



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:48 PM UTC

PDB ID : 8C41 / pdb_00008c41
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

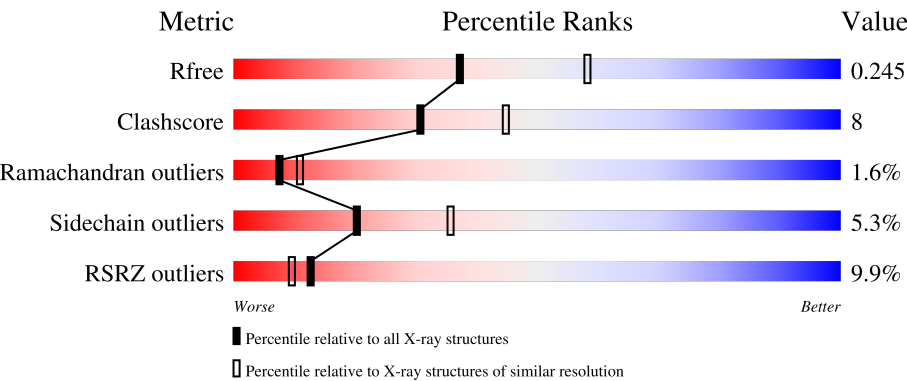
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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.



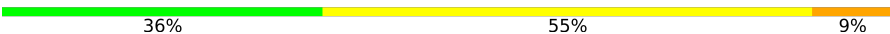
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	11% 73% 20% • •
1	B	742	9% 77% 18% • •
2	E	7	57% 43%
3	F	11	64% 27% 9%

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Mol	Chain	Length	Quality of chain
4	G	7	 43% 57%
5	H	11	 36% 55% 9%

2 Entry composition

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
1	A	720	Total	C	H	N	O	S	321	2	0
			11587	3629	5843	1000	1091	24			
1	B	720	Total	C	H	N	O	S	319	0	0
			11549	3619	5819	996	1091	24			

- 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
2	E	7	Total	C	H	N	O	P	1	0	0
			221	69	80	27	39	6			

- 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
3	F	11	Total	C	H	N	O	P	1	0	0
			351	108	126	39	67	11			

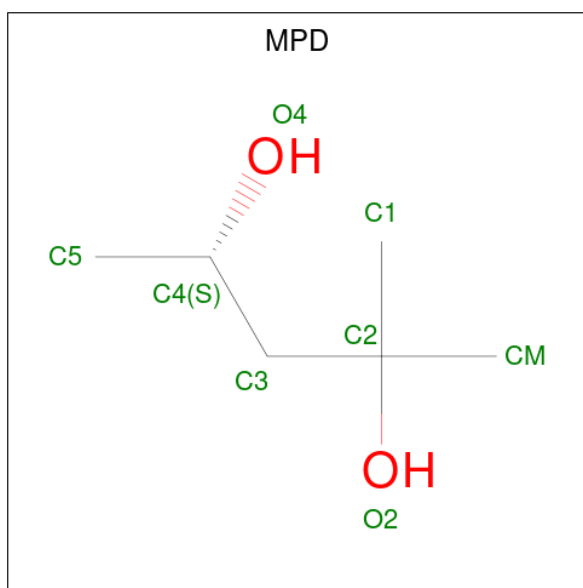
- Molecule 4 is a DNA chain called DNA (5'-D(*CP*GP*TP*GP*CP*AP*T)-3').

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

- 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
5	H	11	Total	C	H	N	O	P	1	0	0
			350	107	124	43	65	11			

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

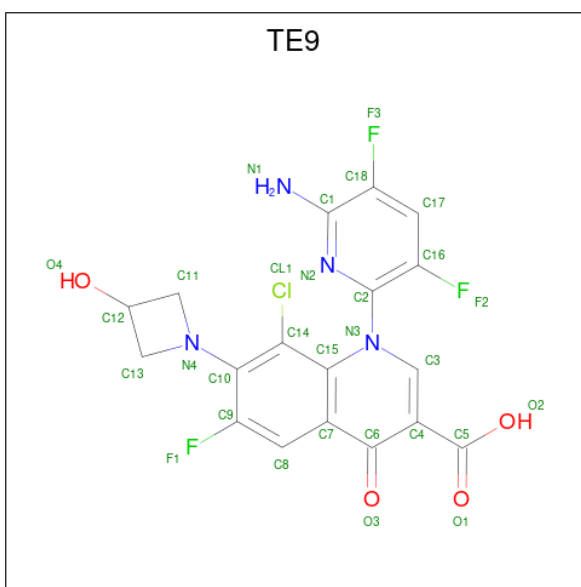
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

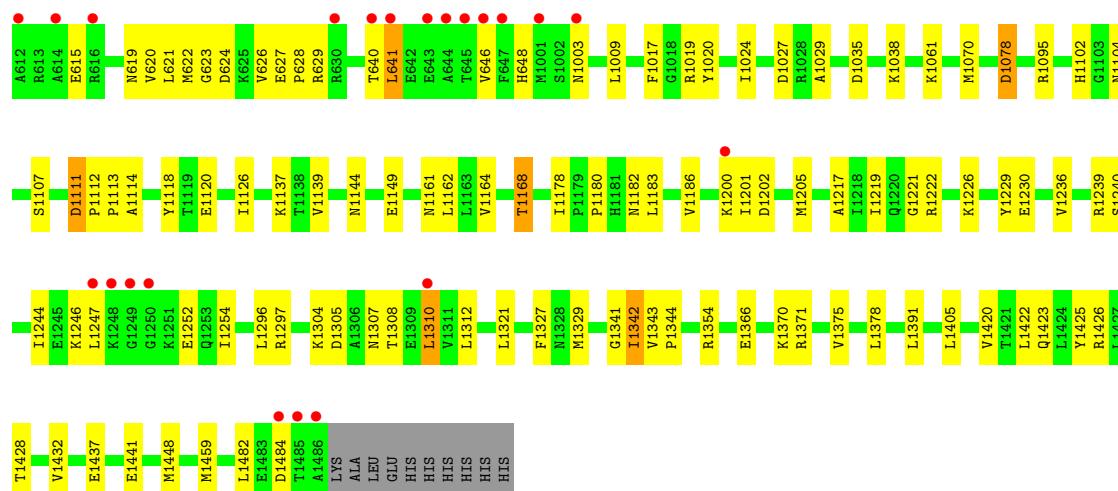
- Molecule 9 is delafloxacin (CCD ID: TE9) (formula: $C_{18}H_{12}ClF_3N_4O_4$) (labeled as "Ligand of Interest" by depositor).



