



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:21 PM UTC

PDB ID : 6SMR / pdb_00006smr
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 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

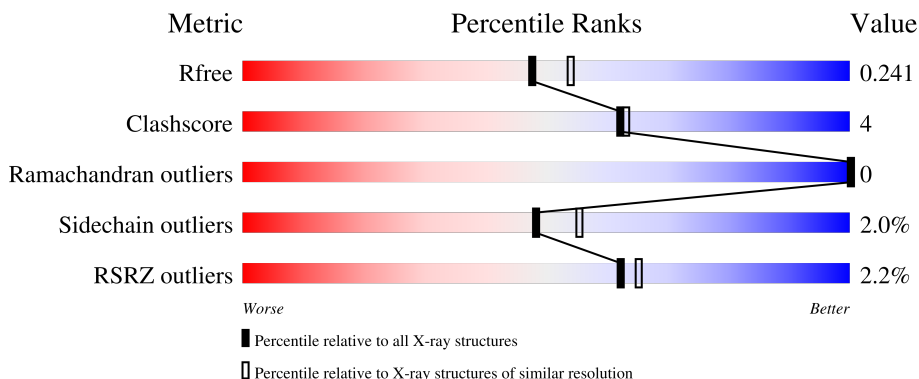
1 Overall quality at a glance

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}	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (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 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	474	 2% 91% 9%
1	B	474	 3% 90% 9%
1	C	474	 3% 86% 13% .
1	D	474	 % 90% 9% ..

2 Entry composition

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.

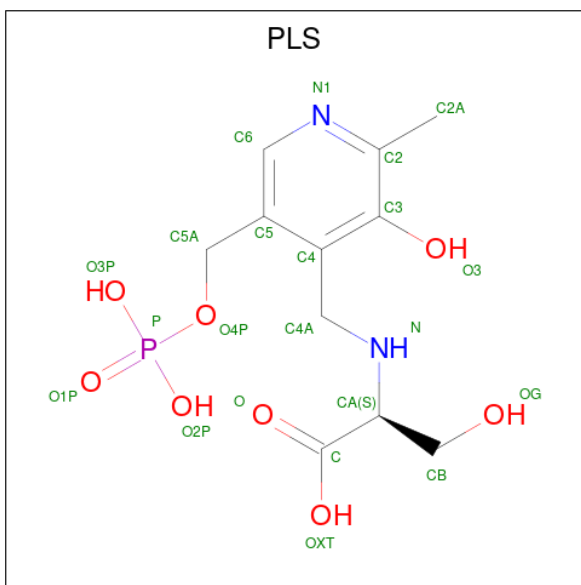
- Molecule 1 is a protein called Serine hydroxymethyltransferase 4.

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

There are 12 discrepancies between the modelled and reference sequences:

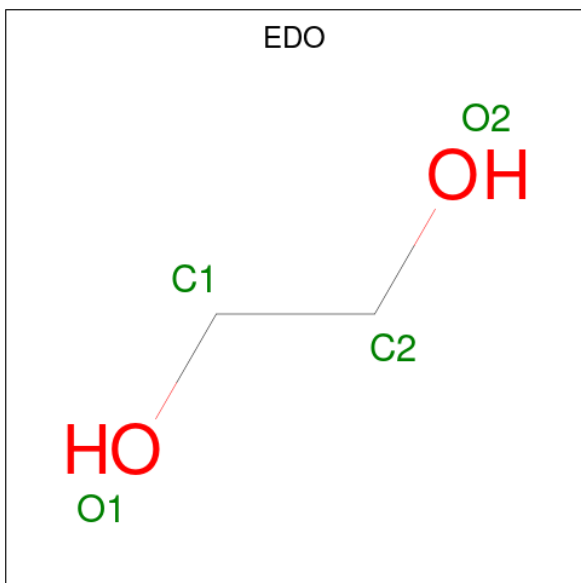
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP O23254
A	-1	ASN	-	expression tag	UNP O23254
A	0	ALA	-	expression tag	UNP O23254
B	-2	SER	-	expression tag	UNP O23254
B	-1	ASN	-	expression tag	UNP O23254
B	0	ALA	-	expression tag	UNP O23254
C	-2	SER	-	expression tag	UNP O23254
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-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (CCD ID: PLS) (formula: C₁₁H₁₇N₂O₈P).



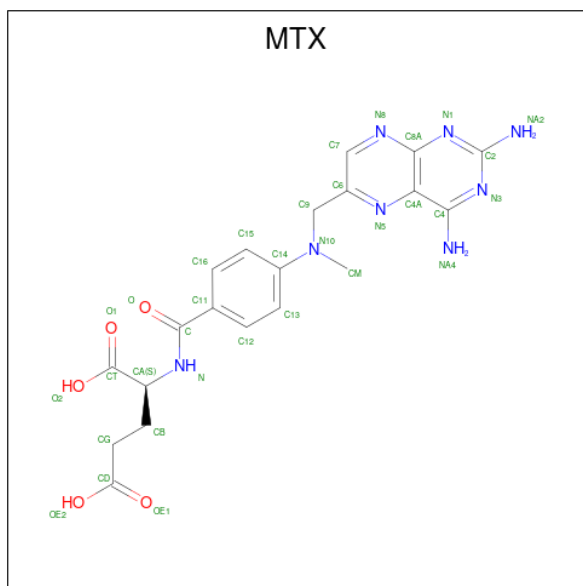
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 22	C 11	N 2	O 8	P 1	0	0
2	B	1	Total 22	C 11	N 2	O 8	P 1	0	0
2	C	1	Total 22	C 11	N 2	O 8	P 1	0	0
2	D	1	Total 22	C 11	N 2	O 8	P 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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 (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



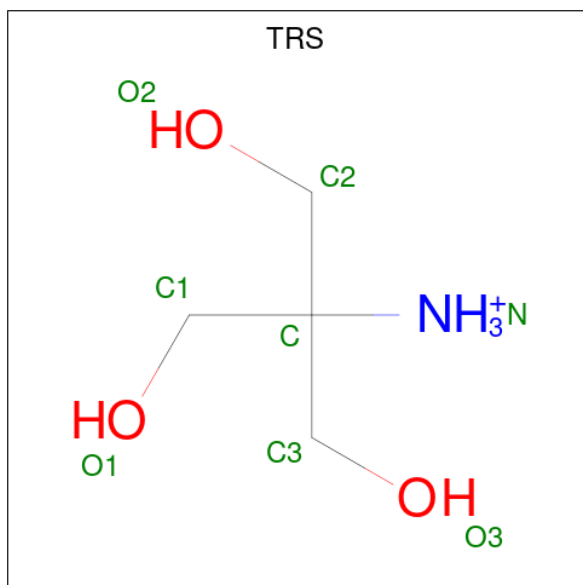
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 33 20 8 5	0	0
4	B	1	Total C N O 33 20 8 5	0	0

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

- Molecule 5 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

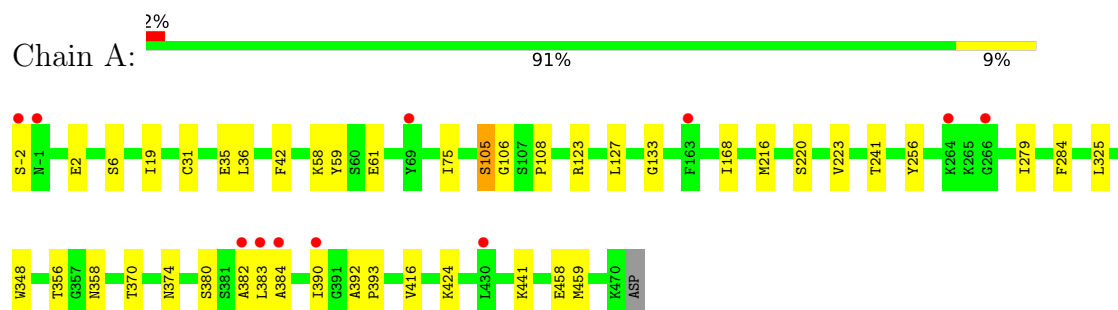
- Molecule 6 is water.

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		

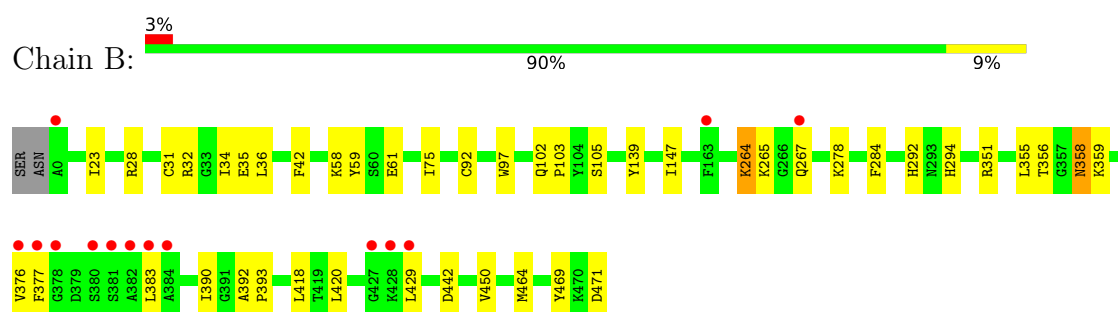
3 Residue-property plots [i](#)

