



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 15, 2024 – 05:36 pm GMT

PDB ID : 8C41
Title : High resolution structure of the Streptococcus pneumoniae topoisomerase IV-DNA complex with the novel fluoroquinolone Delafloxacin
Authors : Najmudin, S.; Pan, X.S.; Wang, B.; Chayen, N.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2022-12-30
Resolution : 2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

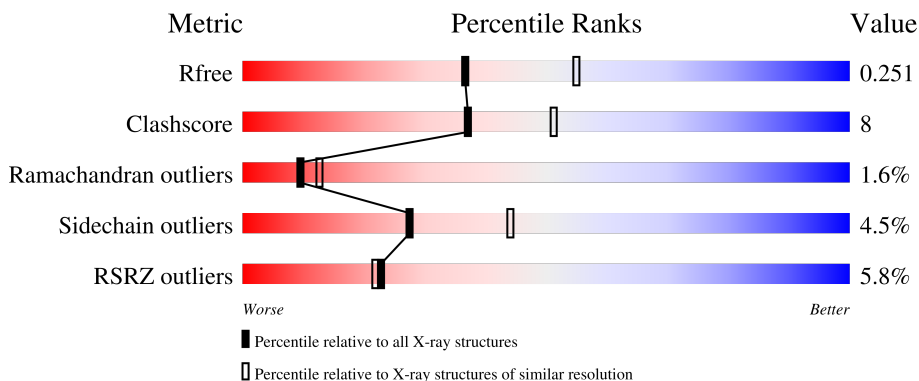
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


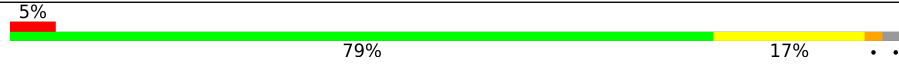
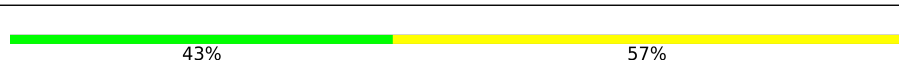
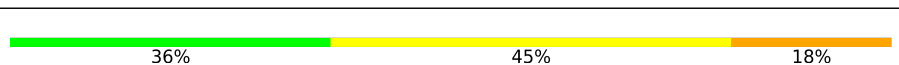
The reported resolution of this entry is 2.39 Å.

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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	742	 6% 74% 20%
1	B	742	 5% 79% 17%
2	E	7	 43% 57%
3	F	11	 36% 45% 18%

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Mol	Chain	Length	Quality of chain		
4	G	7			
5	H	11			

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 24852 atoms, of which 12136 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 Fused ParE30ParC55 CLEAVAGE COMPLEX of the TOPOISOMERASE IV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	720	11587	3629	5843	1000	1091	24	321	2	0
1	B	720	11549	3619	5819	996	1091	24	319	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(*CP*AP*TP*GP*AP*AP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
2	E	7	221	69	80	27	39	6	1	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
3	F	11	351	108	126	39	67	11	1	0	0

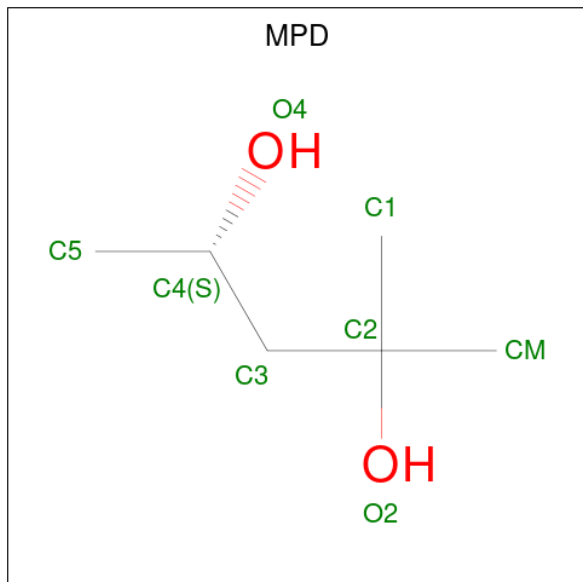
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*GP*CP*AP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
4	G	7	220	68	80	25	41	6	1	0	0

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
5	H	11	350	107	124	43	65	11	1	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
6	A	1	22	6	14	2	1	0
6	A	1	22	6	14	2	1	0
6	B	1	22	6	14	2	1	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

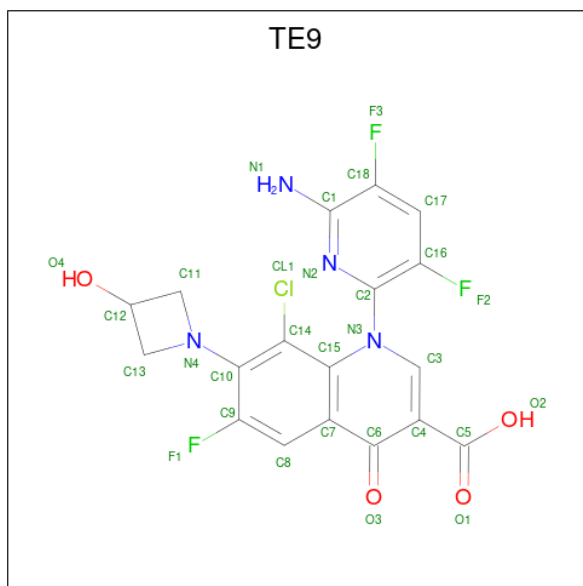
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
7	A	3	3	3	0	0
7	B	3	3	3	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
8	A	1	1	1	0	0
8	B	1	1	1	0	0

- Molecule 9 is delafloxacin (three-letter code: TE9) (formula: C₁₈H₁₂ClF₃N₄O₄) (labeled as

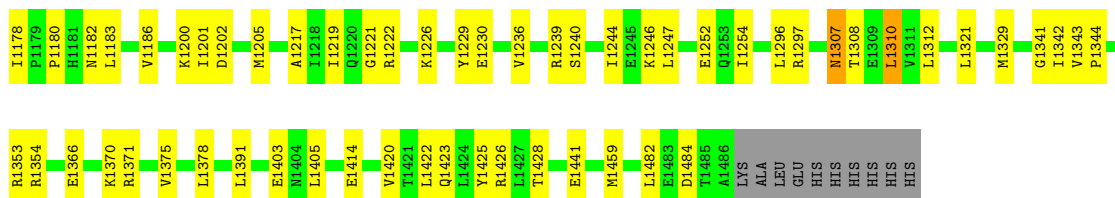
"Ligand of Interest" by depositor).



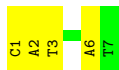
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	Cl	F	H	N			O
9	F	1	41	18	1	3	11	4	4	1	0
9	H	1	41	18	1	3	11	4	4	1	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	195	Total	O	0	0
			195	195		
10	B	195	Total	O	0	0
			195	195		
10	E	10	Total	O	0	0
			10	10		
10	F	7	Total	O	0	0
			7	7		
10	G	7	Total	O	0	0
			7	7		
10	H	4	Total	O	0	0
			4	4		



- Molecule 2: DNA (5'-D(*CP*AP*TP*GP*AP*AP*T)-3')



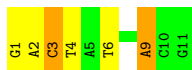
- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3')



- Molecule 4: DNA (5'-D(*CP*GP*TP*GP*CP*AP*T)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.47Å 157.47Å 212.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	115.01 – 2.39 114.75 – 2.39	Depositor EDS
% Data completeness (in resolution range)	58.9 (115.01-2.39) 58.9 (114.75-2.39)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.40Å)	Xtrriage
Refinement program	REFMAC 5.8.0352, PDB-REDO	Depositor
R, R_{free}	0.192 , 0.243 0.201 , 0.251	Depositor DCC
R_{free} test set	3458 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtrriage
Anisotropy	0.423	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	24852	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: TE9, MPD, MG, CL

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	0.45	1/5844 (0.0%)	0.78	4/7879 (0.1%)
1	B	0.45	2/5824 (0.0%)	0.76	1/7854 (0.0%)
2	E	0.81	0/158	1.34	2/242 (0.8%)
3	F	0.92	0/251	1.51	7/385 (1.8%)
4	G	0.87	0/156	1.58	1/239 (0.4%)
5	H	0.85	0/253	1.42	4/388 (1.0%)
All	All	0.49	3/12486 (0.0%)	0.84	19/16987 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	B	0	2
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1403	GLU	CD-OE1	6.60	1.32	1.25
1	B	1414	GLU	CD-OE1	5.42	1.31	1.25
1	A	1185	GLU	CD-OE1	5.34	1.31	1.25

