



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:01 pm BST

PDB ID : 6SMR
Title : A. thaliana serine hydroxymethyltransferase isoform 4 (AtSHMT4) in complex with methotrexate
Authors : Ruszkowski, M.; Sekula, B.; Dauter, Z.
Deposited on : 2019-08-22
Resolution : 2.12 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

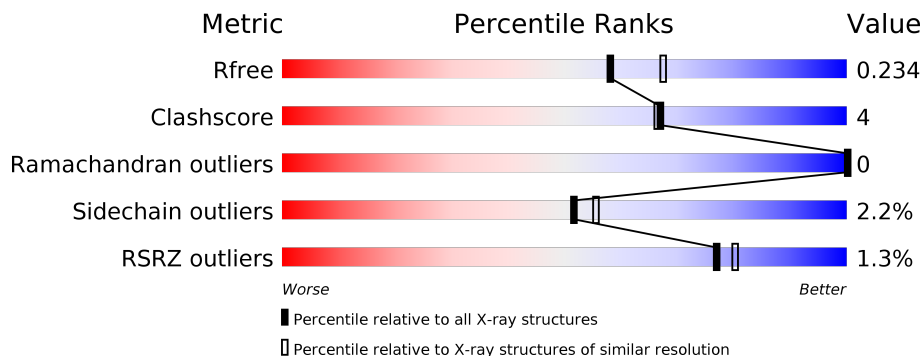
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	
1	B	474	
1	C	474	
1	D	474	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 15779 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 Serine hydroxymethyltransferase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	473	3654	2328	622	687	17	0	0	0
1	B	472	3649	2325	620	687	17	0	0	0
1	C	471	3640	2321	619	683	17	0	0	0
1	D	471	3640	2321	619	683	17	0	0	0

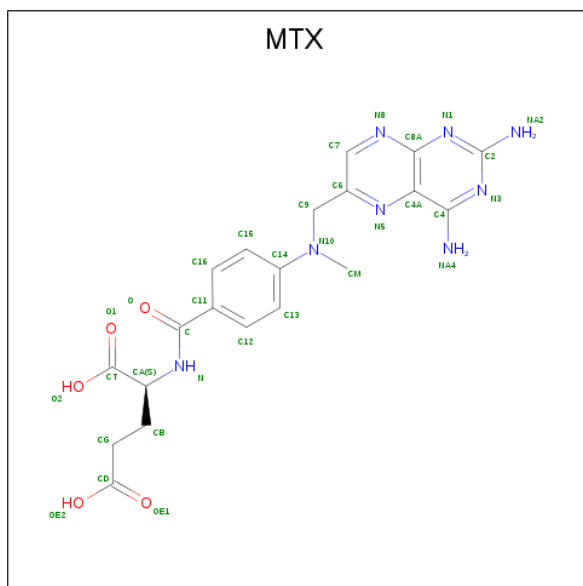
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP O23254
A	-1	ASN	-	expression tag	UNP O23254
A	0	ALA	-	expression tag	UNP O23254
B	-2	SER	-	expression tag	UNP O23254
B	-1	ASN	-	expression tag	UNP O23254
B	0	ALA	-	expression tag	UNP O23254
C	-2	SER	-	expression tag	UNP O23254
C	-1	ASN	-	expression tag	UNP O23254
C	0	ALA	-	expression tag	UNP O23254
D	-2	SER	-	expression tag	UNP O23254
D	-1	ASN	-	expression tag	UNP O23254
D	0	ALA	-	expression tag	UNP O23254

- Molecule 2 is [3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: C₁₁H₁₇N₂O₈P).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅) (labeled as "Ligand of Interest" by author).



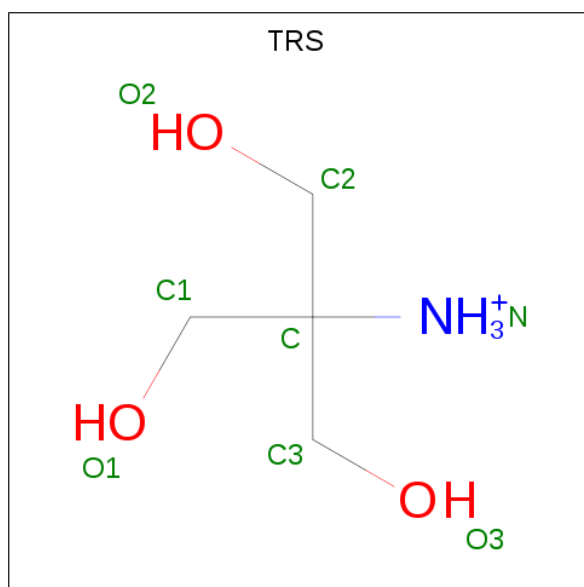
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 33 20 8 5	0	0
4	B	1	Total C N O 33 20 8 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	D	1	33	20	8	5	0	0

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	8	4	1	3	0	0

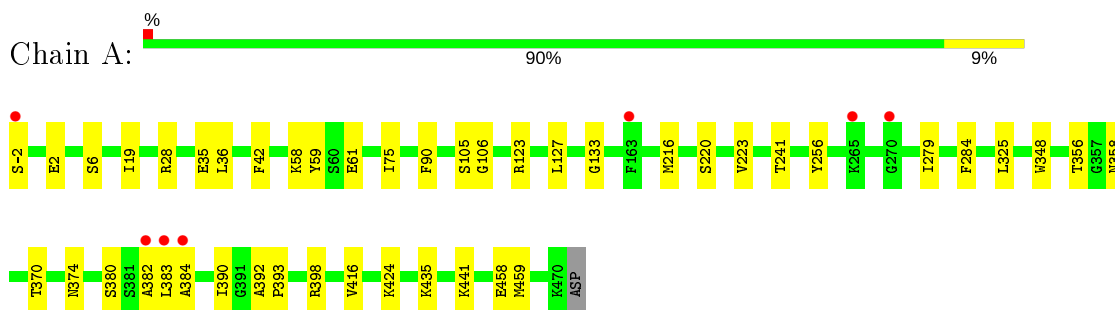
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	227	Total	O	0	0
			227	227		
6	B	259	Total	O	0	0
			259	259		
6	C	230	Total	O	0	0
			230	230		
6	D	249	Total	O	0	0
			249	249		

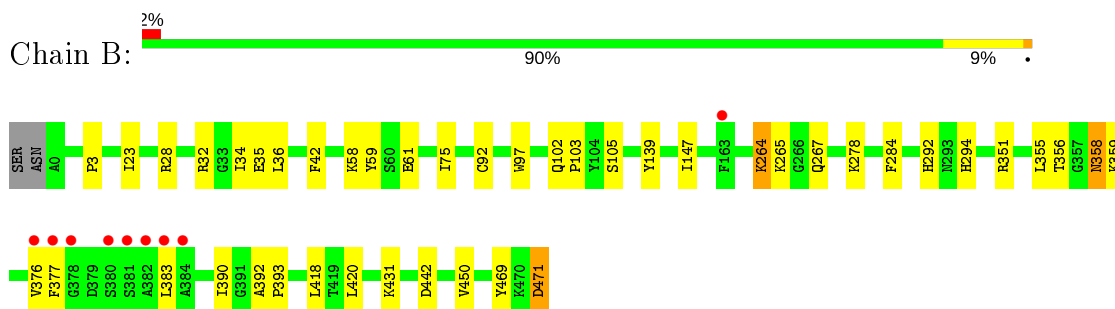
3 Residue-property plots [i](#)

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

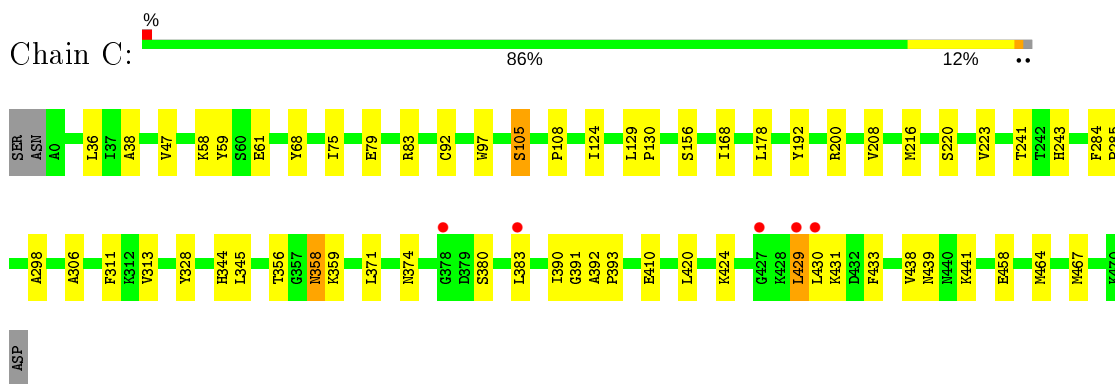
- Molecule 1: Serine hydroxymethyltransferase 4



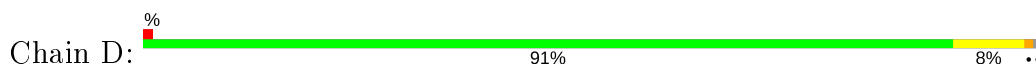
- Molecule 1: Serine hydroxymethyltransferase 4

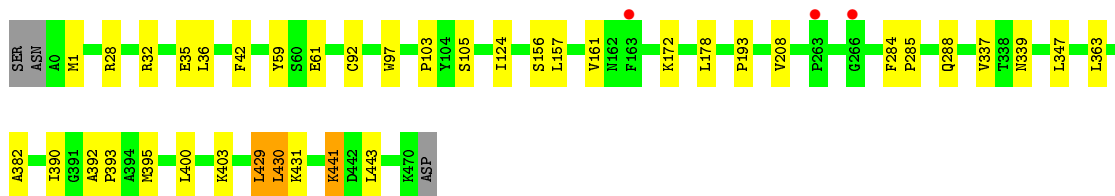


- Molecule 1: Serine hydroxymethyltransferase 4



- Molecule 1: Serine hydroxymethyltransferase 4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.86Å 120.97Å 131.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	88.30 – 2.12 88.27 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.8 (88.30-2.12) 98.8 (88.27-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.12Å)	Xtrriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.173 , 0.234 0.174 , 0.234	Depositor DCC
R_{free} test set	1069 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtrriage
Anisotropy	0.512	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15779	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4816e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MTX, PLS, TRS, EDO

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	0.36	0/3738	0.53	0/5059
1	B	0.36	0/3733	0.53	0/5051
1	C	0.40	0/3724	0.54	0/5040
1	D	0.37	0/3724	0.54	0/5040
All	All	0.37	0/14919	0.54	0/20190

There are no bond length outliers.