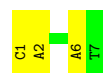
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
9	F	1	Total	C	Cl	F	H	N	O	1	0
			41	18	1	3	11	4	4		
9	H	1	Total	C	Cl	F	H	N	O	1	0
			41	18	1	3	11	4	4		

- 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 – 2.39 115.01 – 2.39	Depositor EDS
% Data completeness (in resolution range)	58.9 (115.01-2.39) 58.9 (115.01-2.39)	Depositor EDS
R_{merge}	0.56	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0352, PDB-REDO	Depositor
R, R_{free}	0.192 , 0.243 0.194 , 0.245	Depositor DCC
R_{free} test set	3458 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.423	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, TE9, MPD

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	0.60	0/5844	1.10	5/7879 (0.1%)
1	B	0.60	0/5824	1.09	5/7854 (0.1%)
2	E	0.56	0/158	1.12	0/242
3	F	0.60	0/251	1.29	2/385 (0.5%)
4	G	0.58	0/156	1.40	3/239 (1.3%)
5	H	0.57	0/253	1.15	3/388 (0.8%)
All	All	0.60	0/12486	1.10	18/16987 (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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	9	DA	O3'-P-O5'	-6.91	93.64	104.00
1	A	1111	ASP	CB-CA-C	6.66	120.66	109.67
1	A	506	ASP	CA-CB-CG	6.59	119.19	112.60
4	G	1	DC	O3'-P-O5'	-6.27	94.60	104.00
1	A	1035	ASP	CA-CB-CG	6.22	118.82	112.60
5	H	7	DG	O3'-P-O5'	-6.13	94.81	104.00
1	B	1111	ASP	CB-CA-C	5.96	118.78	109.42
1	B	1437	GLU	CB-CG-CD	5.55	122.04	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	DA	P-O3'-C3'	-5.53	111.91	120.20
5	H	2	DA	P-O3'-C3'	-5.48	111.98	120.20
1	A	1400	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	1027	ASP	CB-CA-C	-5.32	102.36	111.46
3	F	11	DG	C4-N9-C1'	-5.31	119.04	127.00
4	G	4	DG	P-O3'-C3'	-5.17	112.45	120.20
4	G	6	DA	O3'-P-O5'	-5.15	96.27	104.00
1	B	648	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	1478	ARG	CB-CA-C	-5.08	100.64	109.64
1	B	1327	PHE	CA-CB-CG	5.08	118.88	113.80

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	101	0
1	B	5730	5819	5807	92	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	7	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	202	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 (202) 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
1:B:1205:MET:HE1	1:B:1226:LYS:HA	1.66	0.77
1:B:1178:ILE:HG23	1:B:1329:MET:HE2	1.66	0.77
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
1:A:1235:ARG:HH22	3:F:11:DG:H3'	1.55	0.70
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1205:MET:HE1	1:B:1226:LYS:CA	2.24	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: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: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:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.83	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:1205:MET:HE1	1:B:1226:LYS:CB	2.31	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: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
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:611:LEU:HD13	1:A:611:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:622:MET:HE1	1:A:1017:PHE:CD1	2.43	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: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:A:520:THR:HG21	1:A:622:MET:HG3	1.91	0.52
1:B:1354:ARG:HG3	1:B:1459:MET:HE2	1.91	0.52
1:A:592:TRP:HA	1:A:596:MET:HB2	1.92	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:B:621:LEU:HB3	1:B:622:MET:HE2	1.94	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:A:481:TYR:C	1:A:481:TYR:CD1	2.90	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:621:LEU:HB3	1:A:622:MET:HE2	1.95	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
1:A:602:THR:O	1:A:603:LEU:HD23	2.14	0.48
1:A:480:ILE:HG22	1:A:526:MET:HE3	1.95	0.47
1:A:480:ILE:HG22	1:A:526:MET:CE	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1219:ILE:HG23	1:A:1236:VAL:HG11	1.96	0.47
1:A:1391:LEU:C	1:A:1391:LEU:HD23	2.39	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:A:1459:MET:C	1:A:1459:MET:SD	2.96	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:B:1205:MET:HE1	1:B:1226:LYS:HB2	1.96	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:B:481:TYR:CD1	1:B:481:TYR:C	2.94	0.45
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: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:1381:VAL:O	1:A:1382:ILE:C	2.60	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:615:GLU:CD	1:A:619:ASN:HD21	2.25	0.44
1:A:609:GLU:HG2	1:A:1008:SER:HB3	1.98	0.44
1:A:1425:TYR:C	1:A:1425:TYR:CD1	2.95	0.44
1:A:523:TYR:CD2	1:A:1009:LEU:CD2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1354:ARG:HG3	1:A:1459:MET:HE2	1.99	0.44
1:A:566:GLU:O	1:A:569:LYS:HE3	2.18	0.44
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:B:548:GLY:O	1:B:549:LYS:HB2	2.19	0.43
1:B:1296:LEU:HD23	1:B:1296:LEU:C	2.43	0.43
1:A:1059:TYR:CZ	1:A:1102:HIS:HD2	2.36	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: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:B:622:MET:HE1	1:B:1017:PHE:CD1	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:1107:SER:OG	1:B:1111:ASP:OD1	2.34	0.41
1:A:1392:ILE:O	1:B:1428:THR:HG22	2.21	0.41
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:505:THR:C	1:B:506:ASP:O	2.64	0.41
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.03	0.41
1:B:1304:LYS:O	1:B:1305:ASP:C	2.64	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
1:B:1448:MET:HE3	10:B:1712:HOH:O	2.22	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	720/742 (97%)	664 (92%)	42 (6%)	14 (2%)	6	8
1	B	718/742 (97%)	678 (94%)	31 (4%)	9 (1%)	9	14
All	All	1438/1484 (97%)	1342 (93%)	73 (5%)	23 (2%)	7	11

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	424	PRO

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	578 (94%)	40 (6%)	15	27
1	B	616/635 (97%)	591 (96%)	25 (4%)	27	46
All	All	1234/1270 (97%)	1169 (95%)	65 (5%)	20	36

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	LYS

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Mol	Chain	Res	Type
1	A	424	PRO
1	A	471	LEU
1	A	490	ASP
1	A	492	SER
1	A	516	THR
1	A	542	LEU
1	A	551	LYS
1	A	553	GLU
1	A	569	LYS
1	A	570	GLN
1	A	573	LYS
1	A	576	THR
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	1061	LYS
1	A	1078	ASP
1	A	1139	VAL
1	A	1162	LEU
1	A	1168	THR
1	A	1183	LEU
1	A	1236	VAL
1	A	1279	ASN
1	A	1308	THR
1	A	1321	LEU
1	A	1336	THR
1	A	1342	ILE
1	A	1381	VAL
1	A	1382	ILE
1	A	1383	SER
1	A	1385	LEU
1	A	1386	ASP
1	A	1420	VAL
1	A	1426	ARG
1	A	1433	VAL
1	A	1484	ASP
1	B	470	ILE
1	B	478	THR
1	B	516	THR

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Mol	Chain	Res	Type
1	B	520	THR
1	B	549	LYS
1	B	579	ARG
1	B	595	THR
1	B	600	THR
1	B	604	ILE
1	B	624	ASP
1	B	641	LEU
1	B	1024	ILE
1	B	1061	LYS
1	B	1078	ASP
1	B	1126	ILE
1	B	1139	VAL
1	B	1162	LEU
1	B	1168	THR
1	B	1200	LYS
1	B	1236	VAL
1	B	1310	LEU
1	B	1342	ILE
1	B	1420	VAL
1	B	1432	VAL
1	B	1441	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	420	GLN
1	A	497	ASN
1	A	590	GLN
1	A	619	ASN
1	A	1003	ASN
1	A	1006	ASN
1	A	1102	HIS
1	A	1182	ASN
1	A	1397	ASN
1	B	427	ASN
1	B	473	ASN
1	B	570	GLN
1	B	578	GLN
1	B	1053	ASN
1	B	1094	ASN
1	B	1102	HIS

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Mol	Chain	Res	Type
1	B	1278	ASN
1	B	1313	ASN
1	B	1461	ASN