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1468	ARG	NE-CZ-NH2	-6.63	116.98	120.30
3	F	5	DA	P-O3'-C3'	-6.49	111.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	DA	P-O3'-C3'	-6.43	111.98	119.70
5	H	3	DC	C4'-C3'-C2'	-6.42	97.32	103.10
2	E	3	DT	O5'-P-OP2	-6.29	100.04	105.70
5	H	3	DC	O4'-C4'-C3'	-6.24	102.00	104.50
1	A	1443	ARG	NE-CZ-NH2	-6.08	117.26	120.30
4	G	4	DG	P-O3'-C3'	-6.04	112.45	119.70
3	F	11	DG	C4-N9-C1'	-5.74	119.04	126.50
3	F	11	DG	C8-N9-C1'	5.72	134.44	127.00
1	A	1443	ARG	NE-CZ-NH1	5.60	123.10	120.30
3	F	4	DC	P-O3'-C3'	-5.58	113.01	119.70
3	F	9	DA	O5'-P-OP2	-5.46	100.78	105.70
5	H	9	DA	O3'-P-O5'	-5.45	93.64	104.00
3	F	10	DT	C1'-O4'-C4'	-5.41	104.69	110.10
2	E	3	DT	OP1-P-OP2	5.30	127.56	119.60
3	F	7	DT	OP1-P-O3'	5.19	116.62	105.20
1	B	1353	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	A	1111	ASP	CB-CA-C	5.13	120.66	110.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1276	ARG	Sidechain
1	A	1353	ARG	Sidechain
1	A	1426	ARG	Sidechain
1	A	1457[A]	ARG	Sidechain
1	A	1457[B]	ARG	Sidechain
1	A	447	ARG	Sidechain
1	A	456	ARG	Sidechain
1	B	1239	ARG	Sidechain
1	B	527	ARG	Sidechain

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	5744	5843	5833	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5730	5819	5807	85	0
2	E	141	80	81	2	0
3	F	225	126	126	4	0
4	G	140	80	81	1	0
5	H	226	124	124	5	0
6	A	16	28	28	5	0
6	B	8	14	14	2	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
8	A	1	0	0	1	0
8	B	1	0	0	1	0
9	F	30	11	0	3	0
9	H	30	11	0	3	0
10	A	195	0	0	5	0
10	B	195	0	0	6	0
10	E	10	0	0	0	0
10	F	7	0	0	0	0
10	G	7	0	0	0	0
10	H	4	0	0	1	0
All	All	12716	12136	12094	188	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 8.