There are no bond angle outliers.

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	3654	0	3620	31	0
1	B	3649	0	3613	21	0
1	C	3640	0	3609	38	0
1	D	3640	0	3609	24	0
2	A	22	0	14	0	0
2	B	22	0	14	0	0
2	C	22	0	14	0	0
2	D	22	0	14	0	0
3	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	1	0
3	C	8	0	12	0	0
3	D	8	0	12	1	0
4	A	33	0	19	0	0
4	B	33	0	20	2	0
4	D	33	0	19	1	0
5	C	8	0	12	0	0
6	A	227	0	0	5	0
6	B	259	0	0	1	0
6	C	230	0	0	4	0
6	D	249	0	0	2	0
All	All	15779	0	14631	114	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 4.

All (114) 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:216:MET:SD	6:A:820:HOH:O	2.20	0.99
1:A:216:MET:HE2	1:A:220:SER:HA	1.47	0.94
1:C:216:MET:SD	6:C:825:HOH:O	2.31	0.87
1:B:264:LYS:HG3	1:B:267:GLN:HB2	1.64	0.80
1:A:216:MET:CE	1:A:220:SER:HA	2.18	0.73
1:D:36:LEU:HB3	1:D:390:ILE:HG23	1.74	0.69
1:A:-2:SER:N	6:A:601:HOH:O	2.28	0.65
1:D:430:LEU:H	1:D:430:LEU:HD22	1.63	0.64
1:C:420:LEU:O	1:C:424:LYS:HG2	1.99	0.63
1:C:216:MET:HE1	1:C:223:VAL:HB	1.80	0.61
1:B:58:LYS:HG2	1:B:75:ILE:HG13	1.82	0.61
1:C:216:MET:HE2	1:C:220:SER:HA	1.82	0.60
1:C:58:LYS:HG2	1:C:75:ILE:HG13	1.83	0.60
1:B:278:LYS:NZ	6:B:603:HOH:O	2.35	0.60
1:A:123:ARG:HD2	3:A:502:EDO:H22	1.82	0.59
1:C:216:MET:CE	1:C:220:SER:HA	2.33	0.58
1:C:36:LEU:HB3	1:C:390:ILE:HG23	1.86	0.56
1:D:339:ASN:ND2	6:D:802:HOH:O	2.28	0.55
1:D:337:VAL:HG21	1:D:347:LEU:HD23	1.87	0.55
1:A:398:ARG:HD2	1:A:459:MET:HE1	1.89	0.55
1:D:193:PRO:HG3	1:D:337:VAL:HG23	1.89	0.55
1:C:356:THR:HG23	1:C:359:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:PHE:HE1	1:A:216:MET:HE1	1.73	0.53
1:C:178:LEU:HD23	1:C:208:VAL:HG12	1.90	0.53
1:C:79:GLU:O	1:C:83:ARG:HG3	2.09	0.53
1:A:58:LYS:HG2	1:A:75:ILE:HG13	1.91	0.52
1:C:458:GLU:HA	1:C:464:MET:HE1	1.91	0.52
1:A:358:ASN:ND2	1:A:358:ASN:H	2.08	0.52
1:C:383:LEU:H	1:C:383:LEU:HD12	1.75	0.52
1:B:23:ILE:HG21	3:B:505:EDO:H22	1.92	0.52
1:D:382:ALA:HB2	4:D:703:MTX:C12	2.39	0.51
1:A:127:LEU:O	1:A:133:GLY:HA3	2.10	0.51
1:B:356:THR:HG23	1:B:359:LYS:H	1.74	0.51
1:D:35:GLU:HG3	1:D:42:PHE:HZ	1.75	0.51
1:A:424:LYS:NZ	6:A:604:HOH:O	2.41	0.51
1:C:439:ASN:HB3	6:C:604:HOH:O	2.10	0.51
1:B:355:LEU:HD11	1:B:420:LEU:HG	1.94	0.50
1:D:429:LEU:HB2	6:D:808:HOH:O	2.12	0.50
1:C:429:LEU:HD22	1:C:429:LEU:H	1.76	0.49
1:A:348:TRP:CH2	1:A:416:VAL:HG21	2.47	0.49
1:A:35:GLU:HG3	1:A:42:PHE:HZ	1.78	0.49
1:A:325:LEU:HD21	1:A:390:ILE:HG21	1.95	0.48
1:B:264:LYS:HG3	1:B:267:GLN:CB	2.40	0.48
1:B:358:ASN:N	1:B:358:ASN:OD1	2.46	0.48
1:B:292:HIS:HB3	1:B:294:HIS:CE1	2.49	0.48
1:C:430:LEU:HA	1:C:433:PHE:HB3	1.94	0.48
1:C:47:VAL:HG13	1:C:298:ALA:HB1	1.96	0.47
1:D:441:LYS:H	1:D:441:LYS:NZ	2.12	0.47
1:C:313:VAL:HG12	1:D:1:MET:HG2	1.94	0.47
1:A:256:TYR:HB3	1:A:279:ILE:HD12	1.95	0.47
1:D:395:MET:HB3	1:D:400:LEU:HD22	1.95	0.47
1:C:284:PHE:CD1	1:C:285:PRO:HA	2.49	0.47
1:A:358:ASN:HD22	1:A:358:ASN:H	1.61	0.46
1:D:284:PHE:CD1	1:D:285:PRO:HA	2.49	0.46
1:C:328:TYR:OH	1:C:410:GLU:OE1	2.33	0.46
1:B:32:ARG:NH1	1:B:471:ASP:O	2.48	0.46
1:B:34:ILE:HG13	1:B:450:VAL:HG13	1.97	0.46
1:C:168:ILE:HG13	1:C:192:TYR:CZ	2.51	0.46
1:D:157:LEU:HD21	3:D:701:EDO:H22	1.98	0.46
1:C:200:ARG:NH1	6:C:618:HOH:O	2.48	0.45
1:C:83:ARG:NH1	6:C:613:HOH:O	2.45	0.45
1:B:36:LEU:HB3	1:B:390:ILE:HG23	1.97	0.45
1:C:430:LEU:HD12	1:C:431:LYS:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:CYS:HB3	1:B:97:TRP:HB2	1.98	0.44
1:C:344:HIS:CE1	1:C:345:LEU:HD23	2.52	0.44
1:B:139:TYR:HD2	1:B:147:ILE:HB	1.82	0.44
1:A:61:GLU:HB3	1:A:284:PHE:CZ	2.52	0.44
1:D:392:ALA:N	1:D:393:PRO:CD	2.81	0.44
1:A:435:LYS:NZ	6:A:603:HOH:O	2.40	0.43
1:A:19:ILE:HD13	1:A:19:ILE:HA	1.92	0.43
1:B:61:GLU:HB3	1:B:284:PHE:CZ	2.54	0.43
1:D:337:VAL:HG22	1:D:347:LEU:HB3	2.00	0.43
1:A:35:GLU:HA	1:A:370:THR:CG2	2.48	0.43
1:C:358:ASN:OD1	1:C:358:ASN:N	2.52	0.42
1:B:418:LEU:HD21	1:B:442:ASP:HB3	2.01	0.42
1:C:241:THR:HB	1:C:243:HIS:CE1	2.55	0.42
1:D:363:LEU:HG	1:D:443:LEU:HD11	1.99	0.42
1:B:28:ARG:HD2	1:B:469:TYR:HB3	2.02	0.42
6:A:745:HOH:O	4:B:501:MTX:HG1	2.20	0.42
1:C:392:ALA:N	1:C:393:PRO:CD	2.83	0.42
1:D:61:GLU:HB3	1:D:284:PHE:CZ	2.53	0.42
1:B:35:GLU:HG3	1:B:42:PHE:HZ	1.84	0.42
1:C:420:LEU:HD22	1:C:424:LYS:NZ	2.35	0.42
1:C:124:ILE:O	1:C:156:SER:HA	2.19	0.42
1:A:36:LEU:HB3	1:A:390:ILE:HG23	2.01	0.42
1:C:61:GLU:HB3	1:C:284:PHE:CZ	2.55	0.41
1:A:106:GLY:HA3	1:A:241:THR:HG22	2.03	0.41
1:A:441:LYS:HD3	1:A:441:LYS:HA	1.85	0.41
1:B:102:GLN:N	1:B:103:PRO:CD	2.83	0.41
1:B:351:ARG:HH12	1:B:377:PHE:HD2	1.67	0.41
1:C:68:TYR:CZ	1:C:284:PHE:HE2	2.38	0.41
1:C:92:CYS:HB3	1:C:97:TRP:HB2	2.01	0.41
1:D:92:CYS:HB3	1:D:97:TRP:HB2	2.02	0.41
1:D:103:PRO:HA	1:D:288:GLN:OE1	2.20	0.41
1:B:392:ALA:N	1:B:393:PRO:CD	2.83	0.41
1:D:178:LEU:HD23	1:D:208:VAL:HG12	2.02	0.41
1:A:356:THR:OG1	1:A:358:ASN:ND2	2.54	0.41
1:A:2:GLU:HG2	1:A:6:SER:HB3	2.02	0.41
1:C:306:ALA:HA	1:C:311:PHE:CG	2.56	0.41
1:D:124:ILE:O	1:D:156:SER:HA	2.20	0.41
1:A:382:ALA:HB2	4:B:501:MTX:C12	2.51	0.41
1:D:441:LYS:H	1:D:441:LYS:HZ3	1.67	0.41
1:A:35:GLU:HA	1:A:370:THR:HG22	2.03	0.41
1:A:392:ALA:N	1:A:393:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LYS:HD3	1:D:172:LYS:HA	1.87	0.41
1:C:130:PRO:HG2	1:C:380:SER:HB3	2.01	0.40
1:A:216:MET:HE1	1:A:223:VAL:HB	2.03	0.40
1:A:216:MET:HE3	1:A:223:VAL:HG21	2.04	0.40
1:A:358:ASN:ND2	1:A:384:ALA:HA	2.37	0.40
1:C:105:SER:C	1:C:108:PRO:HD2	2.42	0.40
1:C:464:MET:O	1:C:467:MET:HG2	2.21	0.40
1:D:28:ARG:CZ	1:D:32:ARG:HG3	2.51	0.40
1:C:38:ALA:HA	1:C:391:GLY:HA3	2.03	0.40
1:C:75:ILE:HA	1:C:75:ILE:HD13	1.92	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	471/474 (99%)	457 (97%)	14 (3%)	0	100	100
1	B	470/474 (99%)	451 (96%)	19 (4%)	0	100	100
1	C	469/474 (99%)	454 (97%)	15 (3%)	0	100	100
1	D	469/474 (99%)	454 (97%)	15 (3%)	0	100	100
All	All	1879/1896 (99%)	1816 (97%)	63 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	385/386 (100%)	378 (98%)	7 (2%)	59	63
1	B	384/386 (100%)	374 (97%)	10 (3%)	46	49
1	C	383/386 (99%)	374 (98%)	9 (2%)	50	53
1	D	383/386 (99%)	375 (98%)	8 (2%)	53	57
All	All	1535/1544 (99%)	1501 (98%)	34 (2%)	52	55