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

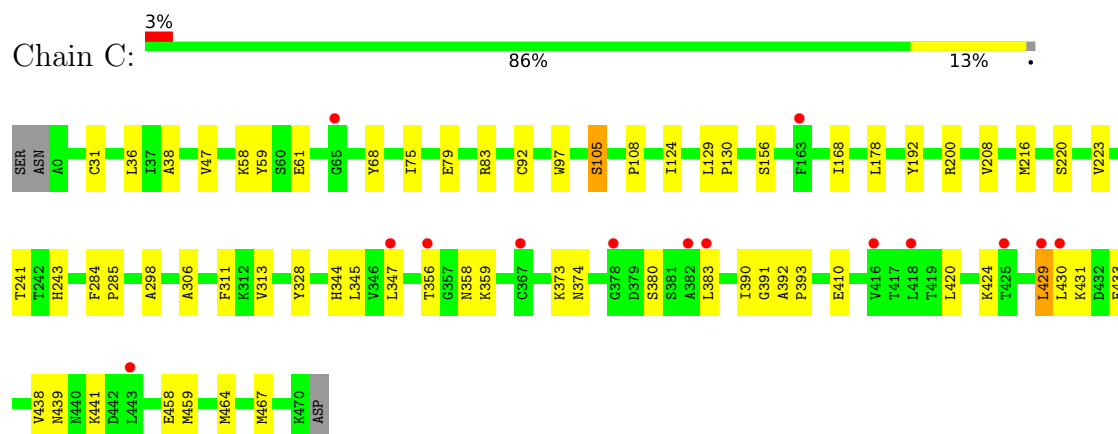
- Molecule 1: Serine hydroxymethyltransferase 4



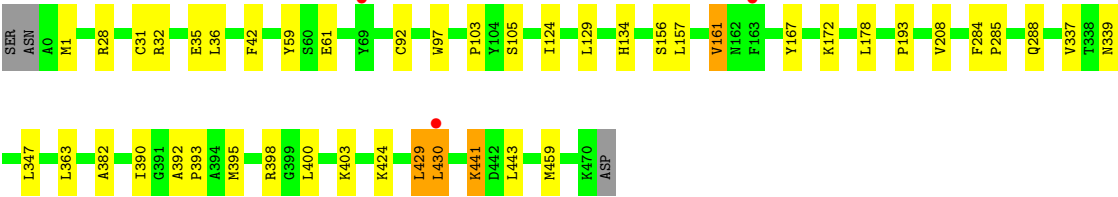
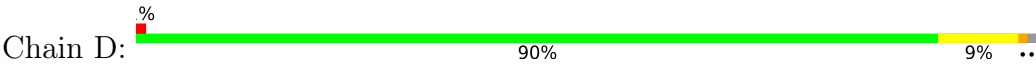
- Molecule 1: Serine hydroxymethyltransferase 4



- 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 88.30 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.8 (88.30-2.12) 98.8 (88.30-2.12)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.15_3459	Depositor
R, R_{free}	0.173 , 0.234 0.183 , 0.241	Depositor DCC
R_{free} test set	1069 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: TRS, MTX, EDO, PLS

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	0.28	0/3738	0.49	0/5059
1	B	0.28	0/3733	0.50	0/5051
1	C	0.37	0/3724	0.51	0/5040
1	D	0.29	0/3724	0.49	0/5040
All	All	0.31	0/14919	0.50	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	30	0
1	B	3649	0	3613	22	0
1	C	3640	0	3609	41	0
1	D	3640	0	3609	27	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	4	0
6	B	259	0	0	1	0
6	C	230	0	0	5	0
6	D	249	0	0	2	0
All	All	15779	0	14631	120	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 (120) 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	1.40	0.99
1:C:216:MET:HE2	1:C:220:SER:HA	1.45	0.96
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:C:216:MET:HE1	1:C:223:VAL:HB	1.62	0.79
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:D:31:CYS:HB3	1:D:459:MET:HE3	1.76	0.66
1:D:430:LEU:HD22	1:D:430:LEU:H	1.63	0.64
1:A:-2:SER:N	6:A:601:HOH:O	2.28	0.63
1:C:420:LEU:O	1:C:424:LYS:HG2	1.99	0.63
1:A:216:MET:HE1	1:A:223:VAL:HB	1.82	0.62
1:B:58:LYS:HG2	1:B:75:ILE:HG13	1.82	0.61
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: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: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:424:LYS:NZ	6:A:604:HOH:O	2.41	0.54
1:C:216:MET:HE1	1:C:223:VAL:CB	2.36	0.53
1:C:31:CYS:HB3	1:C:459:MET:HE3	1.90	0.53
1:C:79:GLU:O	1:C:83:ARG:HG3	2.09	0.53
1:C:178:LEU:HD23	1:C:208:VAL:HG12	1.90	0.53
1:A:58:LYS:HG2	1:A:75:ILE:HG13	1.91	0.52
1:A:358:ASN:ND2	1:A:358:ASN:H	2.08	0.52
1:C:383:LEU:HD12	1:C:383:LEU:H	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: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:A:31:CYS:HB3	1:A:459:MET:HE3	1.94	0.49
1:C:429:LEU:H	1:C:429:LEU:HD22	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:OD1	1:B:358:ASN:N	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:C:458:GLU:HA	1:C:464:MET:HE1	1.95	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:H	1:A:358:ASN:HD22	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:83:ARG:NH1	6:C:613:HOH:O	2.45	0.45
1:C:200:ARG:NH1	6:C:618:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:LEU:HB3	1:B:390:ILE:HG23	1.97	0.45
1:C:105:SER:C	1:C:108:PRO:HD2	2.42	0.45
1:C:216:MET:HE3	1:C:216:MET:HB2	1.56	0.45
1:C:430:LEU:HD12	1:C:431:LYS:N	2.32	0.45
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:D:161:VAL:HG22	1:D:167:TYR:C	2.43	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:C:373:LYS:NZ	6:C:624:HOH:O	2.52	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:129:LEU:HD11	1:D:134:HIS:C	2.44	0.42
1:D:363:LEU:HG	1:D:443:LEU:HD11	1.99	0.42
6:A:745:HOH:O	4:B:501:MTX:HG1	2.20	0.42
1:B:28:ARG:HD2	1:B:469:TYR:HB3	2.02	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:B:31:CYS:SG	1:B:464:MET:HE3	2.60	0.42
1:C:124:ILE:O	1:C:156:SER:HA	2.19	0.42
1:D:398:ARG:NE	1:D:459:MET:HE2	2.35	0.42
1:A:36:LEU:HB3	1:A:390:ILE:HG23	2.01	0.42
1:A:105:SER:C	1:A:108:PRO:HD2	2.45	0.41
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:HA	1:A:441:LYS:HD3	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:A:216:MET:HE3	1:A:216:MET:HB2	1.83	0.41
1:D:103:PRO:HA	1:D:288:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2:GLU:HG2	1:A:6:SER:HB3	2.02	0.41
1:A:356:THR:OG1	1:A:358:ASN:ND2	2.54	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: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
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:358:ASN:ND2	1:A:384:ALA:HA	2.37	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:HD13	1:C:75:ILE:HA	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 ⓘ

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%)	51	59
1	B	384/386 (100%)	376 (98%)	8 (2%)	47	54
1	C	383/386 (99%)	375 (98%)	8 (2%)	47	54
1	D	383/386 (99%)	375 (98%)	8 (2%)	47	54
All	All	1535/1544 (99%)	1504 (98%)	31 (2%)	48	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	105	SER
1	A	168	ILE
1	A	374	ASN
1	A	380	SER
1	A	383	LEU
1	A	458	GLU
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	429	LEU
1	C	59	TYR
1	C	105	SER
1	C	129	LEU
1	C	347	LEU
1	C	374	ASN
1	C	429	LEU
1	C	438	VAL
1	C	441	LYS
1	D	59	TYR

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Mol	Chain	Res	Type
1	D	105	SER
1	D	161	VAL
1	D	403	LYS
1	D	424	LYS
1	D	429	LEU
1	D	430	LEU
1	D	441	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	358	ASN
1	A	374	ASN
1	B	293	ASN
1	B	335	GLN
1	B	439	ASN
1	C	293	ASN
1	C	407	GLN
1	D	119	GLN
1	D	295	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	PLS	C	501	-	22,22,22	2.02	4 (18%)	28,31,31	1.41	5 (17%)
3	EDO	A	502	-	3,3,3	0.38	0	2,2,2	0.40	0
3	EDO	C	504	-	3,3,3	0.42	0	2,2,2	0.53	0
2	PLS	B	502	-	22,22,22	1.99	3 (13%)	28,31,31	1.49	4 (14%)
3	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	B	504	-	3,3,3	0.49	0	2,2,2	0.39	0
3	EDO	D	704	-	3,3,3	0.39	0	2,2,2	0.51	0
4	MTX	D	703	-	35,35,35	2.67	10 (28%)	47,49,49	3.23	22 (46%)
4	MTX	B	501	-	35,35,35	2.57	9 (25%)	47,49,49	1.88	10 (21%)
3	EDO	B	505	-	3,3,3	0.46	0	2,2,2	0.23	0
3	EDO	D	701	-	3,3,3	0.53	0	2,2,2	0.03	0
3	EDO	A	504	-	3,3,3	0.45	0	2,2,2	0.41	0
4	MTX	A	503	-	35,35,35	2.60	9 (25%)	47,49,49	2.30	13 (27%)
2	PLS	A	501	-	22,22,22	1.96	3 (13%)	28,31,31	1.55	6 (21%)
3	EDO	B	503	-	3,3,3	0.38	0	2,2,2	0.54	0
5	TRS	C	503	-	7,7,7	0.28	0	9,9,9	0.62	0
2	PLS	D	702	-	22,22,22	2.00	3 (13%)	28,31,31	1.39	2 (7%)

