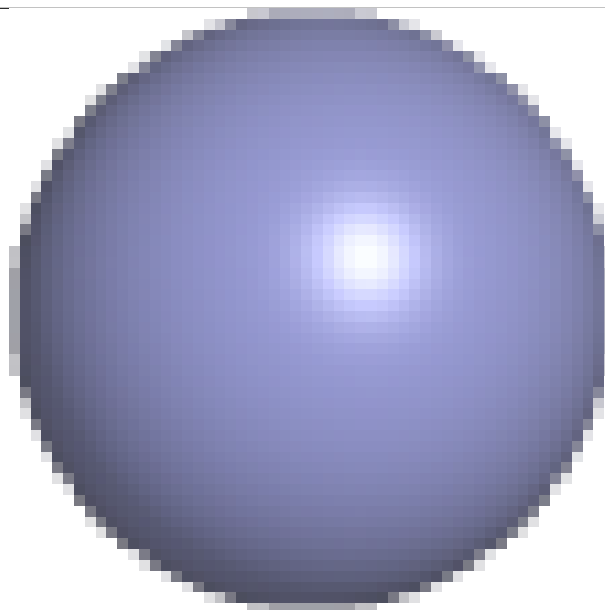
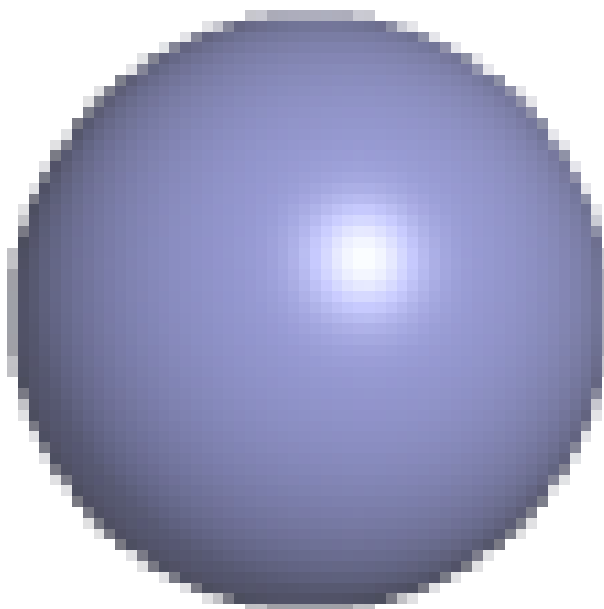
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