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	59	TYR
1	A	105	SER
1	A	374	ASN
1	A	380	SER
1	A	383	LEU
1	A	458	GLU
1	B	3	PRO
1	B	59	TYR
1	B	105	SER
1	B	264	LYS
1	B	265	LYS
1	B	358	ASN
1	B	376	VAL
1	B	383	LEU
1	B	431	LYS
1	B	471	ASP
1	C	59	TYR
1	C	105	SER
1	C	129	LEU
1	C	358	ASN
1	C	371	LEU
1	C	374	ASN
1	C	429	LEU
1	C	438	VAL
1	C	441	LYS
1	D	59	TYR
1	D	105	SER
1	D	161	VAL
1	D	403	LYS

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Mol	Chain	Res	Type
1	D	429	LEU
1	D	430	LEU
1	D	431	LYS
1	D	441	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	358	ASN
1	B	439	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.37	0
3	EDO	B	504	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	D	701	-	3,3,3	0.56	0	2,2,2	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MTX	D	703	-	29,35,35	2.81	8 (27%)	38,49,49	3.87	20 (52%)
3	EDO	C	504	-	3,3,3	0.45	0	2,2,2	0.49	0
3	EDO	D	704	-	3,3,3	0.43	0	2,2,2	0.47	0
5	TRS	C	503	-	7,7,7	0.26	0	9,9,9	0.56	0
4	MTX	B	501	-	29,35,35	2.67	8 (27%)	38,49,49	2.00	9 (23%)
2	PLS	B	502	-	19,22,22	2.08	3 (15%)	25,31,31	1.53	2 (8%)
3	EDO	B	505	-	3,3,3	0.49	0	2,2,2	0.20	0
2	PLS	C	501	-	19,22,22	2.11	3 (15%)	25,31,31	1.46	5 (20%)
2	PLS	A	501	-	19,22,22	2.06	3 (15%)	25,31,31	1.59	6 (24%)
3	EDO	C	502	-	3,3,3	0.46	0	2,2,2	0.30	0
2	PLS	D	702	-	19,22,22	2.08	3 (15%)	25,31,31	1.45	3 (12%)
4	MTX	A	503	-	29,35,35	2.68	8 (27%)	38,49,49	2.90	15 (39%)
3	EDO	A	502	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	B	503	-	3,3,3	0.41	0	2,2,2	0.51	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
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	D	701	-	-	0/1/1/1	-
4	MTX	D	703	-	-	5/19/25/25	0/3/3/3
3	EDO	C	504	-	-	1/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
5	TRS	C	503	-	-	1/9/9/9	-
4	MTX	B	501	-	-	1/19/25/25	0/3/3/3
2	PLS	B	502	-	-	7/13/17/17	0/1/1/1
3	EDO	B	505	-	-	0/1/1/1	-
2	PLS	C	501	-	-	5/13/17/17	0/1/1/1
2	PLS	A	501	-	-	7/13/17/17	0/1/1/1
3	EDO	C	502	-	-	0/1/1/1	-
2	PLS	D	702	-	-	5/13/17/17	0/1/1/1
4	MTX	A	503	-	-	1/19/25/25	0/3/3/3
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	MTX	C2-NA2	7.22	1.48	1.33
2	D	702	PLS	C4A-N	-7.18	1.25	1.46
2	C	501	PLS	C4A-N	-7.14	1.25	1.46
4	A	503	MTX	C2-NA2	7.04	1.48	1.33
2	A	501	PLS	C4A-N	-7.02	1.25	1.46
4	D	703	MTX	C2-NA2	6.93	1.47	1.33
2	B	502	PLS	C4A-N	-6.92	1.26	1.46
4	D	703	MTX	C-N	6.66	1.48	1.34
4	A	503	MTX	C-N	6.64	1.48	1.34
4	B	501	MTX	C-N	6.07	1.47	1.34
4	D	703	MTX	C9-C6	5.20	1.60	1.51
4	A	503	MTX	C9-C6	5.03	1.59	1.51
4	B	501	MTX	C9-C6	4.80	1.59	1.51
4	D	703	MTX	C14-N10	4.74	1.52	1.39
4	A	503	MTX	CM-N10	-4.60	1.38	1.46
4	B	501	MTX	CM-N10	-4.59	1.38	1.46
4	A	503	MTX	C4-NA4	4.55	1.50	1.34
4	B	501	MTX	C4-NA4	4.55	1.50	1.34
4	D	703	MTX	C4-NA4	4.47	1.50	1.34
4	D	703	MTX	CM-N10	-4.39	1.38	1.46
4	B	501	MTX	C14-N10	4.00	1.50	1.39
4	A	503	MTX	C14-N10	3.91	1.50	1.39
4	D	703	MTX	C11-C	3.44	1.57	1.50
2	A	501	PLS	C3-C2	-3.36	1.37	1.40
4	D	703	MTX	O-C	-3.36	1.16	1.23
4	B	501	MTX	O-C	-3.30	1.16	1.23
4	A	503	MTX	O-C	-3.05	1.17	1.23
2	B	502	PLS	C3-C2	-2.93	1.38	1.40
2	C	501	PLS	C5-C4	-2.79	1.36	1.40
2	D	702	PLS	C5-C4	-2.70	1.36	1.40
2	D	702	PLS	C3-C2	-2.64	1.38	1.40
2	B	502	PLS	C5-C4	-2.47	1.36	1.40
4	A	503	MTX	C11-C	2.44	1.55	1.50
2	C	501	PLS	C3-C2	-2.44	1.38	1.40
4	B	501	MTX	C11-C	2.43	1.55	1.50
2	A	501	PLS	C5-C4	-2.18	1.37	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	MTX	CB-CA-N	12.32	128.14	110.19
4	D	703	MTX	C11-C-N	11.05	138.25	117.06
4	D	703	MTX	CA-N-C	10.23	135.53	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	MTX	CB-CA-N	8.86	123.10	110.19
4	D	703	MTX	O-C-N	-6.99	109.59	122.45
4	B	501	MTX	N1-C2-N3	-5.42	119.99	127.22
4	D	703	MTX	N1-C2-N3	-5.33	120.11	127.22
4	A	503	MTX	N1-C2-N3	-5.25	120.22	127.22
4	D	703	MTX	O-C-C11	-5.04	111.95	120.94
2	D	702	PLS	C4A-N-CA	4.67	122.79	113.83
4	D	703	MTX	C2-N1-C8A	4.35	120.33	115.36
4	B	501	MTX	N8-C8A-N1	4.20	120.62	115.82
4	B	501	MTX	C2-N1-C8A	4.16	120.11	115.36
2	B	502	PLS	C4A-N-CA	4.14	121.78	113.83
4	D	703	MTX	N8-C8A-N1	4.09	120.48	115.82
4	A	503	MTX	N8-C8A-N1	4.08	120.47	115.82
4	A	503	MTX	C2-N1-C8A	4.05	119.99	115.36
2	A	501	PLS	C4A-N-CA	3.99	121.49	113.83
4	A	503	MTX	C9-C6-N5	3.92	123.24	116.96
4	D	703	MTX	CG-CB-CA	-3.85	105.26	113.04
4	A	503	MTX	C7-N8-C8A	3.83	120.54	116.69
4	B	501	MTX	C6-C9-N10	-3.71	107.24	113.60
4	D	703	MTX	C7-N8-C8A	3.56	120.27	116.69
4	B	501	MTX	C7-N8-C8A	3.47	120.17	116.69
2	C	501	PLS	C4A-N-CA	3.40	120.36	113.83
4	D	703	MTX	C6-C9-N10	-3.33	107.88	113.60
4	D	703	MTX	C6-C7-N8	-3.30	119.89	123.13
4	B	501	MTX	C6-C7-N8	-3.26	119.93	123.13
4	A	503	MTX	C6-C7-N8	-3.19	120.00	123.13
2	C	501	PLS	C4-C4A-N	3.13	120.39	111.78
2	B	502	PLS	C4-C4A-N	3.05	120.18	111.78
4	D	703	MTX	C15-C14-N10	-3.01	117.30	121.62
4	D	703	MTX	C9-C6-N5	2.94	121.67	116.96
4	B	501	MTX	C9-C6-N5	2.72	121.31	116.96
2	D	702	PLS	C4-C4A-N	2.67	119.14	111.78
4	D	703	MTX	C12-C11-C	2.67	129.26	120.62
2	A	501	PLS	O4P-C5A-C5	2.66	114.42	109.35
4	A	503	MTX	C13-C14-N10	-2.65	117.80	121.62
4	A	503	MTX	CA-N-C	-2.59	119.00	122.34
2	C	501	PLS	O4P-C5A-C5	2.59	114.28	109.35
4	D	703	MTX	CB-CG-CD	-2.56	108.08	113.59
2	A	501	PLS	C4-C4A-N	2.52	118.73	111.78
4	A	503	MTX	C7-C6-N5	-2.51	119.21	120.85
4	D	703	MTX	C16-C11-C	-2.41	112.81	120.62
4	B	501	MTX	C13-C14-N10	-2.35	118.24	121.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	MTX	C7-C6-N5	-2.33	119.32	120.85
2	C	501	PLS	C6-C5-C4	2.33	119.77	118.12
4	A	503	MTX	C9-C6-C7	-2.32	117.55	121.60
2	C	501	PLS	C5-C6-N1	-2.31	119.97	123.82
2	A	501	PLS	O3-C3-C4	2.27	124.78	118.13
4	D	703	MTX	C8A-C4A-N5	-2.25	119.69	122.41
4	A	503	MTX	C8A-C4A-N5	-2.25	119.69	122.41
4	A	503	MTX	CM-N10-C9	2.16	120.58	114.84
2	A	501	PLS	C5-C6-N1	-2.12	120.28	123.82
4	A	503	MTX	C6-C9-N10	-2.12	109.96	113.60
2	D	702	PLS	C5-C6-N1	-2.12	120.29	123.82
4	A	503	MTX	CG-CB-CA	-2.10	108.81	113.04
4	D	703	MTX	C15-C16-C11	2.07	123.19	120.78
4	B	501	MTX	C4A-C4-N3	-2.02	119.69	121.01
2	A	501	PLS	C5A-C5-C6	-2.00	116.08	119.37

