Full wwPDB X-ray Structure Validation Report (i)

Nov 11, 2026 – 07:16 PM JST

PDB ID	:	25UC / pdb_000025uc
Title	:	Crystal structure of SktA in complex with L-tryptophan and Fe2+
Authors	:	Li, H.; Liu, J.; Huang, J.-W.; Chen, C.-C.; Guo, R.-T.
Deposited on	:	2026-04-17
Resolution	:	2.55 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 (i) 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 (i)) were used in the production of this report:

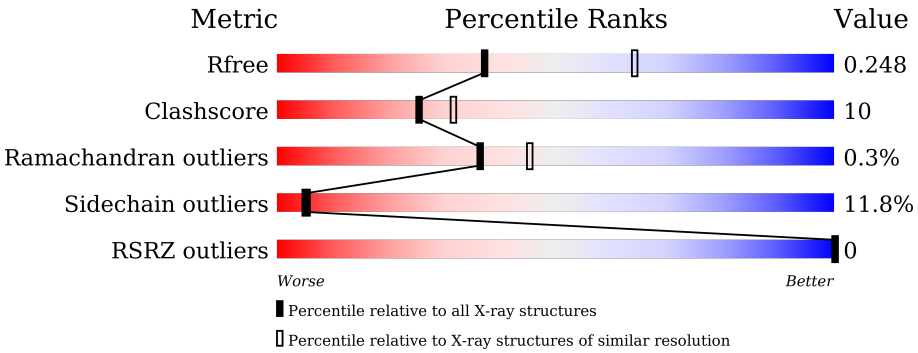
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	248	60% 29% • 8%
1	B	248	67% 21% • 8%
1	C	248	71% 21% • 6%
1	D	248	63% 25% 6% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7811 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 Iron-containing redox enzyme family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	228	Total	C	N	O	S	0	0	0
			1898	1222	313	355	8			
1	C	234	Total	C	N	O	S	0	0	0
			1950	1254	321	367	8			
1	A	227	Total	C	N	O	S	0	0	0
			1890	1217	311	354	8			
1	D	235	Total	C	N	O	S	0	0	0
			1954	1256	322	368	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP A0A367RF96
B	-9	ALA	-	expression tag	UNP A0A367RF96
B	-8	GLY	-	expression tag	UNP A0A367RF96
B	-7	ALA	-	expression tag	UNP A0A367RF96
B	-6	GLY	-	expression tag	UNP A0A367RF96
B	-5	ALA	-	expression tag	UNP A0A367RF96
B	-4	GLY	-	expression tag	UNP A0A367RF96
B	-3	ALA	-	expression tag	UNP A0A367RF96
B	-2	GLY	-	expression tag	UNP A0A367RF96
B	-1	ALA	-	expression tag	UNP A0A367RF96
B	0	GLY	-	expression tag	UNP A0A367RF96
C	-10	GLY	-	expression tag	UNP A0A367RF96
C	-9	ALA	-	expression tag	UNP A0A367RF96
C	-8	GLY	-	expression tag	UNP A0A367RF96
C	-7	ALA	-	expression tag	UNP A0A367RF96
C	-6	GLY	-	expression tag	UNP A0A367RF96
C	-5	ALA	-	expression tag	UNP A0A367RF96
C	-4	GLY	-	expression tag	UNP A0A367RF96
C	-3	ALA	-	expression tag	UNP A0A367RF96
C	-2	GLY	-	expression tag	UNP A0A367RF96
C	-1	ALA	-	expression tag	UNP A0A367RF96

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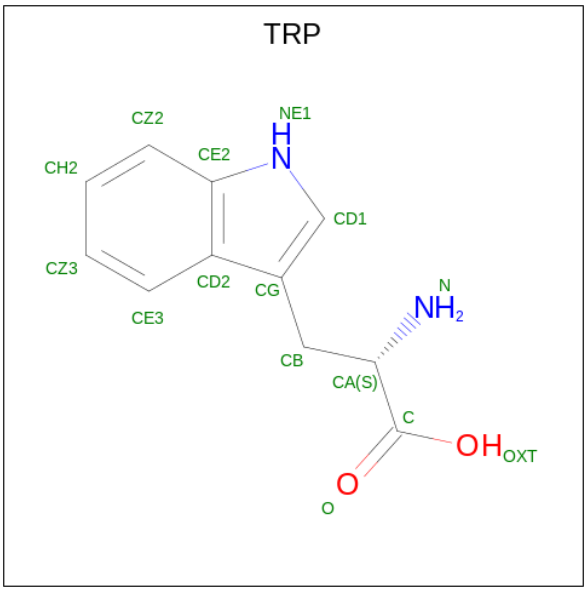
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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP A0A367RF96
A	-10	GLY	-	expression tag	UNP A0A367RF96
A	-9	ALA	-	expression tag	UNP A0A367RF96
A	-8	GLY	-	expression tag	UNP A0A367RF96
A	-7	ALA	-	expression tag	UNP A0A367RF96
A	-6	GLY	-	expression tag	UNP A0A367RF96
A	-5	ALA	-	expression tag	UNP A0A367RF96
A	-4	GLY	-	expression tag	UNP A0A367RF96
A	-3	ALA	-	expression tag	UNP A0A367RF96
A	-2	GLY	-	expression tag	UNP A0A367RF96
A	-1	ALA	-	expression tag	UNP A0A367RF96
A	0	GLY	-	expression tag	UNP A0A367RF96
D	-10	GLY	-	expression tag	UNP A0A367RF96
D	-9	ALA	-	expression tag	UNP A0A367RF96
D	-8	GLY	-	expression tag	UNP A0A367RF96
D	-7	ALA	-	expression tag	UNP A0A367RF96
D	-6	GLY	-	expression tag	UNP A0A367RF96
D	-5	ALA	-	expression tag	UNP A0A367RF96
D	-4	GLY	-	expression tag	UNP A0A367RF96
D	-3	ALA	-	expression tag	UNP A0A367RF96
D	-2	GLY	-	expression tag	UNP A0A367RF96
D	-1	ALA	-	expression tag	UNP A0A367RF96
D	0	GLY	-	expression tag	UNP A0A367RF96

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0

- Molecule 3 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 15 11 2 2	0	0
3	C	1	Total C N O 15 11 2 2	0	0
3	A	1	Total C N O 15 11 2 2	0	0
3	D	1	Total C N O 15 11 2 2	0	0

- Molecule 4 is water.

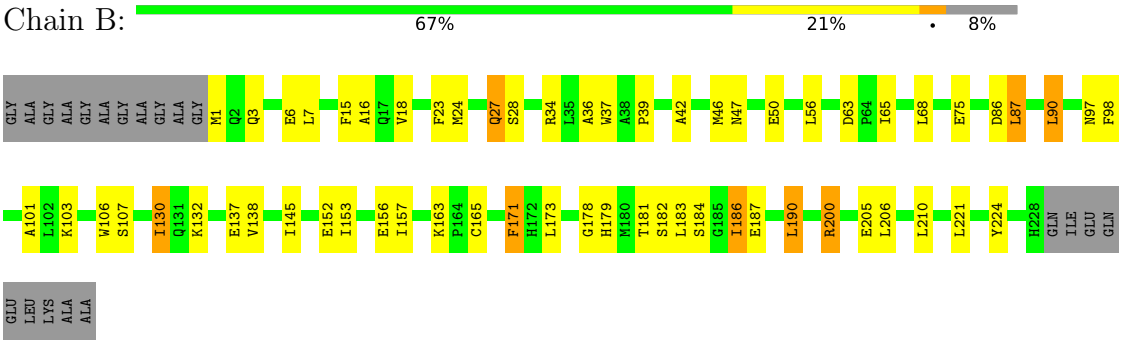
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	14	Total O 14 14	0	0
4	C	14	Total O 14 14	0	0
4	A	13	Total O 13 13	0	0
4	D	10	Total O 10 10	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

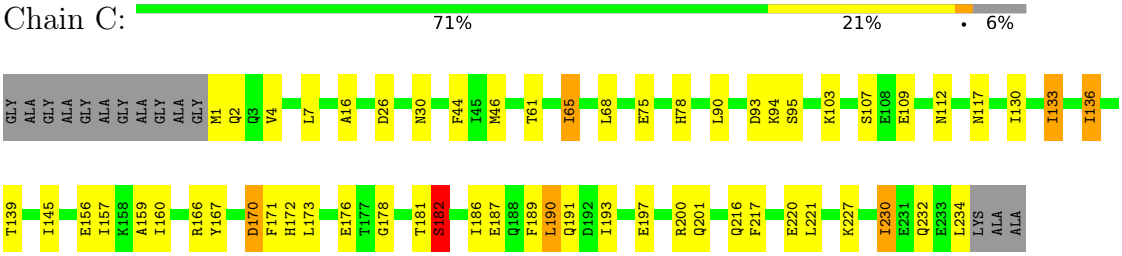
• Molecule 1: Iron-containing redox enzyme family protein

Chain B:



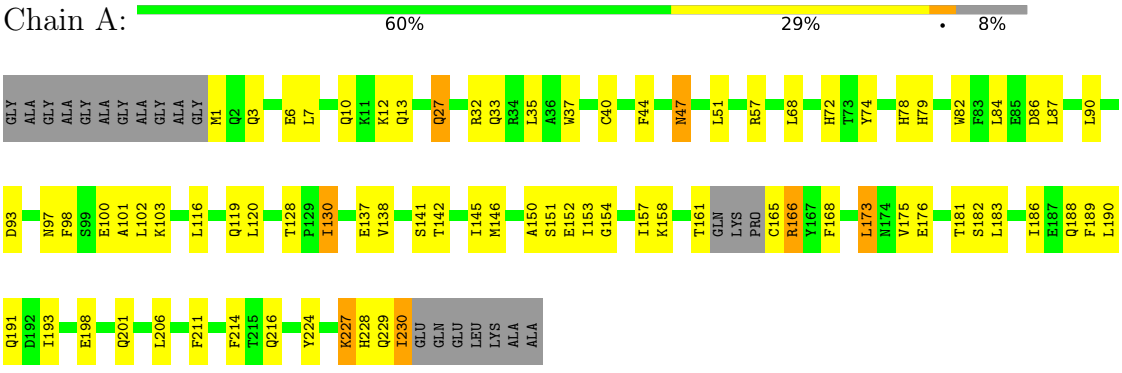
• Molecule 1: Iron-containing redox enzyme family protein

Chain C:



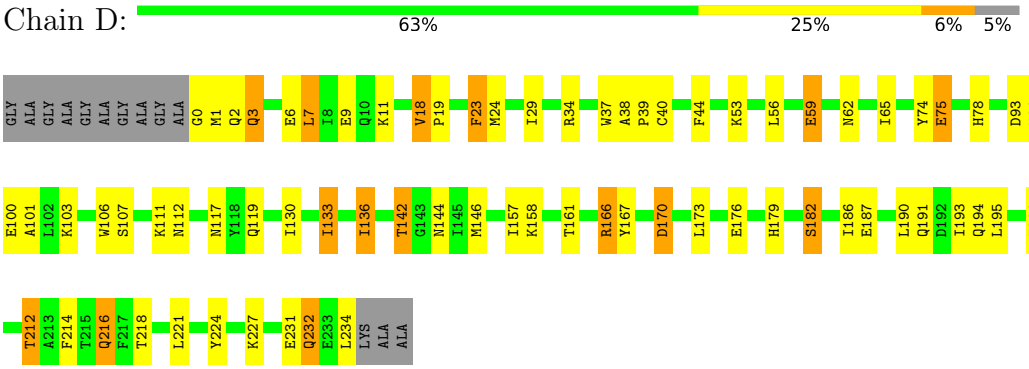
• Molecule 1: Iron-containing redox enzyme family protein

