wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 04:16 AM EDT

PDB ID	:	6SMN
Title	:	A. thaliana serine hydroxymethyltransferase isoform 2 (AtSHMT2) in complex with methotrexate
Authors	:	Ruszkowski, M.; Sekula, B.; Dauter, Z.
Deposited on	:	2019-08-22
Resolution	:	1.63 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

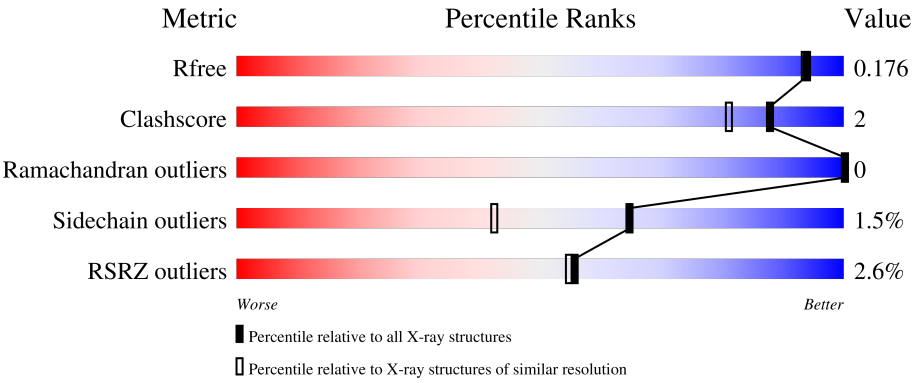
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.63 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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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

Mol	Chain	Length	Quality of chain
1	A	480	2% 93% 5%
1	B	480	3% 94% 5%
1	C	480	% 95%
2	D	480	3% 96%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	607	-	-	X	-
4	EDO	C	609	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17397 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 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	4	0
			3751	2380	641	711	19			
1	B	475	Total	C	N	O	S	0	4	0
			3760	2385	646	711	18			
1	C	475	Total	C	N	O	S	0	8	0
			3782	2396	650	718	18			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	SER	-	expression tag	UNP Q94C74
A	39	ASN	-	expression tag	UNP Q94C74
A	40	ALA	-	expression tag	UNP Q94C74
B	38	SER	-	expression tag	UNP Q94C74
B	39	ASN	-	expression tag	UNP Q94C74
B	40	ALA	-	expression tag	UNP Q94C74
C	38	SER	-	expression tag	UNP Q94C74
C	39	ASN	-	expression tag	UNP Q94C74
C	40	ALA	-	expression tag	UNP Q94C74

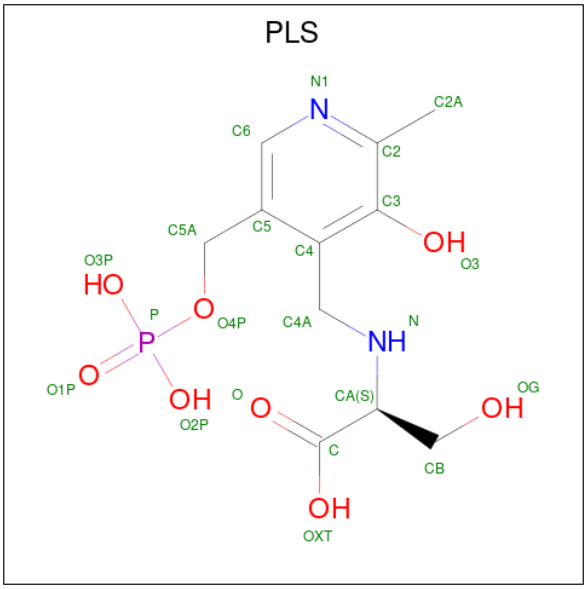
- Molecule 2 is a protein called Serine hydroxymethyltransferase 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	480	Total	C	N	O	P	S	0	1	0
			3785	2400	646	719	1	19			

There are 3 discrepancies between the modelled and reference sequences:

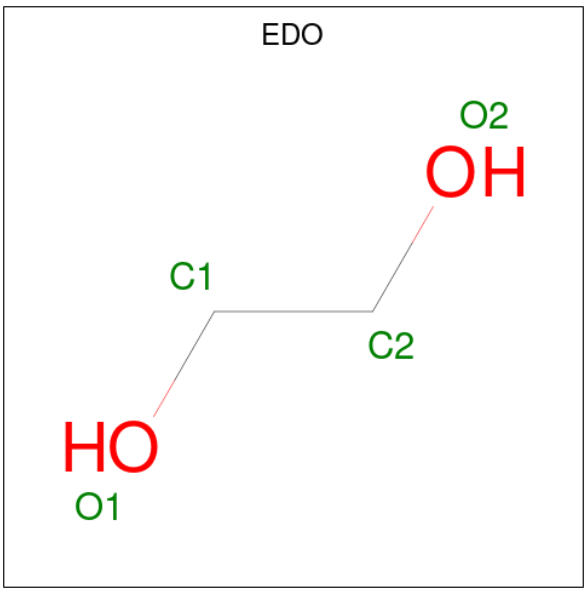
Chain	Residue	Modelled	Actual	Comment	Reference
D	38	SER	-	expression tag	UNP Q94C74
D	39	ASN	-	expression tag	UNP Q94C74
D	40	ALA	-	expression tag	UNP Q94C74

- Molecule 3 is [3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YL METHYL]-SERINE (three-letter code: PLS) (formula: $C_{11}H_{17}N_2O_8P$).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

Continued on next page...

Continued from previous page...

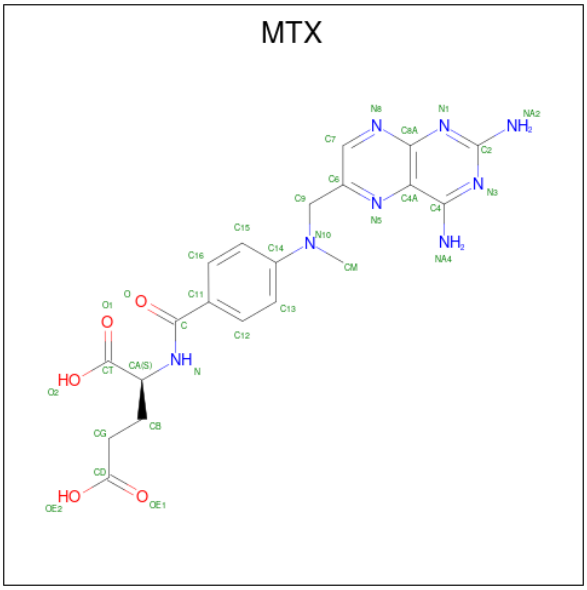
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0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

Continued on next page...

Continued from previous page...

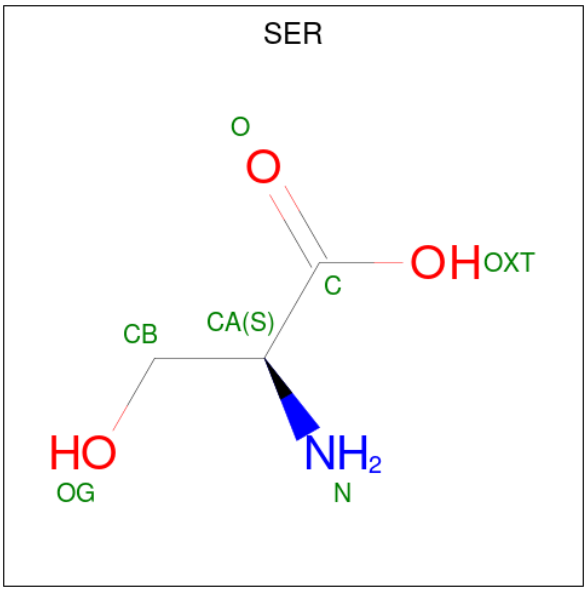
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 6 is SERINE (three-letter code: SER) (formula: $C_3H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	1	Total	C	N	O	0	0
			7	3	1	3		

- Molecule 7 is water.

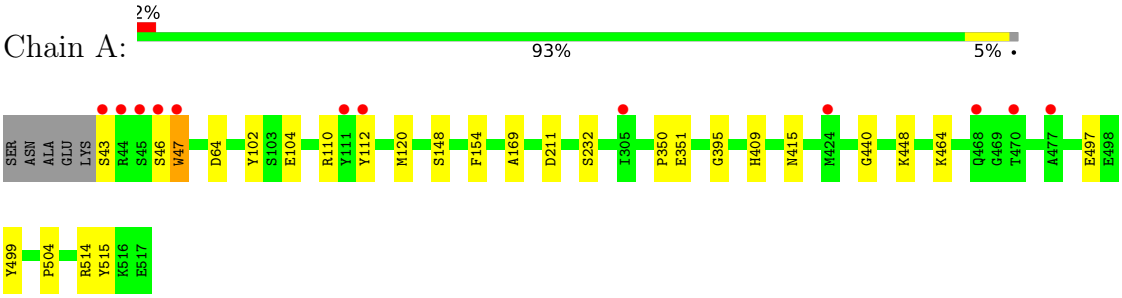
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	506	Total	O	0	0
			506	506		
7	B	461	Total	O	0	0
			461	461		
7	C	517	Total	O	0	0
			517	517		
7	D	438	Total	O	0	0
			438	438		

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.