All (188) 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:A:1222:ARG:NH1	1:A:1484:ASP:OD1	2.04	0.90
1:B:508:ASP:OD2	10:B:1601:HOH:O	1.92	0.87
1:B:579:ARG:HH11	1:B:579:ARG:HB3	1.40	0.87
9:F:101:TE9:CL1	9:F:101:TE9:C2	2.63	0.84
1:A:594:THR:OG1	1:A:595:THR:HG22	1.77	0.83
1:A:504:MET:HA	1:A:538:ALA:HB2	1.60	0.83
1:A:1252:GLU:OE1	1:A:1308:THR:HG21	1.79	0.83
8:B:1505:CL:CL	10:B:1770:HOH:O	2.34	0.81
9:F:101:TE9:CL1	9:F:101:TE9:N2	2.55	0.77
1:A:566:GLU:O	1:A:569:LYS:HG3	1.85	0.76
1:B:1202:ASP:OD1	1:B:1226:LYS:HE3	1.86	0.76
9:H:101:TE9:C2	9:H:101:TE9:CL1	2.72	0.74
9:H:101:TE9:CL1	9:H:101:TE9:N2	2.59	0.73
1:A:1388:VAL:O	1:A:1392:ILE:HG13	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:ARG:HH22	3:F:11:DG:H3'	1.55	0.70
1:A:1426:ARG:NH2	8:A:1506:CL:CL	2.61	0.70
9:F:101:TE9:CL1	9:F:101:TE9:C13	2.77	0.69
1:B:1205:MET:CE	1:B:1226:LYS:HA	2.22	0.69
1:B:1201:ILE:HG13	1:B:1230:GLU:HG3	1.75	0.68
1:A:1211:PRO:O	1:A:1478:ARG:NH2	2.26	0.68
1:A:508:ASP:OD2	10:A:1601:HOH:O	2.11	0.67
1:B:1178:ILE:HG12	1:B:1329:MET:HG2	1.76	0.67
1:B:640:THR:HG23	1:B:641:LEU:HD22	1.76	0.67
1:A:623:GLY:O	1:A:629:ARG:NH2	2.27	0.66
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.77	0.66
1:A:1391:LEU:HD21	1:A:1404:ASN:HB2	1.77	0.66
1:B:1423:GLN:NE2	1:B:1425:TYR:HE2	1.94	0.66
1:B:623:GLY:O	1:B:629:ARG:NH2	2.29	0.66
9:H:101:TE9:CL1	9:H:101:TE9:C13	2.81	0.65
1:B:1118:TYR:HE2	5:H:1:DG:H5'	1.60	0.65
1:A:1229:TYR:CD1	1:A:1342:ILE:HD13	2.32	0.65
1:A:1273:ASP:OD1	1:A:1276:ARG:NH1	2.30	0.64
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.80	0.64
1:B:1205:MET:HE1	1:B:1226:LYS:HA	1.80	0.64
1:B:1252:GLU:OE1	1:B:1308:THR:OG1	2.16	0.63
1:B:516:THR:O	1:B:520:THR:HG23	1.98	0.62
1:B:1118:TYR:CE2	5:H:1:DG:H5'	2.34	0.62
1:A:1384:ILE:O	1:A:1388:VAL:HG23	2.00	0.61
1:B:1205:MET:HE1	1:B:1226:LYS:CB	2.31	0.61
1:A:1118:TYR:HE2	3:F:1:DA:H5'	1.65	0.61
1:B:1341:GLY:O	1:B:1344:PRO:HD2	2.00	0.60
1:B:1423:GLN:HE21	1:B:1425:TYR:HE2	1.50	0.60
1:A:455:LEU:HD23	1:A:475:GLU:OE2	2.02	0.60
1:B:594:THR:OG1	1:B:595:THR:HG22	2.01	0.59
2:E:1:DC:H2''	2:E:2:DA:OP2	2.03	0.59
1:A:605:ARG:NH1	1:A:1006:ASN:HD21	1.99	0.59
1:B:479:MET:O	1:B:483:ILE:HG12	2.03	0.59
1:A:474:GLU:O	1:A:478:THR:HG23	2.04	0.58
1:B:1205:MET:HE1	1:B:1226:LYS:CA	2.35	0.57
1:B:1307:ASN:OD1	1:B:1310:LEU:HD23	2.05	0.57
1:A:611:LEU:HD13	1:A:611:LEU:O	2.04	0.57
1:B:1391:LEU:HD23	1:B:1405:LEU:HD23	1.87	0.57
1:B:474:GLU:O	1:B:478:THR:HG23	2.05	0.56
1:A:560:THR:HG22	1:A:645:THR:CG2	2.35	0.56
1:A:1426:ARG:HH12	6:A:1501:MPD:H11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1422:LEU:HD13	6:B:1501:MPD:H11	1.88	0.56
1:A:1210:GLY:HA2	1:A:1229:TYR:OH	2.06	0.56
1:A:592:TRP:CE2	1:A:597:ASN:HB2	2.42	0.55
1:B:579:ARG:HH11	1:B:579:ARG:CB	2.17	0.55
1:A:560:THR:HG22	1:A:645:THR:HG21	1.89	0.55
1:A:1429:ASN:HB3	6:A:1501:MPD:HM1	1.89	0.54
1:B:1168:THR:HG22	10:B:1696:HOH:O	2.07	0.54
1:A:1096:GLU:HG2	1:A:1126:ILE:HD13	1.88	0.54
1:B:1354:ARG:HG3	1:B:1459:MET:CE	2.38	0.54
1:B:1164:VAL:HG21	1:B:1183:LEU:HD12	1.89	0.54
1:B:579:ARG:HB3	1:B:579:ARG:NH1	2.18	0.54
1:A:1426:ARG:HH11	6:A:1501:MPD:HM3	1.73	0.54
1:A:1240:SER:HB2	1:A:1321:LEU:HD22	1.90	0.53
1:A:1426:ARG:NH1	6:A:1501:MPD:HM3	2.24	0.53
1:A:1271:LYS:HE3	1:A:1319:THR:HA	1.89	0.53
1:B:1205:MET:HE2	1:B:1226:LYS:HA	1.89	0.53
1:B:1182:ASN:O	1:B:1186:VAL:HG23	2.09	0.53
1:B:627:GLU:HB2	1:B:628:PRO:HD3	1.91	0.52
1:B:547:LYS:HG2	1:B:572:GLY:HA3	1.92	0.52
1:B:1246:LYS:O	1:B:1247:LEU:HD23	2.09	0.52
1:A:1118:TYR:CE2	3:F:1:DA:H5'	2.44	0.52
1:B:611:LEU:O	1:B:611:LEU:HD13	2.10	0.52
1:B:1205:MET:HE1	1:B:1226:LYS:HB2	1.91	0.52
1:A:520:THR:HG21	1:A:622:MET:HG3	1.91	0.52
1:A:592:TRP:HA	1:A:596:MET:HB2	1.92	0.51
1:A:611:LEU:HD13	1:A:611:LEU:C	2.31	0.51
1:A:1391:LEU:HD21	1:A:1404:ASN:CB	2.40	0.51
1:A:459:VAL:O	1:A:517:LEU:HD13	2.11	0.50
1:A:516:THR:O	1:A:520:THR:HG23	2.11	0.50
1:B:1070:MET:CE	1:B:1078:ASP:HB3	2.40	0.50
1:A:1019:ARG:NH2	10:A:1607:HOH:O	2.44	0.50
1:B:568:ARG:HG3	1:B:568:ARG:HH11	1.77	0.50
1:B:444:GLY:HA2	1:B:588:ALA:HB1	1.94	0.50
1:B:592:TRP:HA	1:B:596:MET:HB2	1.93	0.50
1:A:1193:MET:CE	1:A:1347:SER:HB3	2.42	0.50
1:A:626:VAL:HG11	3:F:10:DT:OP2	2.13	0.49
1:B:1102:HIS:HB2	1:B:1120:GLU:HG3	1.94	0.49
1:A:1397:ASN:HD21	1:A:1399:ALA:HB3	1.78	0.49
1:B:626:VAL:HG21	10:H:204:HOH:O	2.13	0.49
1:A:546:SER:HB3	1:A:554:GLU:HG2	1.94	0.48
1:B:1144:ASN:ND2	1:B:1149:GLU:HB3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:602:THR:O	1:A:603:LEU:HD23	2.14	0.48
1:A:480:ILE:HG22	1:A:526:MET:CE	2.43	0.47
1:A:1219:ILE:HG23	1:A:1236:VAL:HG11	1.96	0.47
1:B:568:ARG:HH11	1:B:568:ARG:CG	2.27	0.47
1:B:592:TRP:CE2	1:B:597:ASN:HB2	2.49	0.47
1:B:1378:LEU:HD13	6:B:1501:MPD:H52	1.95	0.47
1:A:627:GLU:N	1:A:628:PRO:CD	2.76	0.47
1:B:1219:ILE:HB	1:B:1482:LEU:HD23	1.97	0.47
1:B:1296:LEU:HD23	1:B:1297:ARG:N	2.28	0.47
1:A:1216:GLY:O	1:A:1217:ALA:HB3	2.15	0.46
1:B:1484:ASP:N	10:B:1607:HOH:O	2.47	0.46
1:A:537:ILE:HB	1:A:604:ILE:HB	1.98	0.46
1:A:1222:ARG:NH2	10:A:1611:HOH:O	2.49	0.46
1:A:423:ASN:OD1	1:A:425:ALA:HB3	2.15	0.46
1:B:1229:TYR:CD1	1:B:1342:ILE:HD13	2.51	0.46
1:A:461:ASN:HD21	1:A:622:MET:HB3	1.81	0.46
1:A:1219:ILE:HG23	1:A:1236:VAL:CG1	2.47	0.46
1:B:615:GLU:O	1:B:619:ASN:ND2	2.49	0.46
1:B:1366:GLU:OE2	1:B:1370:LYS:HE2	2.15	0.46
1:A:1319:THR:OG1	1:A:1321:LEU:HB2	2.16	0.45
6:A:1501:MPD:O2	6:A:1501:MPD:H53	2.16	0.45
1:A:481:TYR:C	1:A:481:TYR:CD1	2.90	0.45
1:B:433:GLU:OE2	4:G:7:DT:O3'	2.29	0.45
1:A:615:GLU:O	1:A:619:ASN:ND2	2.50	0.45
1:A:1386:ASP:OD1	1:A:1386:ASP:N	2.48	0.45
1:B:444:GLY:CA	1:B:588:ALA:HB1	2.47	0.45
1:B:527:ARG:N	1:B:528:PRO:CD	2.79	0.45
1:A:558:ALA:HB2	1:A:567:LEU:HD22	1.97	0.45
5:H:3:DC:H2'	5:H:4:DT:C6	2.52	0.45
1:A:1201:ILE:O	1:A:1205:MET:HG3	2.16	0.45
1:A:646:VAL:O	1:A:646:VAL:HG13	2.17	0.45
1:A:1028:ARG:CZ	2:E:6:DA:H4'	2.47	0.45
1:A:1037:LEU:CD1	1:A:1155:LEU:HD12	2.47	0.45
1:A:527:ARG:N	1:A:528:PRO:CD	2.80	0.44
1:A:563:GLU:O	1:A:567:LEU:HB2	2.17	0.44
1:A:609:GLU:HG2	1:A:1008:SER:HB3	1.98	0.44
1:A:523:TYR:CD2	1:A:1009:LEU:CD2	3.00	0.44
1:A:590:GLN:O	1:A:594:THR:HG23	2.18	0.44
1:A:1343:VAL:HB	1:A:1344:PRO:HD3	2.00	0.44
1:B:509:THR:HG22	1:B:1019:ARG:HG2	1.99	0.44
1:A:566:GLU:O	1:A:569:LYS:HE3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1035:ASP:O	1:A:1161:ASN:HB3	2.18	0.43
1:A:630:ARG:NH1	1:A:1173:GLY:O	2.51	0.43
1:A:1387:GLU:O	1:A:1391:LEU:HB2	2.17	0.43
1:B:1240:SER:OG	1:B:1321:LEU:O	2.31	0.43
1:A:1037:LEU:HD11	1:A:1155:LEU:HD12	2.01	0.43
1:A:432:VAL:HA	1:A:504:MET:O	2.19	0.43
1:B:1035:ASP:O	1:B:1161:ASN:HB3	2.19	0.43
1:B:1222:ARG:HB2	1:B:1484:ASP:HA	1.99	0.43
1:B:1343:VAL:HB	1:B:1344:PRO:HD3	2.00	0.43
1:A:1391:LEU:C	1:A:1391:LEU:HD23	2.39	0.43
1:B:548:GLY:O	1:B:549:LYS:HB2	2.19	0.43
1:A:1059:TYR:CZ	1:A:1102:HIS:HD2	2.36	0.43
1:A:1459:MET:C	1:A:1459:MET:SD	2.96	0.43
1:B:523:TYR:CD1	1:B:1009:LEU:CD2	3.02	0.43
1:B:1137:LYS:HA	10:B:1747:HOH:O	2.18	0.43
1:B:1425:TYR:O	1:B:1428:THR:HG23	2.19	0.43
1:B:537:ILE:HB	1:B:604:ILE:HG13	2.00	0.42
1:B:1201:ILE:HG22	1:B:1205:MET:HE3	2.00	0.42
1:B:460:ILE:HA	5:H:6:DT:O3'	2.19	0.42
1:B:591:LEU:HD12	1:B:595:THR:HG23	2.02	0.42
1:A:1089:SER:HA	1:A:1099:VAL:O	2.19	0.42
1:A:1109:ASP:OD1	1:A:1265:LYS:HE3	2.20	0.42
1:B:620:VAL:HG23	1:B:628:PRO:HB2	2.00	0.42
1:B:1029:ALA:O	1:B:1038:LYS:HE2	2.19	0.42
1:B:1104:ASN:HB3	1:B:1114:ALA:HB2	2.01	0.42
1:B:1244:ILE:HD12	1:B:1244:ILE:N	2.34	0.42
1:B:1426:ARG:HD3	1:B:1426:ARG:HA	1.88	0.42
1:A:1185:GLU:OE1	1:A:1478:ARG:NH1	2.53	0.42
1:A:1333:ASP:OD2	1:A:1338:ARG:NH1	2.51	0.42
1:A:1458:THR:HA	10:A:1699:HOH:O	2.20	0.42
1:B:1371:ARG:O	1:B:1375:VAL:HG23	2.19	0.42
1:A:462:THR:HG21	1:A:521:PHE:HD1	1.85	0.42
1:A:1388:VAL:O	1:A:1391:LEU:HB3	2.19	0.42
1:A:627:GLU:HB2	1:A:628:PRO:HD3	2.02	0.42
1:A:1382:ILE:HD12	1:A:1432:VAL:HG22	2.02	0.42
1:B:587:ASN:HB3	10:B:1664:HOH:O	2.20	0.42
1:A:1114:ALA:HB3	1:A:1119:THR:CG2	2.49	0.41
1:A:1316:PHE:CE1	1:A:1321:LEU:HD13	2.54	0.41
1:B:1112:PRO:HA	1:B:1113:PRO:HD2	1.92	0.41
1:B:1254:ILE:HD13	1:B:1312:LEU:HD13	2.02	0.41
1:A:1392:ILE:O	1:B:1428:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1381:VAL:HG21	1:A:1419:ILE:HG12	2.01	0.41
1:B:629:ARG:HH11	5:H:9:DA:P	2.44	0.41
1:B:550:GLY:O	1:B:551:LYS:HB2	2.21	0.41
1:B:577:LEU:HD13	1:B:579:ARG:HG2	2.03	0.41
1:A:488:GLY:O	1:A:489:ALA:CB	2.69	0.41
1:A:1393:ARG:HB2	10:A:1613:HOH:O	2.20	0.41
1:B:481:TYR:CD1	1:B:481:TYR:C	2.94	0.41
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.03	0.41
1:A:1466:GLU:O	1:A:1470:VAL:HG23	2.20	0.40
1:B:513:HIS:HB2	1:B:1020:TYR:CD1	2.57	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	720/742 (97%)	664 (92%)	42 (6%)	14 (2%)	8 10
1	B	718/742 (97%)	678 (94%)	31 (4%)	9 (1%)	12 17
All	All	1438/1484 (97%)	1342 (93%)	73 (5%)	23 (2%)	9 13