Chain A:



• Molecule 1: Iron-containing redox enzyme family protein

Chain D:


63%
25%
6%
5%
GLY ALA GLY ALA GLY ALA GLY ALA GLY ALA GO M1 Q2 Q3 E6 L7 I8 E9 Q10 K11 V18 P19 F23 M24 I29 R34 W37 A38 P39 C40 F44 K53 L56 E59 N62 I65 Y74 E75 H78 D93 K94 N97 F98 S99
E100 A101 L102 K103 W106 S107 K111 N112 N117 Y118 Q119 I130 I133 I136 T142 G143 N144 I145 M146 I157 K158 T161 R166 Y167 D170 L173 E176 H179 S182 I186 E187 L190 Q191 D192 I193 Q194 L195 F204 E205 L206 N209
T212 A213 F214 T215 Q216 F217 T218 L221 Y224 K227 E231 Q232 E233 L234 LYS ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.09Å 66.92Å 69.48Å 73.60° 75.09° 77.08°	Depositor
Resolution (Å)	24.79 – 2.55 24.79 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.0 (24.79-2.55) 96.7 (24.79-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.80 (at 2.53Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.245 0.192 , 0.248	Depositor DCC
R_{free} test set	1442 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	62.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7811	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	1.04	0/1934	1.53	4/2614 (0.2%)
1	B	1.08	0/1944	1.52	3/2629 (0.1%)
1	C	1.09	1/1996 (0.1%)	1.50	3/2699 (0.1%)
1	D	1.06	1/2000 (0.1%)	1.56	6/2704 (0.2%)
All	All	1.07	2/7874 (0.0%)	1.53	16/10646 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	78	HIS	CE1-NE2	8.10	1.40	1.32
1	D	78	HIS	CE1-NE2	7.44	1.40	1.32

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	181	THR	CA-CB-OG1	-7.44	98.44	109.60
1	C	182	SER	CA-C-N	6.20	128.88	120.44
1	C	182	SER	C-N-CA	6.20	128.88	120.44
1	A	128	THR	CA-CB-OG1	-5.52	101.33	109.60
1	B	50	GLU	N-CA-C	-5.29	105.59	111.36
1	D	166	ARG	CA-C-N	5.18	127.48	120.44
1	D	166	ARG	C-N-CA	5.18	127.48	120.44
1	A	154	GLY	CA-C-N	5.15	127.44	120.44
1	A	154	GLY	C-N-CA	5.15	127.44	120.44
1	D	216	GLN	CA-C-N	5.09	127.55	120.63
1	D	216	GLN	C-N-CA	5.09	127.55	120.63
1	B	224	TYR	CA-C-N	5.05	127.05	120.28
1	B	224	TYR	C-N-CA	5.05	127.05	120.28
1	A	44	PHE	N-CA-C	-5.03	105.71	111.14
1	D	182	SER	CA-C-N	5.00	127.26	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	182	SER	C-N-CA	5.00	127.26	120.65

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	1890	0	1842	43	0
1	B	1898	0	1852	32	0
1	C	1950	0	1902	26	0
1	D	1954	0	1905	51	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	15	0	9	1	0
3	B	15	0	9	0	0
3	C	15	0	9	0	0
3	D	15	0	9	1	0
4	A	13	0	0	1	0
4	B	14	0	0	0	0
4	C	14	0	0	0	0
4	D	10	0	0	0	0
All	All	7811	0	7537	147	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 10.

All (147) 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:D:112:ASN:ND2	1:D:216:GLN:HB3	1.92	0.84
1:B:137:GLU:OE1	1:B:183:LEU:HD23	1.81	0.80
1:B:16:ALA:HB2	1:B:145:ILE:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:THR:HG21	1:D:214:PHE:CG	2.23	0.73
1:D:112:ASN:HD22	1:D:216:GLN:HB3	1.55	0.69
1:B:97:ASN:HB3	1:C:93:ASP:OD1	1.93	0.68
1:A:206:LEU:C	1:A:206:LEU:HD23	2.20	0.67
1:B:186:ILE:O	1:B:190:LEU:N	2.28	0.67
1:D:190:LEU:O	1:D:193:ILE:HG22	1.95	0.66
1:D:24:MET:HE3	1:D:37:TRP:HE1	1.60	0.65
1:C:190:LEU:O	1:C:193:ILE:HG22	1.96	0.65
1:C:197:GLU:OE1	1:C:200:ARG:NH2	2.30	0.64
1:A:151:SER:HA	1:A:168:PHE:O	1.99	0.63
1:D:75:GLU:CD	1:D:179:HIS:HE2	2.06	0.62
1:D:103:LYS:O	1:D:107:SER:HB3	1.99	0.61
1:B:165:CYS:O	1:B:171:PHE:CE1	2.54	0.60
1:A:189:PHE:CE1	1:A:193:ILE:HD11	2.38	0.59
1:D:212:THR:HG23	1:D:216:GLN:NE2	2.18	0.59
1:A:173:LEU:HD22	1:A:173:LEU:O	2.04	0.58
1:A:1:MET:HE1	1:A:130:ILE:HD11	1.87	0.57
1:D:59:GLU:OE2	1:D:74:TYR:OH	2.21	0.57
1:B:56:LEU:HA	1:B:132:LYS:HE2	1.87	0.56
1:D:2:GLN:O	1:D:6:GLU:HG3	2.06	0.56
1:A:116:LEU:HD21	1:A:214:PHE:CE1	2.41	0.56
1:C:112:ASN:HD22	1:C:220:GLU:HB2	1.71	0.55
1:B:206:LEU:C	1:B:206:LEU:HD23	2.31	0.55
1:B:42:ALA:O	1:B:46:MET:HG2	2.07	0.54
1:D:65:ILE:HG23	1:D:133:ILE:HG13	1.88	0.54
1:D:187:GLU:O	1:D:191:GLN:HG3	2.08	0.54
1:D:24:MET:HE3	1:D:37:TRP:NE1	2.23	0.53
1:D:112:ASN:HD22	1:D:216:GLN:C	2.18	0.53
1:C:187:GLU:O	1:C:191:GLN:NE2	2.41	0.52
1:C:112:ASN:ND2	1:C:216:GLN:O	2.42	0.52
1:C:197:GLU:O	1:C:201:GLN:HG2	2.10	0.52
1:C:170:ASP:OD2	1:C:170:ASP:N	2.43	0.51
1:A:84:LEU:O	1:A:87:LEU:HB2	2.11	0.51
1:B:27:GLN:H	1:B:27:GLN:HE21	1.59	0.51
1:D:38:ALA:N	1:D:39:PRO:CD	2.74	0.51
1:D:75:GLU:OE2	1:D:179:HIS:NE2	2.39	0.51
1:B:1:MET:HE1	1:B:130:ILE:HD11	1.94	0.50
1:B:183:LEU:O	1:B:186:ILE:HG13	2.12	0.50
1:D:24:MET:O	1:D:34:ARG:HD2	2.10	0.50
1:C:178:GLY:O	1:C:182:SER:OG	2.29	0.50
1:D:232:GLN:N	1:D:232:GLN:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASN:ND2	1:C:220:GLU:HB2	2.26	0.50
1:A:119:GLN:HE21	1:A:119:GLN:HA	1.77	0.49
1:D:119:GLN:NE2	1:D:209:ASN:HB3	2.27	0.49
1:D:167:TYR:OH	3:D:303:TRP:OXT	2.29	0.49
1:C:156:GLU:O	1:C:159:ALA:HB3	2.12	0.49
1:A:97:ASN:HB3	1:D:93:ASP:OD1	2.13	0.49
1:C:103:LYS:O	1:C:107:SER:HB3	2.13	0.49
1:B:90:LEU:HD11	1:B:157:ILE:HG21	1.96	0.48
1:A:33:GLN:OE1	1:A:230:ILE:HG23	2.13	0.48
1:C:16:ALA:HB2	1:C:145:ILE:HD12	1.96	0.48
1:A:27:GLN:HE21	1:A:27:GLN:N	2.11	0.48
1:B:171:PHE:N	1:B:171:PHE:CD2	2.82	0.48
1:C:44:PHE:HA	1:C:117:ASN:HD21	1.79	0.47
1:C:176:GLU:HA	1:C:176:GLU:OE1	2.14	0.47
1:A:224:TYR:O	1:A:227:LYS:HG2	2.14	0.47
1:D:144:ASN:C	1:D:144:ASN:HD22	2.22	0.47
1:A:137:GLU:O	1:A:141:SER:OG	2.29	0.47
1:A:98:PHE:O	1:A:101:ALA:N	2.48	0.47
1:B:178:GLY:O	1:B:182:SER:OG	2.31	0.47
1:A:102:LEU:O	1:A:103:LYS:C	2.58	0.47
1:D:212:THR:HG23	1:D:216:GLN:HE21	1.80	0.47
1:B:23:PHE:CE1	1:B:34:ARG:HA	2.50	0.47
1:C:112:ASN:HD22	1:C:220:GLU:CB	2.27	0.47
1:C:217:PHE:O	1:C:221:LEU:HG	2.15	0.47
1:A:93:ASP:OD2	1:D:99:SER:OG	2.28	0.46
1:D:24:MET:CE	1:D:37:TRP:HZ2	2.28	0.46
1:A:188:GLN:NE2	4:A:402:HOH:O	2.47	0.46
1:B:63:ASP:OD1	1:B:65:ILE:N	2.48	0.46
1:C:109:GLU:O	1:C:220:GLU:CD	2.58	0.46
1:D:24:MET:HE1	1:D:37:TRP:HZ2	1.79	0.46
1:A:12:LYS:HE3	1:A:145:ILE:HD11	1.98	0.46
1:A:79:HIS:CE1	1:A:176:GLU:OE2	2.69	0.46
1:A:188:GLN:O	1:A:191:GLN:HB3	2.15	0.46
1:A:150:ALA:O	1:A:153:ILE:HB	2.17	0.45
1:A:146:MET:HG2	3:A:303:TRP:CZ3	2.51	0.45
1:B:15:PHE:O	1:B:18:VAL:HG22	2.16	0.45
1:A:1:MET:CE	1:A:130:ILE:HD11	2.46	0.45
1:A:47:ASN:ND2	1:D:106:TRP:HE1	2.14	0.45
1:A:74:TYR:O	1:A:78:HIS:CE1	2.70	0.45
1:C:65:ILE:HG23	1:C:133:ILE:HG13	1.98	0.45
1:B:130:ILE:O	1:B:130:ILE:HD13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:LEU:HD22	1:A:168:PHE:CD1	2.52	0.45
1:A:82:TRP:HB3	1:A:166:ARG:HB3	1.99	0.45
1:D:44:PHE:HA	1:D:117:ASN:HD21	1.82	0.45
1:C:26:ASP:OD1	1:C:26:ASP:C	2.59	0.44
1:C:227:LYS:HE3	1:C:227:LYS:HB2	1.84	0.44
1:B:24:MET:HB3	1:B:153:ILE:HD11	2.00	0.44
1:D:37:TRP:HA	1:D:224:TYR:CD1	2.51	0.44
1:A:10:GLN:O	1:A:13:GLN:HB3	2.18	0.44
1:D:56:LEU:HD13	1:D:136:ILE:HD11	2.00	0.44
1:B:200:ARG:CG	1:B:200:ARG:HH11	2.29	0.44
1:A:86:ASP:O	1:A:90:LEU:HB2	2.18	0.44
1:A:230:ILE:H	1:A:230:ILE:HD13	1.82	0.44
1:D:18:VAL:HG22	1:D:19:PRO:CD	2.48	0.44
1:D:1:MET:CE	1:D:195:LEU:HD21	2.48	0.43
1:D:37:TRP:CE3	1:D:37:TRP:C	2.96	0.43
1:C:167:TYR:CE2	1:C:172:HIS:CE1	3.06	0.43
1:B:1:MET:HE1	1:B:130:ILE:CD1	2.49	0.43
1:D:0:GLY:HA2	1:D:3:GLN:HE22	1.83	0.43
1:A:51:LEU:HD22	1:A:120:LEU:HD13	2.00	0.43
1:A:142:THR:HG21	1:A:214:PHE:CD2	2.53	0.43
1:B:86:ASP:O	1:B:90:LEU:HB2	2.19	0.42
1:A:206:LEU:C	1:A:206:LEU:CD2	2.91	0.42
1:D:23:PHE:CD1	1:D:23:PHE:C	2.97	0.42
1:B:184:SER:HA	1:B:187:GLU:HB2	2.00	0.42
1:A:157:ILE:O	1:A:161:THR:HG22	2.19	0.42
1:C:186:ILE:O	1:C:189:PHE:N	2.53	0.42
1:D:170:ASP:OD2	1:D:170:ASP:N	2.52	0.42
1:C:136:ILE:HA	1:C:139:THR:OG1	2.20	0.42
1:B:36:ALA:O	1:B:39:PRO:HD2	2.19	0.42
1:B:138:VAL:HG11	1:B:210:LEU:HB3	2.02	0.42
1:D:7:LEU:HD22	1:D:11:LYS:HG3	2.01	0.42
1:A:227:LYS:HG3	1:A:228:HIS:CD2	2.54	0.42
1:D:37:TRP:C	1:D:39:PRO:HD2	2.45	0.42
1:B:103:LYS:O	1:B:107:SER:HB3	2.20	0.41
1:D:7:LEU:HD12	1:D:204:PHE:CD1	2.54	0.41
1:D:119:GLN:HE21	1:D:209:ASN:HB3	1.85	0.41
1:D:194:GLN:C	1:D:195:LEU:HD22	2.45	0.41
1:D:218:THR:O	1:D:221:LEU:HB2	2.20	0.41
1:D:0:GLY:CA	1:D:3:GLN:HE22	2.33	0.41
1:A:138:VAL:HG22	1:A:211:PHE:CE2	2.55	0.41
1:D:18:VAL:HG22	1:D:19:PRO:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:TRP:CZ2	1:D:146:MET:HE1	2.56	0.41
1:D:176:GLU:OE2	1:D:176:GLU:HA	2.20	0.41
1:B:179:HIS:O	1:B:183:LEU:HD13	2.20	0.41
1:A:119:GLN:HA	1:A:119:GLN:NE2	2.36	0.41
1:A:97:ASN:HB2	1:A:100:GLU:HG2	2.02	0.41
1:A:130:ILE:O	1:A:130:ILE:HD13	2.21	0.41
1:B:86:ASP:OD2	1:B:165:CYS:SG	2.78	0.41
1:A:72:HIS:NE2	1:A:182:SER:HB2	2.36	0.41
1:A:84:LEU:O	1:A:87:LEU:N	2.54	0.41
1:B:87:LEU:HD22	1:B:87:LEU:HA	1.93	0.41
1:A:37:TRP:O	1:A:40:CYS:N	2.53	0.41
1:D:1:MET:HB2	1:D:195:LEU:HD21	2.02	0.41
1:D:37:TRP:O	1:D:40:CYS:HB3	2.21	0.41
1:A:188:GLN:O	1:A:191:GLN:CB	2.69	0.40
1:B:106:TRP:CE2	1:C:46:MET:HB3	2.57	0.40
1:C:30:ASN:ND2	1:C:230:ILE:CD1	2.84	0.40
1:B:37:TRP:CE3	1:B:221:LEU:HD13	2.56	0.40
1:B:98:PHE:O	1:B:101:ALA:N	2.54	0.40
1:D:24:MET:CE	1:D:37:TRP:CZ2	3.04	0.40
1:D:206:LEU:C	1:D:206:LEU:HD23	2.46	0.40
1:D:98:PHE:O	1:D:101:ALA:HB3	2.22	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	223/248 (90%)	203 (91%)	20 (9%)	0	100 100
1	B	226/248 (91%)	213 (94%)	12 (5%)	1 (0%)	30 39
1	C	232/248 (94%)	217 (94%)	13 (6%)	2 (1%)	14 20
1	D	233/248 (94%)	217 (93%)	16 (7%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	914/992 (92%)	850 (93%)	61 (7%)	3 (0%)	36 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	GLU
1	C	230	ILE
1	C	160	ILE