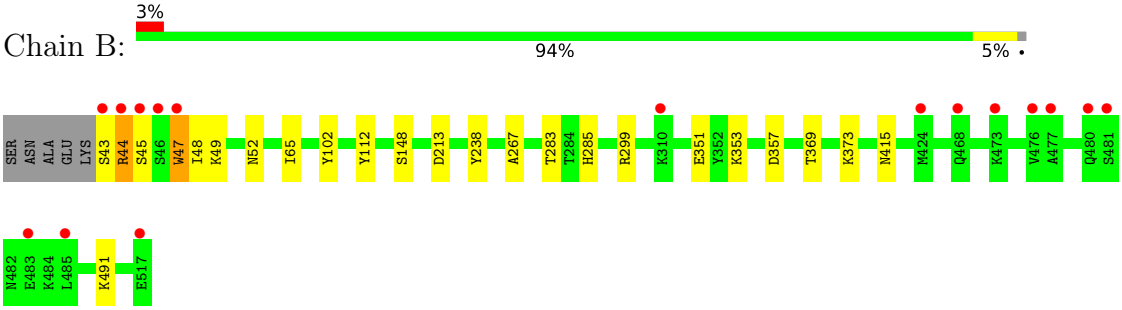
• Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial

Chain A:



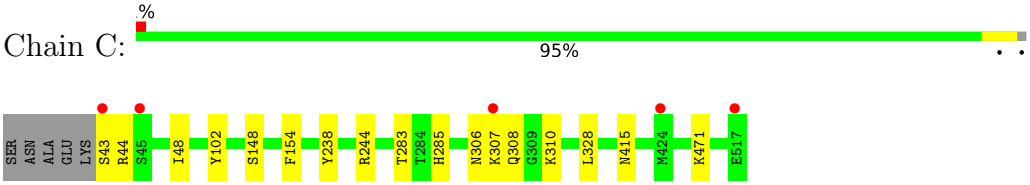
• Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial

Chain B:



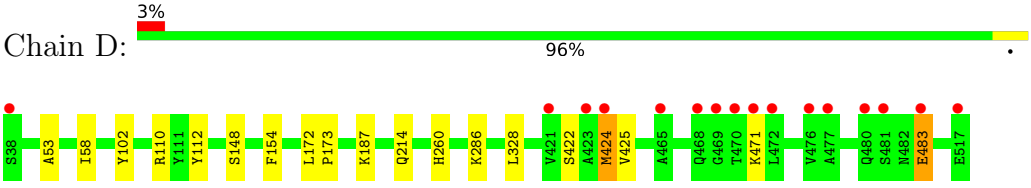
• Molecule 1: Serine hydroxymethyltransferase 2, mitochondrial

Chain C:



• Molecule 2: Serine hydroxymethyltransferase 2, mitochondrial

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.03Å 130.40Å 150.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	80.00 – 1.63 75.41 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.8 (80.00-1.63) 99.8 (75.41-1.63)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.63Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.125 , 0.177 0.125 , 0.176	Depositor DCC
R_{free} test set	1397 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å^2)	18.2	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	17397	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MTX, EDO, PLS, LLP

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	0.34	0/3825	0.51	0/5159
1	B	0.33	0/3835	0.51	0/5173
1	C	0.35	0/3857	0.52	0/5202
2	D	0.35	0/3834	0.52	0/5170
All	All	0.34	0/15351	0.52	0/20704

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

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	3751	0	3754	24	0
1	B	3760	0	3759	16	0
1	C	3782	0	3776	7	0
2	D	3785	0	3781	12	0
3	A	22	0	14	3	0
3	B	22	0	14	2	0
3	C	22	0	14	1	0
4	A	60	0	90	9	0
4	B	40	0	60	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	60	0	90	7	0
4	D	32	0	48	0	0
5	A	33	0	20	1	0
5	B	33	0	20	2	0
5	C	66	0	40	1	0
6	D	7	0	4	0	0
7	A	506	0	0	4	0
7	B	461	0	0	3	0
7	C	517	0	0	2	0
7	D	438	0	0	5	0
All	All	17397	0	15484	63	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 2.

The worst 5 of 63 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:504:PRO:HA	4:A:607:EDO:H21	1.64	0.78
1:C:471:LYS:HB3	4:C:606:EDO:H12	1.76	0.66
1:A:440:GLY:O	1:B:44:ARG:NH1	2.30	0.65
1:A:504:PRO:HG2	1:B:48:ILE:HD13	1.79	0.63
1:B:299[B]:ARG:NH1	7:B:2503:HOH:O	2.28	0.62

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	477/480 (99%)	463 (97%)	14 (3%)	0	100	100
1	B	477/480 (99%)	465 (98%)	12 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	481/480 (100%)	469 (98%)	12 (2%)	0	100	100
2	D	478/480 (100%)	468 (98%)	10 (2%)	0	100	100
All	All	1913/1920 (100%)	1865 (98%)	48 (2%)	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	401/401 (100%)	397 (99%)	4 (1%)	76	59
1	B	401/401 (100%)	395 (98%)	6 (2%)	65	42
1	C	405/401 (101%)	398 (98%)	7 (2%)	60	36
2	D	401/400 (100%)	394 (98%)	7 (2%)	60	36
All	All	1608/1603 (100%)	1584 (98%)	24 (2%)	65	42

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	307	LYS
2	D	102	TYR
1	C	415	ASN
2	D	148	SER
1	B	102	TYR

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

Mol	Chain	Res	Type
1	A	50	GLN
1	C	308	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

1 non-standard protein/DNA/RNA residue is 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	LLP	D	286	2	23,24,25	2.50	6 (26%)	25,32,34	1.59	3 (12%)

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	LLP	D	286	2	-	2/16/17/19	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	286	LLP	C4-C4'	7.91	1.61	1.46
2	D	286	LLP	C4'-NZ	5.13	1.44	1.27
2	D	286	LLP	C2'-C2	3.49	1.56	1.50
2	D	286	LLP	C4-C5	-3.11	1.38	1.42
2	D	286	LLP	C6-N1	2.79	1.40	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	286	LLP	OP4-C5'-C5	4.75	118.40	109.35
2	D	286	LLP	C4-C4'-NZ	-3.45	108.47	124.31
2	D	286	LLP	C5'-C5-C6	-2.39	115.45	119.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	286	LLP	C4-C4'-NZ-CE
2	D	286	LLP	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