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
2	PLS	C	501	-	-	6/17/17/17	0/1/1/1
3	EDO	A	502	-	-	0/1/1/1	-
3	EDO	C	504	-	-	1/1/1/1	-
2	PLS	B	502	-	-	7/17/17/17	0/1/1/1
3	EDO	C	502	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	D	704	-	-	1/1/1/1	-
4	MTX	D	703	-	-	8/25/25/25	0/3/3/3
4	MTX	B	501	-	-	4/25/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	505	-	-	0/1/1/1	-
3	EDO	D	701	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
4	MTX	A	503	-	-	7/25/25/25	0/3/3/3
2	PLS	A	501	-	-	7/17/17/17	0/1/1/1
3	EDO	B	503	-	-	0/1/1/1	-
5	TRS	C	503	-	-	2/9/9/9	-
2	PLS	D	702	-	-	5/17/17/17	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	702	PLS	C4A-N	-7.28	1.25	1.46
4	B	501	MTX	C2-NA2	7.25	1.48	1.33
2	C	501	PLS	C4A-N	-7.23	1.25	1.46
2	A	501	PLS	C4A-N	-7.11	1.25	1.46
4	A	503	MTX	C2-NA2	7.07	1.48	1.33
2	B	502	PLS	C4A-N	-7.01	1.26	1.46
4	D	703	MTX	C2-NA2	6.96	1.47	1.33
4	D	703	MTX	C-N	6.24	1.48	1.34
4	A	503	MTX	C-N	6.22	1.48	1.34
4	B	501	MTX	C-N	5.69	1.47	1.34
4	D	703	MTX	C9-C6	5.07	1.60	1.51
4	D	703	MTX	C14-N10	4.99	1.52	1.38
4	A	503	MTX	C9-C6	4.91	1.59	1.51
4	A	503	MTX	CM-N10	-4.90	1.38	1.46
4	B	501	MTX	CM-N10	-4.89	1.38	1.46
4	A	503	MTX	CG-CD	4.73	1.61	1.50
4	B	501	MTX	C9-C6	4.69	1.59	1.51
4	D	703	MTX	CM-N10	-4.67	1.38	1.46
4	A	503	MTX	C4-NA4	4.64	1.50	1.34
4	B	501	MTX	C4-NA4	4.63	1.50	1.34
4	B	501	MTX	CG-CD	4.58	1.61	1.50
4	D	703	MTX	C4-NA4	4.56	1.50	1.34
4	B	501	MTX	C14-N10	4.22	1.50	1.38
4	A	503	MTX	C14-N10	4.12	1.50	1.38
4	D	703	MTX	CG-CD	4.07	1.60	1.50
2	A	501	PLS	C3-C2	-3.30	1.37	1.41
4	D	703	MTX	C11-C	3.26	1.57	1.50
4	D	703	MTX	O-C	-2.95	1.16	1.23
4	B	501	MTX	O-C	-2.89	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	PLS	C3-C2	-2.89	1.38	1.41
2	C	501	PLS	C5-C4	-2.82	1.36	1.40
2	D	702	PLS	C5-C4	-2.73	1.36	1.40
4	A	503	MTX	O-C	-2.68	1.17	1.23
2	D	702	PLS	C3-C2	-2.61	1.38	1.41
2	B	502	PLS	C5-C4	-2.50	1.36	1.40
2	C	501	PLS	C3-C2	-2.41	1.38	1.41
4	A	503	MTX	C11-C	2.31	1.55	1.50
4	B	501	MTX	C11-C	2.29	1.55	1.50
2	A	501	PLS	C5-C4	-2.21	1.37	1.40
2	C	501	PLS	C2A-C2	2.12	1.53	1.50
4	D	703	MTX	C13-C12	2.05	1.42	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	MTX	C11-C-N	11.44	138.25	117.04
4	A	503	MTX	CB-CA-N	8.70	128.14	110.91
4	D	703	MTX	O-C-N	-6.77	109.59	122.47
4	D	703	MTX	CB-CA-N	6.16	123.10	110.91
4	D	703	MTX	CA-N-C	5.82	135.53	121.56
4	B	501	MTX	N1-C2-N3	-5.68	119.99	127.21
4	D	703	MTX	N1-C2-N3	-5.59	120.11	127.21
4	A	503	MTX	N1-C2-N3	-5.50	120.22	127.21
2	D	702	PLS	C4A-N-CA	4.77	122.79	113.84
4	D	703	MTX	O-C-C11	-4.52	111.95	120.90
4	D	703	MTX	C2-N1-C8A	4.49	120.33	115.48
4	B	501	MTX	N8-C8A-N1	4.45	120.62	115.77
4	D	703	MTX	N8-C8A-N1	4.33	120.48	115.77
4	A	503	MTX	N8-C8A-N1	4.32	120.47	115.77
4	B	501	MTX	C2-N1-C8A	4.29	120.11	115.48
4	D	703	MTX	CG-CB-CA	-4.28	105.26	113.16
2	B	502	PLS	C4A-N-CA	4.23	121.78	113.84
4	D	703	MTX	CT-CA-N	4.19	120.28	110.57
4	A	503	MTX	C2-N1-C8A	4.18	119.99	115.48
2	A	501	PLS	C4A-N-CA	4.08	121.49	113.84
4	A	503	MTX	C9-C6-N5	3.79	123.24	117.09
2	C	501	PLS	C4A-N-CA	3.47	120.36	113.84
4	D	703	MTX	C6-C7-N8	-3.38	119.89	123.14
4	B	501	MTX	C6-C7-N8	-3.34	119.93	123.14
4	B	501	MTX	C6-C9-N10	-3.33	107.24	112.95
4	A	503	MTX	C6-C7-N8	-3.27	120.00	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	MTX	C15-C14-N10	-3.08	117.30	121.59
4	D	703	MTX	C6-C9-N10	-2.96	107.88	112.95
4	D	703	MTX	C9-C6-N5	2.82	121.67	117.09
4	D	703	MTX	O2-CT-O1	-2.73	117.89	124.08
4	A	503	MTX	C13-C14-N10	-2.71	117.80	121.59
2	A	501	PLS	O4P-C5A-C5	2.70	114.42	109.36
4	D	703	MTX	C12-C11-C	2.67	129.26	120.60
2	C	501	PLS	O4P-C5A-C5	2.63	114.28	109.36
4	B	501	MTX	C9-C6-N5	2.60	121.31	117.09
4	A	503	MTX	C7-C6-N5	-2.56	119.21	120.87
4	D	703	MTX	C16-C11-C	-2.40	112.81	120.60
4	A	503	MTX	C7-N8-C8A	2.40	120.54	117.20
4	B	501	MTX	C13-C14-N10	-2.40	118.24	121.59
4	D	703	MTX	C7-C6-N5	-2.38	119.32	120.87
4	D	703	MTX	C8A-C4A-N5	-2.38	119.69	122.35
4	A	503	MTX	C8A-C4A-N5	-2.38	119.69	122.35
2	C	501	PLS	C5-C6-N1	-2.38	119.97	123.83
2	B	502	PLS	OXT-C-CA	2.36	121.50	113.51
4	A	503	MTX	CG-CB-CA	-2.36	108.81	113.16
2	C	501	PLS	OXT-C-CA	2.36	121.50	113.51
2	A	501	PLS	O3-C3-C4	2.28	124.78	118.18
2	C	501	PLS	C6-C5-C4	2.25	119.77	118.06
4	D	703	MTX	C15-C16-C11	2.24	123.19	120.80
2	B	502	PLS	OXT-C-O	-2.23	119.03	124.08
4	D	703	MTX	C7-N8-C8A	2.21	120.27	117.20
2	A	501	PLS	C5-C6-N1	-2.18	120.28	123.83
2	D	702	PLS	C5-C6-N1	-2.18	120.29	123.83
4	B	501	MTX	C7-N8-C8A	2.14	120.17	117.20
4	B	501	MTX	O2-CT-CA	2.11	120.66	113.51
4	A	503	MTX	C9-C6-C7	-2.11	117.55	121.38
4	A	503	MTX	CM-N10-C9	2.10	120.58	115.11
2	B	502	PLS	C2A-C2-N1	2.09	121.57	117.64
4	D	703	MTX	C13-C14-N10	2.05	124.45	121.59
4	B	501	MTX	O2-CT-O1	-2.03	119.46	124.08
2	A	501	PLS	OXT-C-CA	2.02	120.33	113.51
2	A	501	PLS	C5A-C5-C6	-2.01	116.08	119.36