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 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	B	1501	-	7,7,7	0.29	0	9,10,10	0.68	0
6	MPD	A	1501	-	7,7,7	0.24	0	9,10,10	0.48	0
9	TE9	F	101	7	32,33,33	1.13	4 (12%)	38,51,51	1.23	2 (5%)
9	TE9	H	101	7	32,33,33	1.20	2 (6%)	38,51,51	1.37	6 (15%)
6	MPD	A	1502	-	7,7,7	0.17	0	9,10,10	0.75	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	B	1501	-	-	3/5/5/5	-
6	MPD	A	1501	-	-	4/5/5/5	-
9	TE9	F	101	7	-	7/11/20/20	0/4/4/4
9	TE9	H	101	7	-	3/11/20/20	0/4/4/4
6	MPD	A	1502	-	-	3/5/5/5	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	TE9	C2-C16	-2.93	1.38	1.42
9	H	101	TE9	C1-C18	2.67	1.42	1.39
9	H	101	TE9	C2-C16	-2.63	1.39	1.42
9	F	101	TE9	C1-C18	2.36	1.42	1.39
9	F	101	TE9	C4-C5	2.24	1.52	1.48
9	F	101	TE9	O1-C5	2.13	1.27	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	101	TE9	C17-C18-C1	-3.09	119.66	121.68
9	F	101	TE9	C17-C18-C1	-2.91	119.77	121.68
9	H	101	TE9	C4-C3-N3	-2.77	120.54	123.81
9	H	101	TE9	O1-C5-C4	-2.48	117.54	122.67
9	H	101	TE9	C15-N3-C2	2.47	123.58	119.11
9	F	101	TE9	C4-C3-N3	-2.39	120.99	123.81
9	H	101	TE9	C3-C4-C6	2.24	121.58	119.94
9	H	101	TE9	C17-C16-C2	-2.01	120.37	121.69

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1502	MPD	C2-C3-C4-O4
6	A	1502	MPD	C2-C3-C4-C5
9	F	101	TE9	N2-C2-N3-C3
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	C1-C2-C3-C4
6	A	1501	MPD	CM-C2-C3-C4

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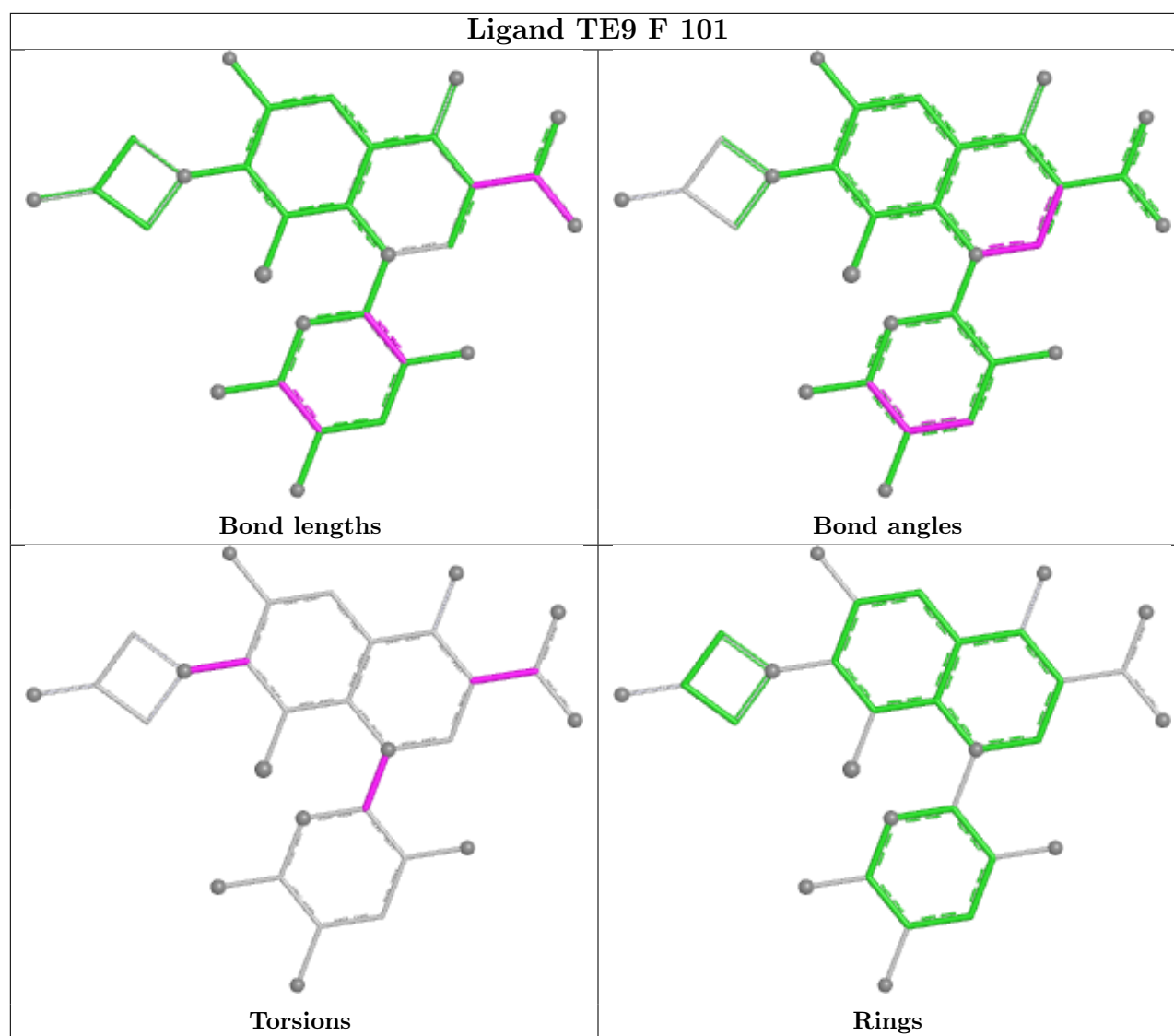
Mol	Chain	Res	Type	Atoms
6	B	1501	MPD	CM-C2-C3-C4
6	A	1501	MPD	C2-C3-C4-C5
9	F	101	TE9	C3-C4-C5-O2
9	F	101	TE9	C14-C10-N4-C11
9	H	101	TE9	C14-C10-N4-C11
9	F	101	TE9	C16-C2-N3-C15
9	H	101	TE9	C16-C2-N3-C15
6	A	1501	MPD	O2-C2-C3-C4
6	A	1502	MPD	O2-C2-C3-C4
6	B	1501	MPD	O2-C2-C3-C4
6	B	1501	MPD	C1-C2-C3-C4