56 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	$\#\|Z\| > 2$
4	EDO	B	2406	-	3,3,3	0.43	0	2,2,2	0.35	0
4	EDO	D	703	-	3,3,3	0.43	0	2,2,2	0.51	0
6	SER	D	702	-	5,6,6	0.99	1 (20%)	5,7,7	1.76	2 (40%)
4	EDO	A	602	-	3,3,3	0.51	0	2,2,2	0.29	0
4	EDO	C	613	-	3,3,3	0.32	0	2,2,2	0.71	0
4	EDO	C	616	-	3,3,3	0.51	0	2,2,2	0.27	0
3	PLS	C	601	-	22,22,22	1.89	3 (13%)	27,31,31	1.65	6 (22%)
4	EDO	B	2408	-	3,3,3	0.48	0	2,2,2	0.24	0
4	EDO	D	704	-	3,3,3	0.51	0	2,2,2	0.22	0
5	MTX	B	2404	-	35,35,35	2.59	9 (25%)	46,49,49	1.87	12 (26%)
4	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	C	611	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	C	605	-	3,3,3	0.43	0	2,2,2	0.48	0
4	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	EDO	B	2407	-	3,3,3	0.45	0	2,2,2	0.35	0
3	PLS	A	601	-	22,22,22	1.89	4 (18%)	27,31,31	1.60	6 (22%)
4	EDO	B	2405	-	3,3,3	0.47	0	2,2,2	0.49	0
4	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.30	0
4	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.53	0
4	EDO	B	2411	-	3,3,3	0.46	0	2,2,2	0.32	0
4	EDO	C	614	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	A	612	-	3,3,3	0.46	0	2,2,2	0.23	0
5	MTX	C	617	-	35,35,35	2.59	9 (25%)	46,49,49	1.79	10 (21%)
4	EDO	C	606	-	3,3,3	0.49	0	2,2,2	0.25	0
5	MTX	A	603	-	35,35,35	2.56	9 (25%)	46,49,49	1.97	12 (26%)
4	EDO	C	602	-	3,3,3	0.47	0	2,2,2	0.33	0
4	EDO	A	611	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.27	0
4	EDO	D	706	-	3,3,3	0.43	0	2,2,2	0.39	0
4	EDO	D	708	-	3,3,3	0.46	0	2,2,2	0.43	0
4	EDO	C	608	-	3,3,3	0.46	0	2,2,2	0.37	0
4	EDO	A	614	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	D	705	-	3,3,3	0.46	0	2,2,2	0.35	0
4	EDO	D	701	-	3,3,3	0.48	0	2,2,2	0.30	0
4	EDO	C	612	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	B	2410	-	3,3,3	0.44	0	2,2,2	0.29	0
4	EDO	A	606	-	3,3,3	0.34	0	2,2,2	0.48	0
4	EDO	D	709	-	3,3,3	0.45	0	2,2,2	0.47	0
5	MTX	C	603	-	35,35,35	2.60	9 (25%)	46,49,49	1.87	12 (26%)
4	EDO	C	607	-	3,3,3	0.54	0	2,2,2	0.27	0
4	EDO	C	604	-	3,3,3	0.41	0	2,2,2	0.43	0
4	EDO	A	608	-	3,3,3	0.42	0	2,2,2	0.39	0
4	EDO	A	617	-	3,3,3	0.48	0	2,2,2	0.37	0
4	EDO	B	2401	-	3,3,3	0.47	0	2,2,2	0.34	0
4	EDO	C	618	-	3,3,3	0.48	0	2,2,2	0.29	0
4	EDO	B	2409	-	3,3,3	0.42	0	2,2,2	0.55	0
4	EDO	B	2403	-	3,3,3	0.51	0	2,2,2	0.17	0
4	EDO	A	610	-	3,3,3	0.46	0	2,2,2	0.29	0
3	PLS	B	2402	-	22,22,22	1.89	3 (13%)	27,31,31	1.69	4 (14%)
4	EDO	D	707	-	3,3,3	0.47	0	2,2,2	0.26	0
4	EDO	C	610	-	3,3,3	0.42	0	2,2,2	0.41	0
4	EDO	A	615	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	C	609	-	3,3,3	0.36	0	2,2,2	0.52	0
4	EDO	A	613	-	3,3,3	0.43	0	2,2,2	0.33	0
4	EDO	C	615	-	3,3,3	0.49	0	2,2,2	0.29	0
4	EDO	B	2412	-	3,3,3	0.45	0	2,2,2	0.36	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
4	EDO	B	2406	-	-	0/1/1/1	-
4	EDO	D	703	-	-	0/1/1/1	-
6	SER	D	702	-	-	2/6/6/6	-
4	EDO	A	602	-	-	1/1/1/1	-
4	EDO	C	613	-	-	0/1/1/1	-
4	EDO	C	616	-	-	1/1/1/1	-
3	PLS	C	601	-	-	5/17/17/17	0/1/1/1
4	EDO	B	2408	-	-	0/1/1/1	-
4	EDO	D	704	-	-	0/1/1/1	-
5	MTX	B	2404	-	-	9/25/25/25	0/3/3/3
4	EDO	A	609	-	-	0/1/1/1	-
4	EDO	C	611	-	-	1/1/1/1	-
4	EDO	C	605	-	-	0/1/1/1	-
4	EDO	A	616	-	-	0/1/1/1	-
4	EDO	B	2407	-	-	0/1/1/1	-
3	PLS	A	601	-	-	4/17/17/17	0/1/1/1
4	EDO	B	2405	-	-	0/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	A	604	-	-	0/1/1/1	-
4	EDO	B	2411	-	-	0/1/1/1	-
4	EDO	C	614	-	-	0/1/1/1	-
4	EDO	A	612	-	-	0/1/1/1	-
5	MTX	C	617	-	-	2/25/25/25	0/3/3/3
4	EDO	C	606	-	-	1/1/1/1	-
5	MTX	A	603	-	-	7/25/25/25	0/3/3/3
4	EDO	C	602	-	-	1/1/1/1	-
4	EDO	A	611	-	-	0/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	D	706	-	-	1/1/1/1	-
4	EDO	D	708	-	-	0/1/1/1	-
4	EDO	C	608	-	-	0/1/1/1	-
4	EDO	A	614	-	-	0/1/1/1	-
4	EDO	D	705	-	-	0/1/1/1	-
4	EDO	D	701	-	-	1/1/1/1	-
4	EDO	C	612	-	-	0/1/1/1	-
4	EDO	B	2410	-	-	0/1/1/1	-
4	EDO	A	606	-	-	0/1/1/1	-
4	EDO	D	709	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MTX	C	603	-	-	10/25/25/25	0/3/3/3
4	EDO	C	607	-	-	0/1/1/1	-
4	EDO	C	604	-	-	0/1/1/1	-
4	EDO	A	608	-	-	0/1/1/1	-
4	EDO	A	617	-	-	1/1/1/1	-
4	EDO	B	2401	-	-	1/1/1/1	-
4	EDO	C	618	-	-	1/1/1/1	-
4	EDO	B	2409	-	-	0/1/1/1	-
4	EDO	B	2403	-	-	0/1/1/1	-
4	EDO	A	610	-	-	0/1/1/1	-
3	PLS	B	2402	-	-	4/17/17/17	0/1/1/1
4	EDO	D	707	-	-	0/1/1/1	-
4	EDO	C	610	-	-	0/1/1/1	-
4	EDO	A	615	-	-	0/1/1/1	-
4	EDO	C	609	-	-	0/1/1/1	-
4	EDO	A	613	-	-	0/1/1/1	-
4	EDO	C	615	-	-	0/1/1/1	-
4	EDO	B	2412	-	-	0/1/1/1	-

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	617	MTX	C2-NA2	7.22	1.48	1.33
5	B	2404	MTX	C2-NA2	7.06	1.48	1.33
5	C	603	MTX	C2-NA2	7.05	1.48	1.33
3	C	601	PLS	C4A-N	-6.87	1.26	1.46
3	A	601	PLS	C4A-N	-6.87	1.26	1.46

The worst 5 of 64 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2402	PLS	C4A-N-CA	5.55	124.43	113.92
5	B	2404	MTX	N1-C2-N3	-5.45	119.96	127.22
5	C	617	MTX	N1-C2-N3	-5.40	120.01	127.22
5	C	603	MTX	N1-C2-N3	-5.35	120.09	127.22
5	A	603	MTX	N1-C2-N3	-5.15	120.35	127.22

There are no chirality outliers.

5 of 55 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	PLS	CB-CA-N-C4A
3	A	601	PLS	C-CA-N-C4A
3	A	601	PLS	C3-C4-C4A-N
3	A	601	PLS	C5-C4-C4A-N
3	B	2402	PLS	CB-CA-N-C4A

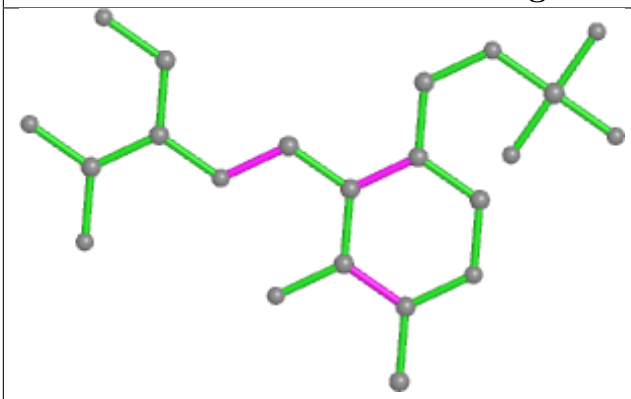
There are no ring outliers.

19 monomers are involved in 30 short contacts:

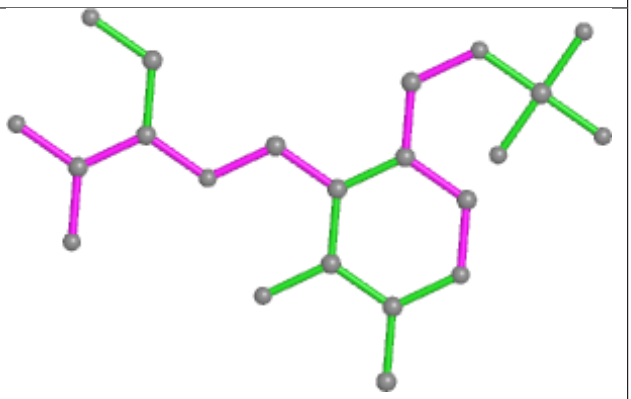
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	EDO	1	0
4	C	616	EDO	1	0
3	C	601	PLS	1	0
5	B	2404	MTX	2	0
4	A	609	EDO	1	0
4	B	2407	EDO	2	0
3	A	601	PLS	3	0
4	A	607	EDO	4	0
4	A	612	EDO	1	0
4	C	606	EDO	1	0
5	A	603	MTX	1	0
4	B	2410	EDO	1	0
4	A	606	EDO	1	0
5	C	603	MTX	1	0
4	B	2401	EDO	1	0
4	C	618	EDO	1	0
3	B	2402	PLS	2	0
4	C	609	EDO	4	0
4	A	613	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