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLS	C5-C4-C4A-N

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Mol	Chain	Res	Type	Atoms
2	A	501	PLS	C5A-O4P-P-O3P
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	C-CA-N-C4A
2	C	501	PLS	C5-C4-C4A-N
2	D	702	PLS	C5-C4-C4A-N
2	D	702	PLS	C5A-O4P-P-O2P
4	D	703	MTX	O-C-N-CA
5	C	503	TRS	N-C-C2-O2
4	D	703	MTX	C11-C-N-CA
4	D	703	MTX	CT-CA-CB-CG
2	C	501	PLS	C3-C4-C4A-N
4	D	703	MTX	CA-CB-CG-CD
4	A	503	MTX	CT-CA-CB-CG
4	D	703	MTX	N-CA-CT-O1
4	D	703	MTX	N-CA-CT-O2
2	A	501	PLS	C5A-O4P-P-O2P
2	B	502	PLS	C5A-O4P-P-O3P
2	A	501	PLS	CB-CA-N-C4A
2	B	502	PLS	CB-CA-N-C4A
2	D	702	PLS	CB-CA-N-C4A
2	A	501	PLS	C3-C4-C4A-N
2	C	501	PLS	C4-C5-C5A-O4P
2	D	702	PLS	C3-C4-C4A-N
2	A	501	PLS	C-CA-N-C4A
2	B	502	PLS	C-CA-N-C4A
2	D	702	PLS	C-CA-N-C4A
4	A	503	MTX	CB-CA-CT-O2
3	D	704	EDO	O1-C1-C2-O2
2	A	501	PLS	C5A-O4P-P-O1P
4	A	503	MTX	CB-CA-CT-O1
3	C	504	EDO	O1-C1-C2-O2
4	D	703	MTX	OE1-CD-CG-CB
4	D	703	MTX	OE2-CD-CG-CB
2	C	501	PLS	C6-C5-C5A-O4P
4	A	503	MTX	OE2-CD-CG-CB
4	A	503	MTX	OE1-CD-CG-CB
4	A	503	MTX	CT-CA-N-C
2	B	502	PLS	C5A-O4P-P-O2P
5	C	503	TRS	C1-C-C2-O2
2	C	501	PLS	CB-CA-N-C4A

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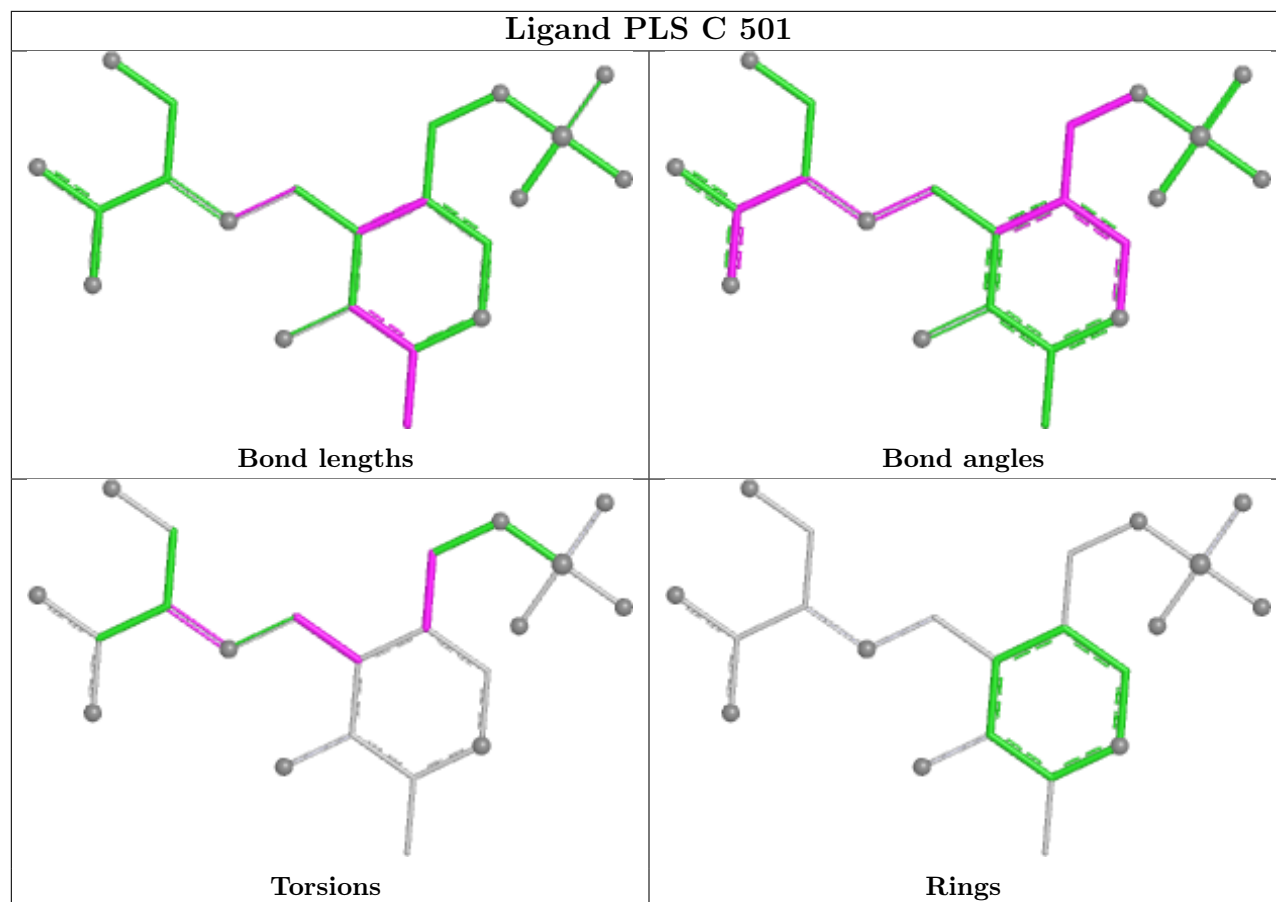
Mol	Chain	Res	Type	Atoms
3	B	504	EDO	O1-C1-C2-O2
4	A	503	MTX	N-CA-CT-O1
4	B	501	MTX	CA-CB-CG-CD
4	B	501	MTX	CB-CA-CT-O2
4	B	501	MTX	CB-CA-CT-O1
4	B	501	MTX	OE2-CD-CG-CB

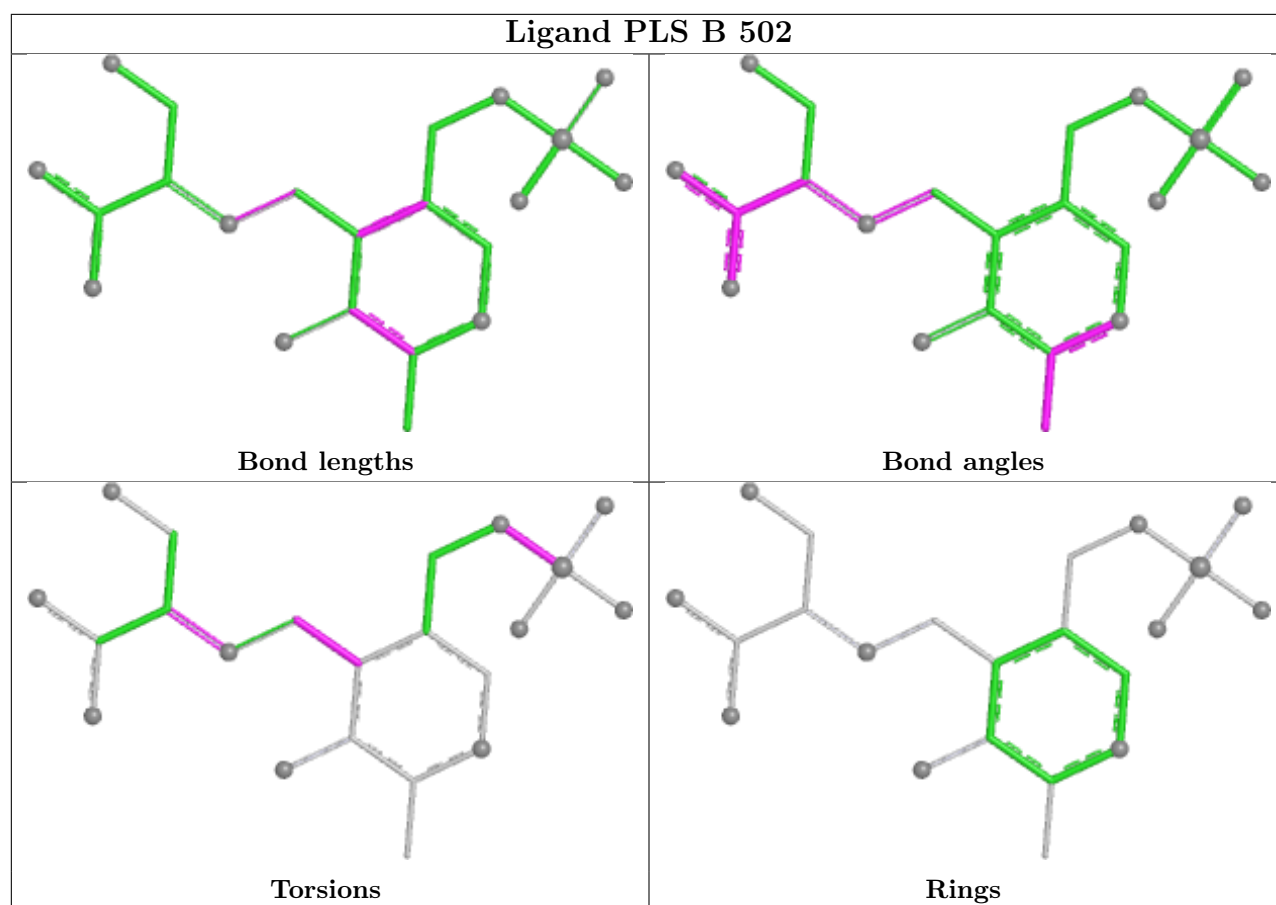
There are no ring outliers.