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	208/216 (96%)	183 (88%)	25 (12%)	5 5
1	B	209/216 (97%)	189 (90%)	20 (10%)	8 9
1	C	215/216 (100%)	192 (89%)	23 (11%)	6 7
1	D	215/216 (100%)	183 (85%)	32 (15%)	3 2
All	All	847/864 (98%)	747 (88%)	100 (12%)	5 5

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	6	GLU
1	B	7	LEU
1	B	27	GLN
1	B	28	SER
1	B	47	ASN
1	B	68	LEU
1	B	75	GLU
1	B	87	LEU
1	B	90	LEU
1	B	130	ILE
1	B	152	GLU

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Mol	Chain	Res	Type
1	B	163	LYS
1	B	171	PHE
1	B	173	LEU
1	B	181	THR
1	B	186	ILE
1	B	190	LEU
1	B	200	ARG
1	B	205	GLU
1	C	1	MET
1	C	2	GLN
1	C	4	VAL
1	C	7	LEU
1	C	61	THR
1	C	65	ILE
1	C	68	LEU
1	C	75	GLU
1	C	90	LEU
1	C	94	LYS
1	C	95	SER
1	C	130	ILE
1	C	133	ILE
1	C	136	ILE
1	C	157	ILE
1	C	166	ARG
1	C	170	ASP
1	C	171	PHE
1	C	173	LEU
1	C	182	SER
1	C	190	LEU
1	C	232	GLN
1	C	234	LEU
1	A	3	GLN
1	A	6	GLU
1	A	7	LEU
1	A	27	GLN
1	A	32	ARG
1	A	47	ASN
1	A	57	ARG
1	A	68	LEU
1	A	130	ILE
1	A	152	GLU
1	A	158	LYS

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Mol	Chain	Res	Type
1	A	165	CYS
1	A	166	ARG
1	A	173	LEU
1	A	175	VAL
1	A	181	THR
1	A	183	LEU
1	A	186	ILE
1	A	190	LEU
1	A	198	GLU
1	A	201	GLN
1	A	216	GLN
1	A	227	LYS
1	A	229	GLN
1	A	230	ILE
1	D	3	GLN
1	D	7	LEU
1	D	9	GLU
1	D	18	VAL
1	D	23	PHE
1	D	29	ILE
1	D	53	LYS
1	D	59	GLU
1	D	62	ASN
1	D	75	GLU
1	D	94	LYS
1	D	97	ASN
1	D	100	GLU
1	D	111	LYS
1	D	130	ILE
1	D	133	ILE
1	D	136	ILE
1	D	142	THR
1	D	157	ILE
1	D	158	LYS
1	D	161	THR
1	D	166	ARG
1	D	170	ASP
1	D	173	LEU
1	D	182	SER
1	D	186	ILE
1	D	205	GLU
1	D	212	THR

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Mol	Chain	Res	Type
1	D	227	LYS
1	D	231	GLU
1	D	232	GLN
1	D	234	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	13	GLN
1	B	27	GLN
1	B	47	ASN
1	B	97	ASN
1	B	112	ASN
1	B	117	ASN
1	B	162	GLN
1	B	174	ASN
1	C	17	GLN
1	C	27	GLN
1	C	47	ASN
1	C	52	ASN
1	C	72	HIS
1	C	112	ASN
1	C	117	ASN
1	C	174	ASN
1	C	188	GLN
1	C	228	HIS
1	C	232	GLN
1	A	27	GLN
1	A	30	ASN
1	A	47	ASN
1	A	119	GLN
1	A	174	ASN
1	A	201	GLN
1	A	228	HIS
1	A	229	GLN
1	D	2	GLN
1	D	3	GLN
1	D	112	ASN
1	D	117	ASN
1	D	174	ASN
1	D	191	GLN
1	D	201	GLN

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Mol	Chain	Res	Type
1	D	209	ASN
1	D	216	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	TRP	C	303	2	14,16,16	0.48	0	20,22,22	1.11	3 (15%)
3	TRP	B	303	2	14,16,16	0.65	0	20,22,22	1.10	3 (15%)
3	TRP	D	303	2	14,16,16	0.61	0	20,22,22	0.70	0
3	TRP	A	303	2	14,16,16	0.66	0	20,22,22	1.07	2 (10%)

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
3	TRP	C	303	2	-	1/8/8/8	0/2/2/2
3	TRP	B	303	2	-	1/8/8/8	0/2/2/2
3	TRP	D	303	2	-	0/8/8/8	0/2/2/2
3	TRP	A	303	2	-	2/8/8/8	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	303	TRP	OXT-C-O	-3.19	116.84	124.09
3	C	303	TRP	OXT-C-CA	3.15	124.12	113.38
3	B	303	TRP	OXT-C-O	-2.85	117.63	124.09
3	B	303	TRP	OXT-C-CA	2.54	122.05	113.38
3	A	303	TRP	OXT-C-CA	2.52	121.98	113.38
3	C	303	TRP	O-C-CA	-2.24	114.22	122.14
3	B	303	TRP	CA-CB-CG	2.22	117.73	113.50
3	C	303	TRP	CA-CB-CG	2.01	117.33	113.50

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	303	TRP	OXT-C-CA-CB
3	A	303	TRP	O-C-CA-CB
3	B	303	TRP	N-CA-CB-CG
3	C	303	TRP	O-C-CA-N

There are no ring outliers.