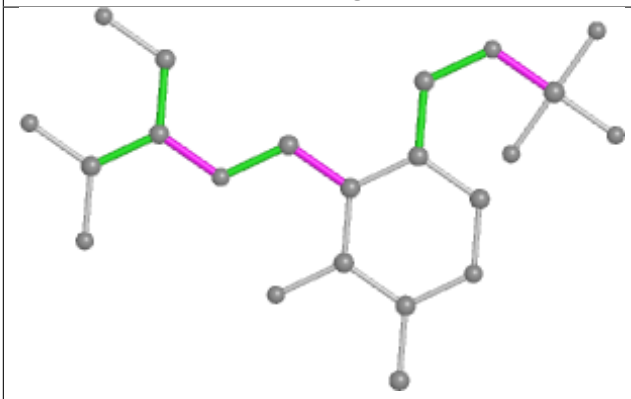
Ligand PLS C 601



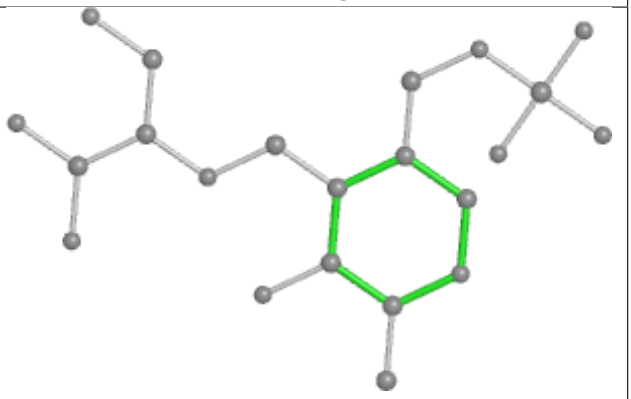
Bond lengths



Bond angles

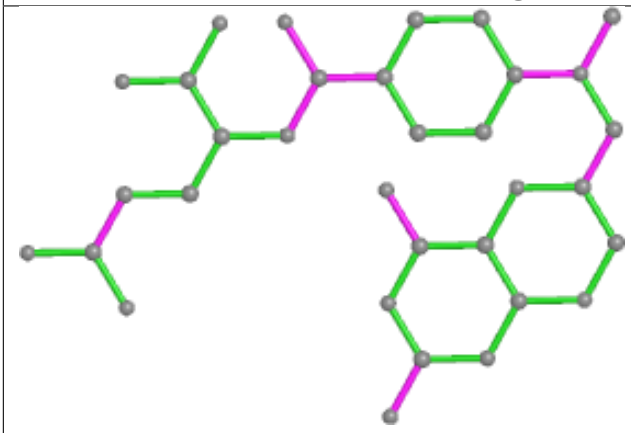


Torsions

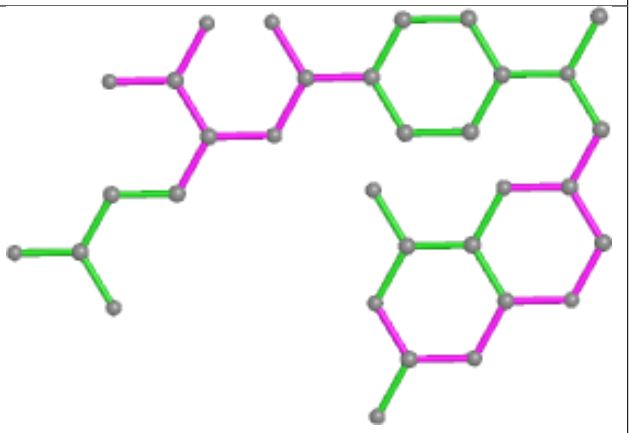


Rings

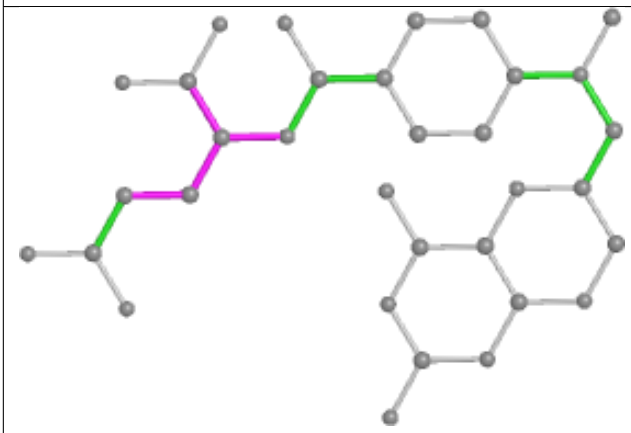
Ligand MTX B 2404



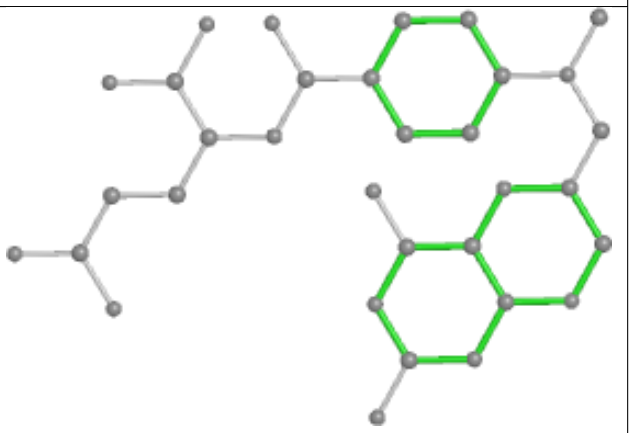
Bond lengths



Bond angles

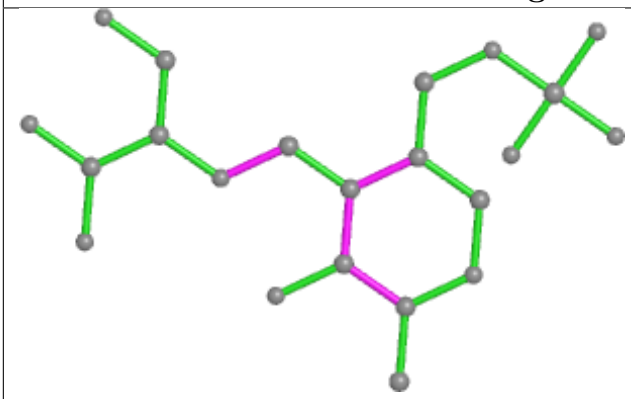


Torsions

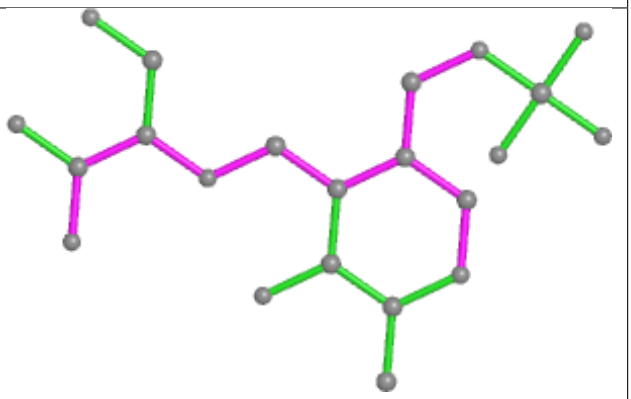


Rings

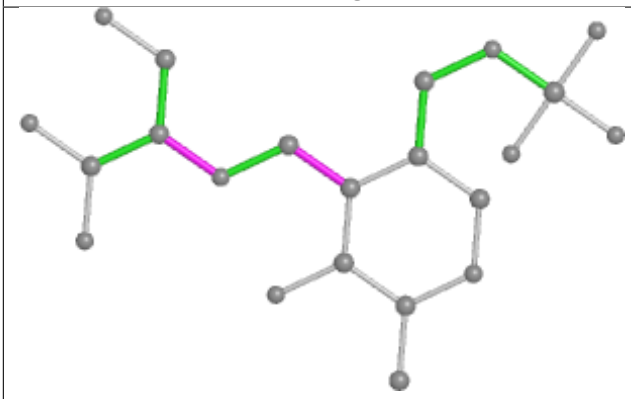
Ligand PLS A 601



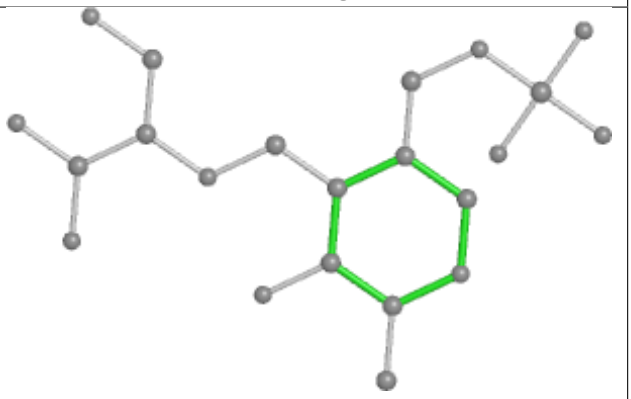
Bond lengths



Bond angles

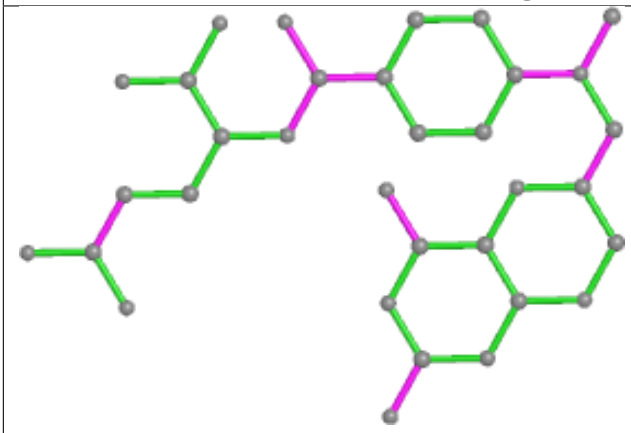


Torsions

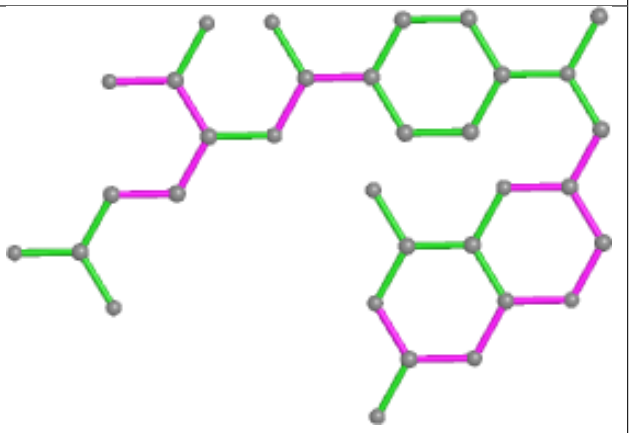


Rings

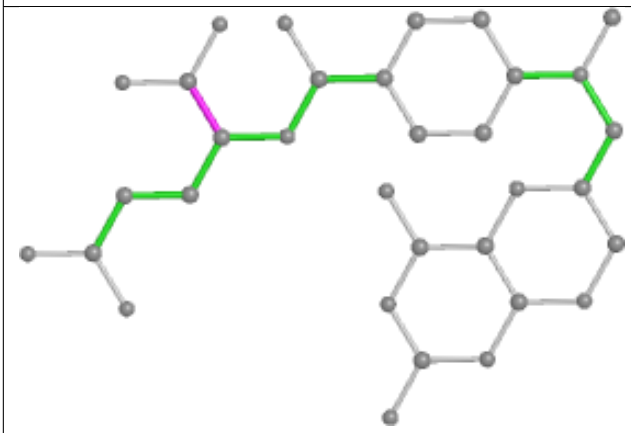
Ligand MTX C 617



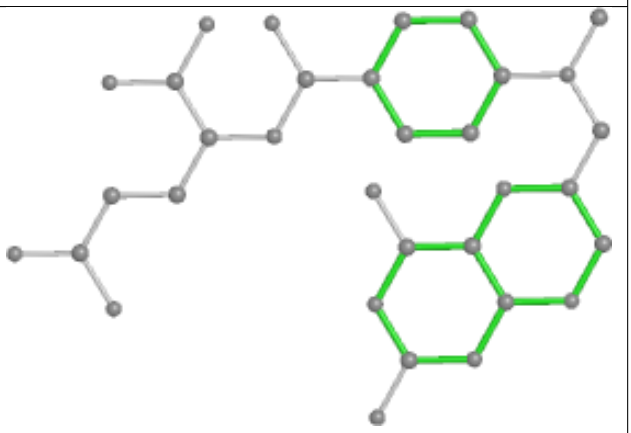
Bond lengths



Bond angles

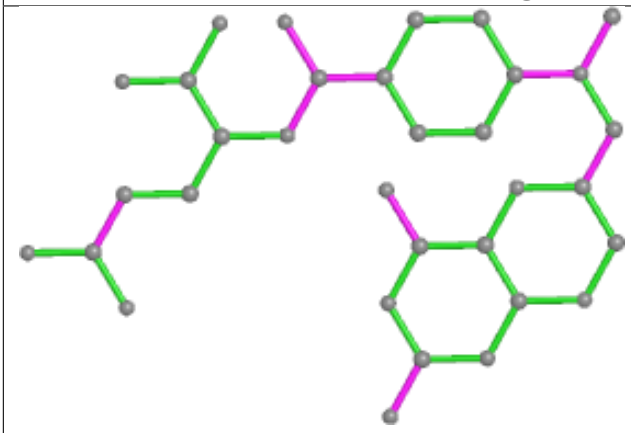


Torsions

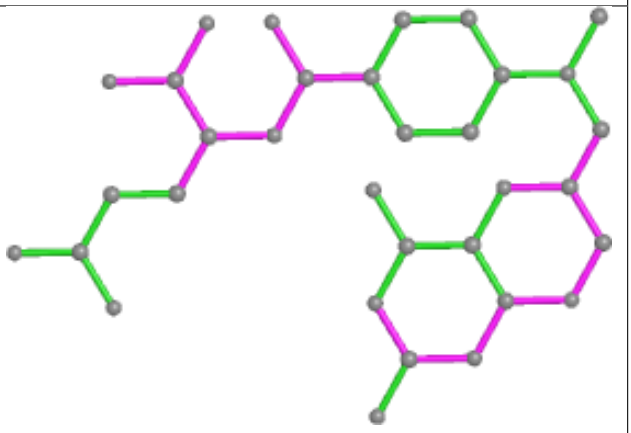


Rings

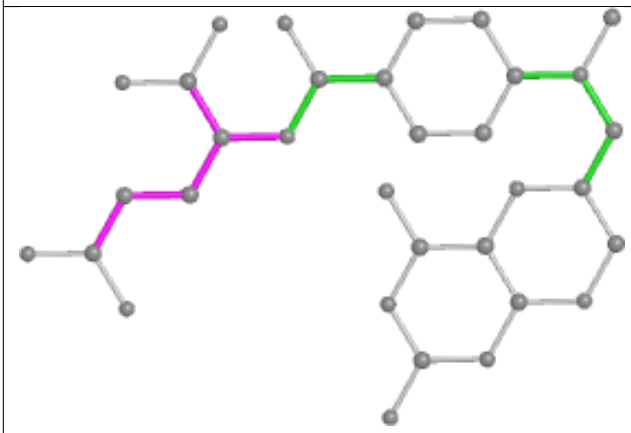
Ligand MTX A 603



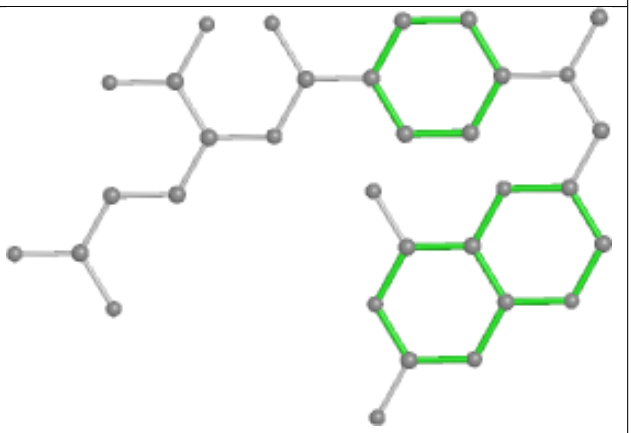
Bond lengths



Bond angles

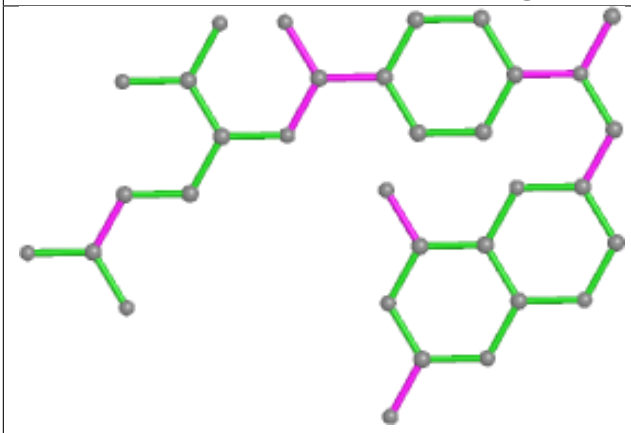


Torsions

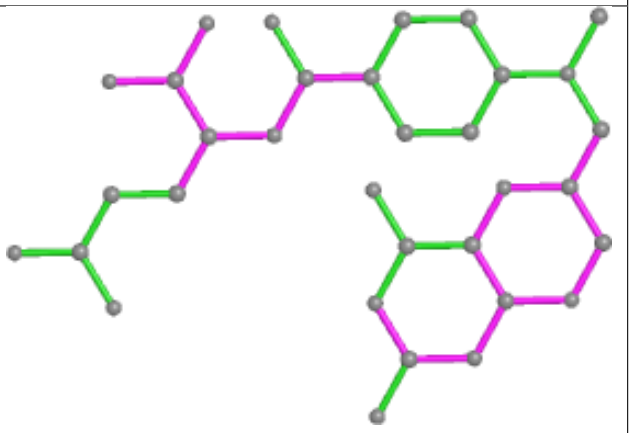


Rings

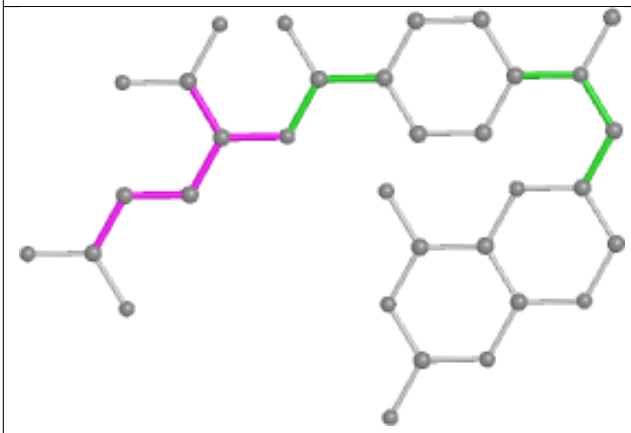
Ligand MTX C 603