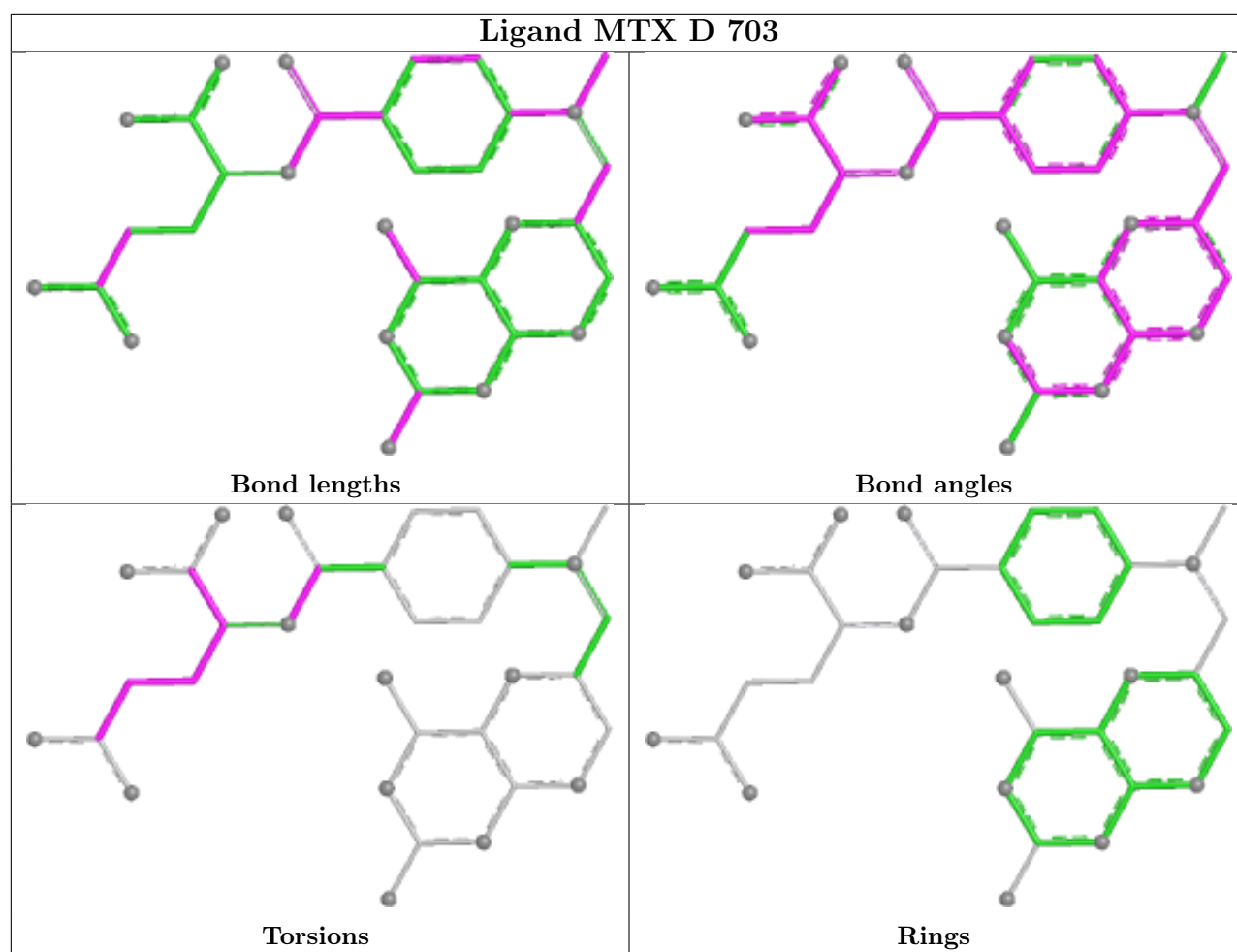
5 monomers are involved in 6 short contacts:

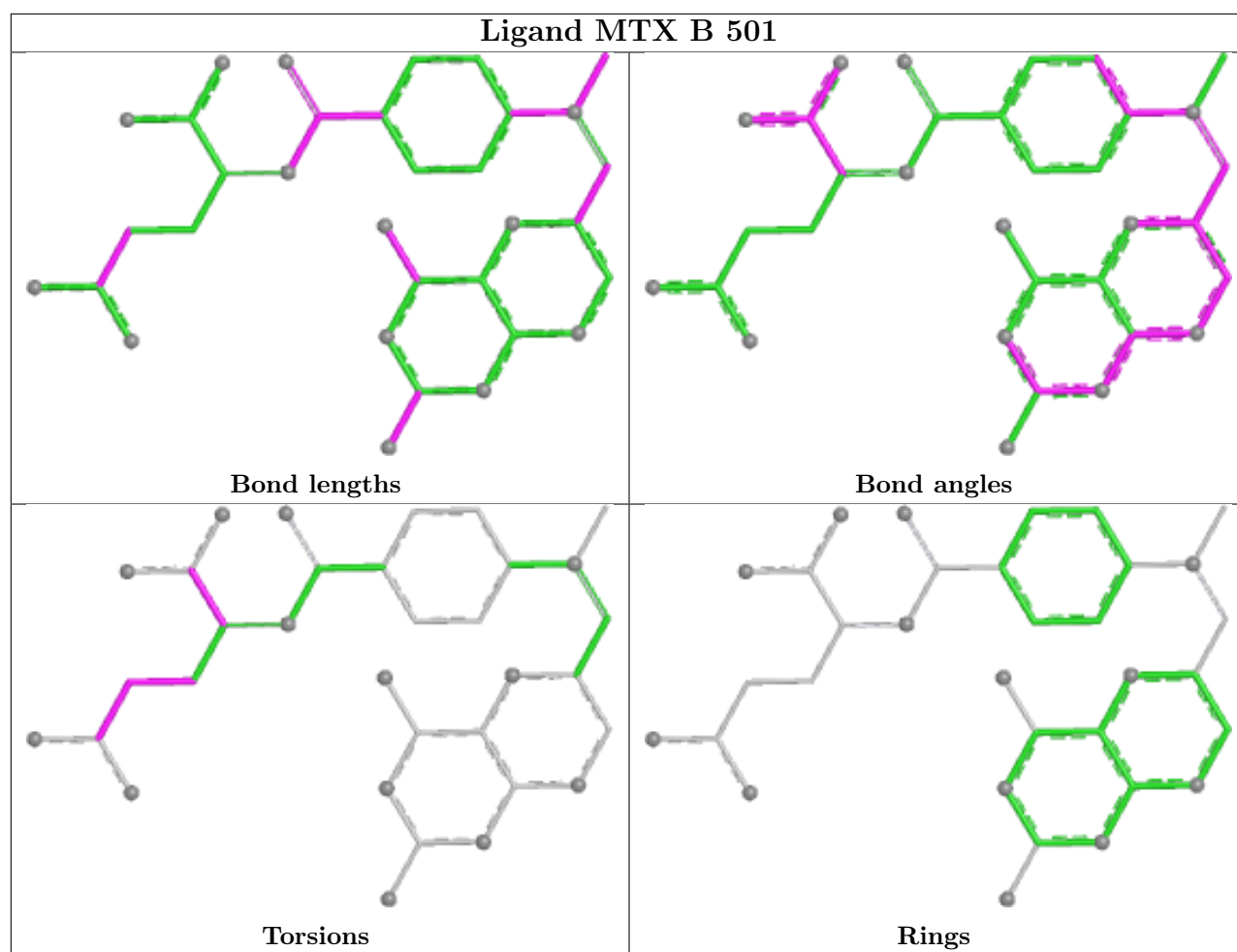
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	1	0
4	D	703	MTX	1	0
4	B	501	MTX	2	0
3	B	505	EDO	1	0
3	D	701	EDO	1	0

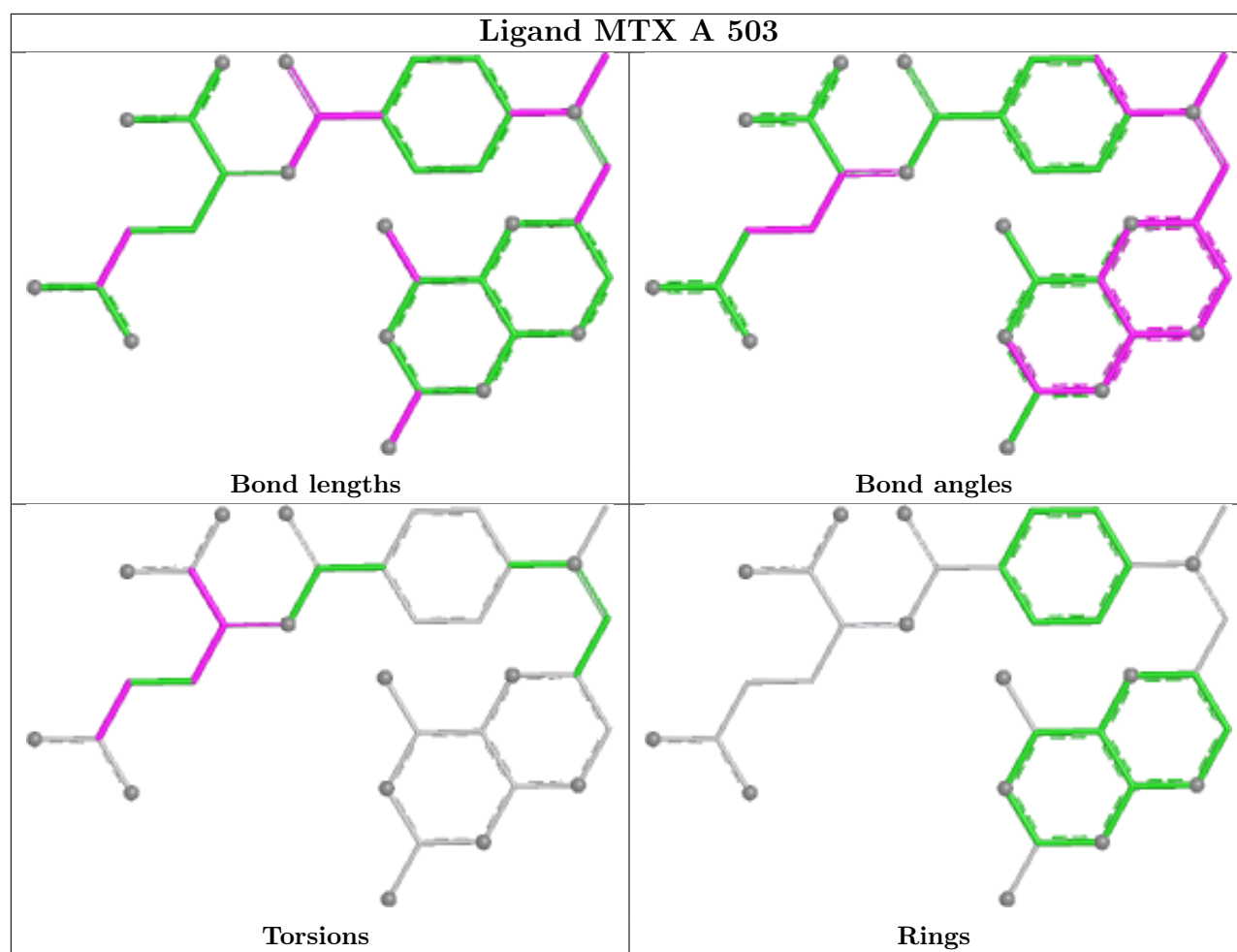
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