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	PRO
1	A	466	LYS
1	A	467	MET
1	A	489	ALA
1	A	549	LYS
1	A	1003	ASN
1	B	551	LYS
1	B	569	LYS

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Mol	Chain	Res	Type
1	A	546	SER
1	A	571	PHE
1	B	466	LYS
1	B	467	MET
1	B	549	LYS
1	B	1217	ALA
1	A	526	MET
1	A	1217	ALA
1	A	1262	GLU
1	A	570	GLN
1	A	572	GLY
1	A	1221	GLY
1	B	646	VAL
1	B	1003	ASN
1	B	1221	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	618/635 (97%)	580 (94%)	38 (6%)	18	30
1	B	616/635 (97%)	597 (97%)	19 (3%)	40	60
All	All	1234/1270 (97%)	1177 (95%)	57 (5%)	27	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LYS
1	A	424	PRO
1	A	447	ARG
1	A	471	LEU
1	A	472	LYS
1	A	481	TYR
1	A	490	ASP
1	A	492	SER

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Mol	Chain	Res	Type
1	A	516	THR
1	A	551	LYS
1	A	553	GLU
1	A	569	LYS
1	A	570	GLN
1	A	573	LYS
1	A	579	ARG
1	A	595	THR
1	A	602	THR
1	A	616	ARG
1	A	1027	ASP
1	A	1058	SER
1	A	1078	ASP
1	A	1139	VAL
1	A	1162	LEU
1	A	1168	THR
1	A	1200	LYS
1	A	1222	ARG
1	A	1236	VAL
1	A	1279	ASN
1	A	1308	THR
1	A	1321	LEU
1	A	1336	THR
1	A	1367[A]	LYS
1	A	1367[B]	LYS
1	A	1383	SER
1	A	1385	LEU
1	A	1386	ASP
1	A	1426	ARG
1	A	1484	ASP
1	B	478	THR
1	B	516	THR
1	B	520	THR
1	B	579	ARG
1	B	595	THR
1	B	600	THR
1	B	624	ASP
1	B	1024	ILE
1	B	1061	LYS
1	B	1078	ASP
1	B	1162	LEU
1	B	1168	THR

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Mol	Chain	Res	Type
1	B	1171	SER
1	B	1200	LYS
1	B	1236	VAL
1	B	1307	ASN
1	B	1310	LEU
1	B	1420	VAL
1	B	1441	GLU

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

Mol	Chain	Res	Type
1	A	497	ASN
1	A	570	GLN
1	A	590	GLN
1	A	619	ASN
1	A	1005	GLN
1	A	1102	HIS
1	B	619	ASN
1	B	1102	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 8 are monoatomic - leaving 5 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
6	MPD	A	1501	-	7,7,7	0.22	0	9,10,10	0.50	0
9	TE9	H	101	7	31,33,33	1.17	2 (6%)	37,51,51	1.31	5 (13%)
6	MPD	A	1502	-	7,7,7	0.14	0	9,10,10	0.78	0
9	TE9	F	101	7	31,33,33	1.20	4 (12%)	37,51,51	1.21	2 (5%)
6	MPD	B	1501	-	7,7,7	0.28	0	9,10,10	0.68	0

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
6	MPD	A	1501	-	-	4/5/5/5	-
9	TE9	H	101	7	-	4/11/20/20	0/4/4/4
6	MPD	A	1502	-	-	2/5/5/5	-
9	TE9	F	101	7	-	7/11/20/20	0/4/4/4
6	MPD	B	1501	-	-	2/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	TE9	C2-C16	-3.00	1.38	1.42
9	H	101	TE9	C2-C16	-2.69	1.39	1.42
9	H	101	TE9	C1-C18	2.69	1.42	1.40
9	F	101	TE9	C3-N3	2.53	1.42	1.37
9	F	101	TE9	C1-C18	2.35	1.42	1.40
9	F	101	TE9	C4-C5	2.09	1.52	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	101	TE9	C17-C18-C1	-3.13	119.66	121.70
9	F	101	TE9	C17-C18-C1	-2.95	119.77	121.70
9	H	101	TE9	C4-C3-N3	-2.60	120.54	123.75
9	H	101	TE9	C3-C4-C6	2.28	121.58	119.88
9	H	101	TE9	O1-C5-C4	-2.24	117.54	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	TE9	C4-C3-N3	-2.23	120.99	123.75
9	H	101	TE9	C17-C16-C2	-2.12	120.37	121.73

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1502	MPD	C2-C3-C4-O4
9	F	101	TE9	C16-C2-N3-C15
9	F	101	TE9	N2-C2-N3-C3
9	H	101	TE9	C16-C2-N3-C15
9	H	101	TE9	N2-C2-N3-C3
9	F	101	TE9	C6-C4-C5-O1
9	F	101	TE9	C3-C4-C5-O1
9	F	101	TE9	C6-C4-C5-O2
6	A	1501	MPD	O2-C2-C3-C4
6	A	1501	MPD	C2-C3-C4-C5
6	A	1502	MPD	C2-C3-C4-C5
6	A	1501	MPD	C1-C2-C3-C4
6	A	1501	MPD	CM-C2-C3-C4
6	B	1501	MPD	CM-C2-C3-C4
6	B	1501	MPD	O2-C2-C3-C4
9	F	101	TE9	C3-C4-C5-O2
9	F	101	TE9	C14-C10-N4-C11
9	H	101	TE9	C14-C10-N4-C11
9	H	101	TE9	N2-C2-N3-C15

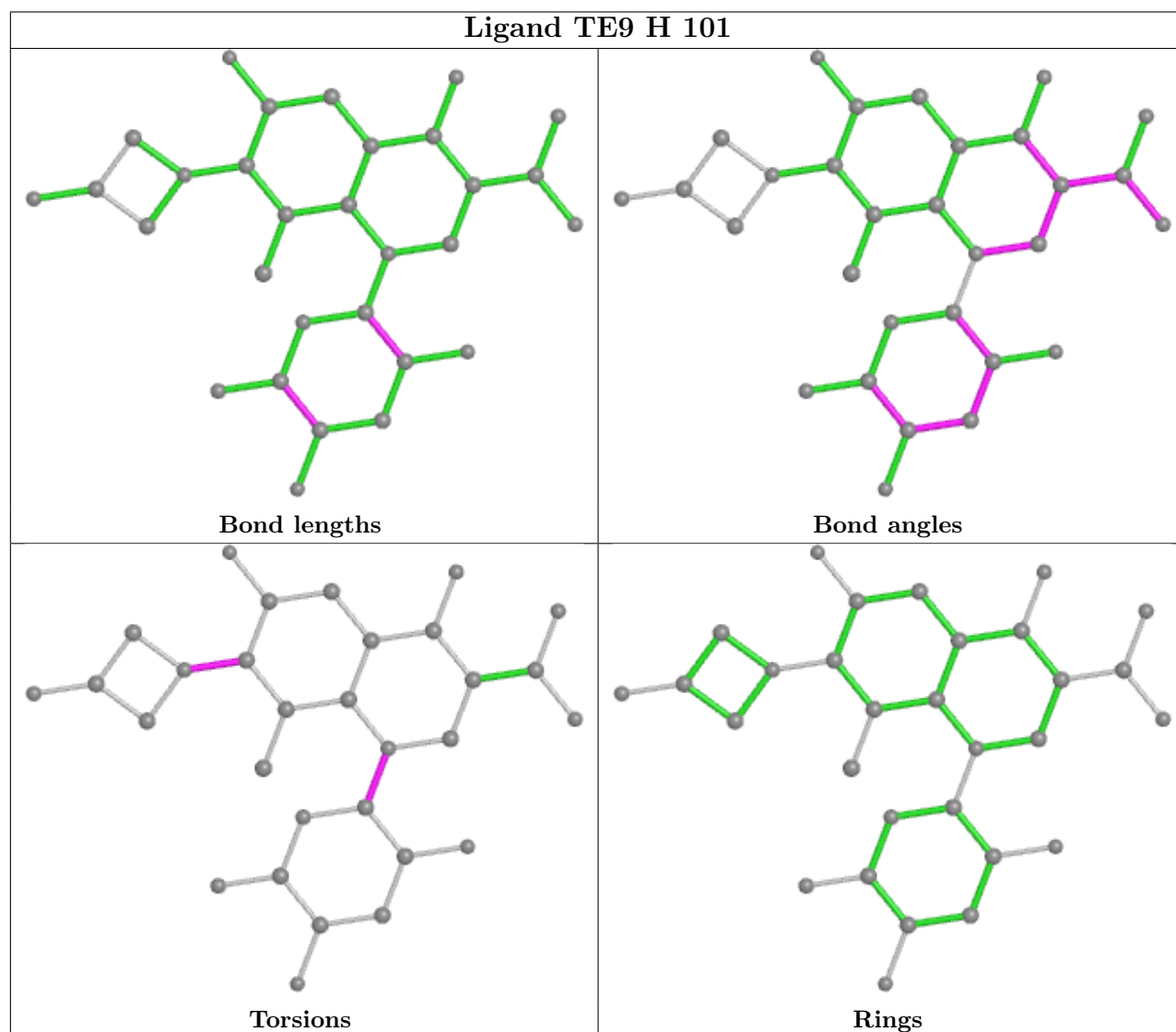
There are no ring outliers.