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	703	MTX	O-C-N-CA
4	D	703	MTX	CT-CA-CB-CG
4	D	703	MTX	CA-CB-CG-CD
5	C	503	TRS	N-C-C2-O2
2	B	502	PLS	C3-C4-C4A-N
2	B	502	PLS	C5-C4-C4A-N
2	B	502	PLS	C5A-O4P-P-O1P
2	C	501	PLS	C5-C4-C4A-N
2	A	501	PLS	C5-C4-C4A-N
2	A	501	PLS	C5A-O4P-P-O3P
2	D	702	PLS	C5-C4-C4A-N
2	D	702	PLS	C5A-O4P-P-O2P
4	A	503	MTX	CT-CA-N-C
4	D	703	MTX	C11-C-N-CA
2	C	501	PLS	C3-C4-C4A-N
4	D	703	MTX	CT-CA-N-C
3	C	504	EDO	O1-C1-C2-O2
2	B	502	PLS	C5A-O4P-P-O3P
2	A	501	PLS	C5A-O4P-P-O2P
4	B	501	MTX	CA-CB-CG-CD
2	C	501	PLS	C4-C5-C5A-O4P
3	D	704	EDO	O1-C1-C2-O2

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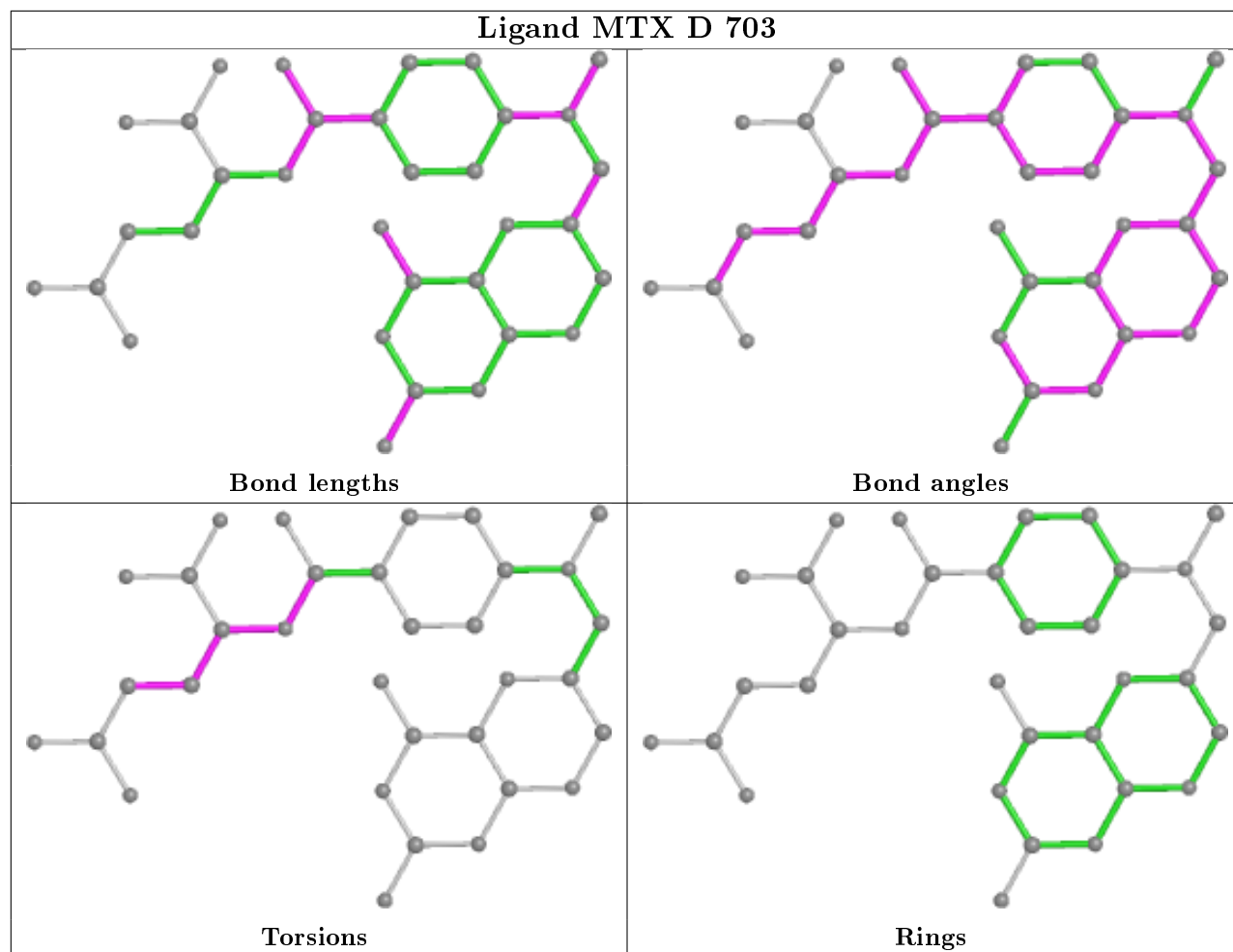
Mol	Chain	Res	Type	Atoms
2	B	502	PLS	CB-CA-N-C4A
2	A	501	PLS	CB-CA-N-C4A
2	D	702	PLS	CB-CA-N-C4A
2	A	501	PLS	C5A-O4P-P-O1P
2	B	502	PLS	C-CA-N-C4A
2	A	501	PLS	C-CA-N-C4A
2	D	702	PLS	C-CA-N-C4A
2	A	501	PLS	C3-C4-C4A-N
2	D	702	PLS	C3-C4-C4A-N
2	C	501	PLS	C6-C5-C5A-O4P
2	B	502	PLS	C5A-O4P-P-O2P
3	B	504	EDO	O1-C1-C2-O2
2	C	501	PLS	C-CA-N-C4A