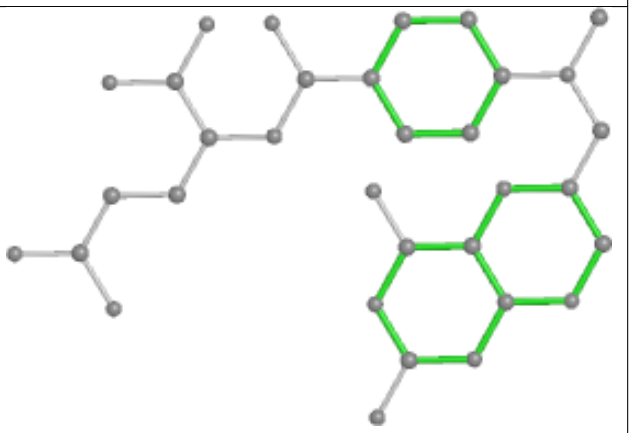
Bond lengths



Bond angles

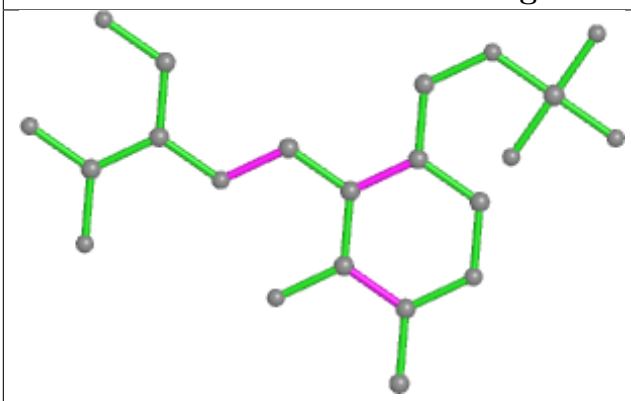


Torsions

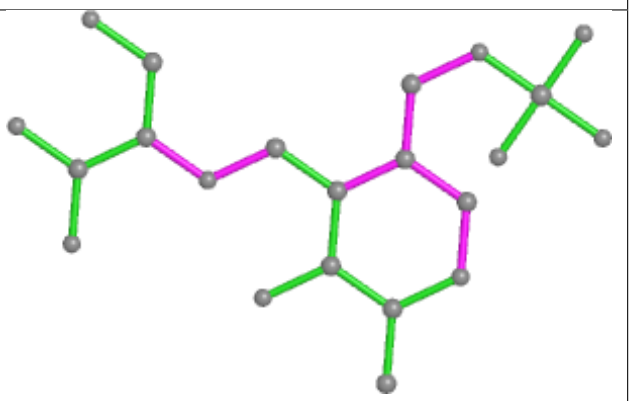


Rings

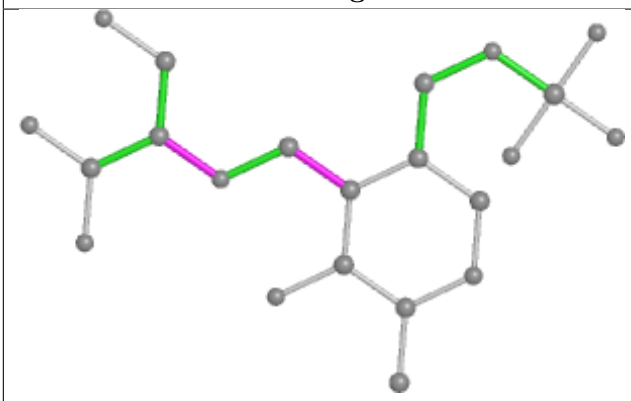
Ligand PLS B 2402



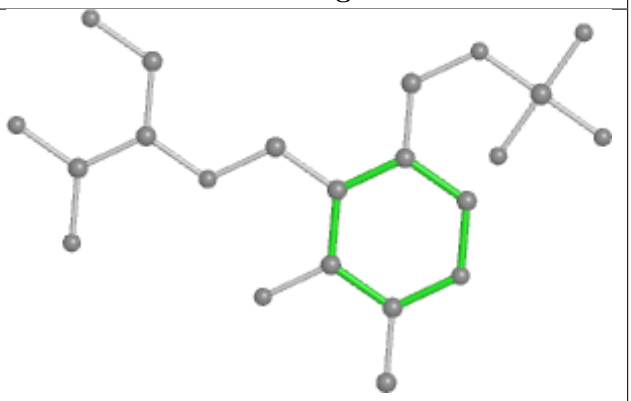
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	475/480 (98%)	-0.37	12 (2%)	57	56	14, 19, 49, 87	0
1	B	475/480 (98%)	-0.29	16 (3%)	45	43	13, 22, 55, 86	0
1	C	475/480 (98%)	-0.36	5 (1%)	80	81	13, 19, 41, 87	0
2	D	479/480 (99%)	-0.23	16 (3%)	46	44	13, 22, 55, 90	0
All	All	1904/1920 (99%)	-0.31	49 (2%)	56	55	13, 21, 51, 90	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	468	GLN	7.0
2	D	421	VAL	6.1
1	B	43	SER	5.9
1	A	43	SER	5.9
1	A	46	SER	5.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LLP	D	286	24/25	0.98	0.08	15,18,22,24	0

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	607	4/4	0.50	0.40	75,76,76,77	0
4	EDO	C	611	4/4	0.57	0.28	74,75,75,75	0
4	EDO	C	615	4/4	0.57	0.14	75,75,76,76	0
5	MTX	C	603	33/33	0.66	0.27	38,55,76,77	33
4	EDO	B	2408	4/4	0.67	0.16	83,84,85,85	0
5	MTX	B	2404	33/33	0.69	0.23	41,51,70,71	33
4	EDO	D	704	4/4	0.74	0.14	59,59,61,61	0
4	EDO	A	602	4/4	0.74	0.20	51,53,57,58	0
4	EDO	C	606	4/4	0.74	0.15	40,44,46,47	0