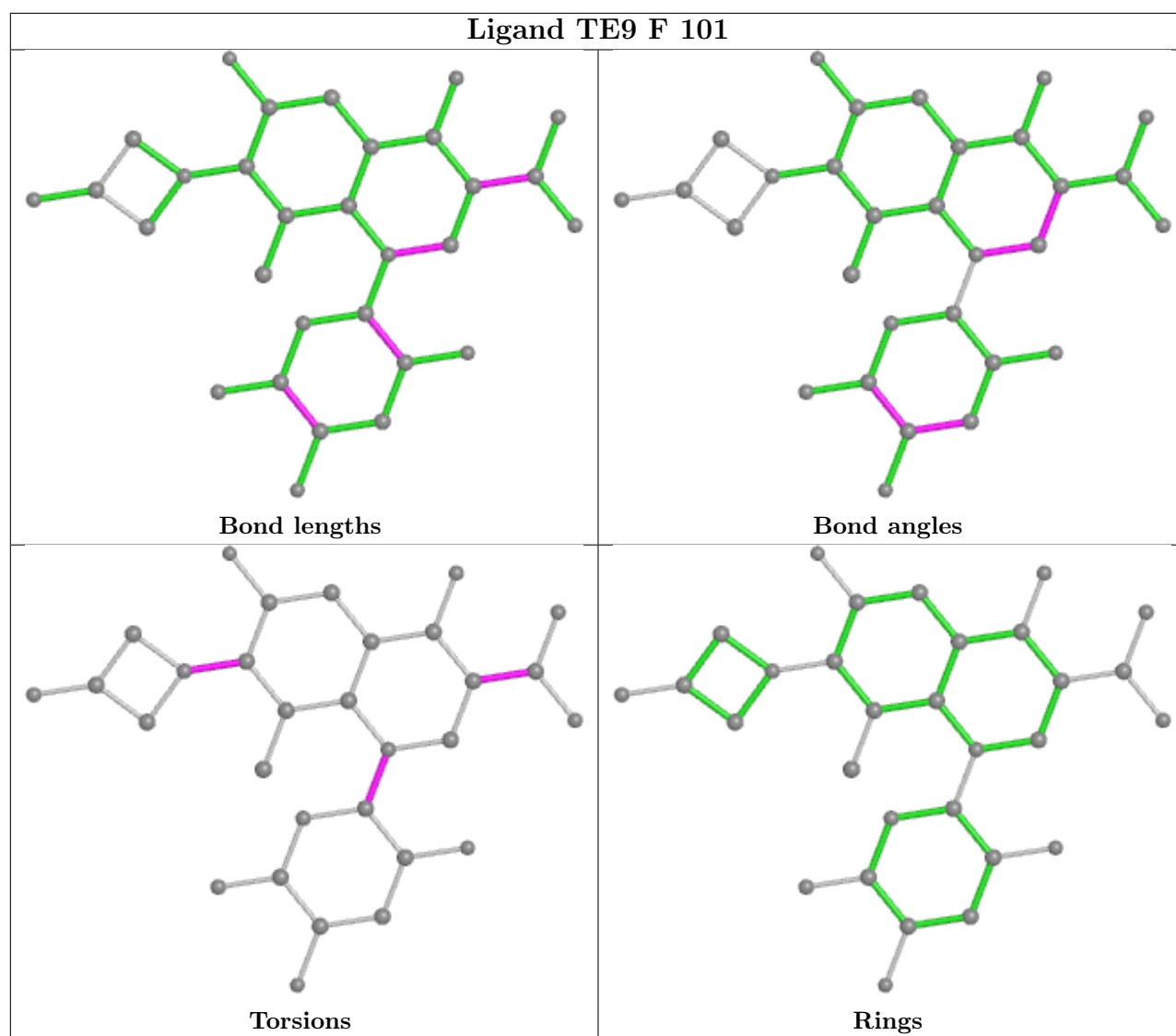
4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1501	MPD	5	0
9	H	101	TE9	3	0
9	F	101	TE9	3	0
6	B	1501	MPD	2	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 than 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.





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, 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	720/742 (97%)	0.39	48 (6%) 17 16	27, 46, 108, 155	0
1	B	720/742 (97%)	0.32	37 (5%) 28 26	27, 44, 105, 154	0
2	E	7/7 (100%)	0.10	0 100 100	42, 44, 65, 91	0
3	F	11/11 (100%)	0.08	0 100 100	46, 61, 93, 97	0
4	G	7/7 (100%)	0.06	0 100 100	37, 39, 67, 89	0
5	H	11/11 (100%)	0.18	0 100 100	48, 61, 91, 97	0
All	All	1476/1520 (97%)	0.35	85 (5%) 23 22	27, 46, 107, 155	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	GLY	13.1
1	A	571	PHE	12.4
1	B	571	PHE	9.7
1	A	553	GLU	9.3
1	A	549	LYS	9.1
1	B	548	GLY	7.8
1	B	552	LYS	7.5
1	A	550	GLY	6.9
1	B	550	GLY	6.7
1	A	1001	MET	6.4
1	A	573	LYS	6.0
1	A	551	LYS	6.0
1	A	547	LYS	5.9
1	A	496	ALA	5.9
1	A	574	GLY	5.7
1	B	575	ALA	5.6
1	A	552	LYS	5.4
1	B	553	GLU	5.4
1	A	645	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	A	647	PHE	5.2
1	B	551	LYS	4.8
1	B	647	PHE	4.4
1	B	489	ALA	4.0
1	B	573	LYS	3.9
1	B	574	GLY	3.8
1	A	468	ALA	3.8
1	B	1001	MET	3.7
1	B	471	LEU	3.7
1	A	471	LEU	3.6
1	B	572	GLY	3.5
1	B	554	GLU	3.3
1	A	467	MET	3.3
1	B	549	LYS	3.3
1	A	466	LYS	3.2
1	B	570	GLN	3.2
1	A	546	SER	3.2
1	A	570	GLN	3.2
1	A	469	ASP	3.1
1	A	539	LEU	3.0
1	B	522	PHE	3.0
1	A	648	HIS	3.0
1	A	606	VAL	2.9
1	B	532	ALA	2.8
1	A	560	THR	2.8
1	B	555	VAL	2.8
1	A	489	ALA	2.7
1	A	554	GLU	2.7
1	A	644	ALA	2.7
1	A	426	LYS	2.6
1	A	1003	ASN	2.6
1	A	522	PHE	2.6
1	B	466	LYS	2.6
1	B	468	ALA	2.6
1	A	577	LEU	2.5
1	A	575	ALA	2.5
1	A	534	HIS	2.5
1	B	481	TYR	2.4
1	A	480	ILE	2.4
1	B	483	ILE	2.4
1	B	493	ILE	2.4
1	A	493	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	501	ILE	2.3
1	B	607	THR	2.3
1	A	555	VAL	2.3
1	B	576	THR	2.3
1	A	612	ALA	2.3
1	B	467	MET	2.3
1	B	646	VAL	2.2
1	A	416	LEU	2.2
1	B	1003	ASN	2.2
1	B	494	GLU	2.2
1	A	564	LEU	2.2
1	B	416	LEU	2.2
1	A	523	TYR	2.2
1	A	484	GLY	2.2
1	B	603	LEU	2.2
1	A	646	VAL	2.2
1	A	532	ALA	2.1
1	A	481	TYR	2.1
1	B	472	LYS	2.1
1	A	576	THR	2.1
1	A	641	LEU	2.0
1	B	1012	ILE	2.0
1	B	491	PHE	2.0
1	B	645	THR	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](#)