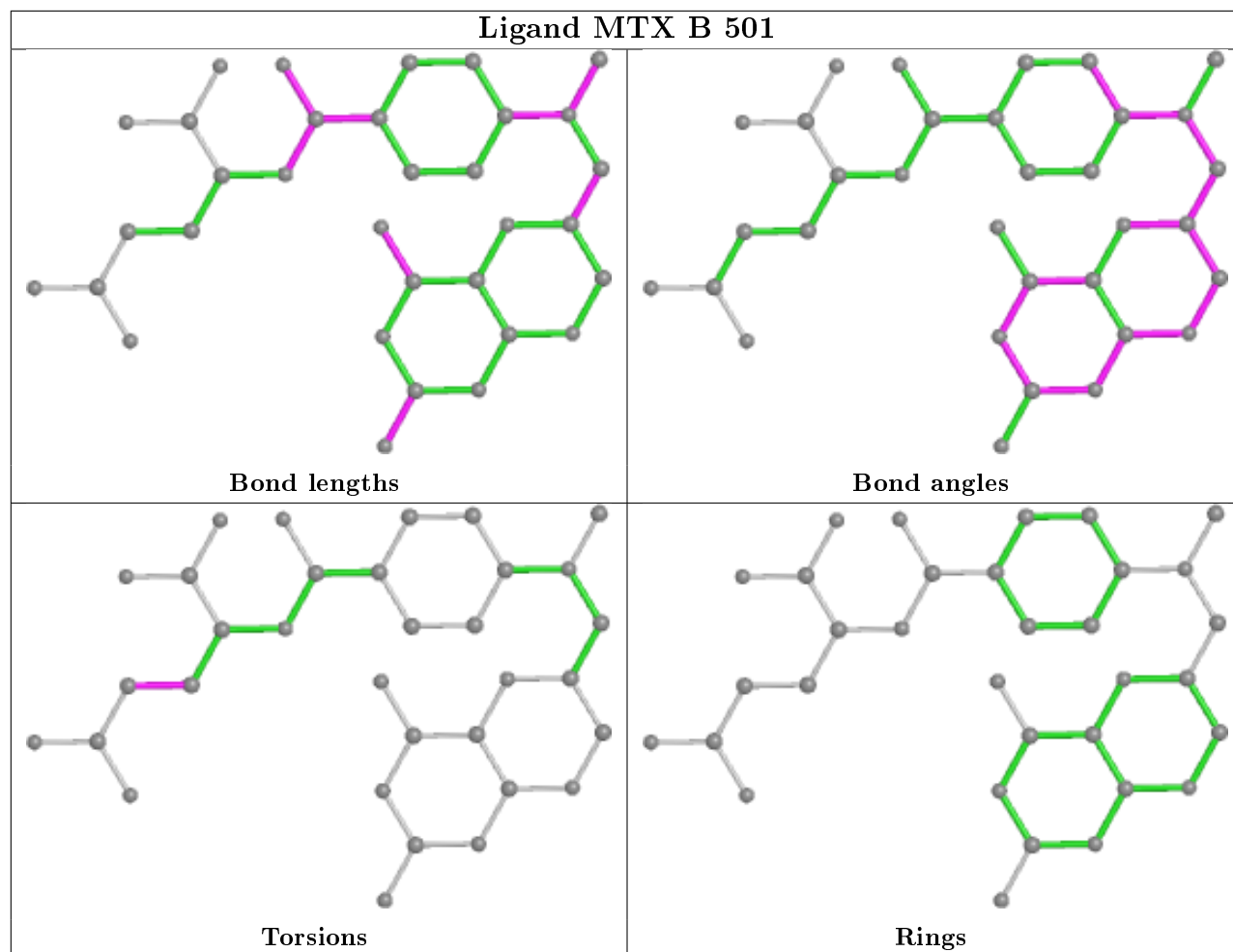
There are no ring outliers.

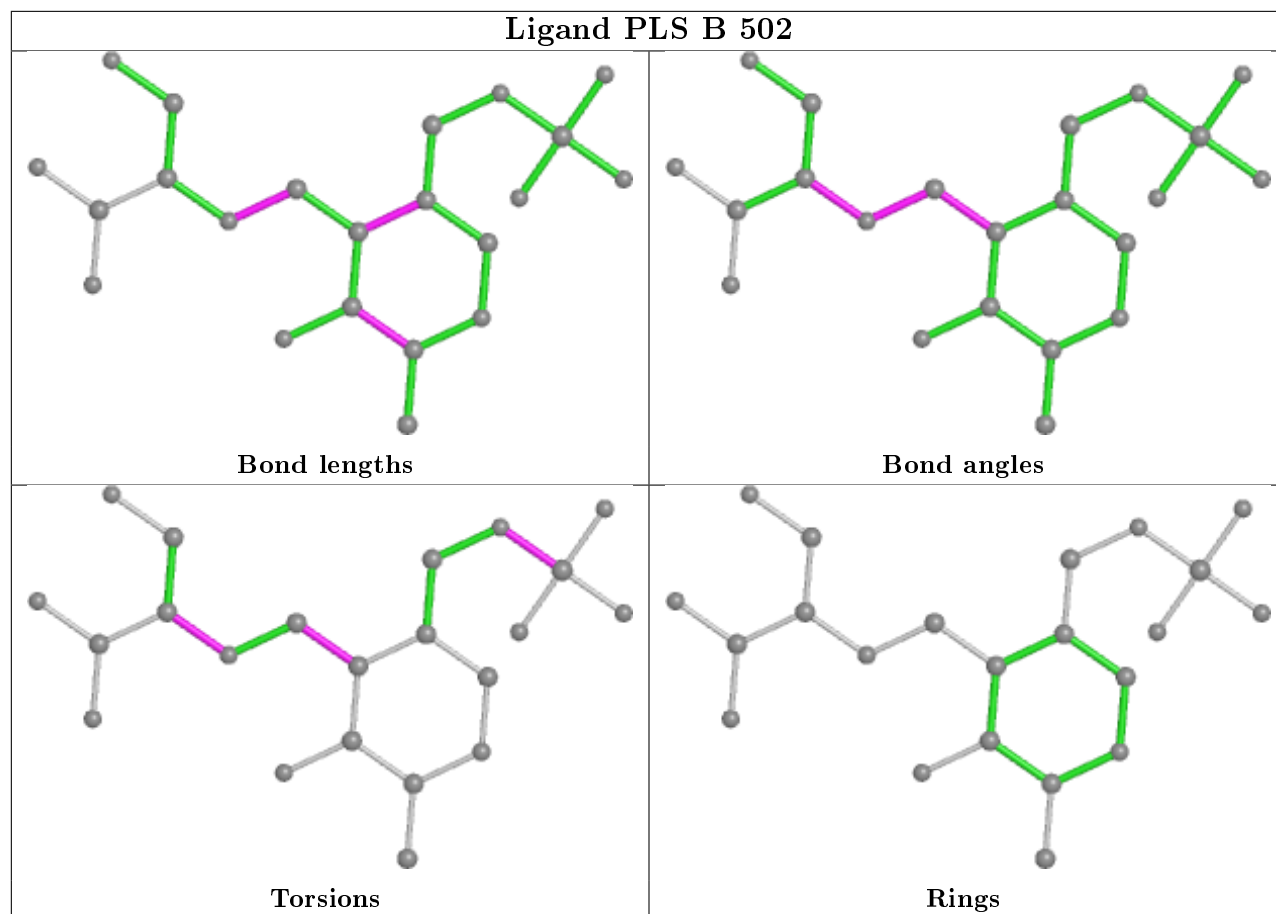
5 monomers are involved in 6 short contacts:

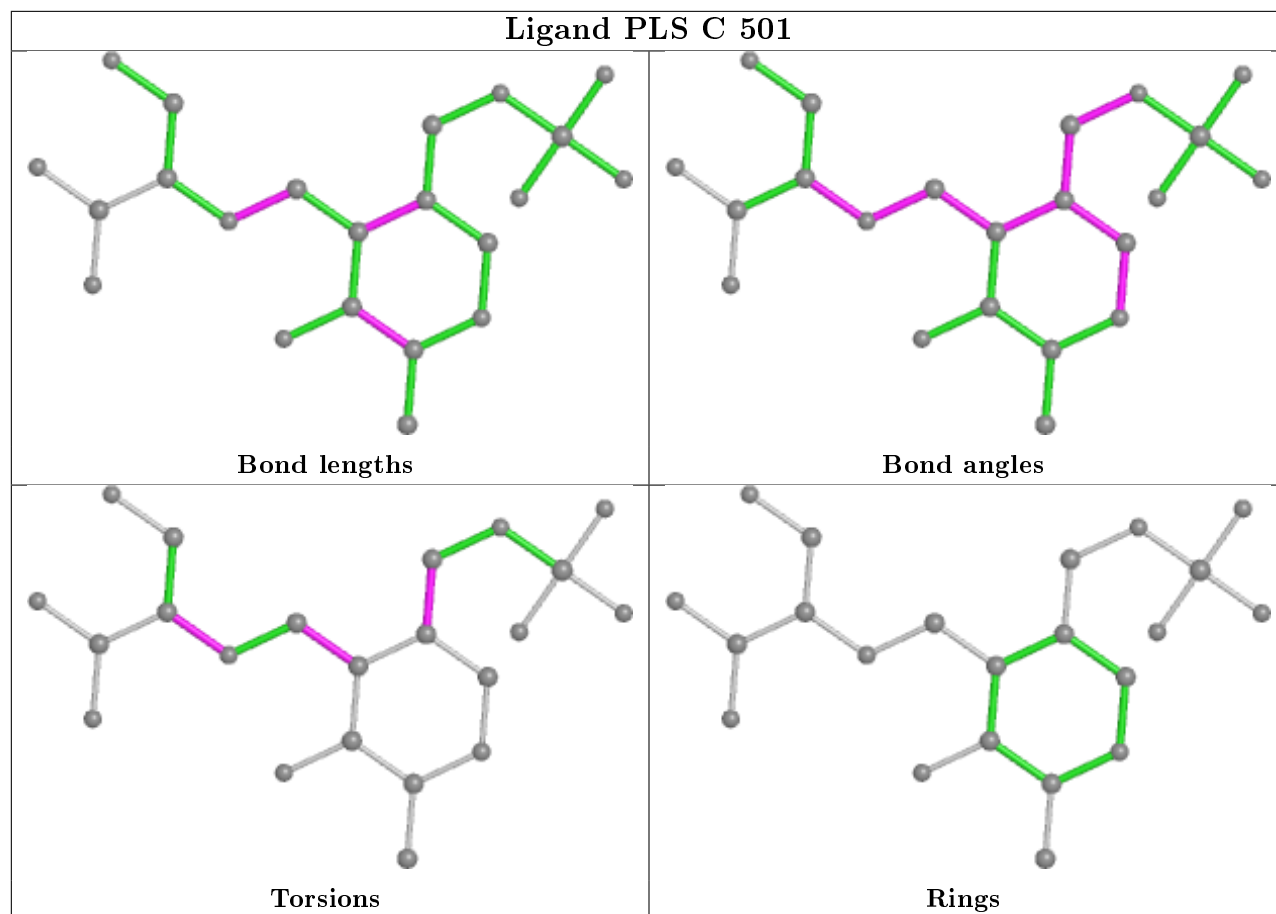
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	701	EDO	1	0
4	D	703	MTX	1	0
4	B	501	MTX	2	0
3	B	505	EDO	1	0
3	A	502	EDO	1	0