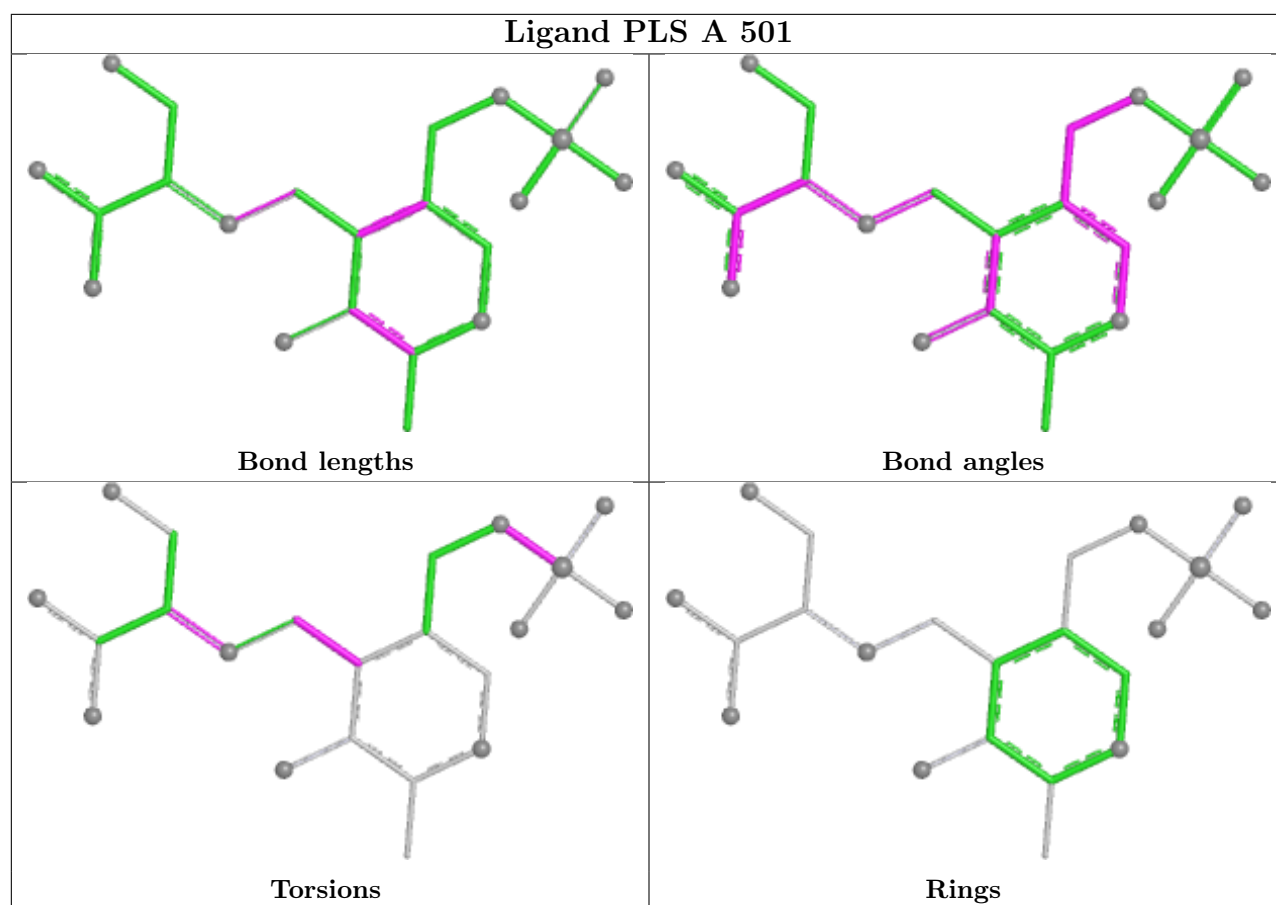


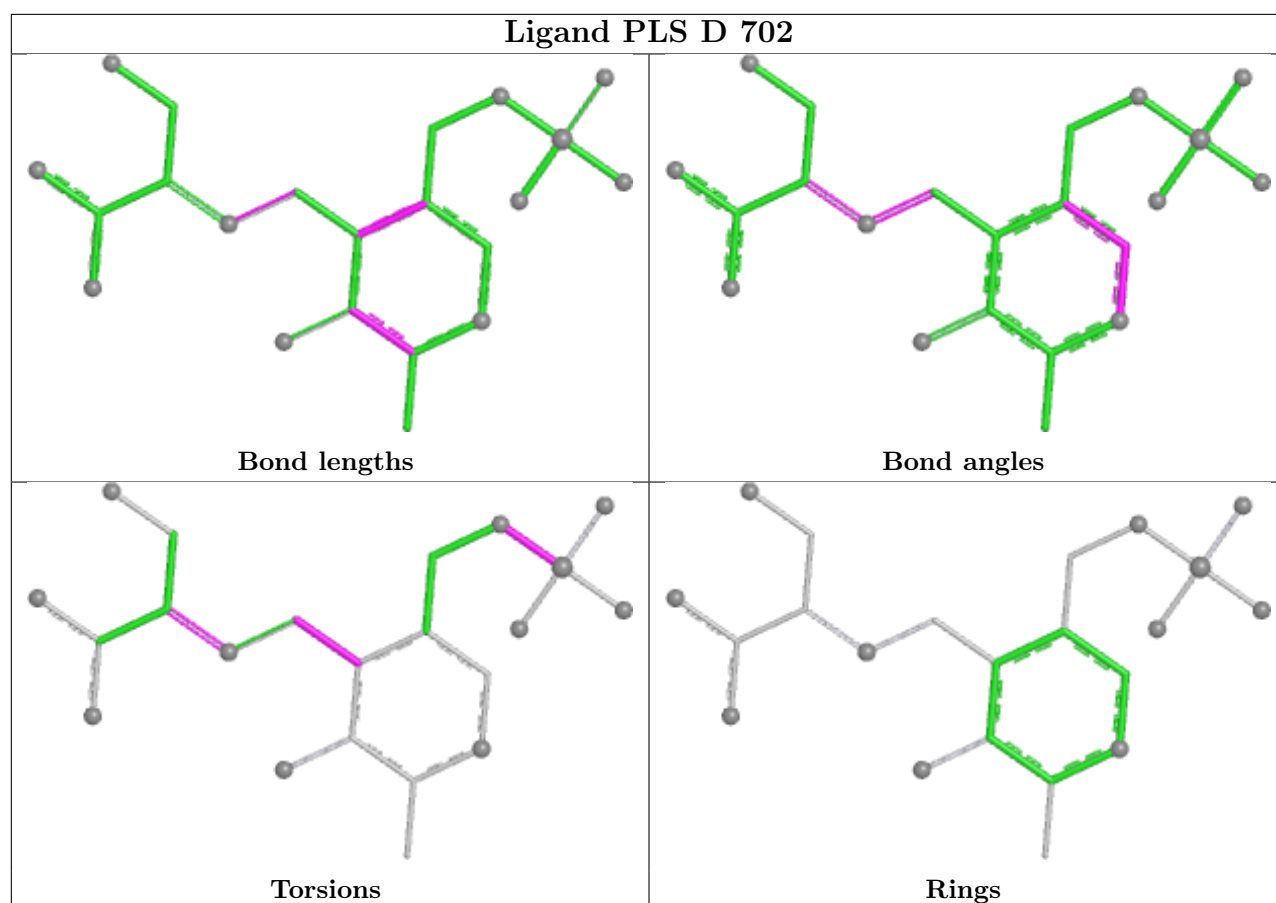












5.7 Other polymers [i](#)

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%)	-0.13	11 (2%) 61 64	21, 35, 63, 103	0
1	B	472/474 (99%)	-0.15	14 (2%) 52 55	21, 33, 68, 127	0
1	C	471/474 (99%)	0.00	14 (2%) 52 55	22, 36, 76, 107	0
1	D	471/474 (99%)	-0.21	3 (0%) 85 87	23, 34, 52, 99	0
All	All	1887/1896 (99%)	-0.12	42 (2%) 62 65	21, 35, 66, 127	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	378	GLY	5.1
1	B	377	PHE	5.0
1	B	380	SER	4.1
1	B	383	LEU	4.0
1	B	382	ALA	3.9
1	A	-2	SER	3.7
1	A	163	PHE	3.5
1	B	376	VAL	3.4
1	B	429	LEU	3.4
1	A	384	ALA	3.3
1	B	384	ALA	3.2
1	C	163	PHE	3.2
1	C	378	GLY	3.2
1	A	382	ALA	3.1
1	C	429	LEU	3.0
1	D	430	LEU	3.0
1	A	69	TYR	2.9
1	C	430	LEU	2.9
1	A	390	ILE	2.8
1	B	381	SER	2.7
1	D	163	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	383	LEU	2.6
1	C	383	LEU	2.6
1	D	69	TYR	2.6
1	B	427	GLY	2.5
1	B	163	PHE	2.5
1	C	425	THR	2.4
1	C	382	ALA	2.3
1	C	356	THR	2.2
1	B	428	LYS	2.2
1	B	0	ALA	2.2
1	B	267	GLN	2.1
1	A	430	LEU	2.1
1	C	367	CYS	2.1
1	C	65	GLY	2.1
1	A	264	LYS	2.1
1	C	416	VAL	2.1
1	A	-1	ASN	2.0
1	C	347	LEU	2.0
1	C	418	LEU	2.0
1	C	443	LEU	2.0
1	A	266	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 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.