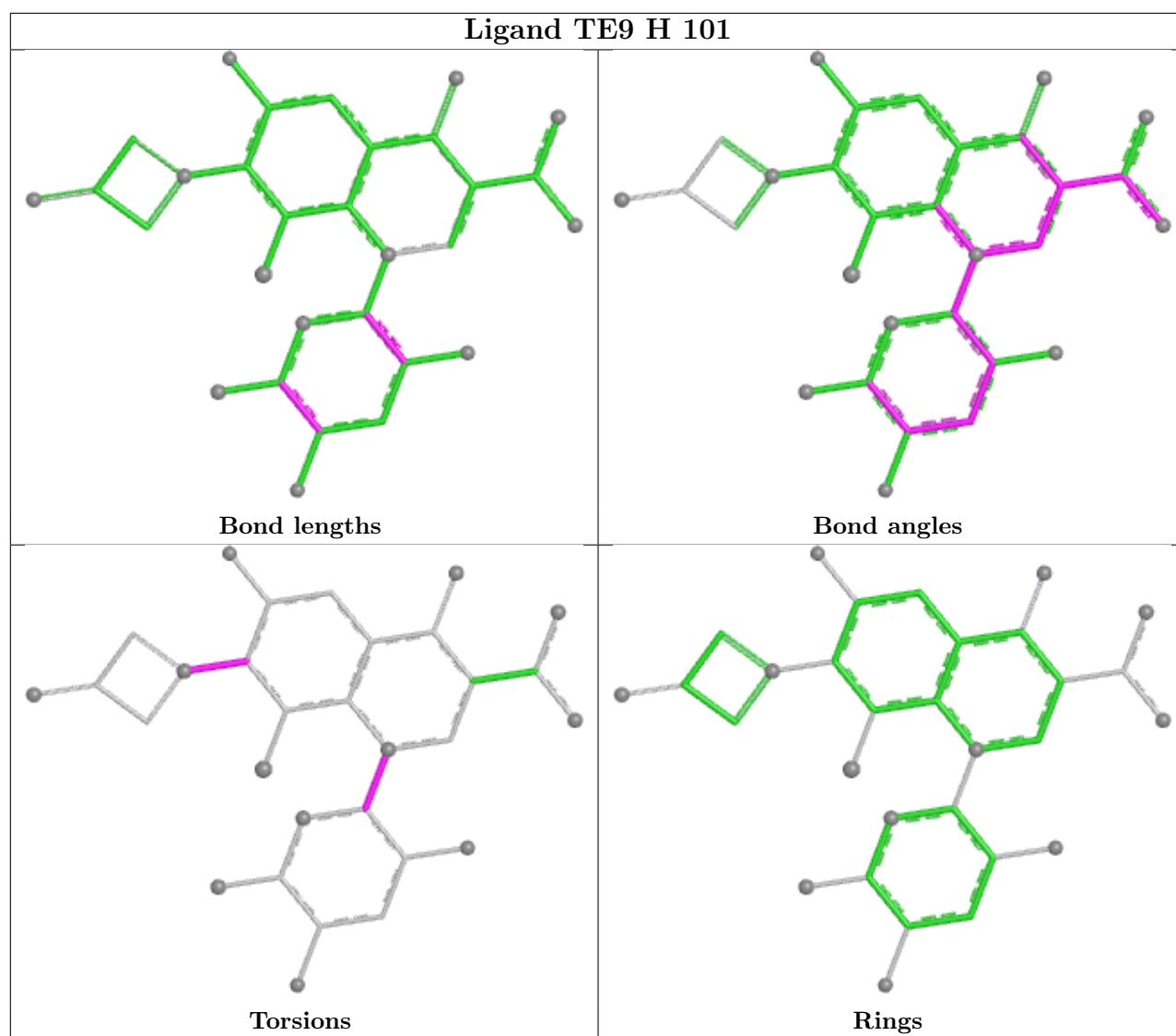
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1501	MPD	2	0
6	A	1501	MPD	5	0
9	F	101	TE9	3	0
9	H	101	TE9	3	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%)	0.41	80 (11%) 10 7	15, 45, 107, 156	2 (0%)
1	B	720/742 (97%)	0.31	66 (9%) 14 12	23, 43, 103, 155	0
2	E	7/7 (100%)	-0.47	0 100 100	41, 43, 62, 92	0
3	F	11/11 (100%)	0.00	0 100 100	46, 61, 91, 95	0
4	G	7/7 (100%)	-0.47	0 100 100	37, 38, 65, 90	0
5	H	11/11 (100%)	0.37	0 100 100	47, 59, 90, 95	0
All	All	1476/1520 (97%)	0.35	146 (9%) 13 9	15, 45, 104, 156	2 (0%)

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1486	ALA	11.8
1	A	1486	ALA	11.6
1	A	571	PHE	9.8
1	A	572	GLY	8.1
1	A	647	PHE	7.6
1	B	571	PHE	7.5
1	B	647	PHE	7.3
1	A	646	VAL	6.2
1	B	548	GLY	6.1
1	A	641	LEU	5.6
1	B	574	GLY	5.5
1	A	549	LYS	5.4
1	A	574	GLY	5.4
1	B	467	MET	5.3
1	B	471	LEU	5.1
1	A	644	ALA	4.9
1	B	646	VAL	4.9
1	A	550	GLY	4.8
1	B	1250	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	1485	THR	4.7
1	B	1485	THR	4.7
1	A	553	GLU	4.6
1	B	575	ALA	4.5
1	A	551	LYS	4.3
1	B	1310	LEU	4.2
1	A	573	LYS	4.2
1	A	496	ALA	4.2
1	B	466	LYS	4.2
1	B	552	LYS	4.2
1	A	564	LEU	4.2
1	B	584	GLY	4.1
1	A	611	LEU	4.0
1	A	466	LYS	3.9
1	A	1457[A]	ARG	3.9
1	A	468	ALA	3.9
1	B	645	THR	3.9
1	B	573	LYS	3.8
1	B	468	ALA	3.8
1	A	471	LEU	3.8
1	A	577	LEU	3.8
1	B	641	LEU	3.8
1	B	644	ALA	3.7
1	A	467	MET	3.7
1	A	422	LYS	3.6
1	A	575	ALA	3.6
1	A	562	GLY	3.6
1	B	1249	GLY	3.6
1	A	416	LEU	3.5
1	A	469	ASP	3.5
1	A	555	VAL	3.4
1	A	487	VAL	3.4
1	A	522	PHE	3.3
1	B	561	ASP	3.3
1	A	546	SER	3.2
1	B	547	LYS	3.2
1	A	547	LYS	3.2
1	A	539	LEU	3.2
1	A	432	VAL	3.1
1	A	616	ARG	3.1
1	A	474	GLU	3.1
1	B	522	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	584	GLY	3.1
1	B	518	LEU	3.1
1	B	481	TYR	3.1
1	A	1001	MET	3.1
1	B	550	GLY	3.1
1	B	551	LYS	3.1
1	A	538	ALA	3.0
1	B	1001	MET	3.0
1	B	1248	LYS	3.0
1	A	453	LEU	3.0
1	B	470	ILE	3.0
1	A	543	TYR	3.0
1	A	1003	ASN	3.0
1	A	567	LEU	2.9
1	B	572	GLY	2.9
1	A	493	ILE	2.9
1	B	616	ARG	2.9
1	B	643	GLU	2.9
1	A	645	THR	2.9
1	A	1484	ASP	2.9
1	A	552	LYS	2.8
1	A	438	GLY	2.8
1	B	612	ALA	2.8
1	B	472	LYS	2.8
1	B	465	ALA	2.7
1	A	488	GLY	2.7
1	B	567	LEU	2.7
1	A	568	ARG	2.7
1	B	614	ALA	2.6
1	B	569	LYS	2.6
1	B	1484	ASP	2.6
1	A	561	ASP	2.6
1	B	576	THR	2.6
1	B	489	ALA	2.6
1	B	577	LEU	2.5
1	A	1386	ASP	2.5
1	A	1249	GLY	2.5
1	A	570	GLN	2.5
1	A	501	ILE	2.5
1	B	1003	ASN	2.5
1	B	1200	LYS	2.5
1	A	581	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	611	LEU	2.4
1	B	554	GLU	2.4
1	A	1390	ALA	2.4
1	A	625	LYS	2.4
1	A	1004	ILE	2.4
1	B	416	LEU	2.4
1	A	429	LEU	2.4
1	B	1247	LEU	2.4
1	A	491	PHE	2.3
1	A	569	LYS	2.3
1	B	568	ARG	2.3
1	A	480	ILE	2.3
1	A	1407	VAL	2.3
1	A	1383	SER	2.3
1	A	643	GLU	2.3
1	B	475	GLU	2.3
1	B	476	ILE	2.3
1	B	469	ASP	2.2
1	B	491	PHE	2.2
1	B	493	ILE	2.2
1	A	1305	ASP	2.2
1	A	486	GLY	2.2
1	B	549	LYS	2.2
1	B	478	THR	2.2
1	B	606	VAL	2.2
1	A	472	LYS	2.2
1	A	559	TRP	2.1
1	A	521	PHE	2.1
1	A	612	ALA	2.1
1	B	640	THR	2.1
1	B	494	GLU	2.1
1	B	565	GLU	2.1
1	B	553	GLU	2.1
1	A	424	PRO	2.1
1	B	630	ARG	2.1
1	A	556	ALA	2.1
1	A	548	GLY	2.1
1	A	1250	GLY	2.1
1	B	422	LYS	2.0
1	A	489	ALA	2.0
1	B	562	GLY	2.0
1	A	642	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1396	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