4	EDO	D	706	4/4	0.77	0.22	67,68,69,69	0
4	EDO	B	2410	4/4	0.78	0.17	70,70,70,71	0
5	MTX	C	617	33/33	0.78	0.20	58,62,74,76	33
4	EDO	C	610	4/4	0.79	0.16	62,62,63,64	0
4	EDO	B	2411	4/4	0.81	0.19	66,66,66,67	0
4	EDO	C	612	4/4	0.81	0.10	66,66,66,66	0
4	EDO	A	615	4/4	0.82	0.09	55,55,55,56	0
4	EDO	A	612	4/4	0.85	0.15	53,56,59,62	0
4	EDO	A	609	4/4	0.87	0.20	52,53,54,56	0
4	EDO	B	2403	4/4	0.87	0.18	51,51,54,56	0
5	MTX	A	603	33/33	0.87	0.15	21,37,76,78	33
4	EDO	B	2409	4/4	0.88	0.13	48,49,50,52	0
4	EDO	A	611	4/4	0.88	0.09	62,62,62,63	0
4	EDO	C	608	4/4	0.89	0.12	47,49,50,52	0
4	EDO	D	708	4/4	0.89	0.09	47,48,48,49	0
4	EDO	B	2407	4/4	0.90	0.14	51,52,52,53	0
4	EDO	C	602	4/4	0.90	0.17	42,45,47,51	0
4	EDO	C	604	4/4	0.90	0.14	47,48,49,50	0
4	EDO	A	613	4/4	0.90	0.23	84,84,84,85	0
4	EDO	A	616	4/4	0.91	0.09	52,52,52,53	0
4	EDO	D	709	4/4	0.91	0.12	48,49,49,51	0
4	EDO	D	707	4/4	0.91	0.10	56,57,57,57	0
4	EDO	A	614	4/4	0.92	0.22	44,46,49,52	0
4	EDO	C	613	4/4	0.92	0.12	33,36,37,38	0
4	EDO	B	2406	4/4	0.92	0.17	48,48,50,50	0
4	EDO	C	607	4/4	0.92	0.10	30,31,31,33	0
4	EDO	B	2412	4/4	0.93	0.12	72,73,74,74	0
4	EDO	C	616	4/4	0.93	0.08	34,37,37,41	0

Continued on next page...

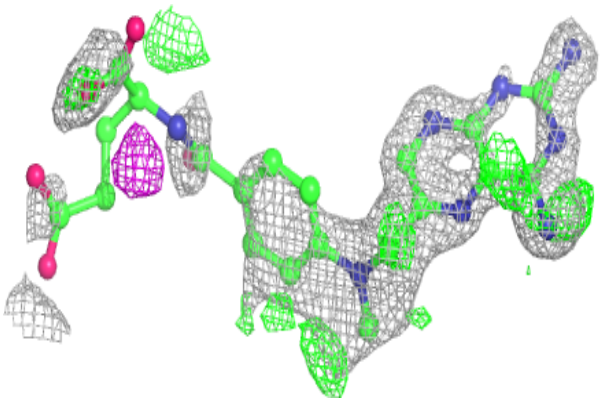
Continued from previous page...