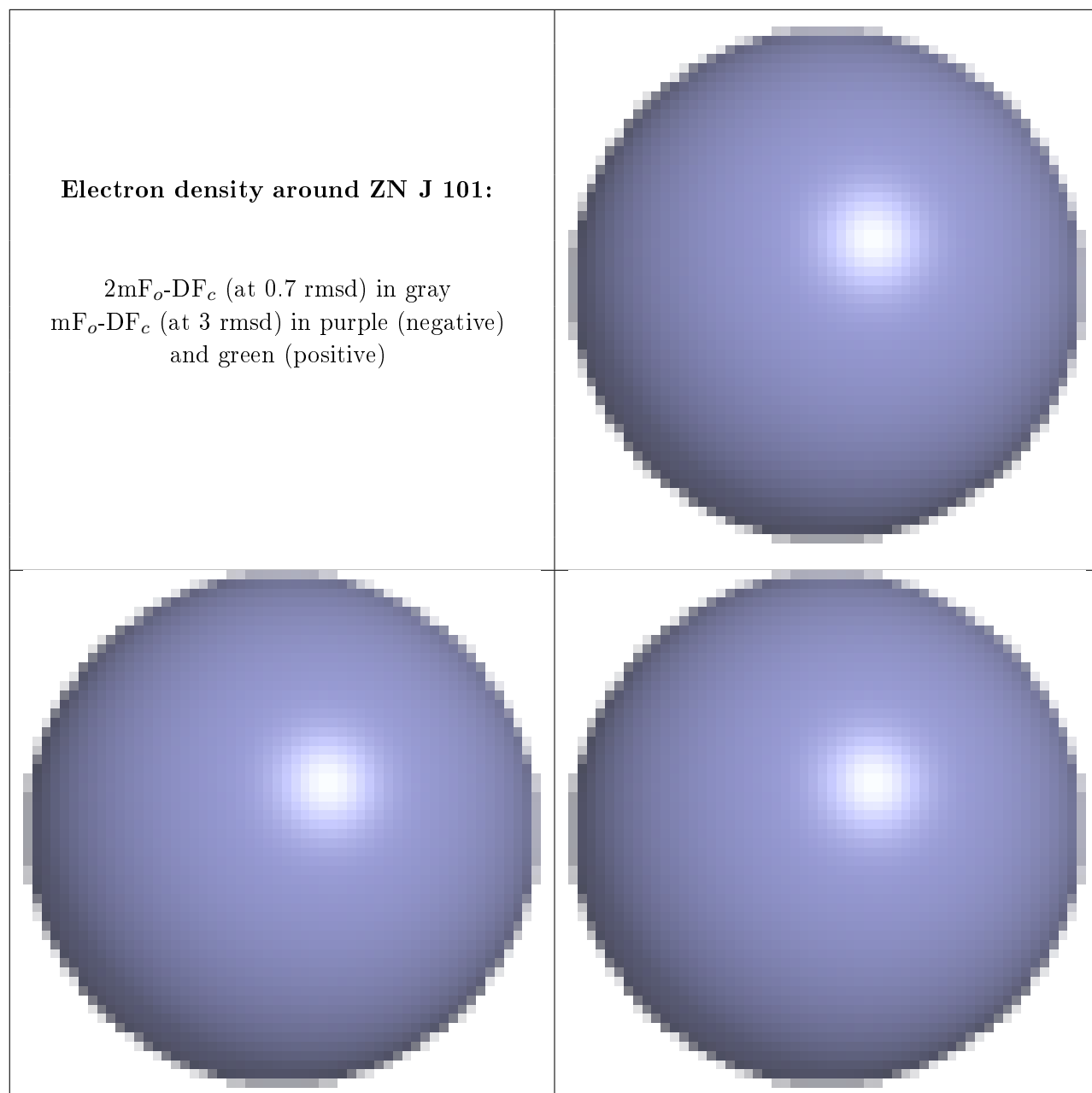


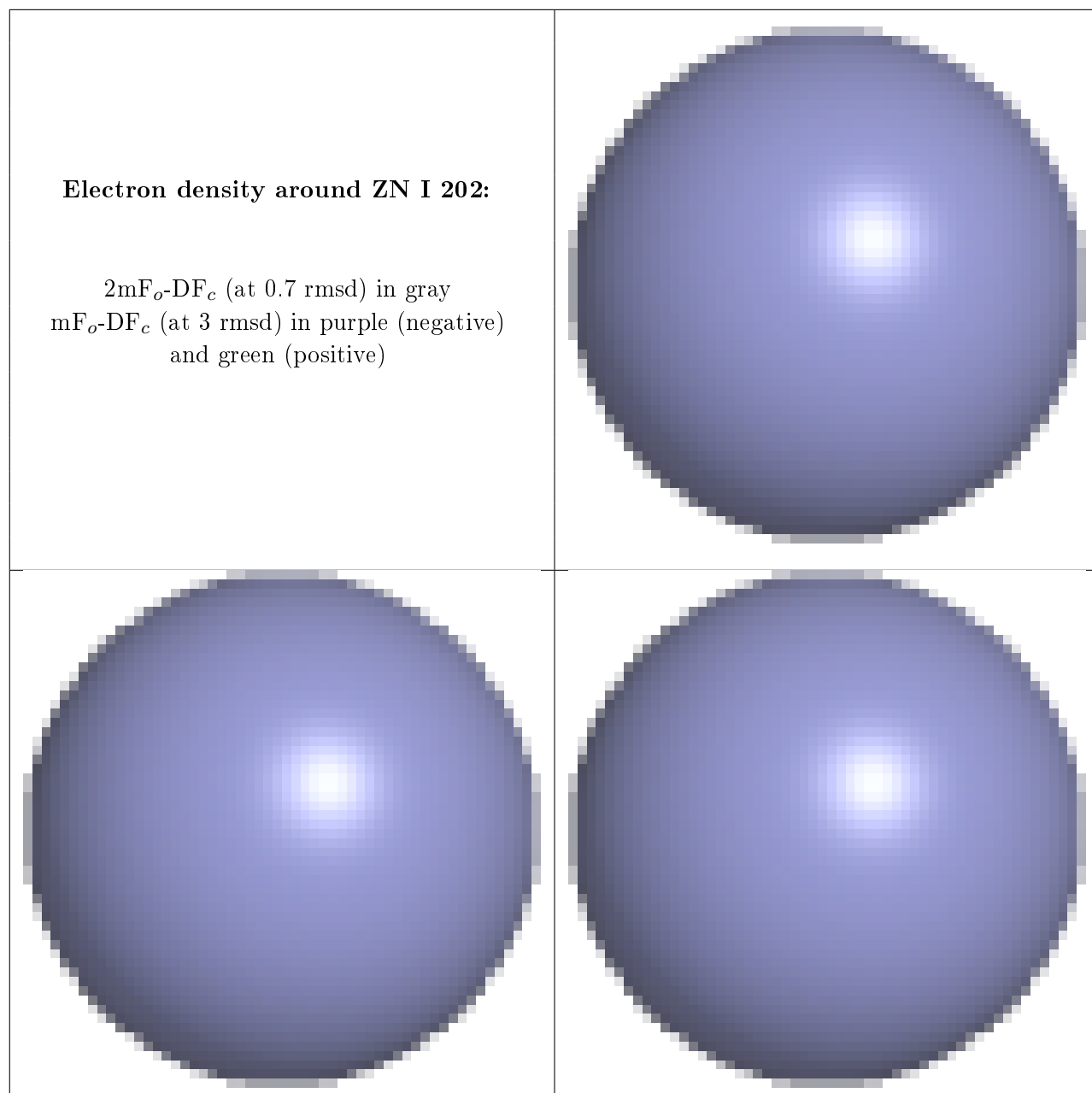


Electron density around ZN C 401:

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







6.5 Other polymers ⓘ

There are no such residues in this entry.