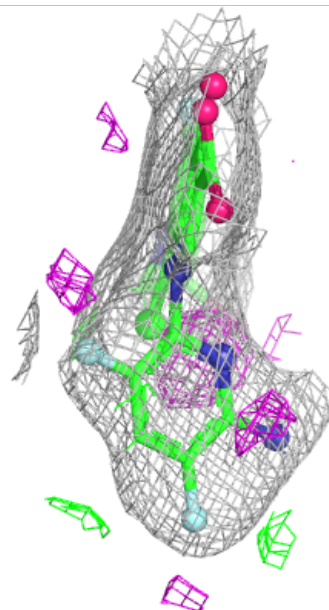
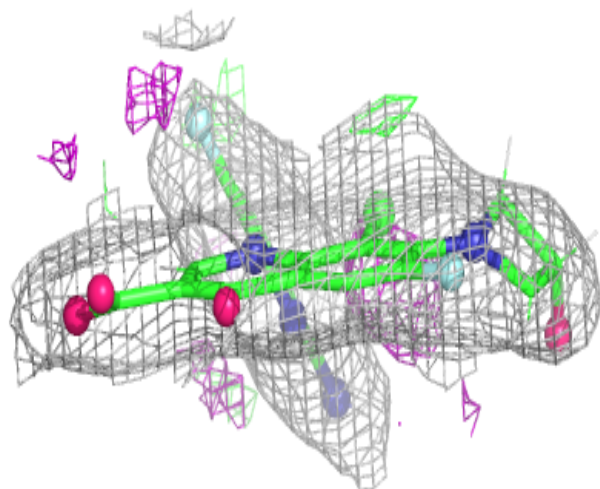
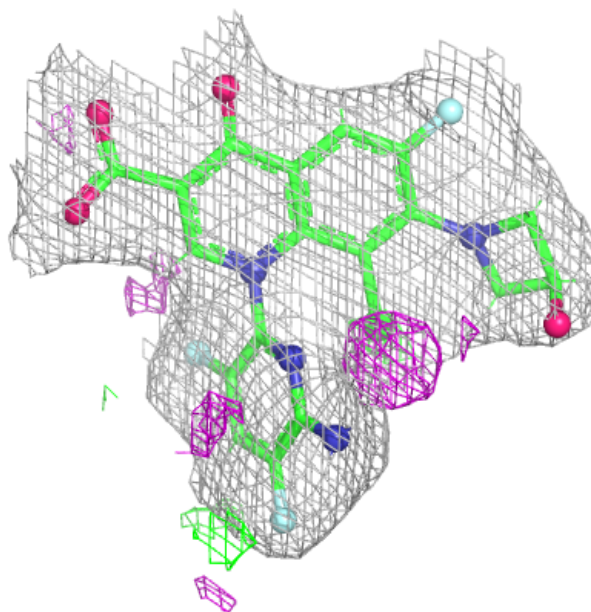
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MPD	A	1502	8/8	0.90	0.19	62,74,77,78	1
6	MPD	A	1501	8/8	0.93	0.12	46,48,48,49	1
8	CL	A	1506	1/1	0.93	0.12	51,51,51,51	0
6	MPD	B	1501	8/8	0.95	0.09	31,31,32,34	1
9	TE9	F	101	30/30	0.95	0.08	49,60,62,65	1
9	TE9	H	101	30/30	0.95	0.07	50,54,60,62	1
7	MG	A	1505	1/1	0.97	0.06	39,39,39,39	0
7	MG	B	1503	1/1	0.97	0.04	26,26,26,26	0
7	MG	B	1504	1/1	0.97	0.04	27,27,27,27	0
7	MG	A	1503	1/1	0.98	0.05	19,19,19,19	0
8	CL	B	1505	1/1	0.98	0.04	47,47,47,47	0
7	MG	A	1504	1/1	0.99	0.05	8,8,8,8	0
7	MG	B	1502	1/1	0.99	0.07	31,31,31,31	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.

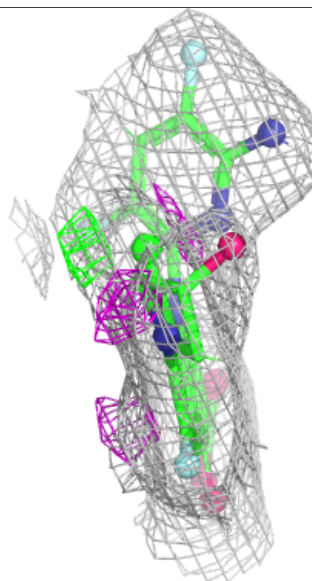
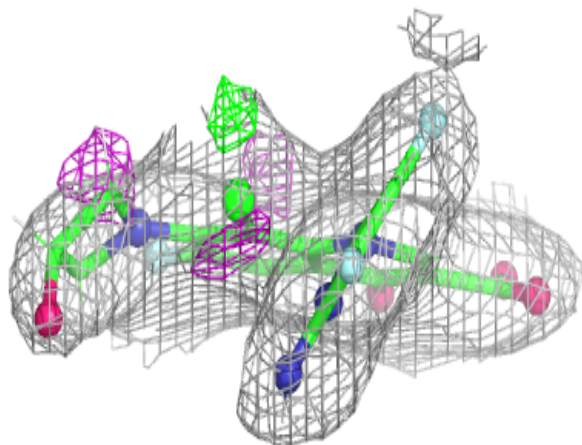
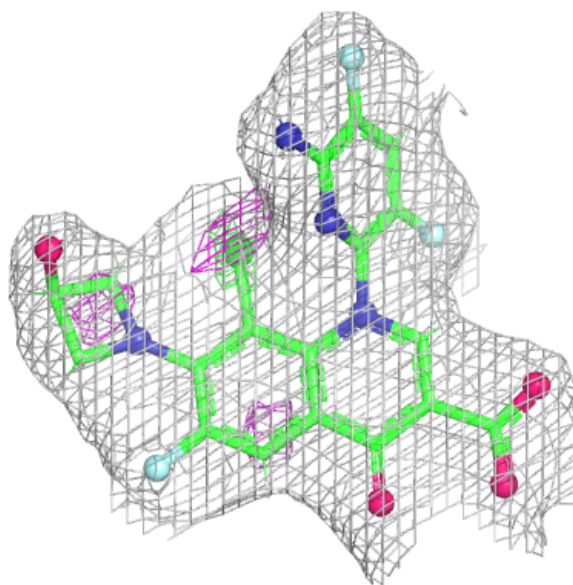
Electron density around TE9 F 101:

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



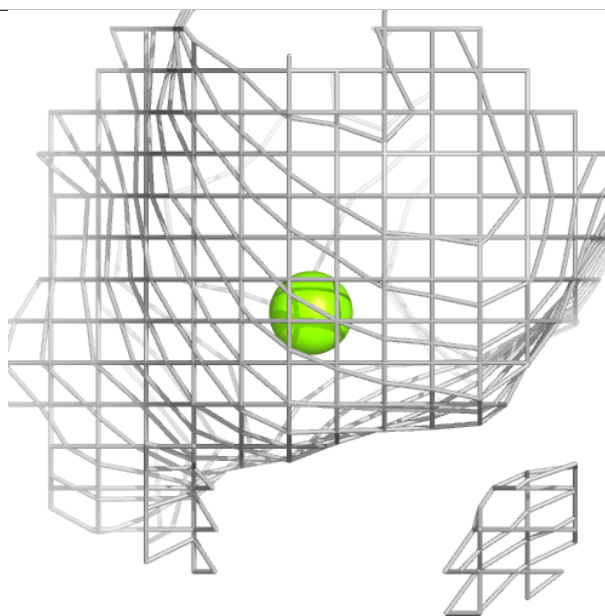
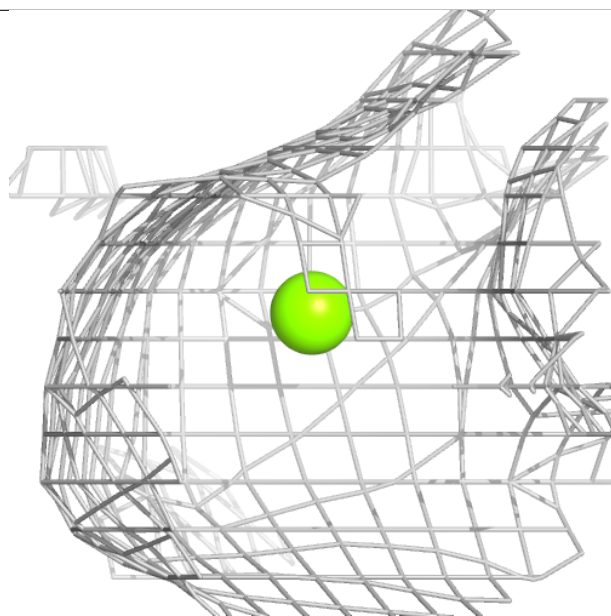
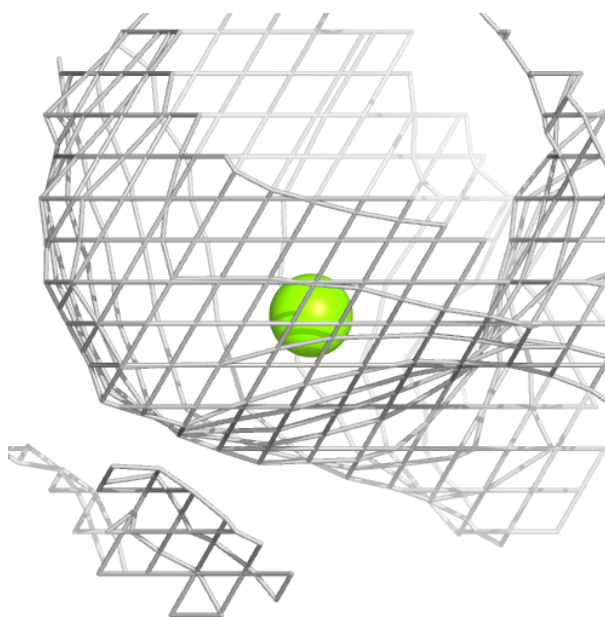
Electron density around TE9 H 101:

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



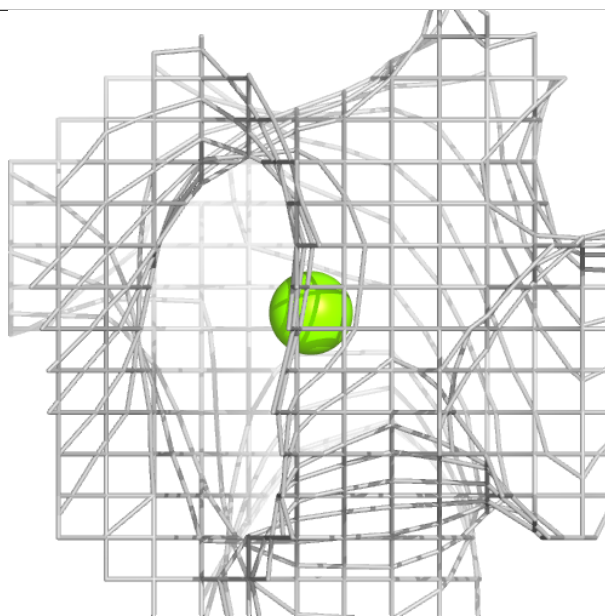
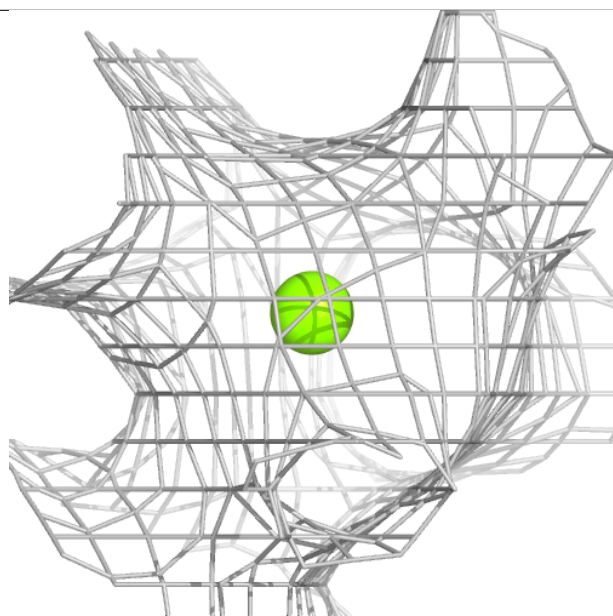
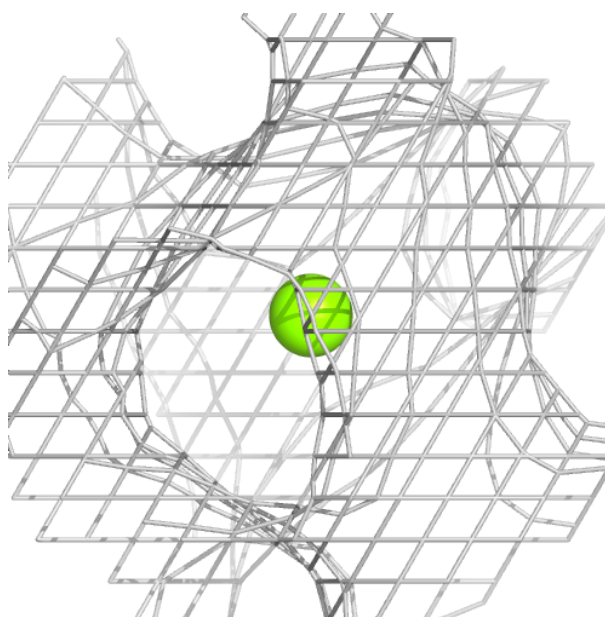
Electron density around MG A 1505:

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



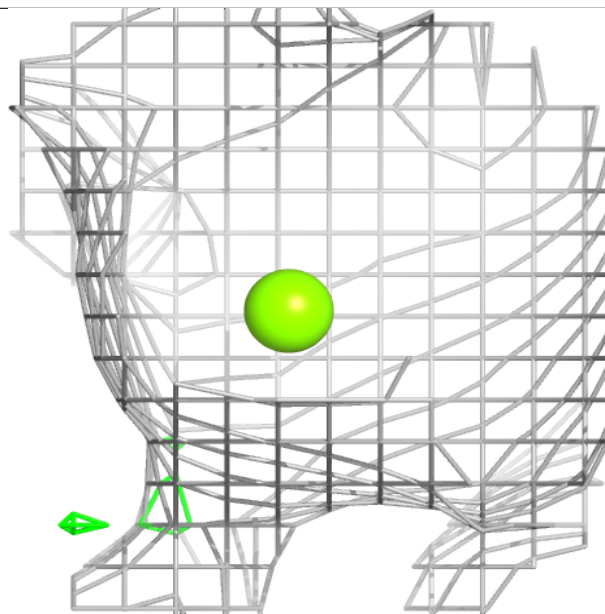
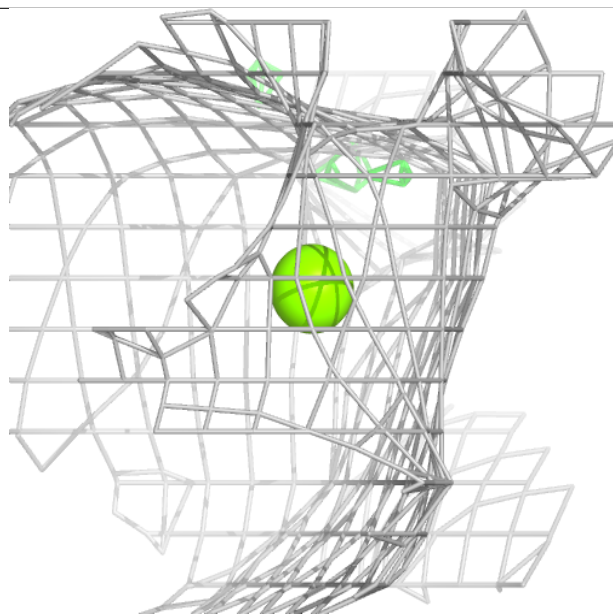
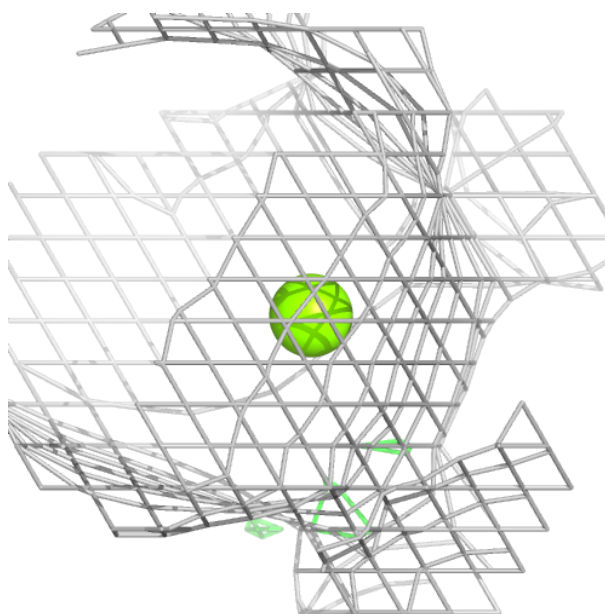
Electron density around MG B 1503:

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



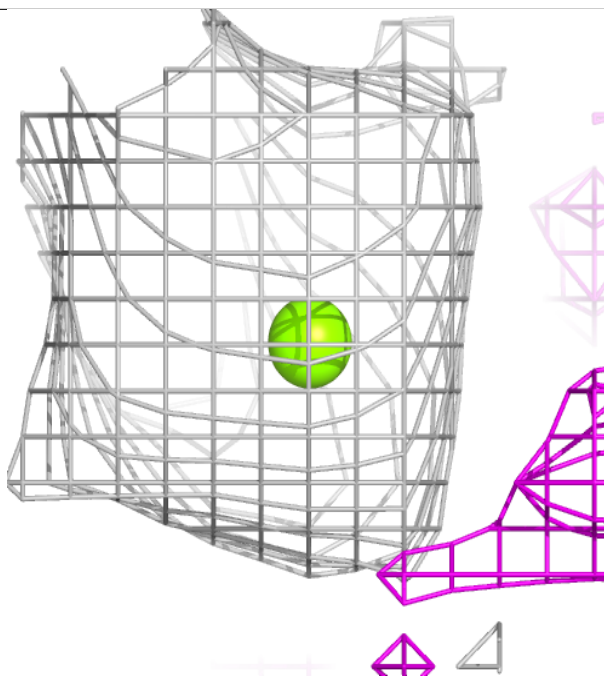
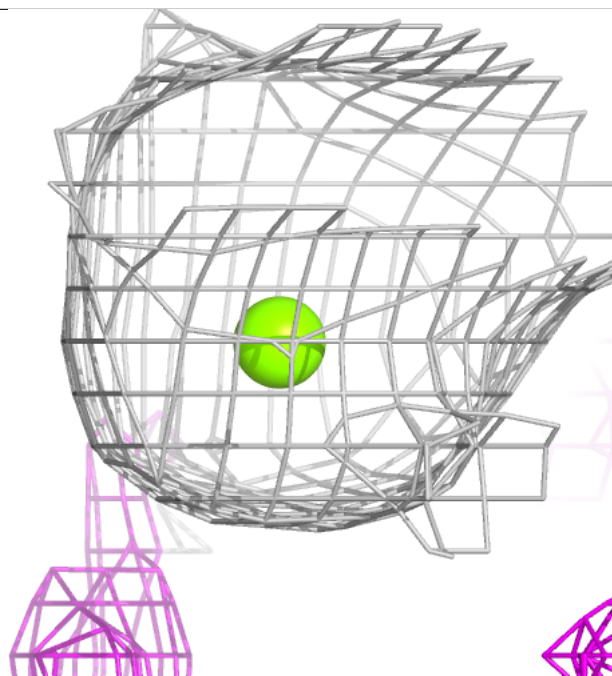
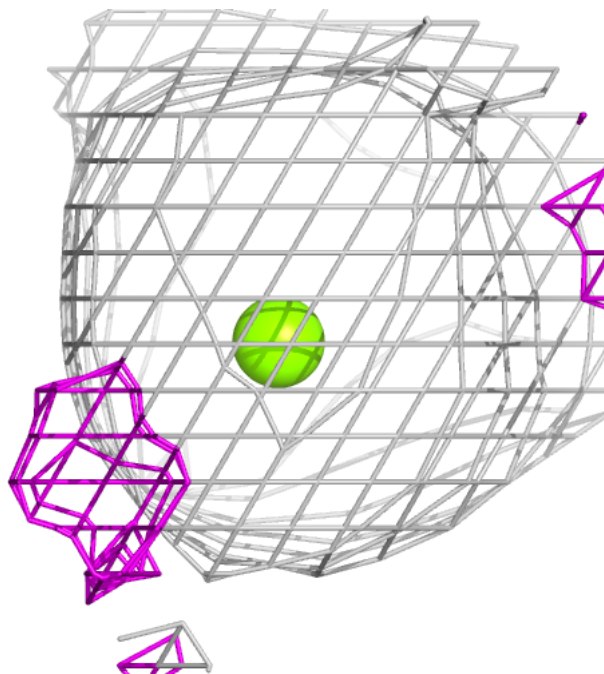
Electron density around MG B 1504:

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



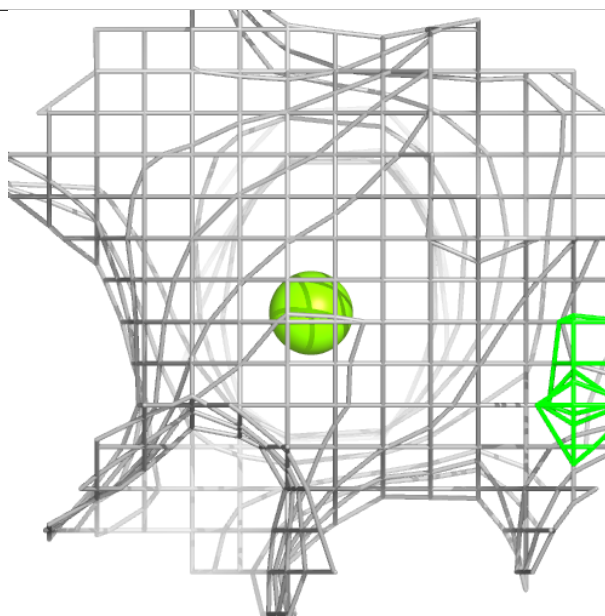
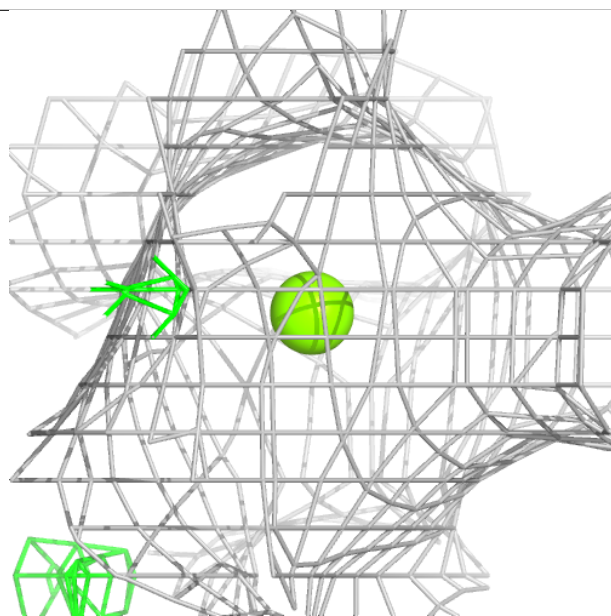
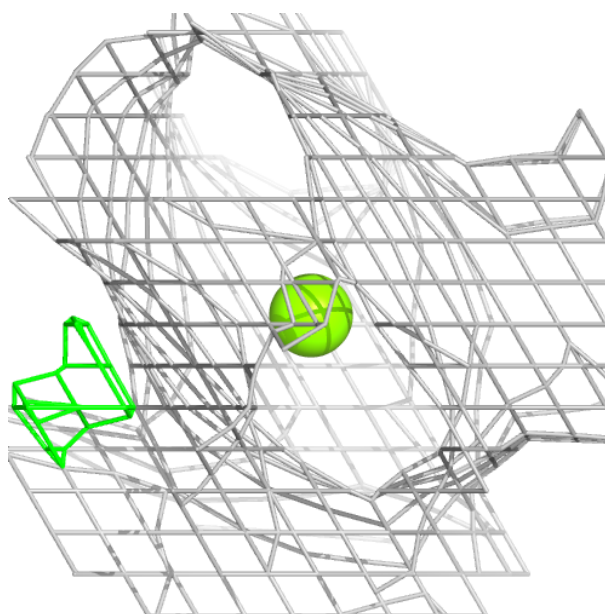
Electron density around MG A 1503:

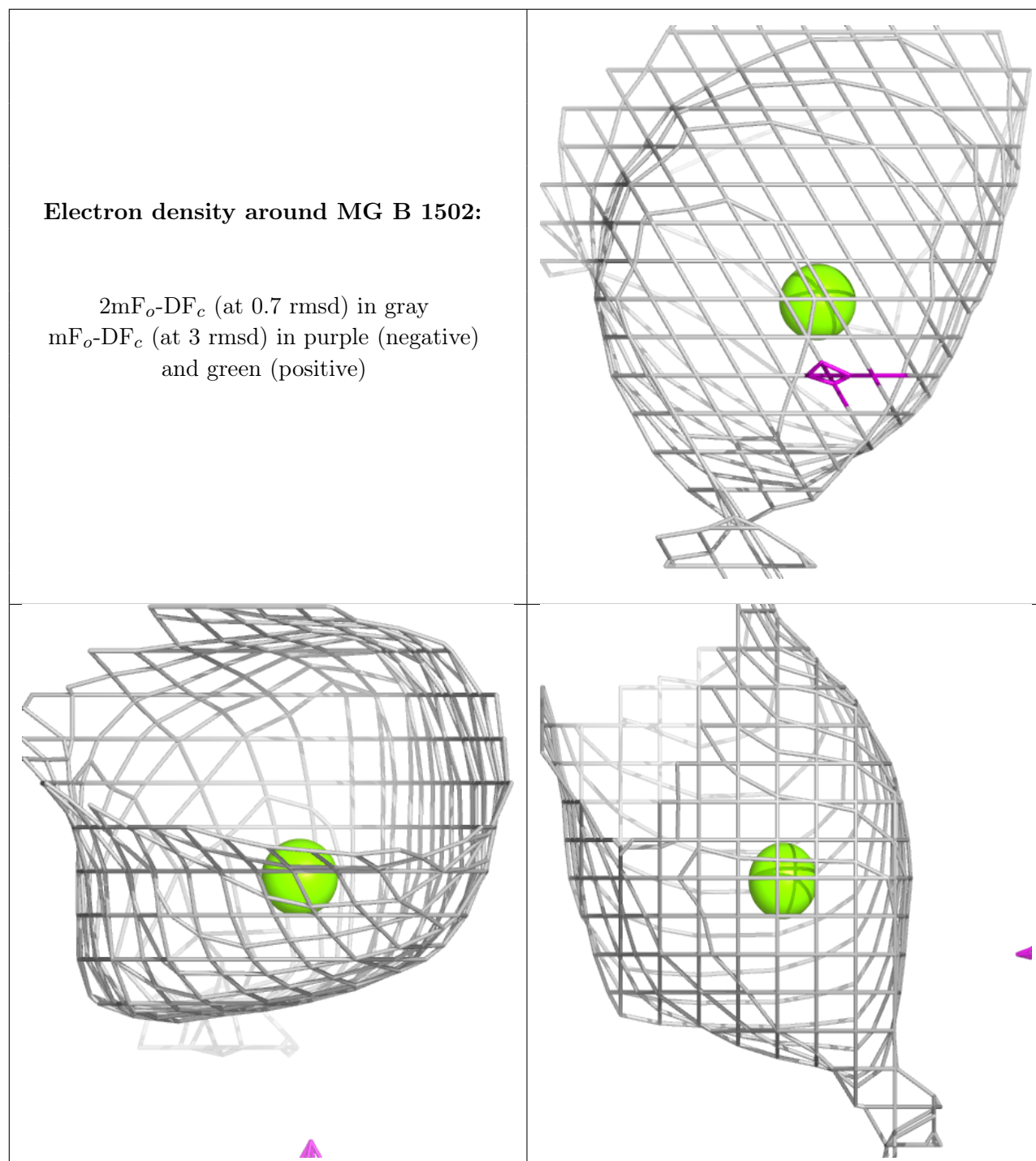
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1504:

$2mF_o-DF_c$ (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.