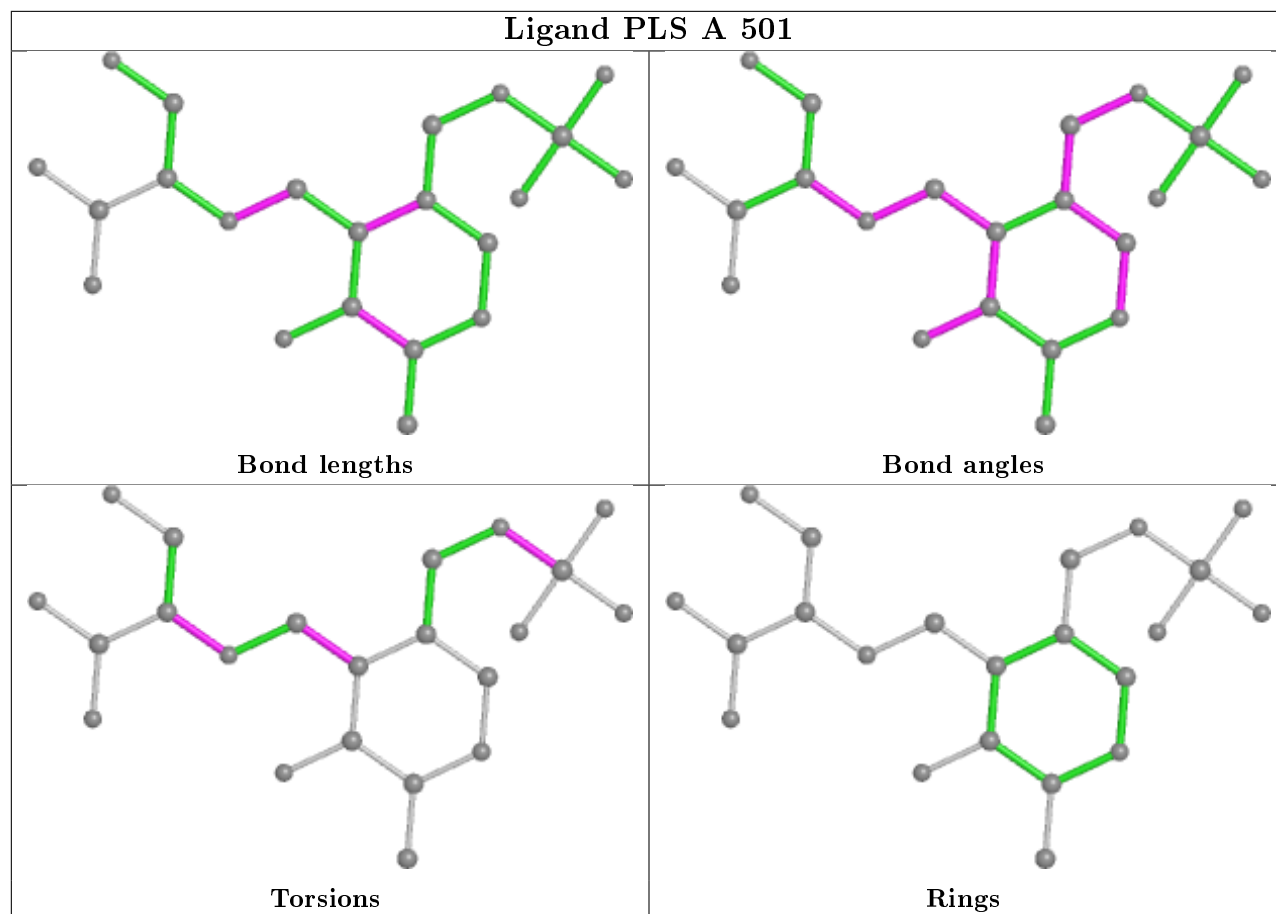
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