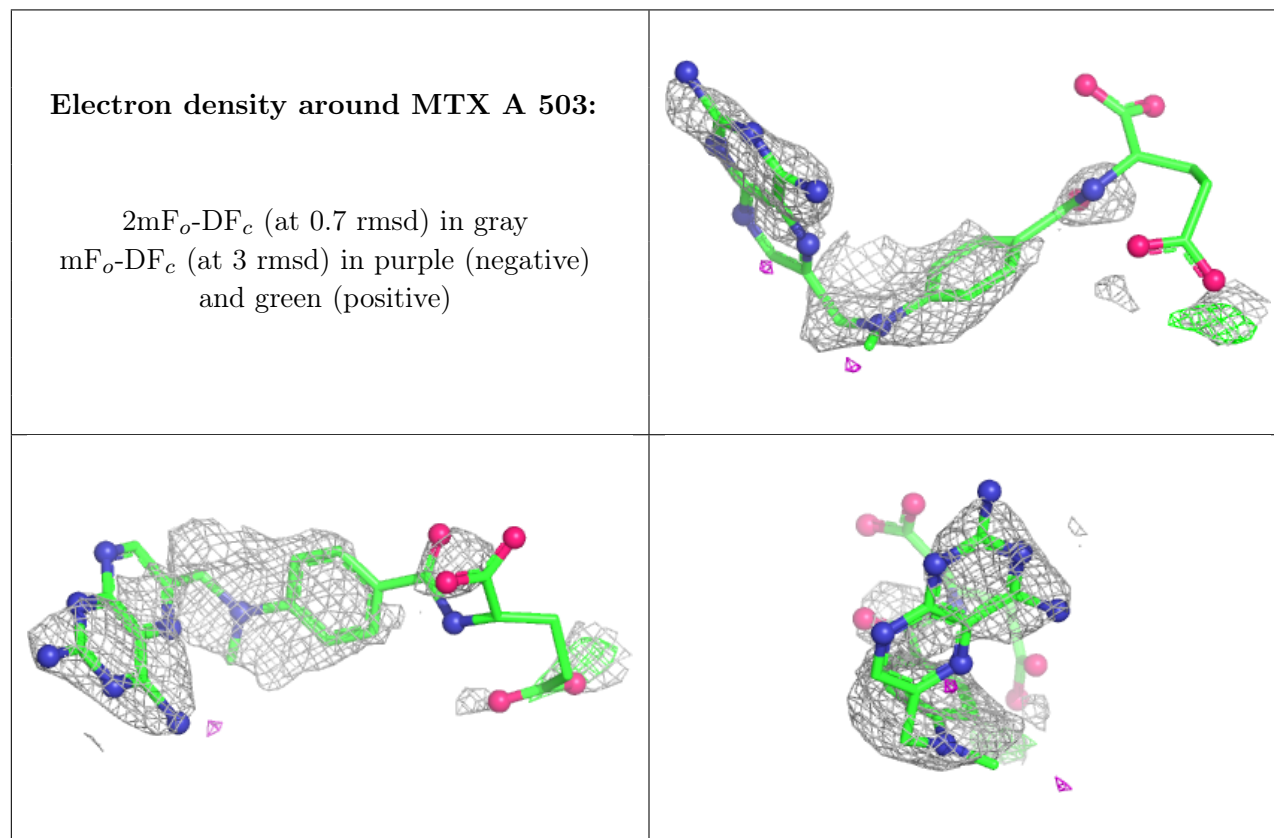
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MTX	A	503	33/33	0.64	0.18	107,112,135,139	0
4	MTX	D	703	33/33	0.82	0.13	50,62,75,78	0

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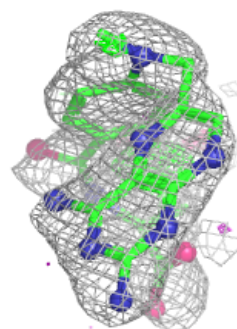
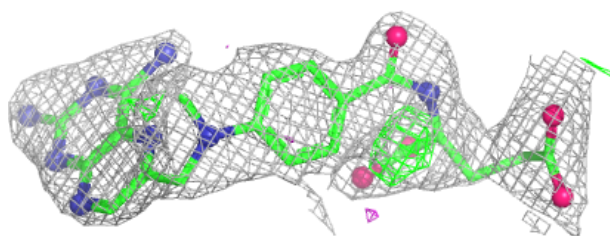
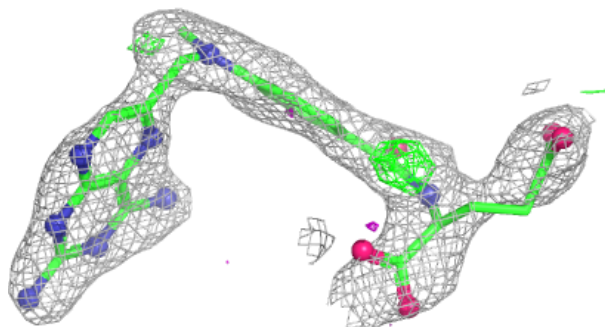
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MTX	B	501	33/33	0.83	0.14	76,81,100,102	0
3	EDO	D	701	4/4	0.87	0.12	42,43,47,48	0
3	EDO	A	504	4/4	0.87	0.15	42,43,49,49	0
3	EDO	B	505	4/4	0.89	0.13	54,54,55,56	0
3	EDO	D	704	4/4	0.91	0.15	46,47,47,52	0
3	EDO	C	504	4/4	0.91	0.11	34,36,36,41	0
3	EDO	A	502	4/4	0.93	0.09	42,43,45,48	0
3	EDO	B	504	4/4	0.94	0.08	33,35,38,45	0
3	EDO	B	503	4/4	0.94	0.10	27,32,33,35	0
3	EDO	C	502	4/4	0.94	0.09	36,45,46,47	0
5	TRS	C	503	8/8	0.94	0.07	33,41,45,47	0
2	PLS	B	502	22/22	0.97	0.05	17,27,32,34	0
2	PLS	C	501	22/22	0.97	0.06	22,29,38,42	0
2	PLS	D	702	22/22	0.97	0.05	21,30,34,36	0
2	PLS	A	501	22/22	0.97	0.06	18,29,34,37	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.

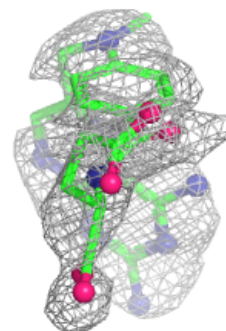
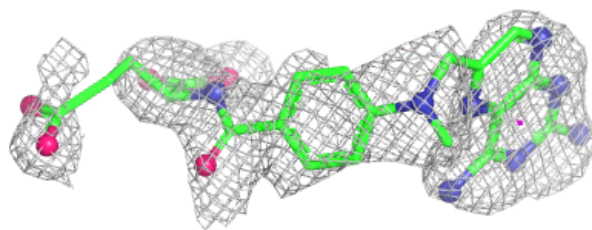
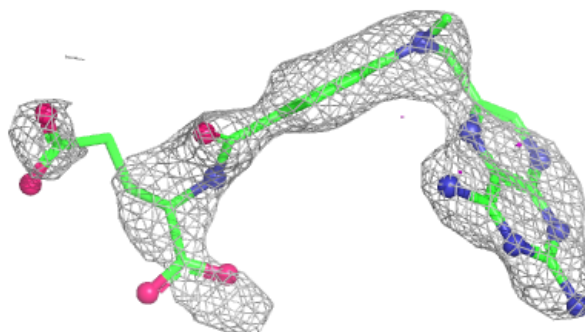


Electron density around MTX D 703:

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

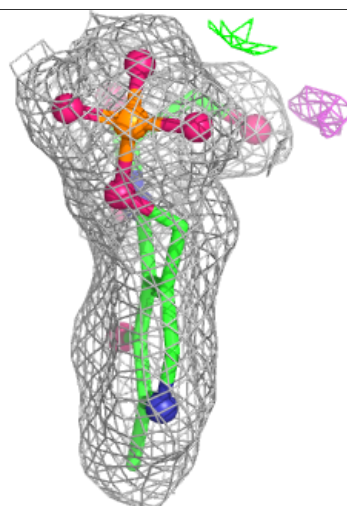
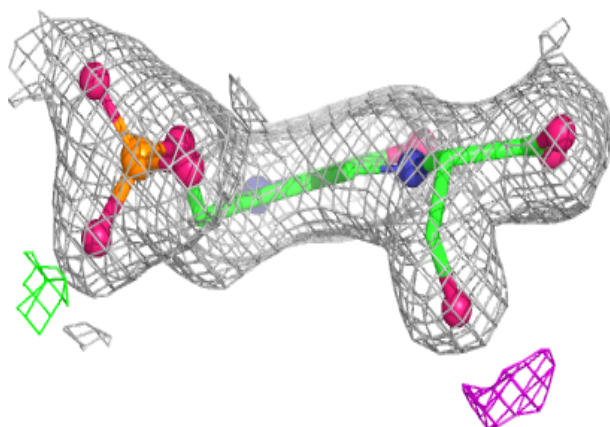
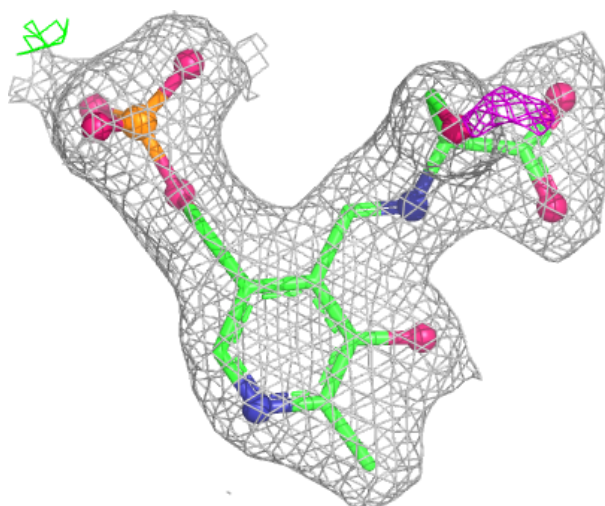
**Electron density around MTX B 501:**

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



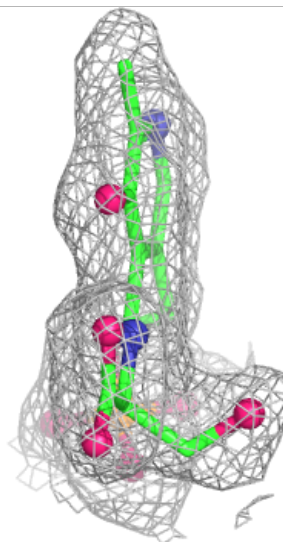
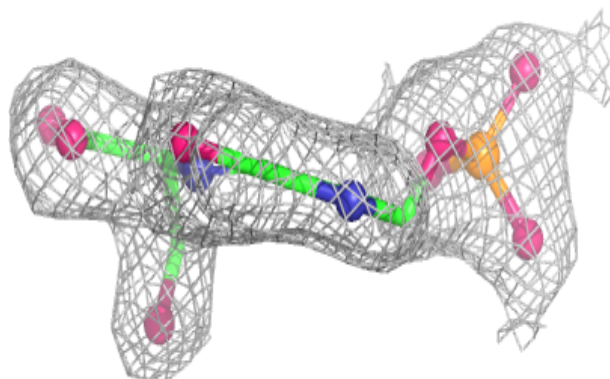
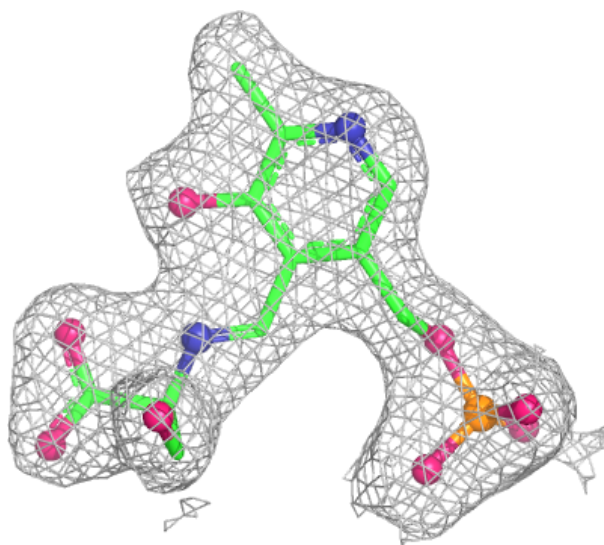
Electron density around PLS B 502:

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



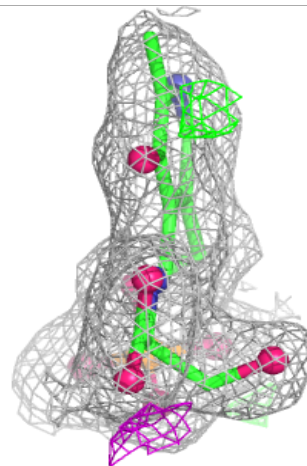
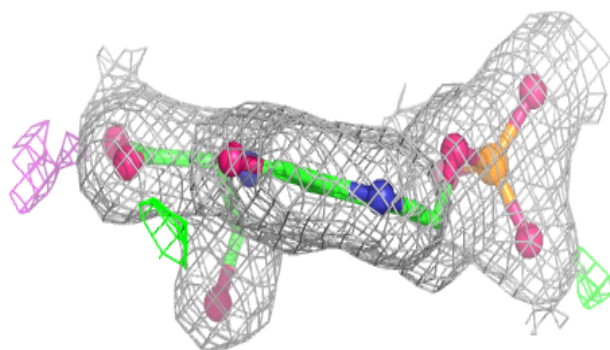
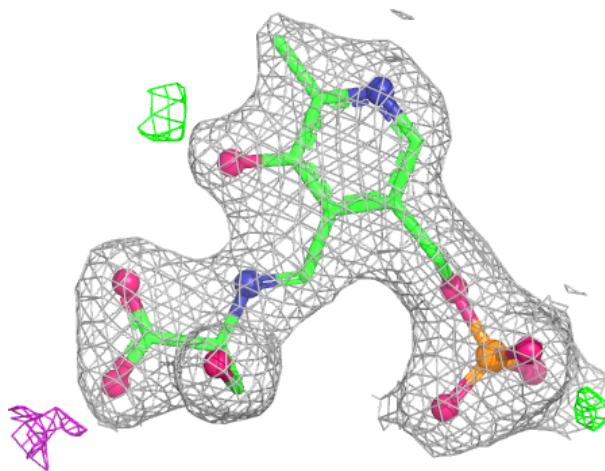
Electron density around PLS C 501:

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



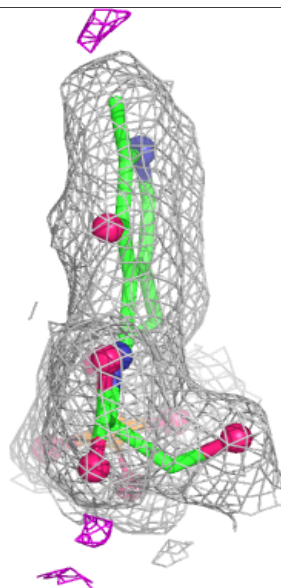
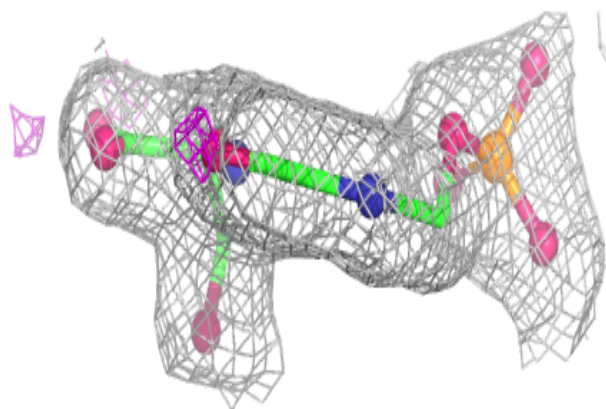
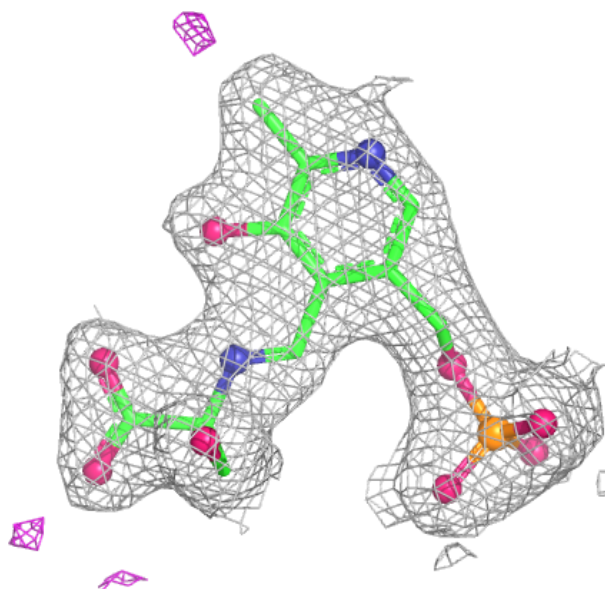
Electron density around PLS D 702:

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



Electron density around PLS A 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.