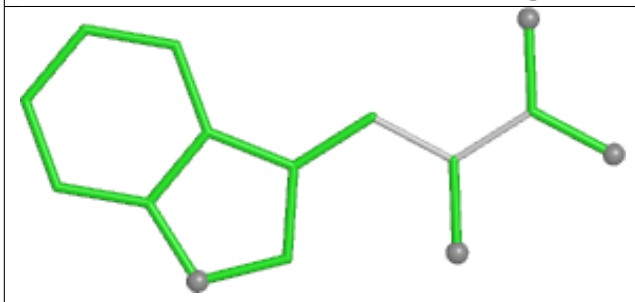
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	303	TRP	1	0
3	A	303	TRP	1	0

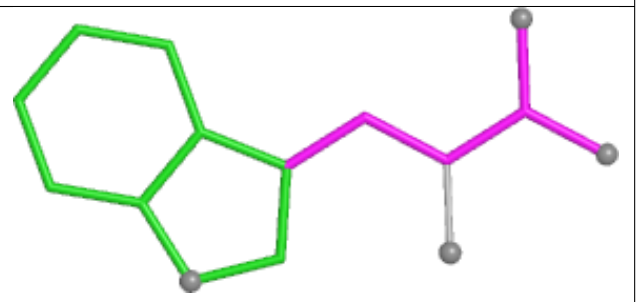
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

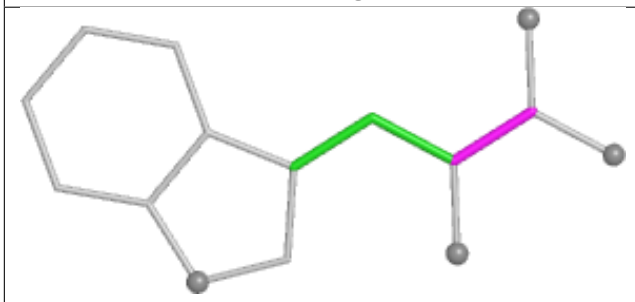
Ligand TRP C 303



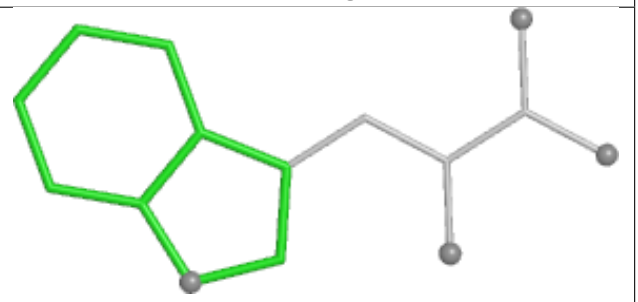
Bond lengths



Bond angles

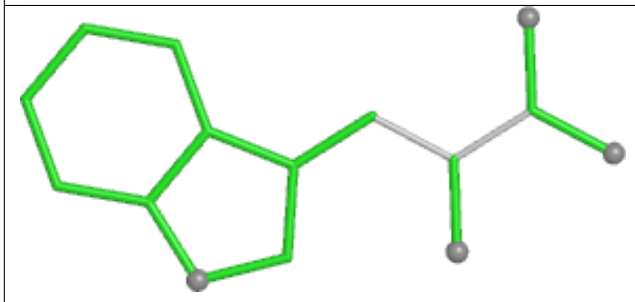


Torsions

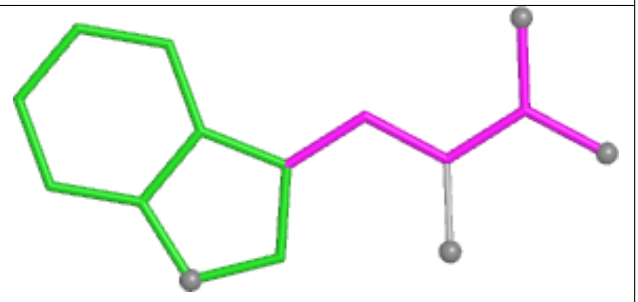


Rings

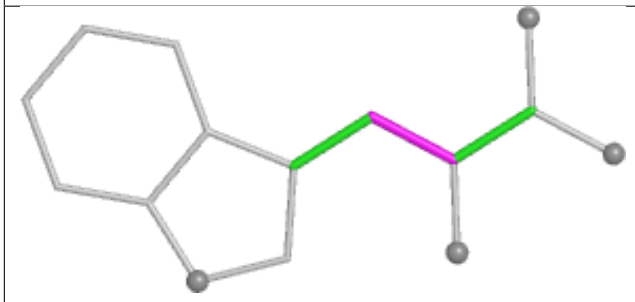
Ligand TRP B 303



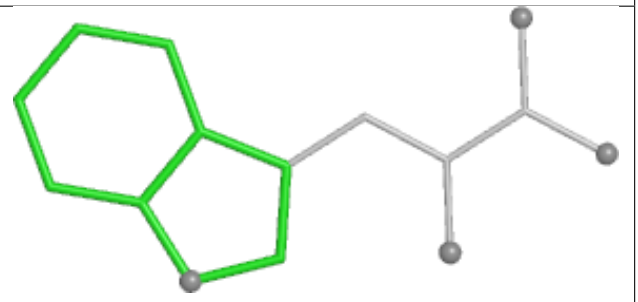
Bond lengths



Bond angles

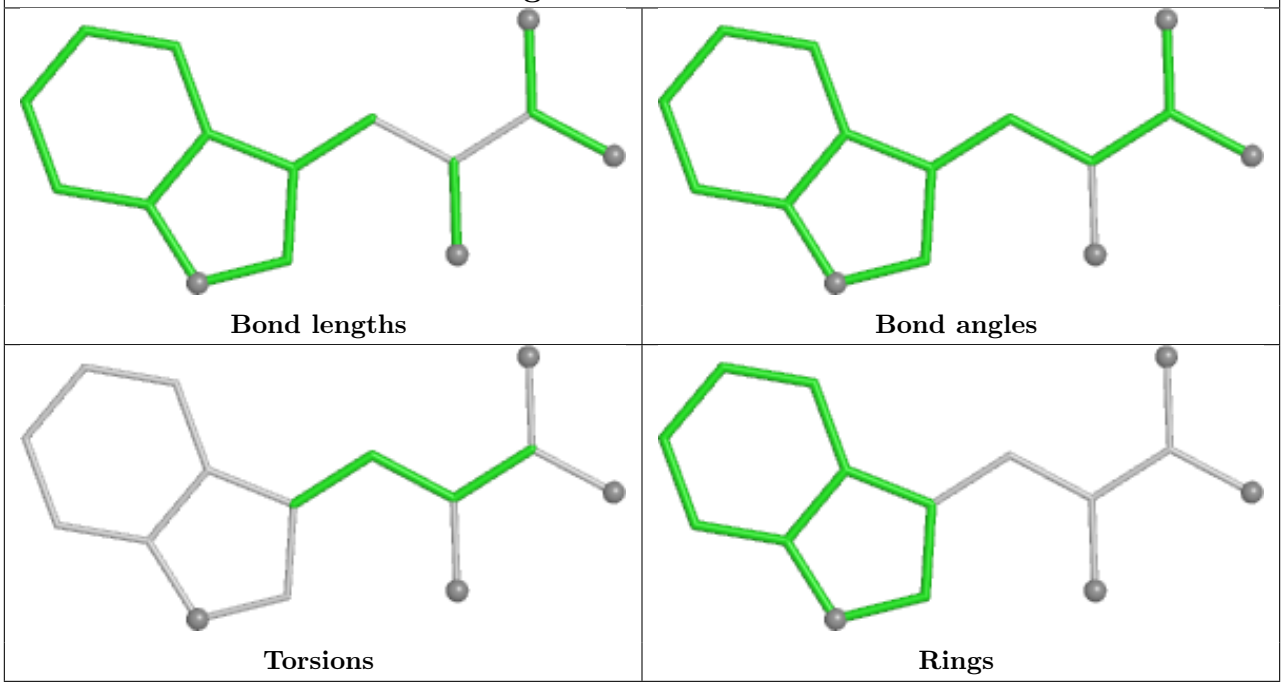


Torsions

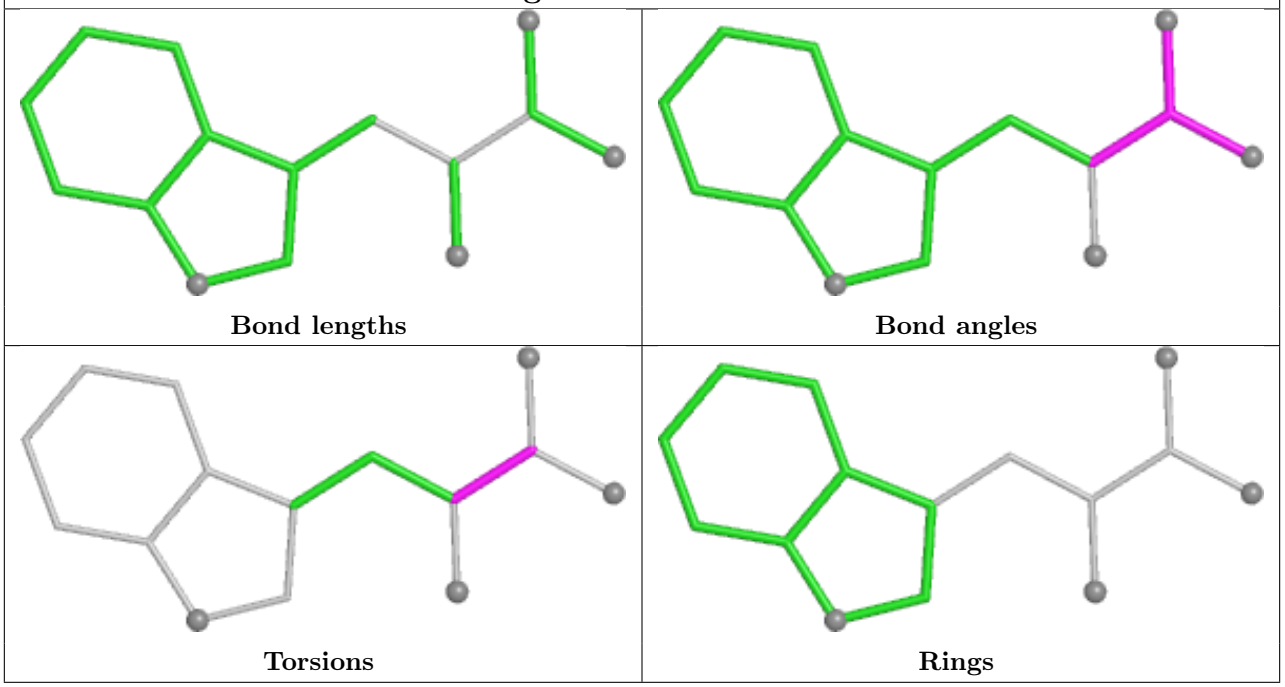


Rings

Ligand TRP D 303



Ligand TRP A 303



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	227/248 (91%)	-0.36	0	100	100	45, 77, 110, 134	0
1	B	228/248 (91%)	-0.36	0	100	100	42, 68, 98, 133	0
1	C	234/248 (94%)	-0.52	0	100	100	41, 61, 98, 118	0
1	D	235/248 (94%)	-0.36	0	100	100	45, 76, 107, 134	0
All	All	924/992 (93%)	-0.40	0	100	100	41, 71, 105, 134	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands