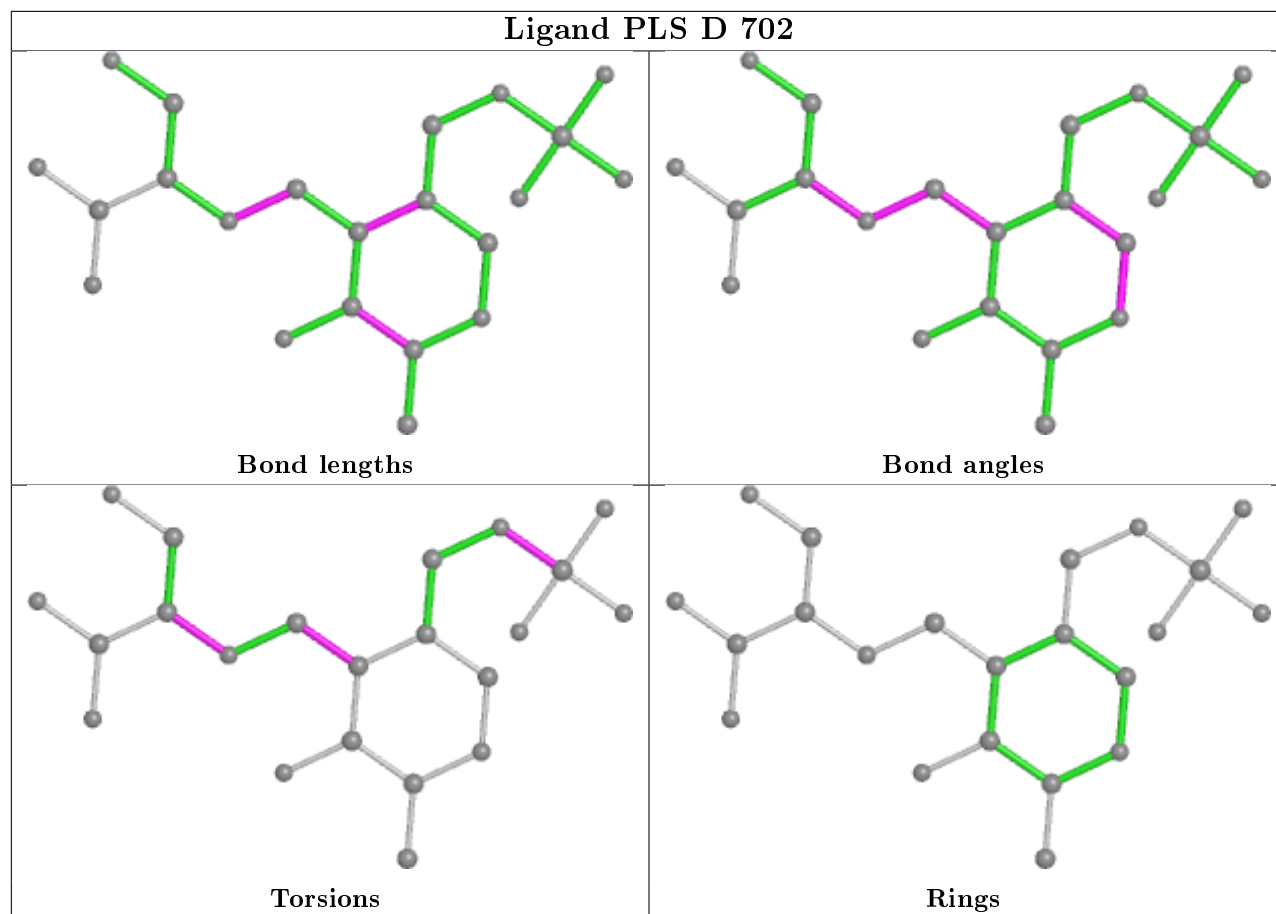


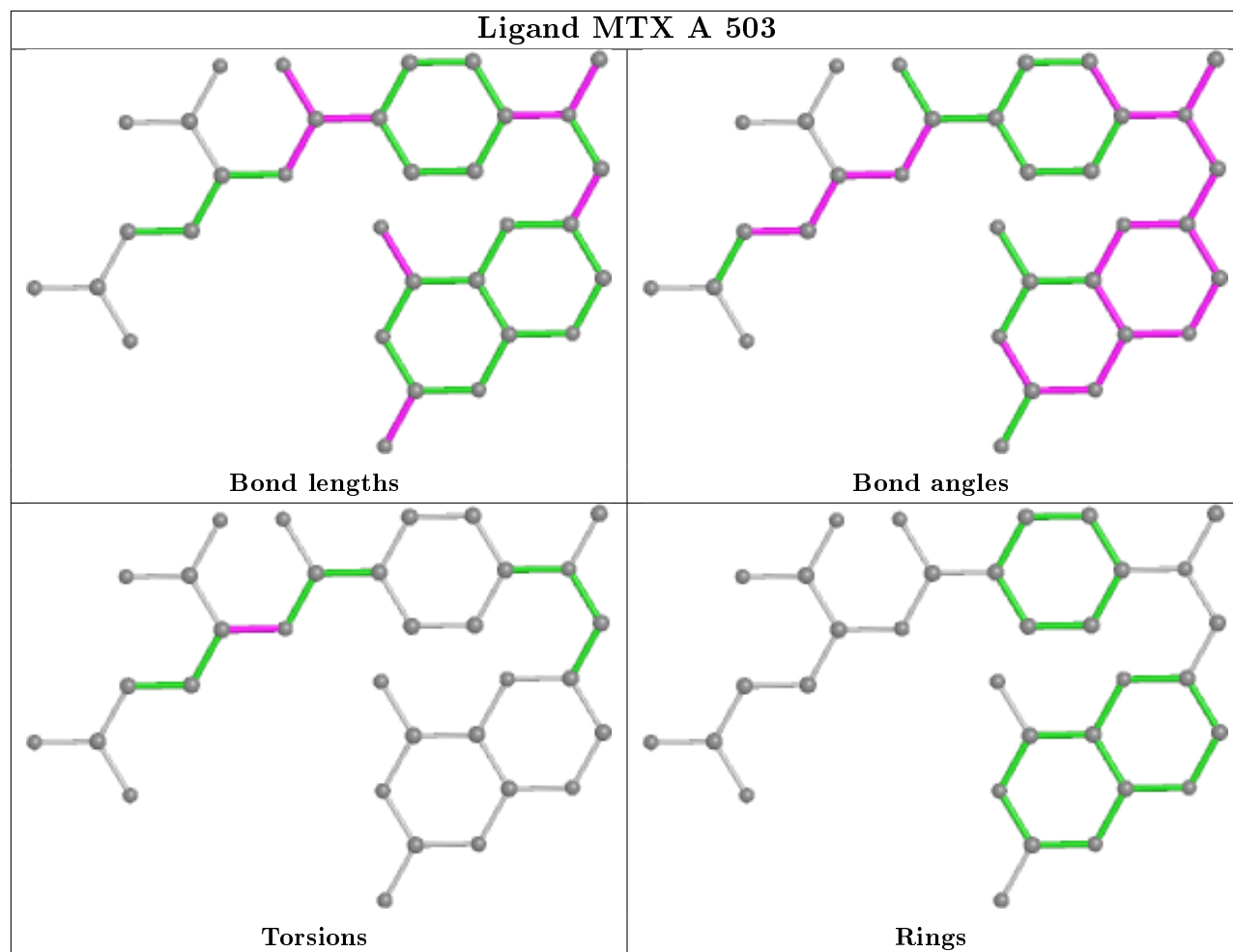












5.7 Other polymers [\(i\)](#)

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	473/474 (99%)	-0.39	7 (1%) 73 77	21, 35, 63, 103	0
1	B	472/474 (99%)	-0.30	9 (1%) 66 71	21, 33, 68, 127	0
1	C	471/474 (99%)	-0.29	5 (1%) 80 84	22, 36, 76, 107	0
1	D	471/474 (99%)	-0.46	3 (0%) 89 91	23, 34, 52, 99	0
All	All	1887/1896 (99%)	-0.36	24 (1%) 77 80	21, 35, 66, 127	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	LEU	9.4
1	B	380	SER	8.6
1	A	-2	SER	5.5
1	C	383	LEU	5.4
1	B	377	PHE	5.4
1	B	376	VAL	4.5
1	A	265	LYS	4.3
1	B	378	GLY	3.9
1	C	429	LEU	3.9
1	B	381	SER	3.4
1	A	163	PHE	3.1
1	A	383	LEU	3.0
1	C	427	GLY	3.0
1	A	382	ALA	2.9
1	B	382	ALA	2.9
1	A	384	ALA	2.9
1	B	384	ALA	2.8
1	B	163	PHE	2.4
1	C	430	LEU	2.3
1	D	163	PHE	2.2
1	D	266	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	270	GLY	2.1
1	D	263	PRO	2.0
1	C	378	GLY	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 carbohydrates in this entry.

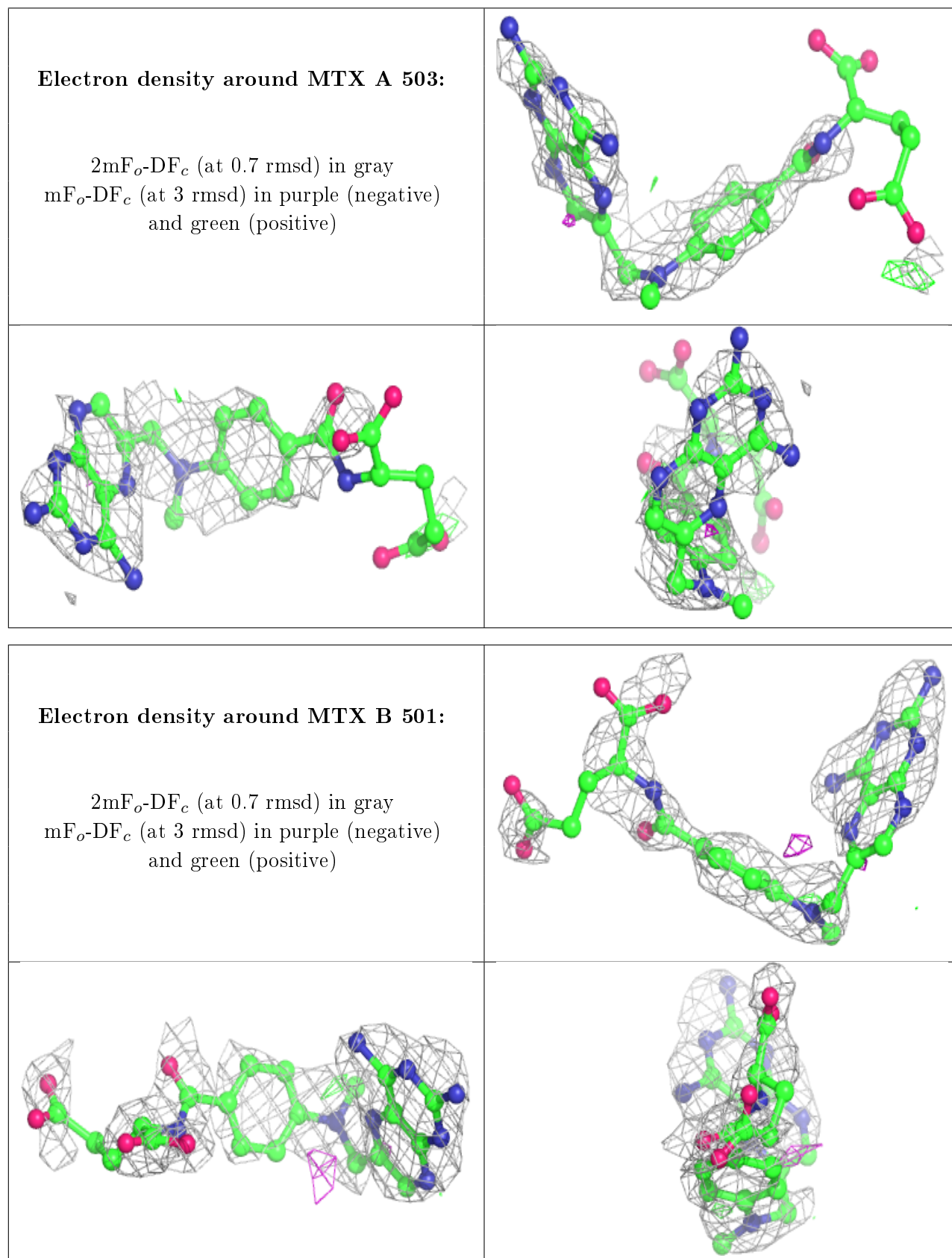
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	MTX	A	503	33/33	0.65	0.37	107,112,135,139	0
4	MTX	B	501	33/33	0.81	0.22	76,81,100,102	0
4	MTX	D	703	33/33	0.83	0.17	50,62,75,78	0
3	EDO	D	701	4/4	0.86	0.13	42,43,47,48	0
3	EDO	A	504	4/4	0.89	0.16	42,43,49,49	0
3	EDO	D	704	4/4	0.89	0.22	46,47,47,52	0
3	EDO	B	505	4/4	0.92	0.15	54,54,55,56	0
5	TRS	C	503	8/8	0.93	0.10	33,41,45,47	0
3	EDO	C	504	4/4	0.94	0.17	34,36,36,41	0
3	EDO	B	504	4/4	0.94	0.10	33,35,38,45	0
3	EDO	C	502	4/4	0.96	0.15	36,45,46,47	0
3	EDO	A	502	4/4	0.96	0.12	42,43,45,48	0
2	PLS	B	502	22/22	0.98	0.10	17,27,32,34	0
2	PLS	D	702	22/22	0.98	0.09	21,30,34,36	0
2	PLS	C	501	22/22	0.98	0.10	22,29,38,42	0
2	PLS	A	501	22/22	0.98	0.09	18,29,34,37	0
3	EDO	B	503	4/4	0.98	0.12	27,32,33,35	0

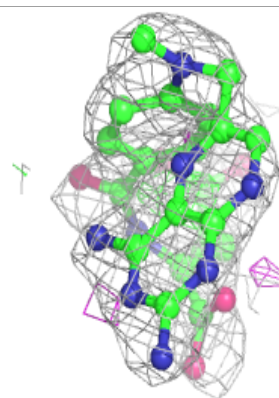
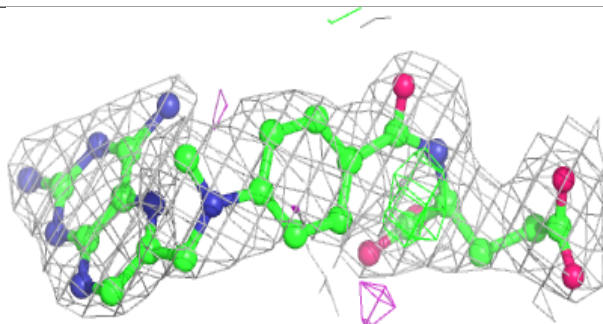
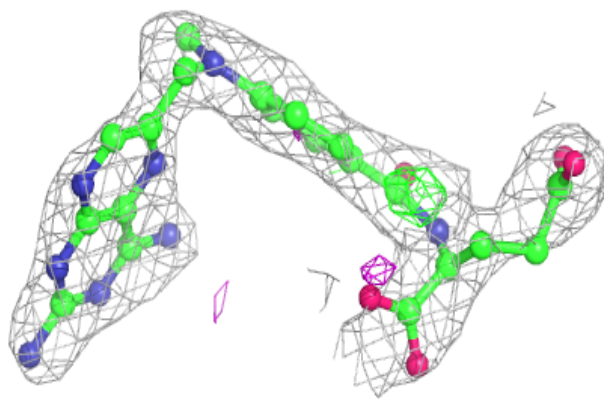
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