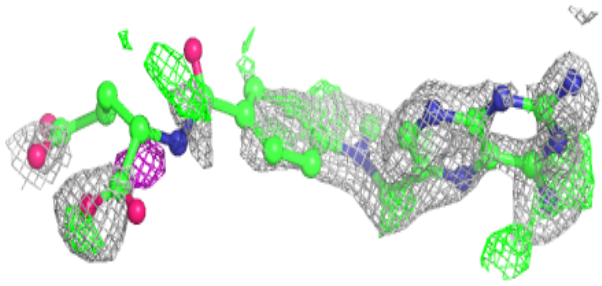
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	D	701	4/4	0.93	0.12	41,44,47,49	0
4	EDO	A	608	4/4	0.93	0.12	49,49,49,51	0
4	EDO	A	617	4/4	0.94	0.08	40,43,44,45	0
4	EDO	C	605	4/4	0.94	0.12	38,38,39,39	0
4	EDO	A	606	4/4	0.94	0.24	37,38,38,38	0
6	SER	D	702	7/7	0.94	0.13	38,39,41,43	0
4	EDO	A	610	4/4	0.95	0.10	39,43,46,48	0
4	EDO	B	2401	4/4	0.95	0.10	44,46,47,48	0
4	EDO	C	618	4/4	0.95	0.09	34,38,40,42	0
4	EDO	C	614	4/4	0.95	0.16	48,49,49,50	0
4	EDO	D	703	4/4	0.95	0.10	22,26,30,33	0
4	EDO	A	605	4/4	0.96	0.15	22,27,29,31	0
4	EDO	B	2405	4/4	0.96	0.21	22,27,32,36	0
4	EDO	D	705	4/4	0.96	0.10	34,37,38,40	0
4	EDO	A	604	4/4	0.96	0.08	23,26,31,34	0
4	EDO	C	609	4/4	0.97	0.13	37,37,37,38	0
3	PLS	B	2402	22/22	0.97	0.07	15,17,25,36	0
3	PLS	C	601	22/22	0.98	0.08	14,17,26,37	0
3	PLS	A	601	22/22	0.98	0.07	13,16,19,30	0

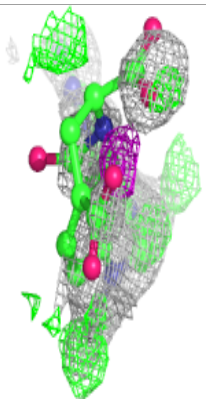
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTX C 603:

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

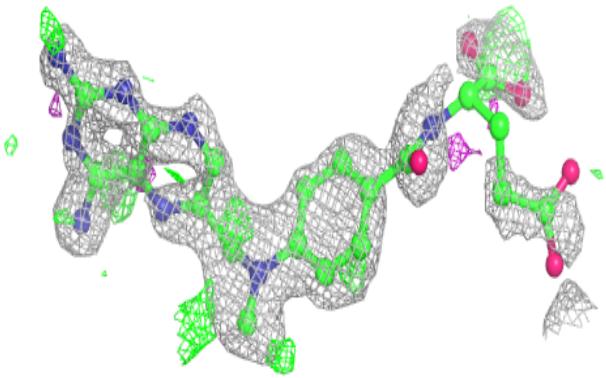


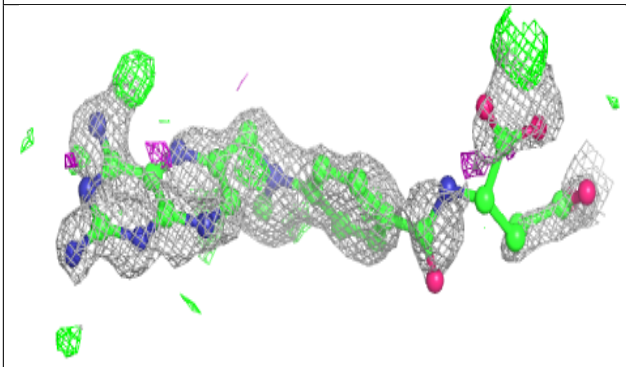


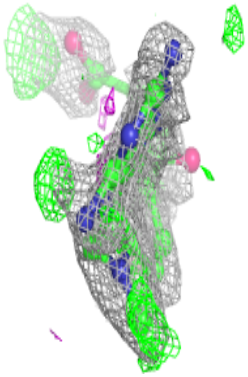


Electron density around MTX B 2404:

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

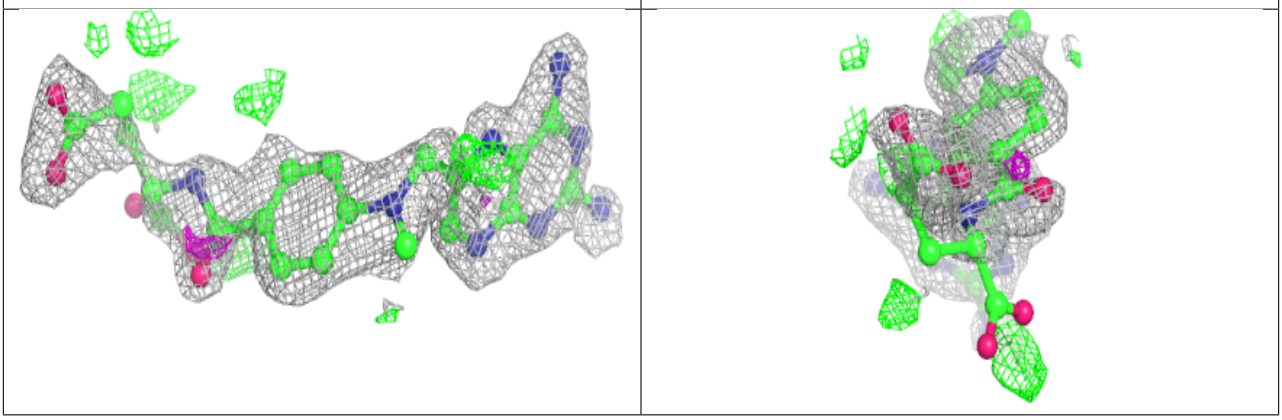






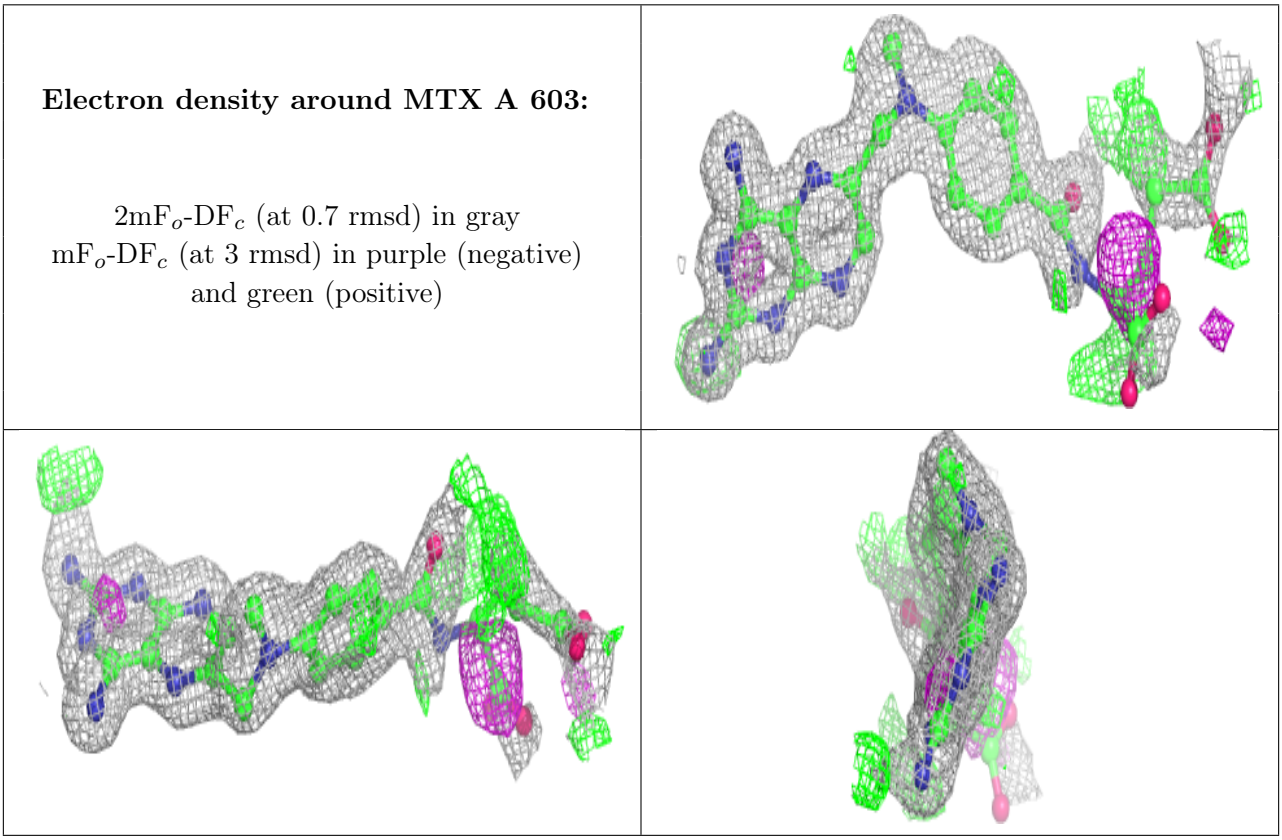
Electron density around MTX C 617:

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



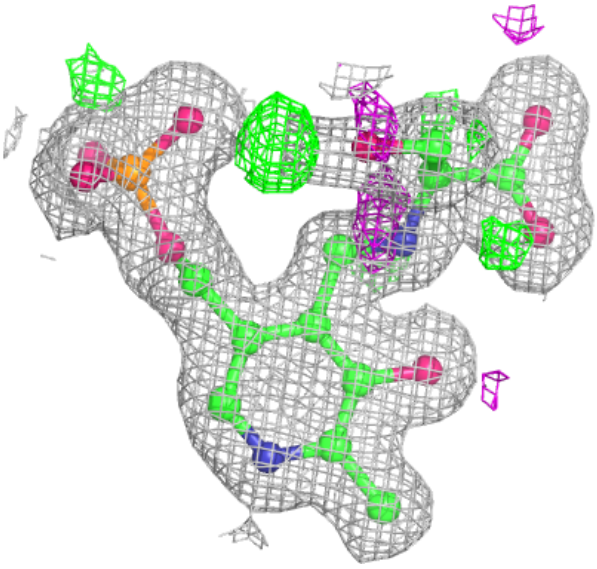
Electron density around MTX A 603:

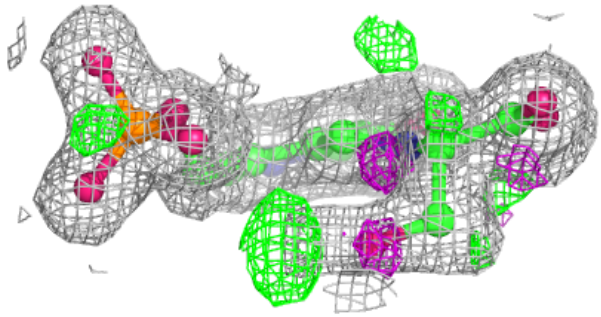
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

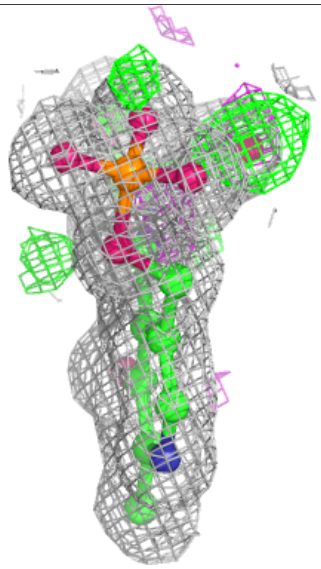


Electron density around PLS B 2402:

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

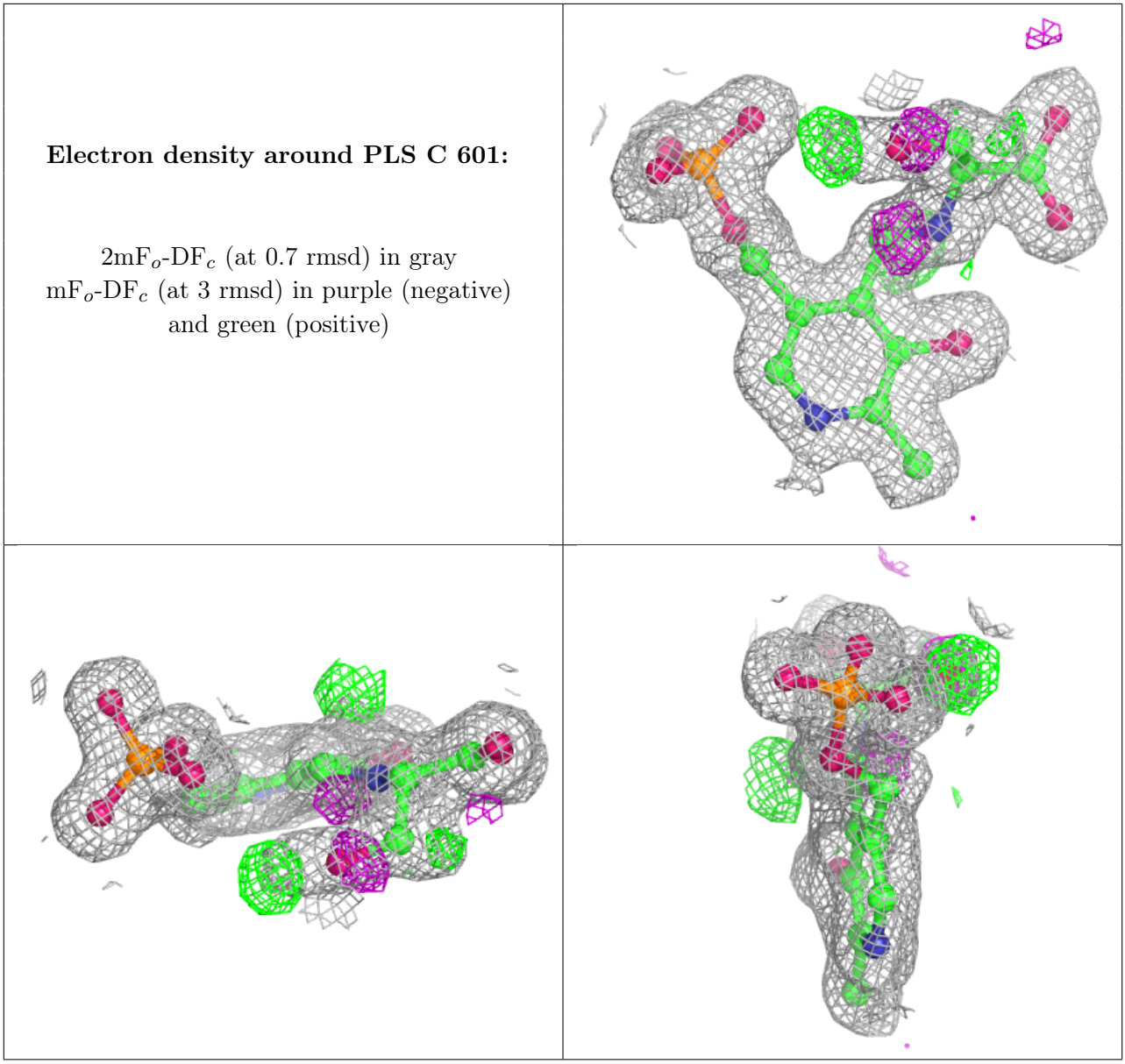






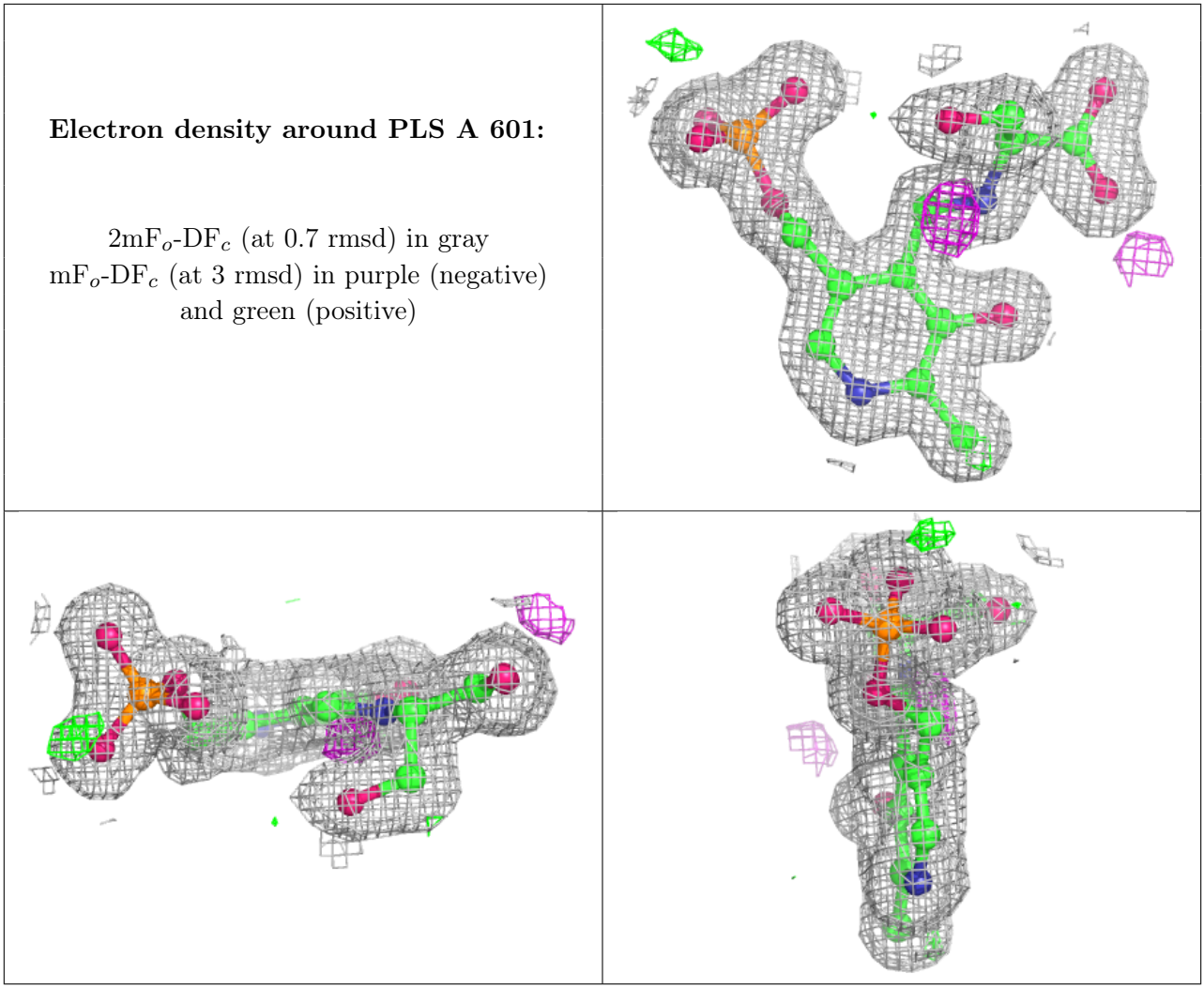
Electron density around PLS C 601:

$2mF_o$-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 601:

$2mF_o$-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.