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	TRP	A	303	15/15	0.92	0.07	49,54,79,84	0
3	TRP	B	303	15/15	0.95	0.06	37,44,69,77	0
3	TRP	D	303	15/15	0.95	0.07	54,60,65,65	0
3	TRP	C	303	15/15	0.97	0.05	39,47,50,51	0

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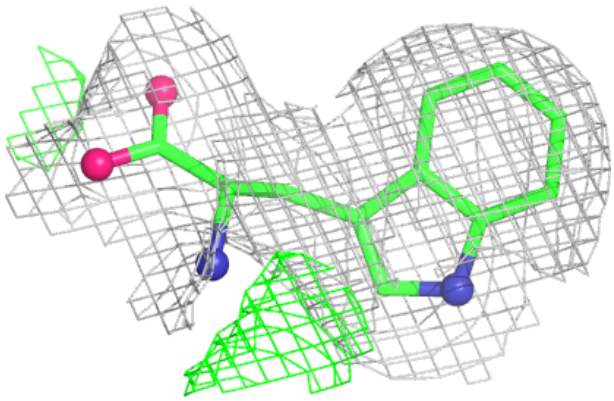
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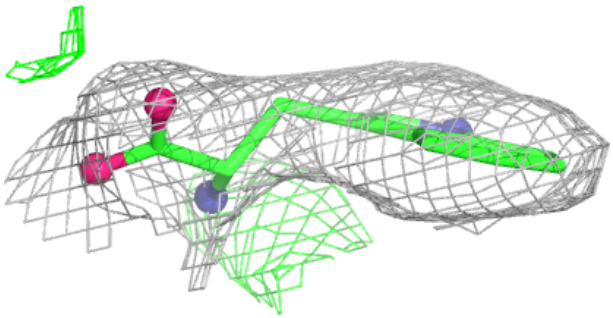
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE2	A	302	1/1	0.99	0.04	67,67,67,67	0
2	FE2	D	302	1/1	0.99	0.02	62,62,62,62	0
2	FE2	B	302	1/1	0.99	0.02	67,67,67,67	0
2	FE2	C	301	1/1	1.00	0.01	53,53,53,53	0
2	FE2	C	302	1/1	1.00	0.01	52,52,52,52	0
2	FE2	A	301	1/1	1.00	0.02	76,76,76,76	0
2	FE2	B	301	1/1	1.00	0.02	71,71,71,71	0
2	FE2	D	301	1/1	1.00	0.01	69,69,69,69	0

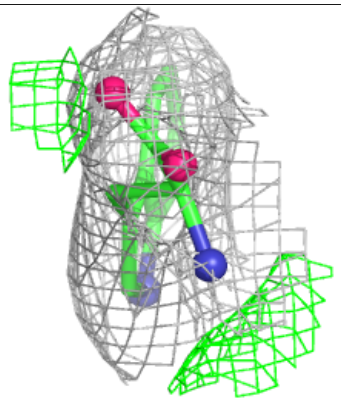
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TRP A 303:

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

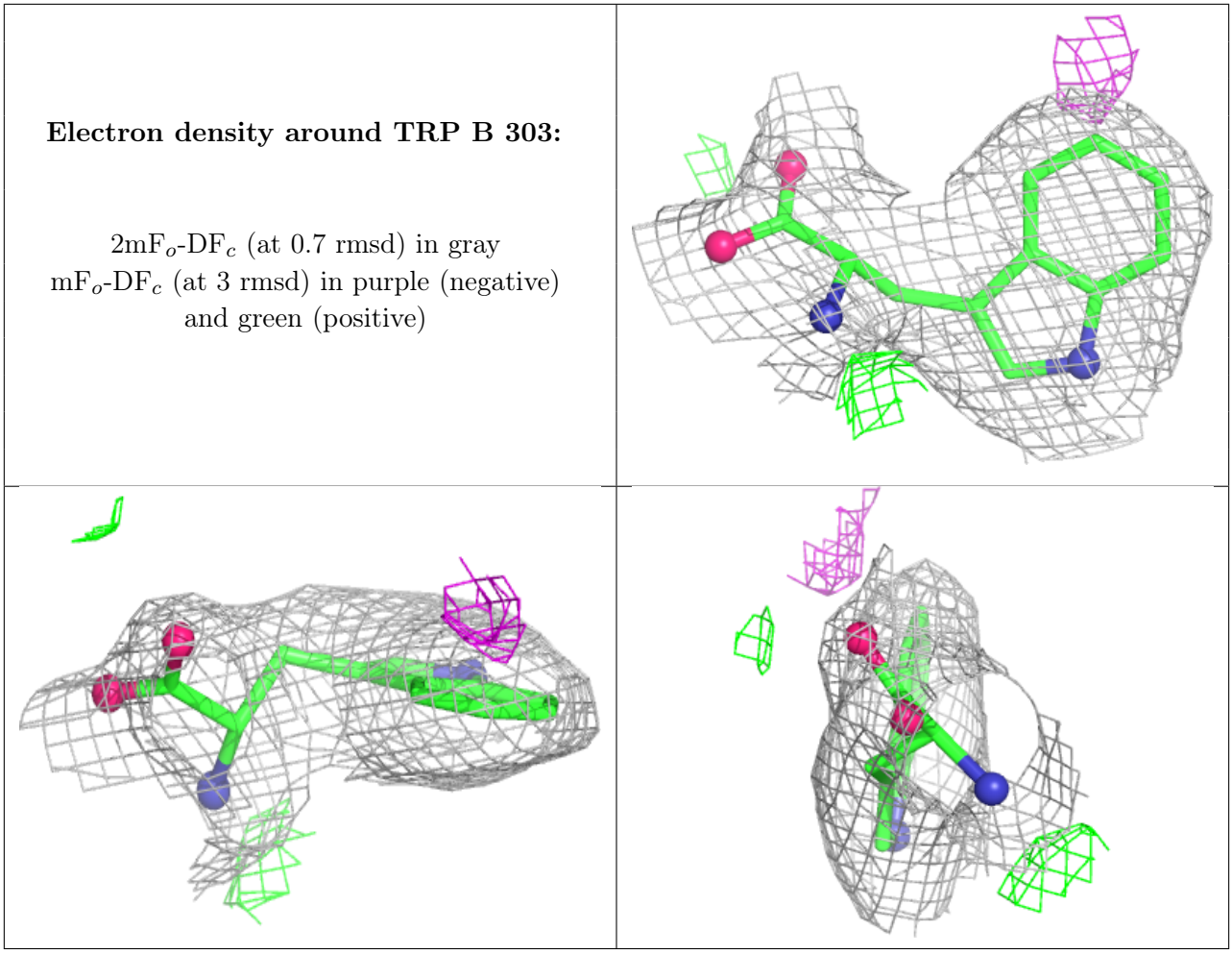






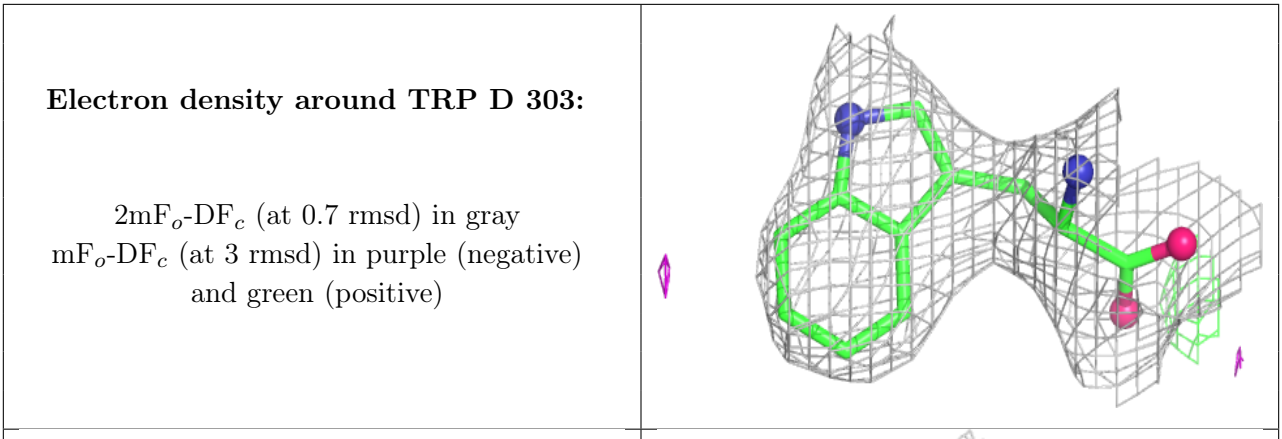
Electron density around TRP B 303:

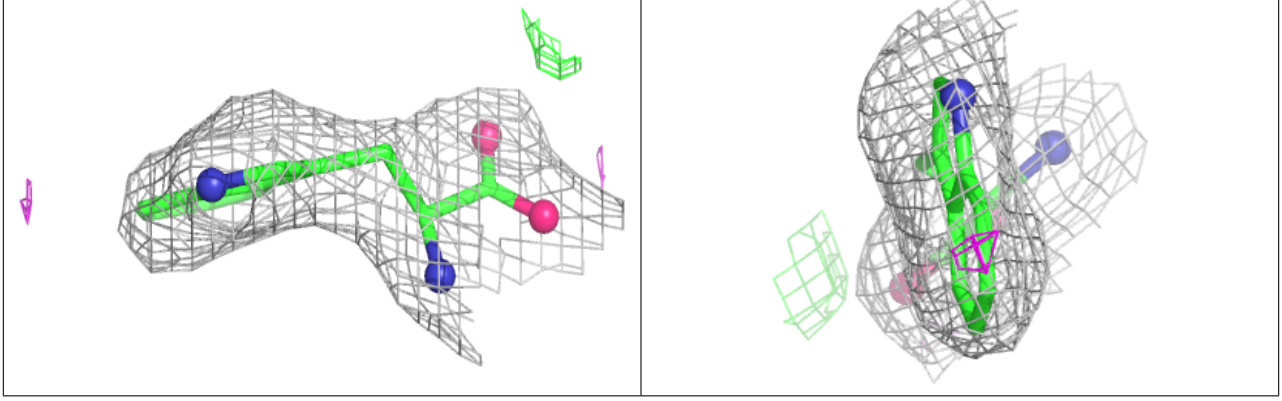
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around TRP D 303:

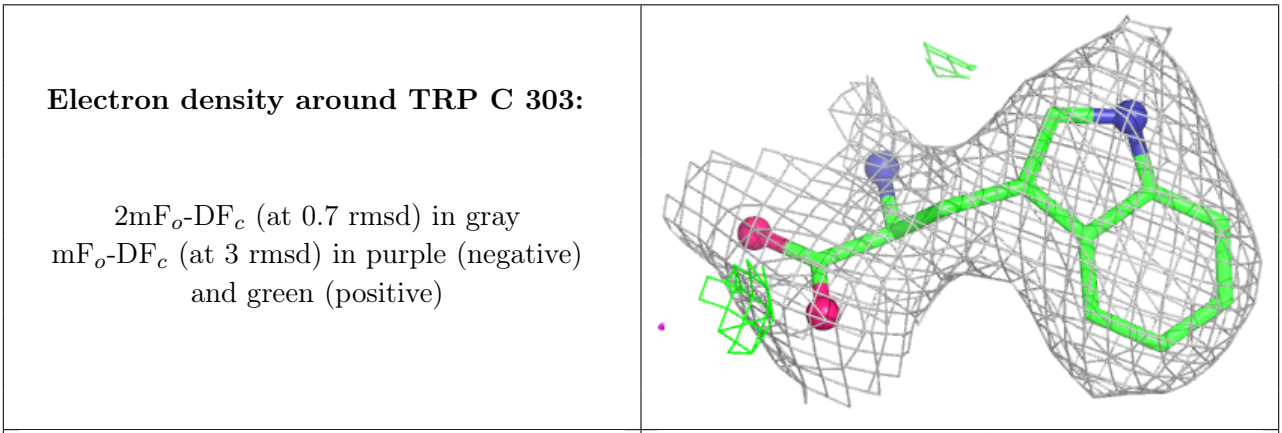
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