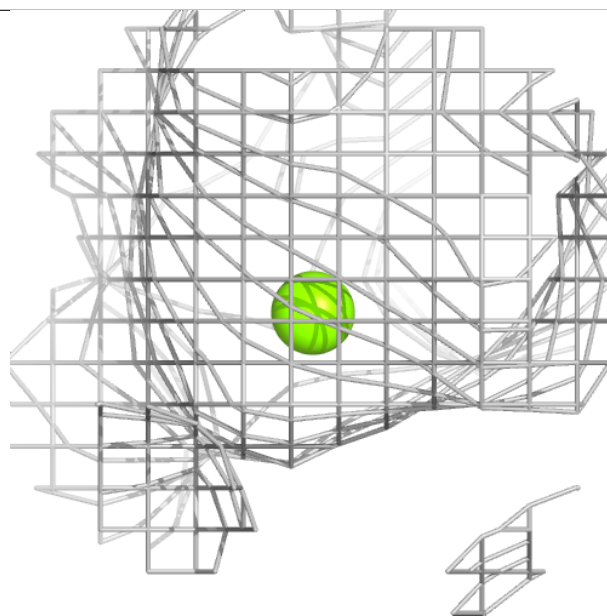
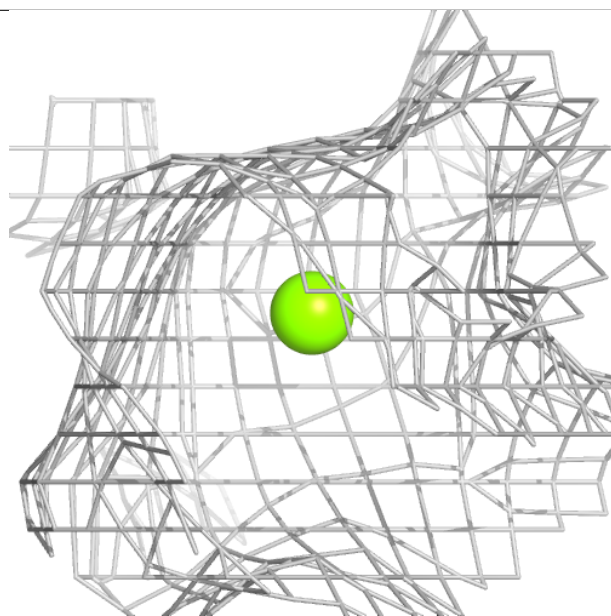
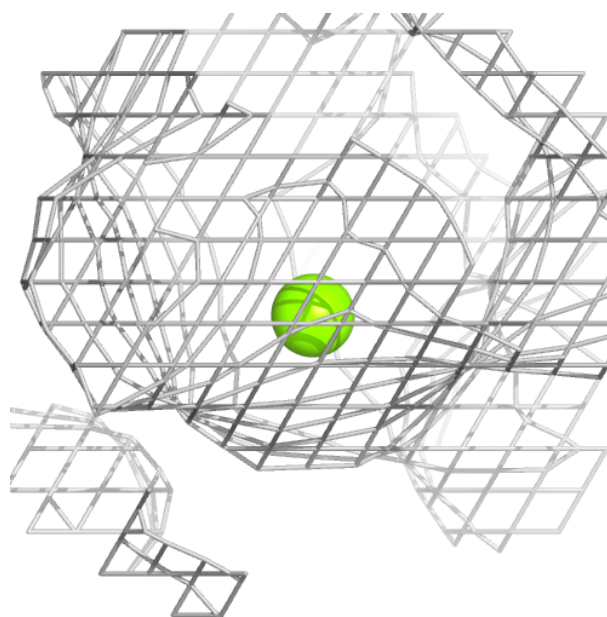
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MPD	A	1502	8/8	0.90	0.24	62,74,77,78	1
6	MPD	A	1501	8/8	0.95	0.19	46,48,48,49	1
6	MPD	B	1501	8/8	0.95	0.19	31,31,32,34	1
8	CL	A	1506	1/1	0.95	0.07	51,51,51,51	0
7	MG	A	1505	1/1	0.96	0.05	39,39,39,39	0
9	TE9	F	101	30/30	0.96	0.17	49,60,62,65	1
9	TE9	H	101	30/30	0.96	0.16	50,54,60,62	1
7	MG	B	1504	1/1	0.98	0.07	27,27,27,27	0
7	MG	A	1503	1/1	0.98	0.05	19,19,19,19	0
7	MG	B	1502	1/1	0.98	0.04	31,31,31,31	0
7	MG	B	1503	1/1	0.98	0.07	26,26,26,26	0
8	CL	B	1505	1/1	0.99	0.11	47,47,47,47	0
7	MG	A	1504	1/1	1.00	0.09	8,8,8,8	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.

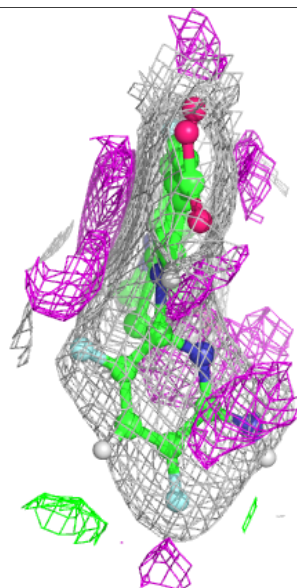
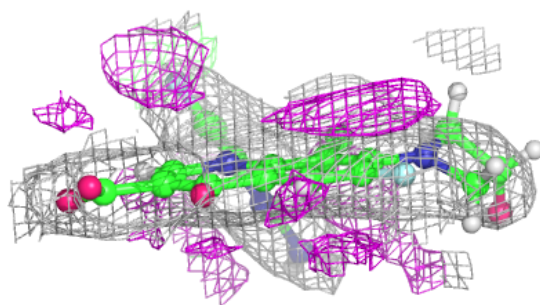
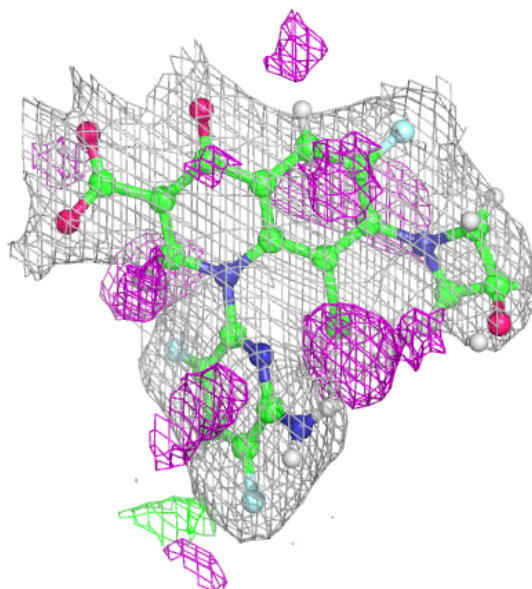
Electron density around MG A 1505:

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



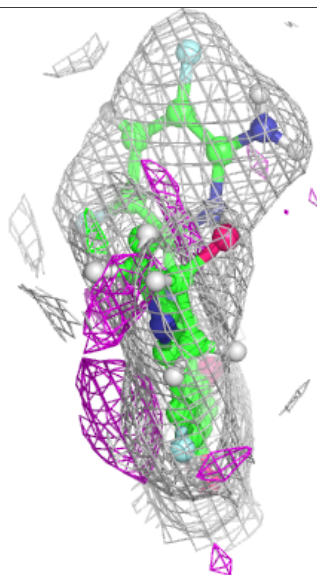
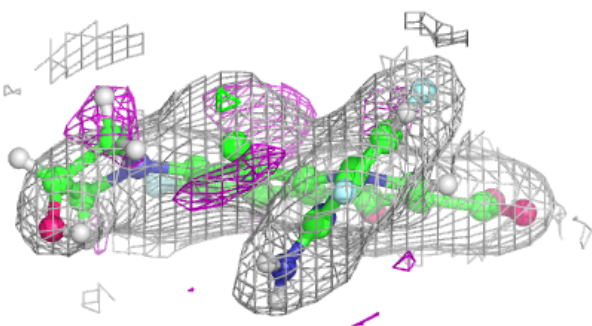
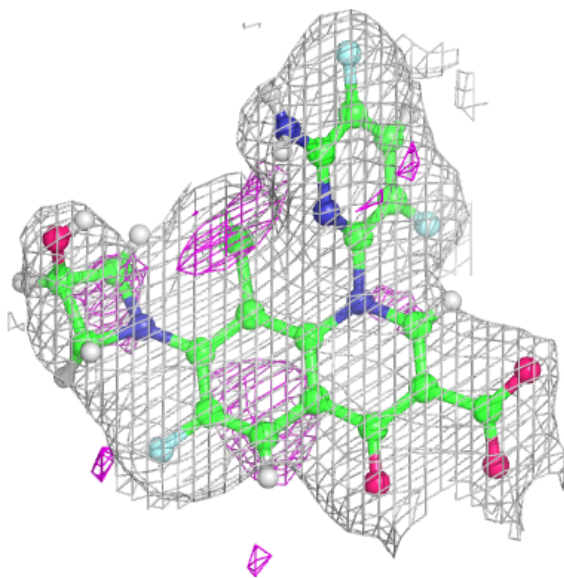
Electron density around TE9 F 101:

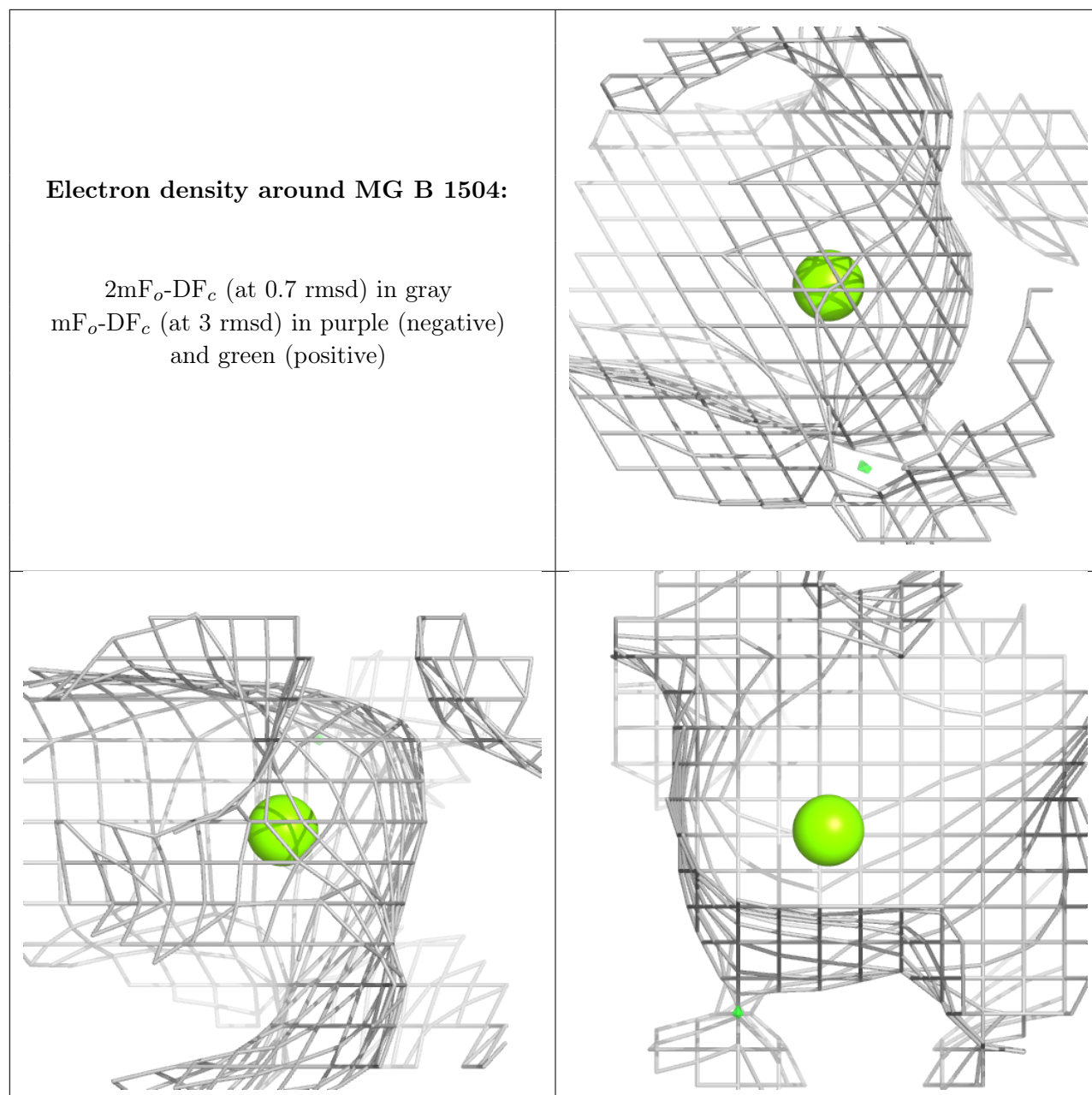
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around TE9 H 101:

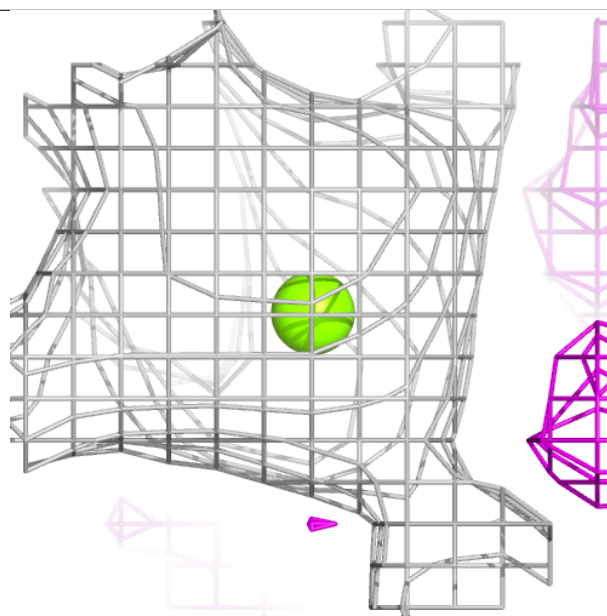
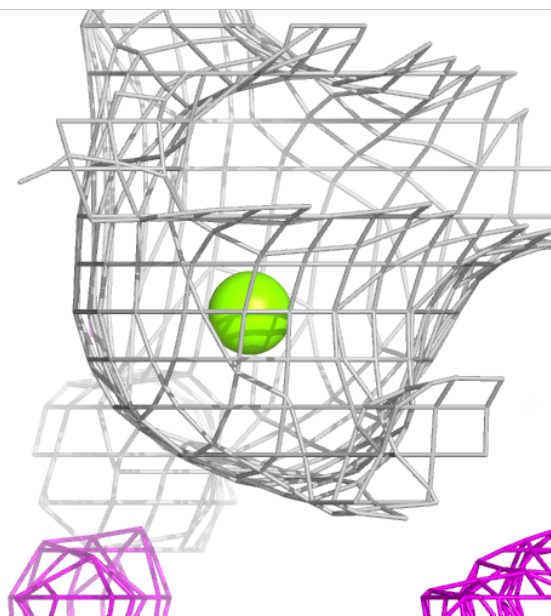
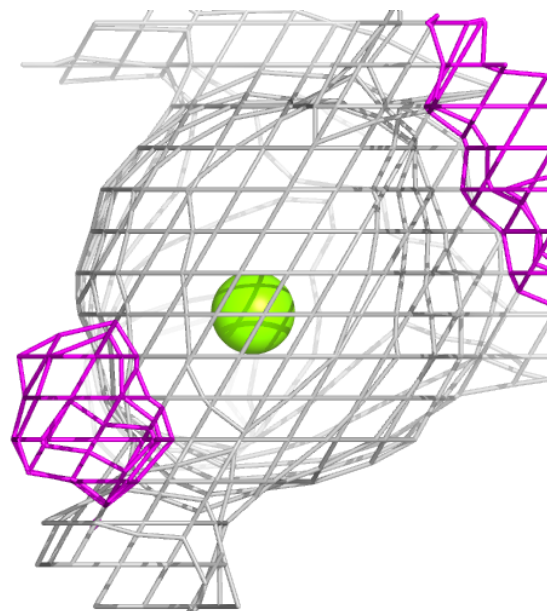
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