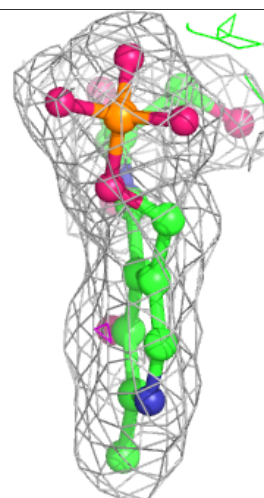
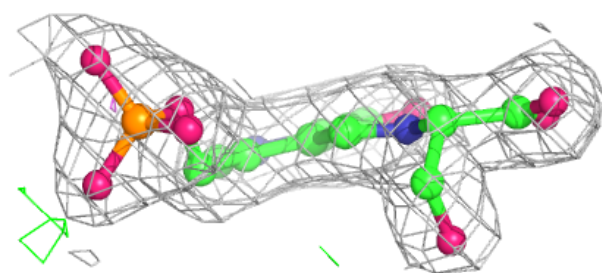
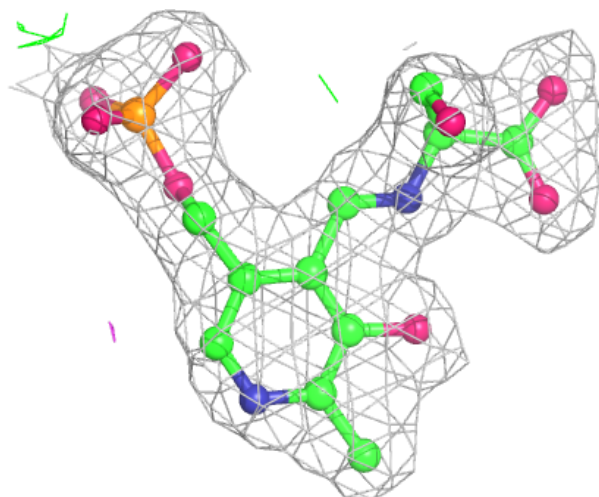
Electron density around MTX D 703:

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



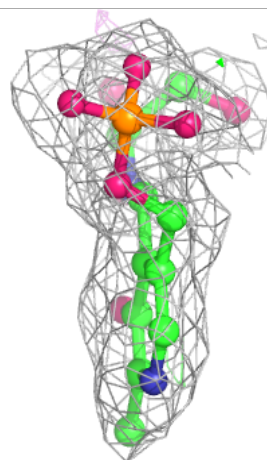
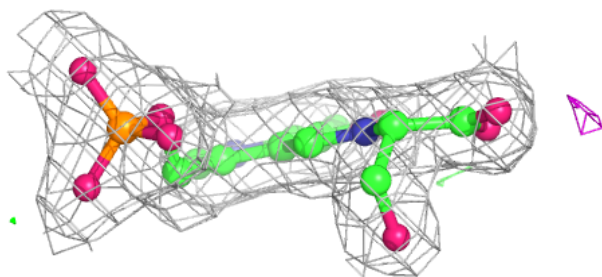
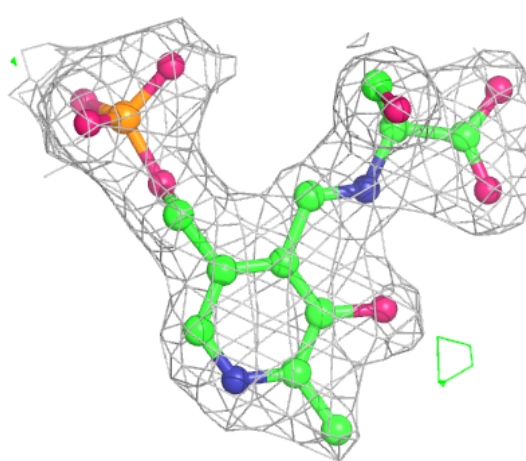
Electron density around PLS B 502:

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



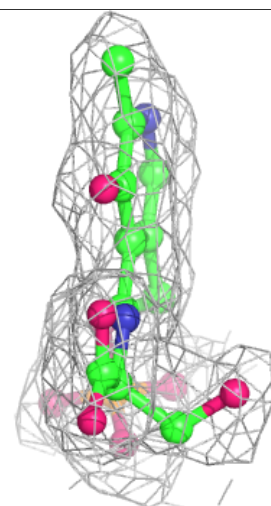
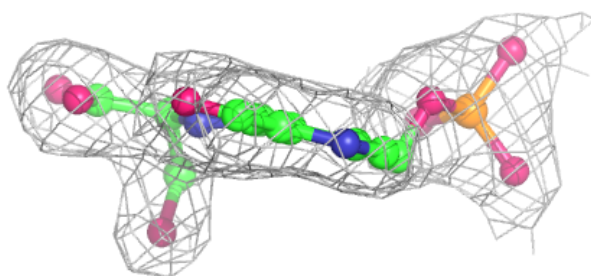
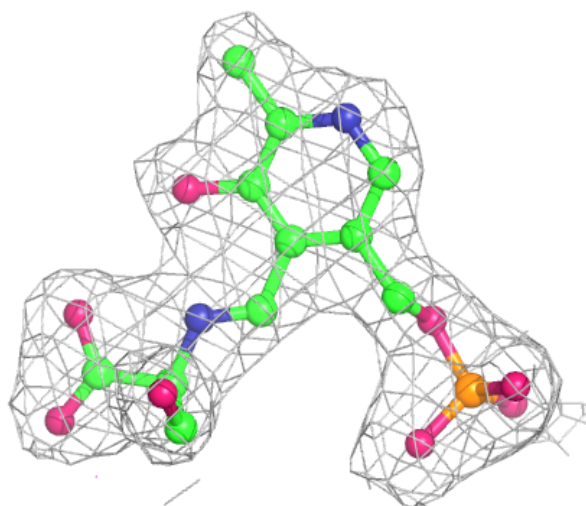
Electron density around PLS D 702:

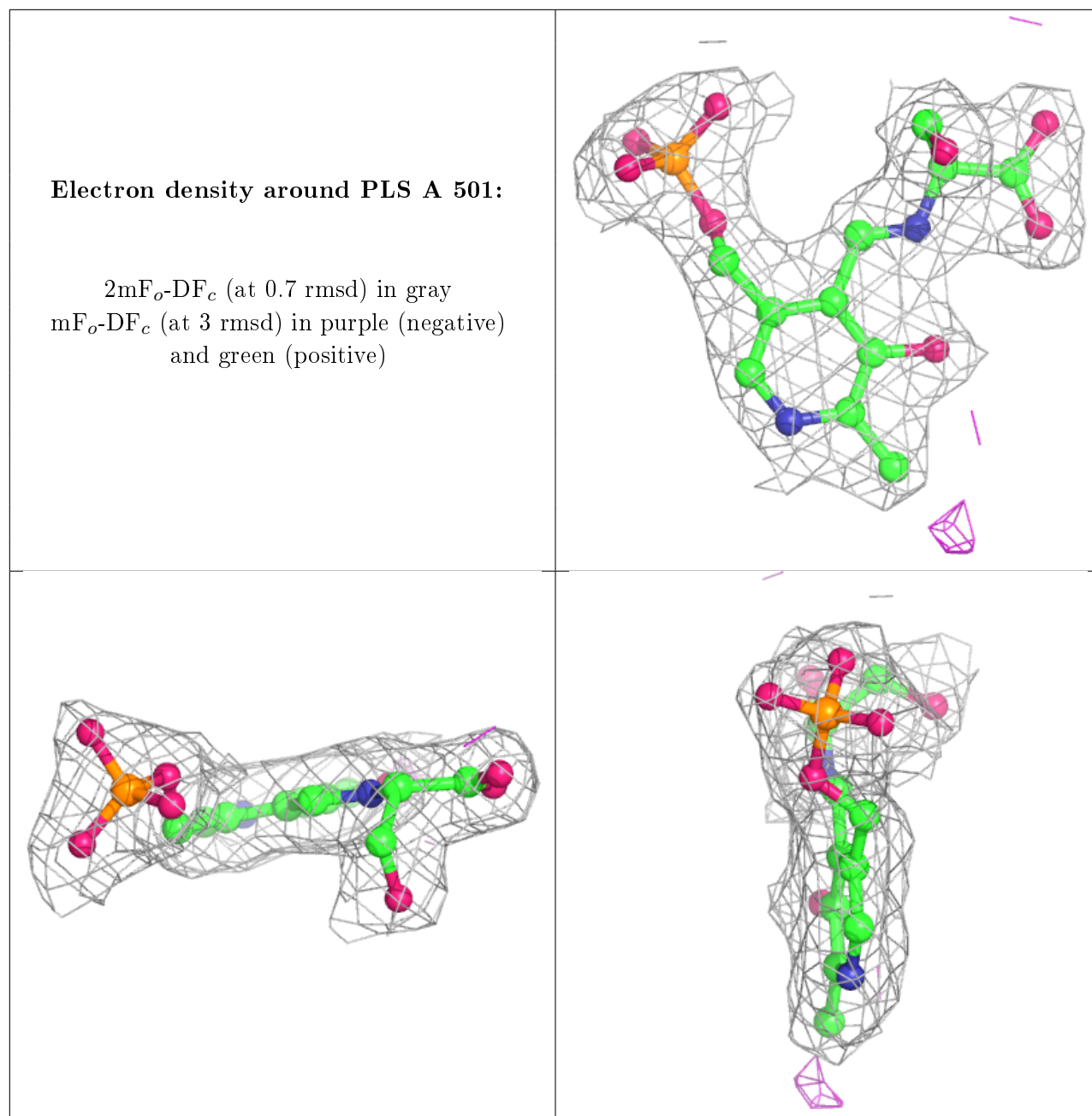
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLS C 501:

$2mF_o-DF_c$ (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.