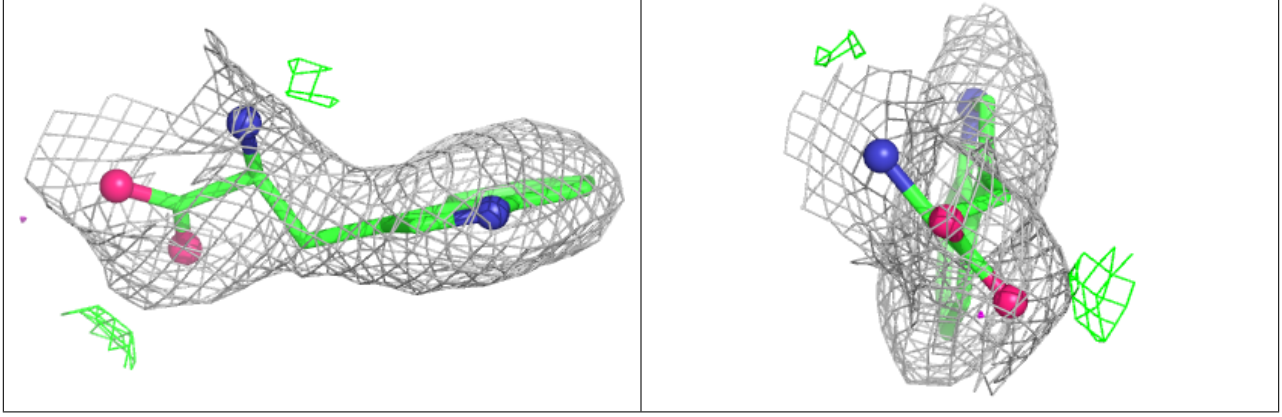




Electron density around TRP C 303:

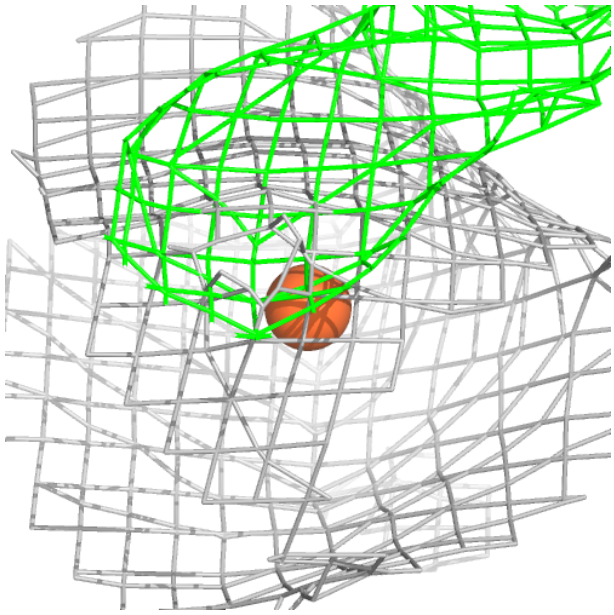
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

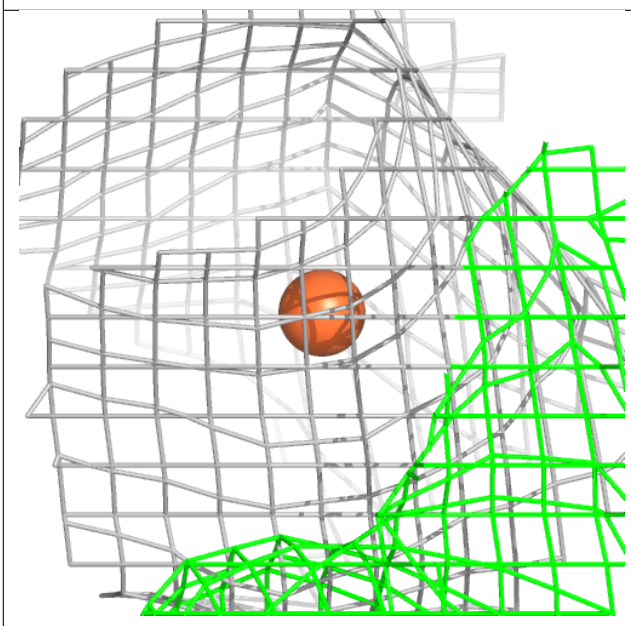


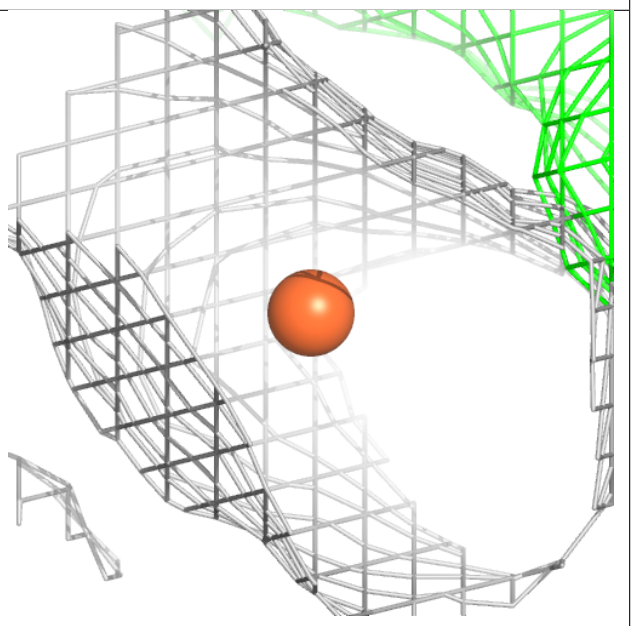


Electron density around FE2 A 302:

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

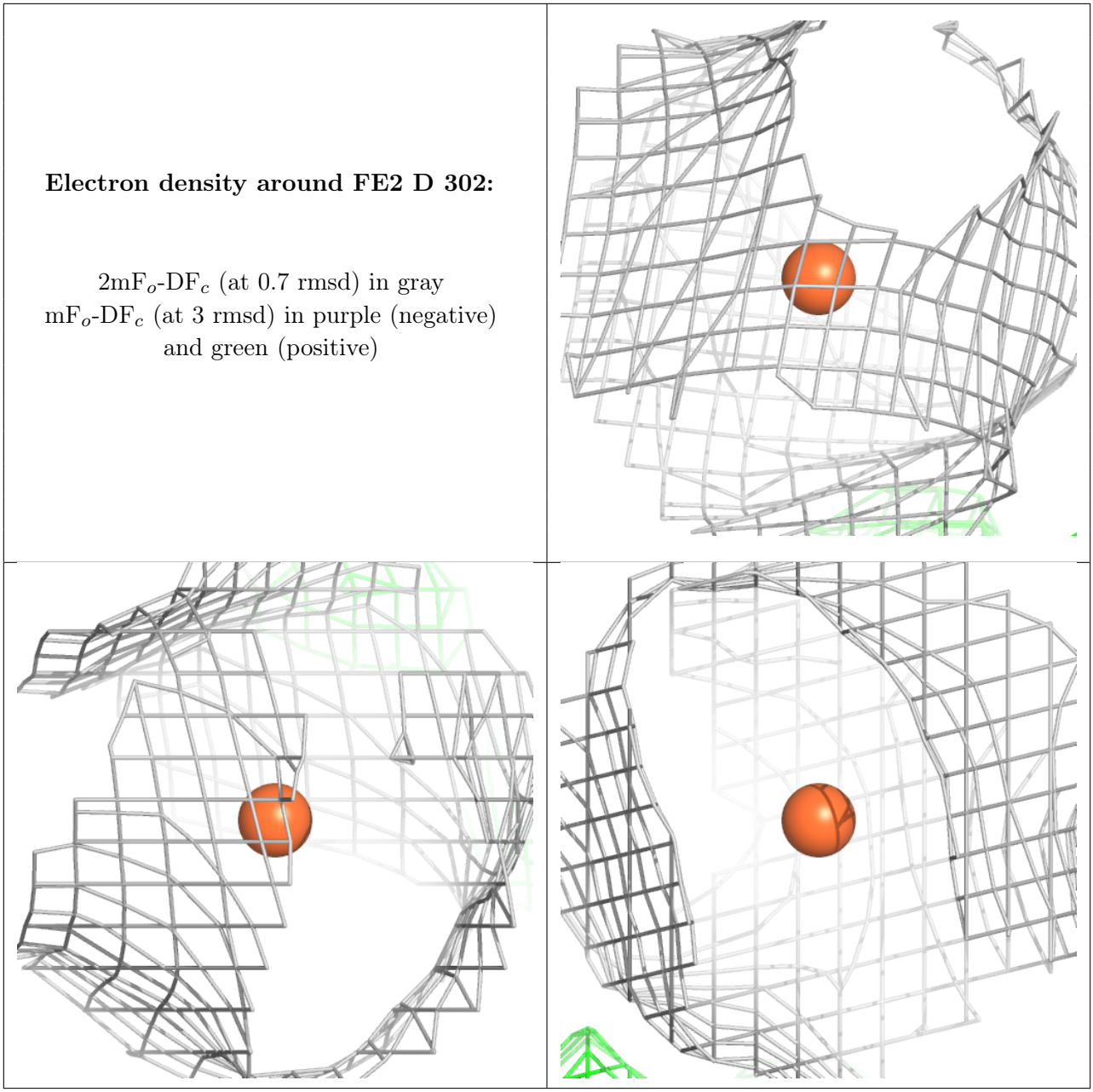






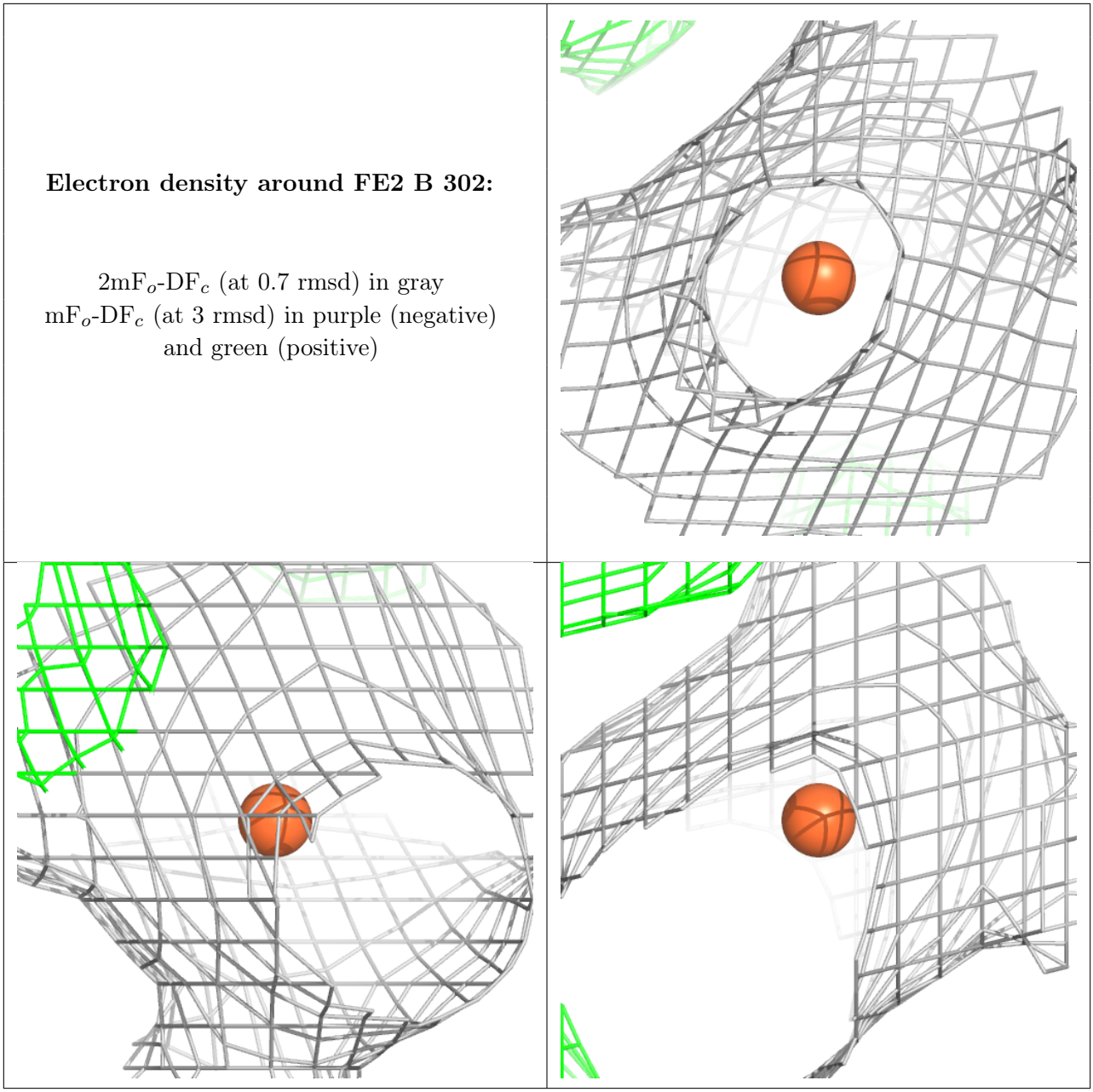
Electron density around FE2 D 302:

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



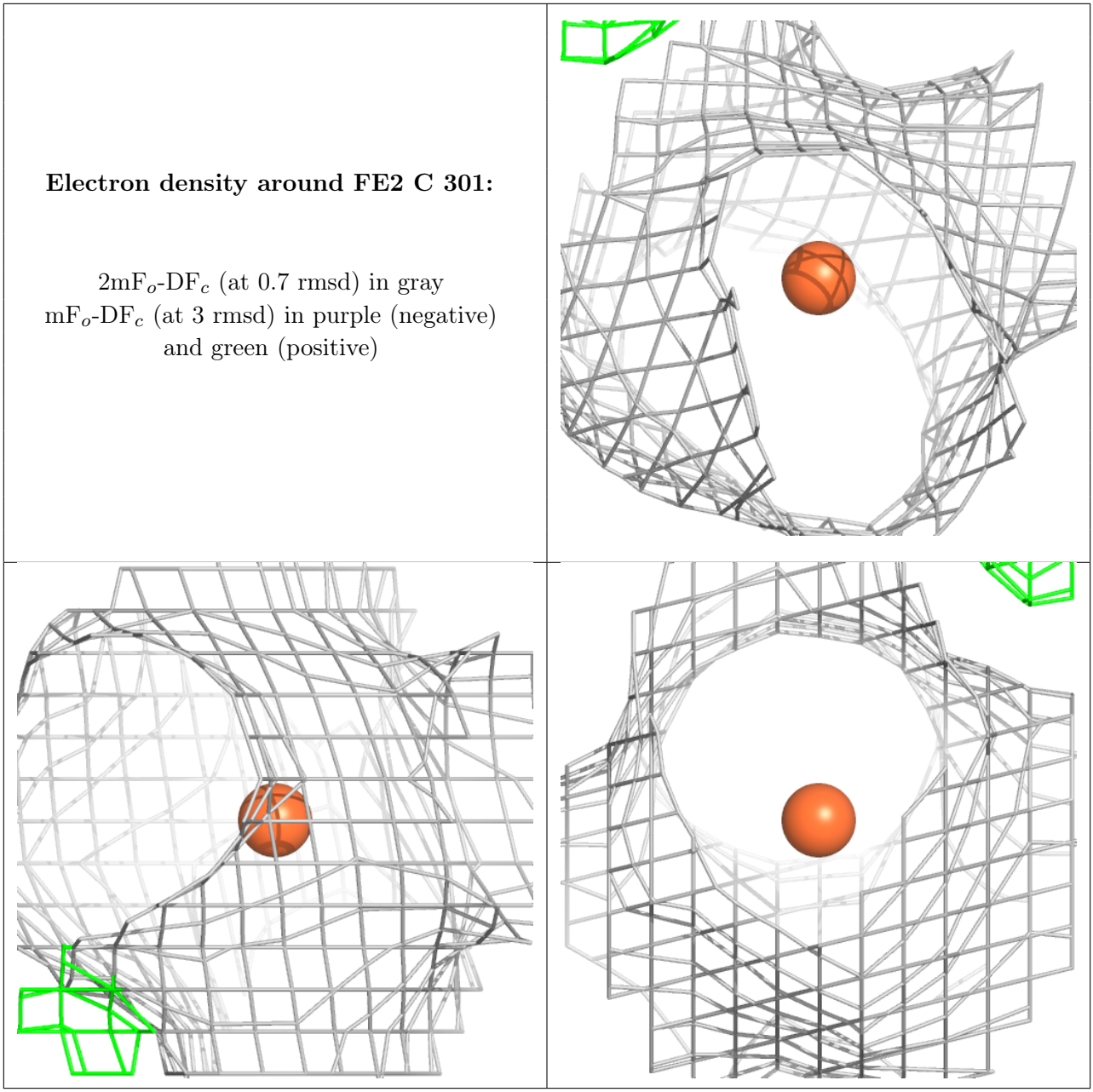
Electron density around FE2 B 302:

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



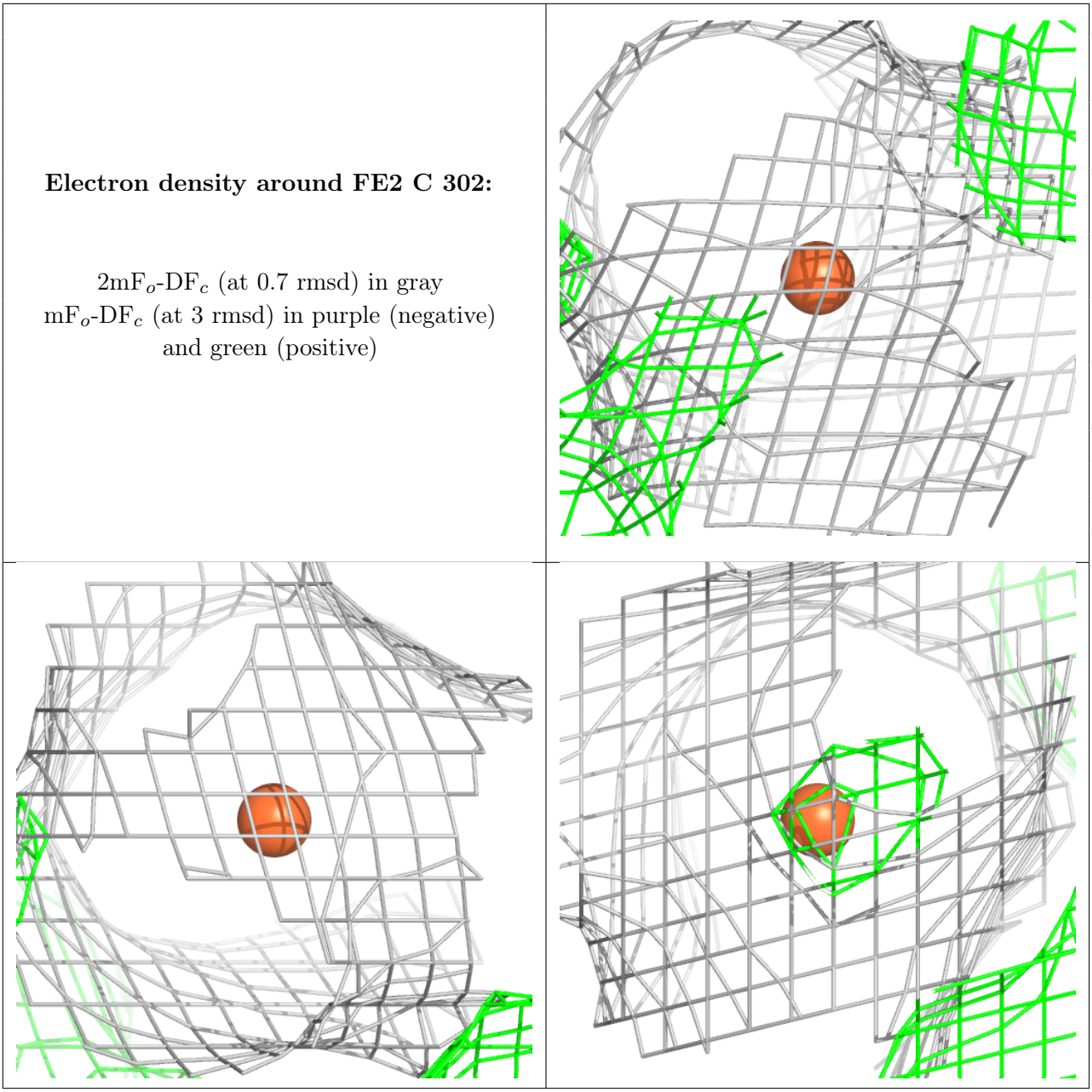
Electron density around FE2 C 301:

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



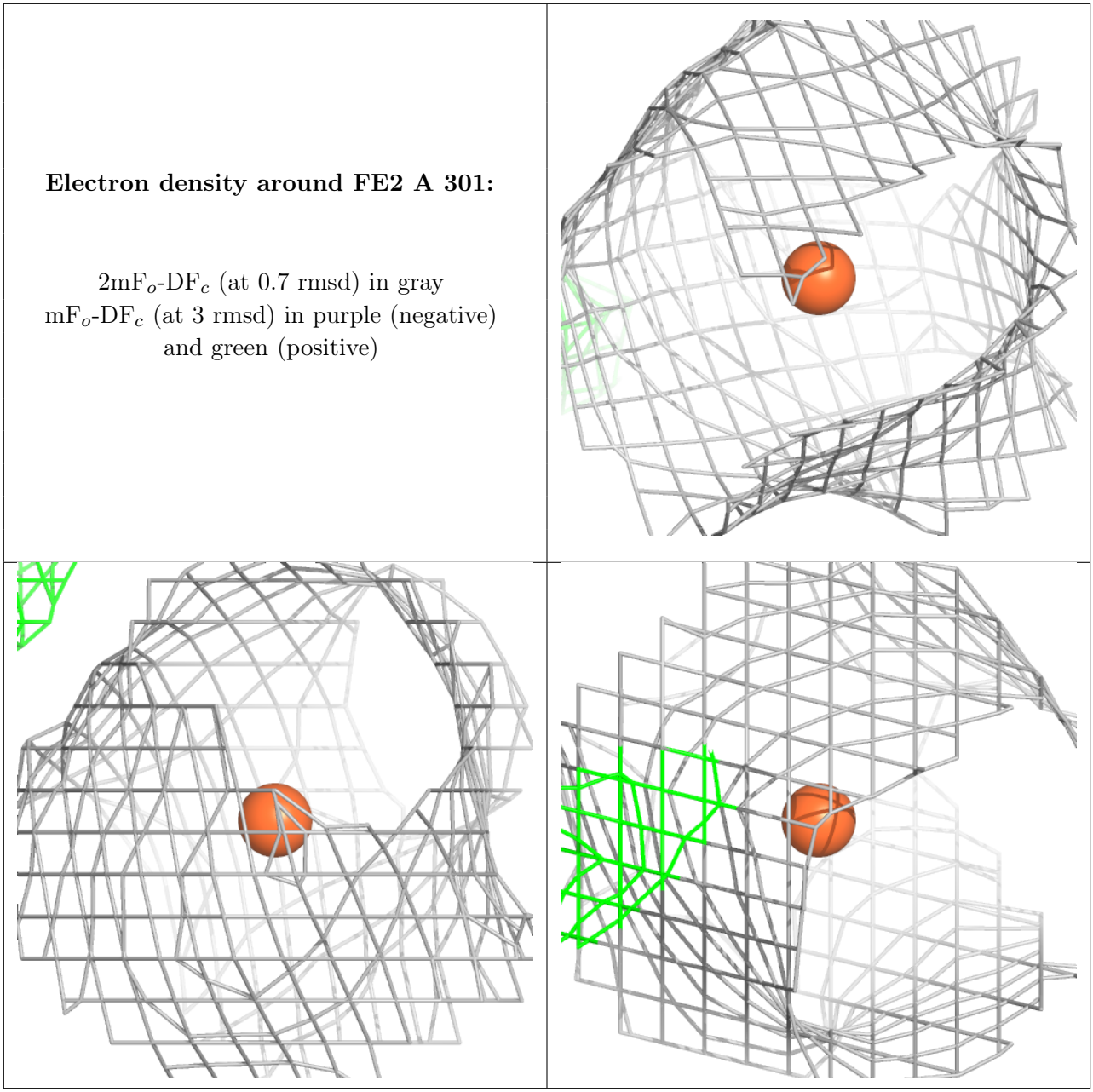
Electron density around FE2 C 302:

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



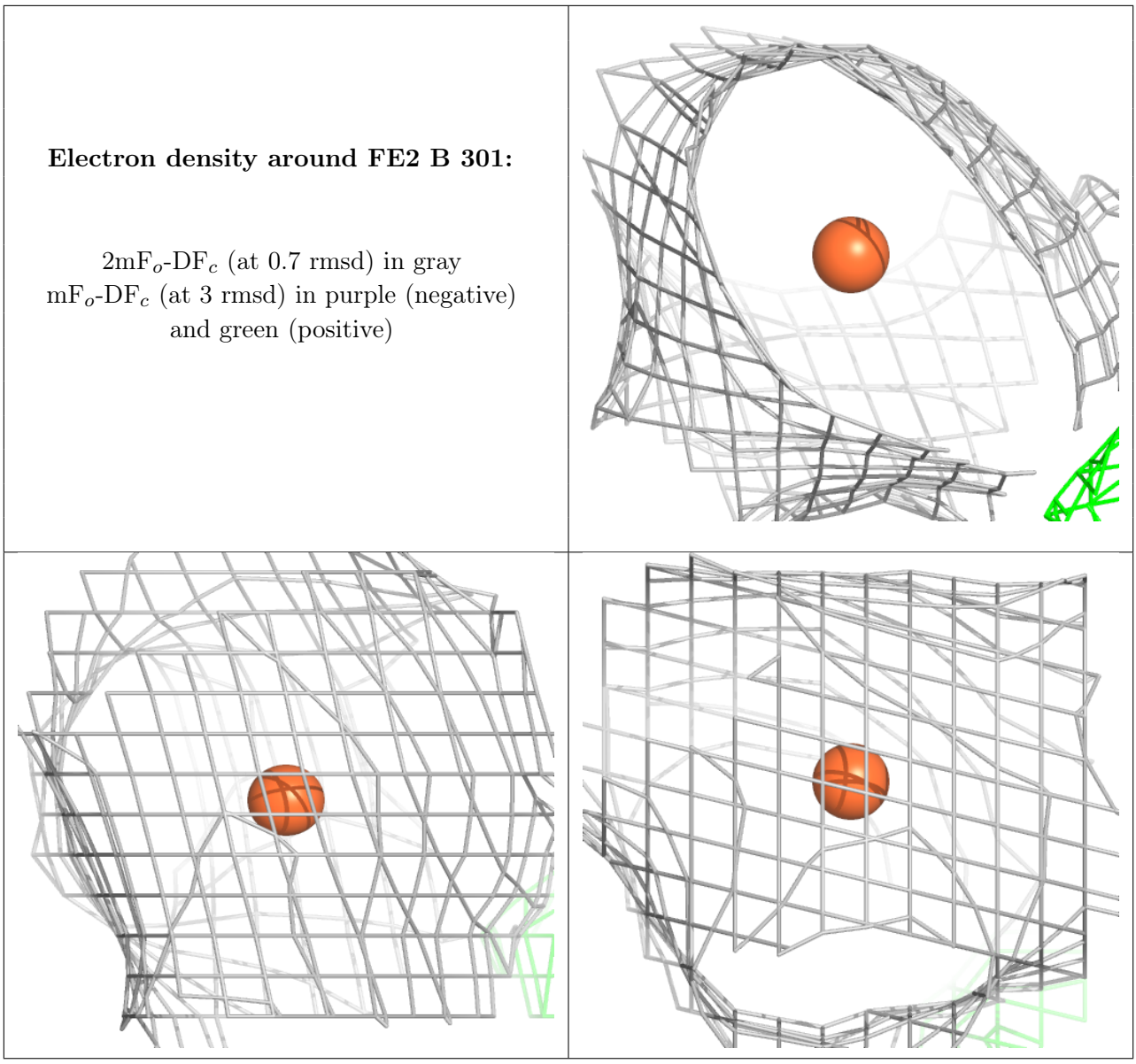
Electron density around FE2 A 301:

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



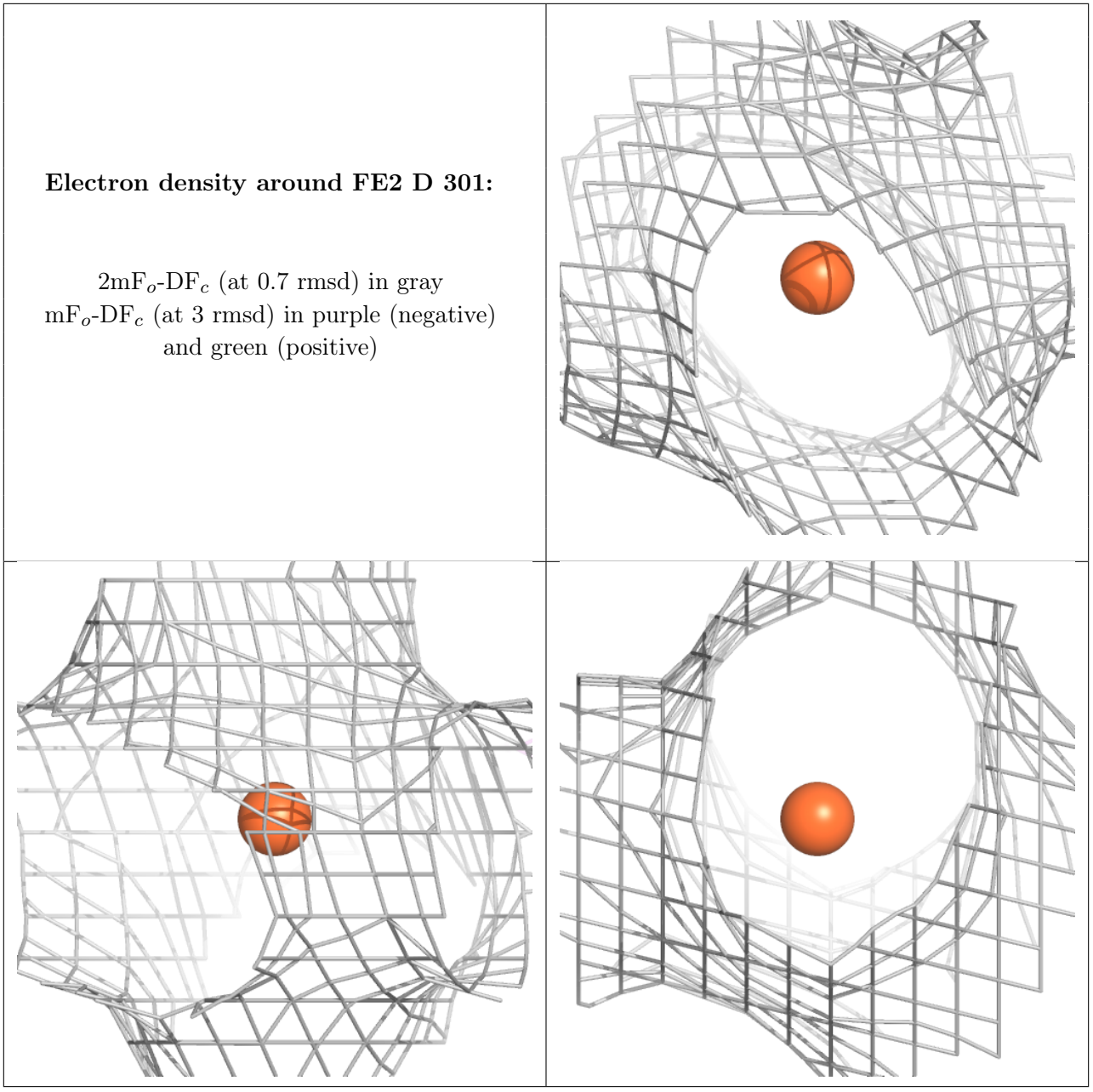
Electron density around FE2 B 301:

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



Electron density around FE2 D 301:

$2mF_o$-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.