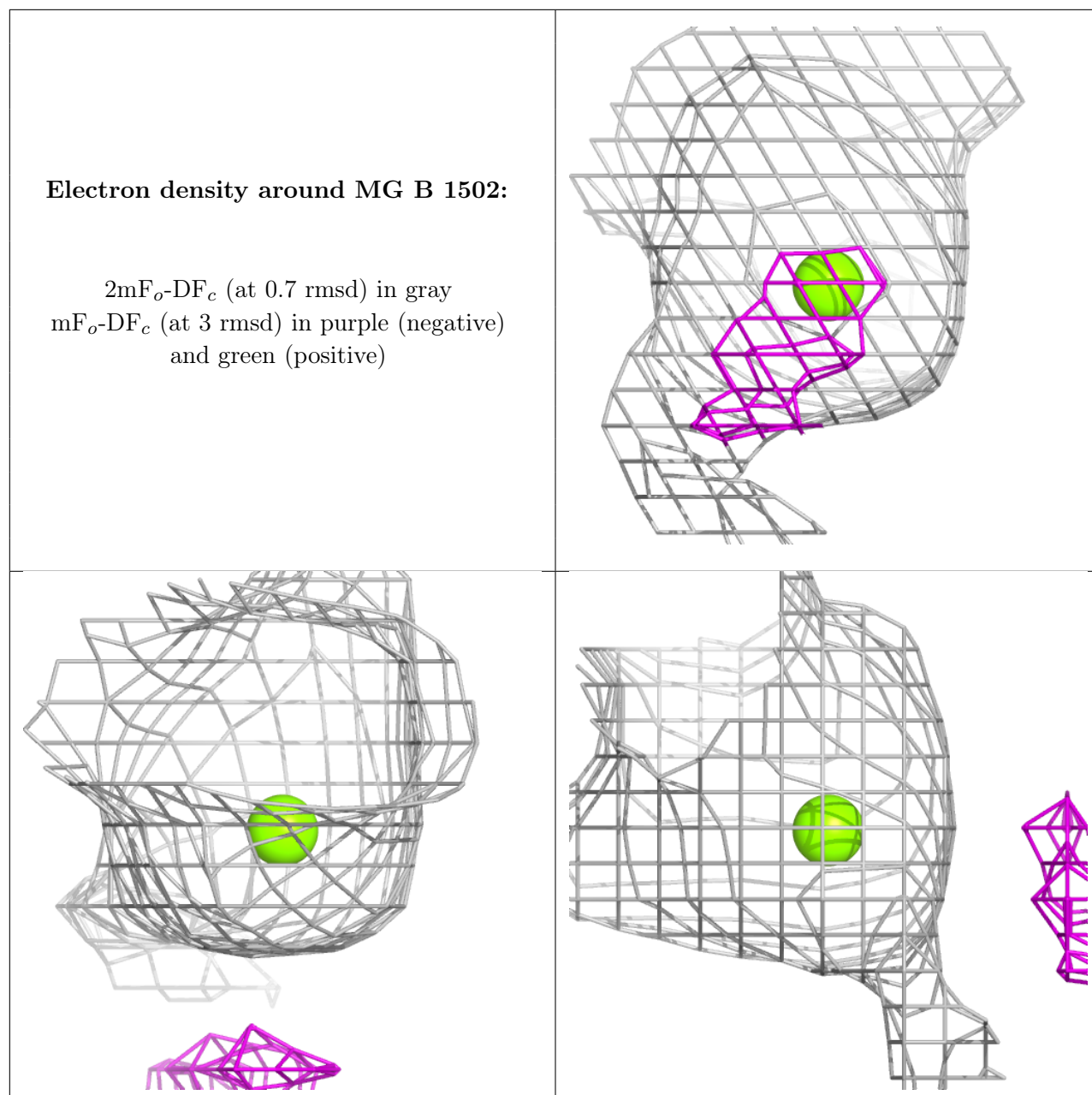


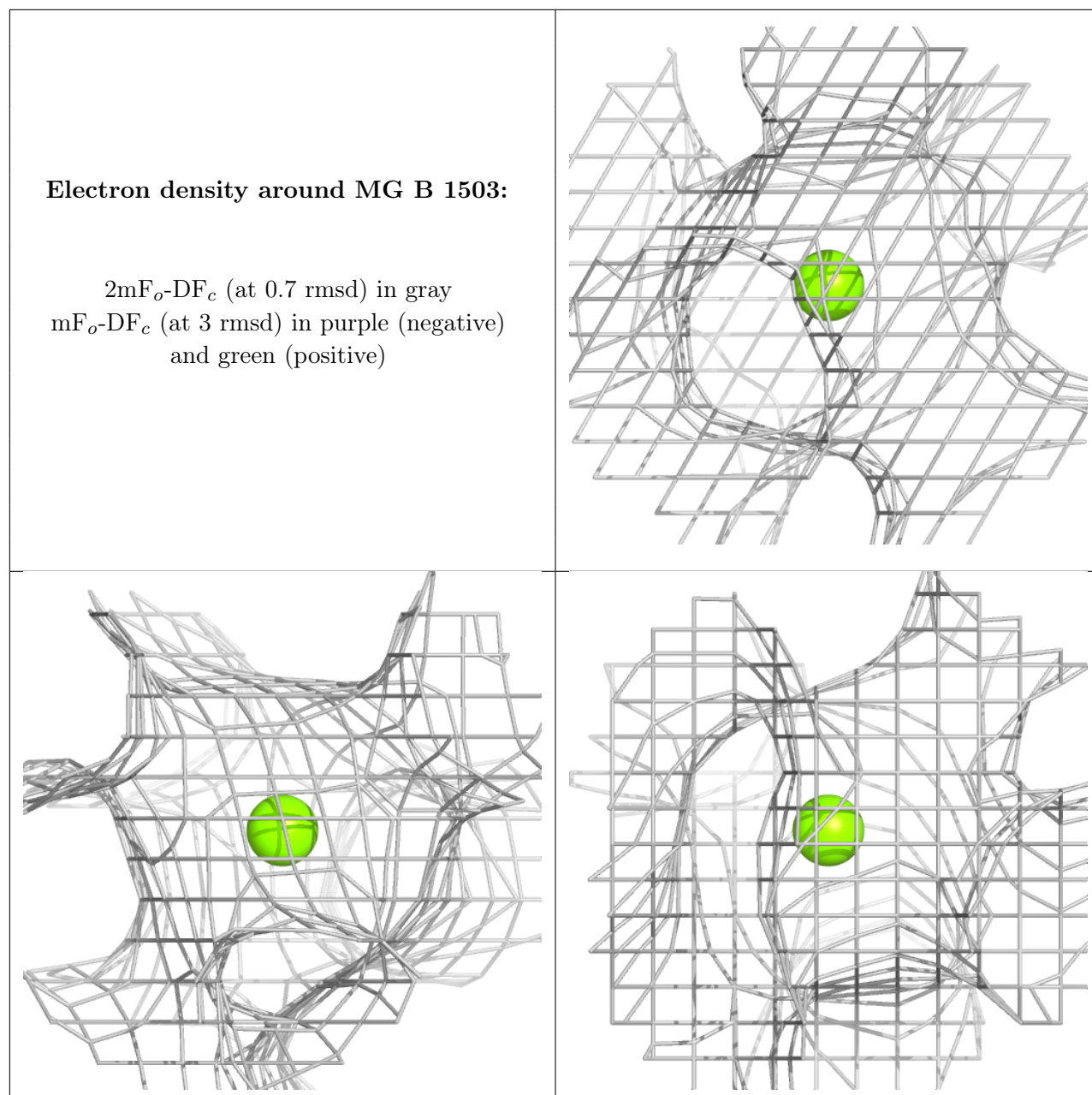


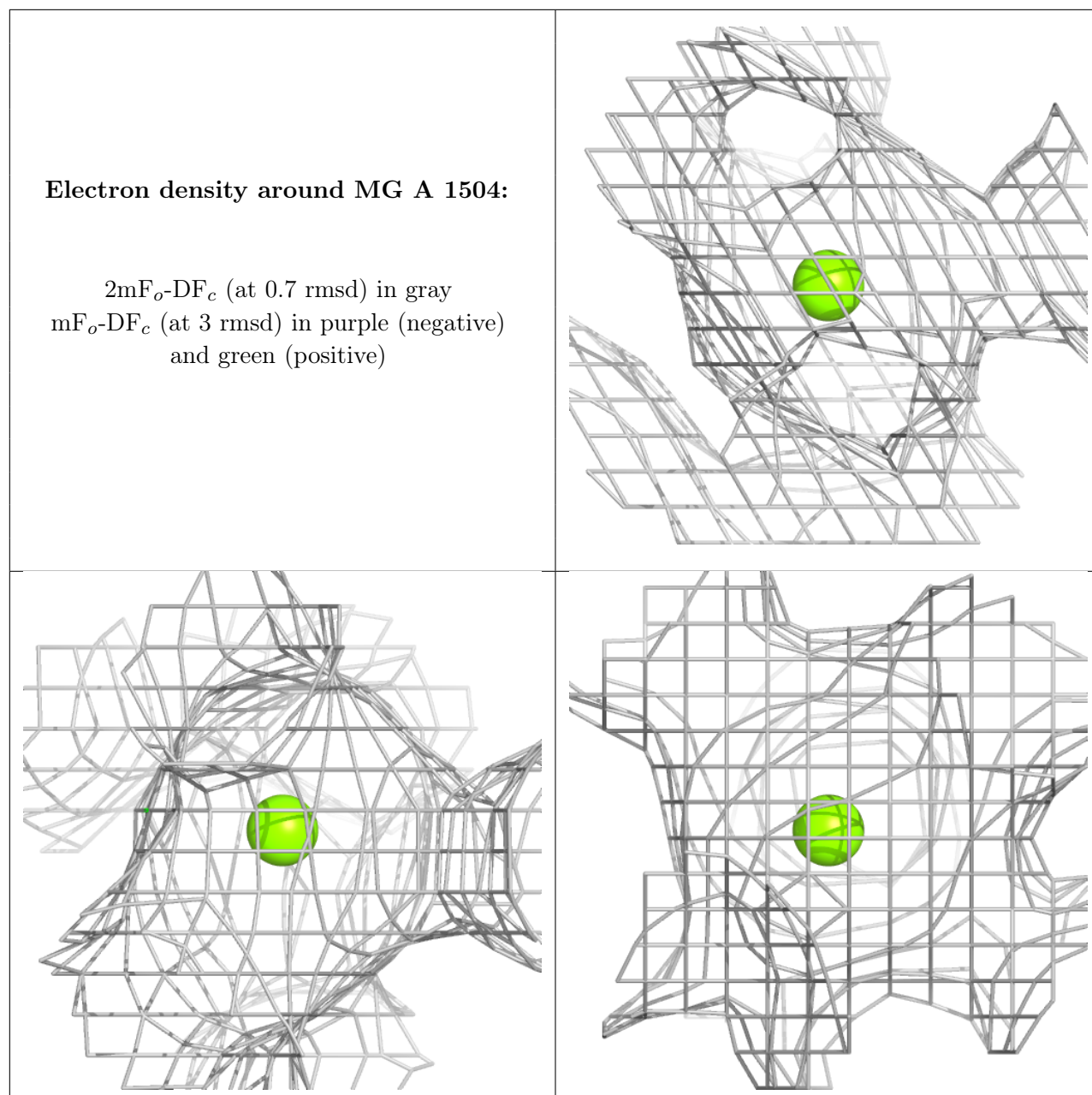
Electron density around MG A 1503:

$2mF_o-DF_c$ (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.