Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:46 PM EDT

PDB ID	:	5J7W
Title	:	Enterococcus faecalis thymidylate synthase complex with methotrexate
Authors	:	Mangani, S.; Pozzi, C.
Deposited on	:	2016-04-07
Resolution	:	2.50 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 (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:

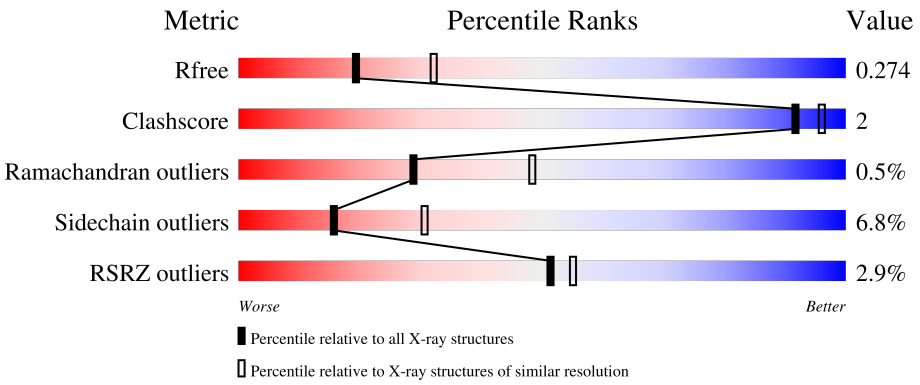
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	315	7%, 79%, 9%, •, 11%
1	B	315	3%, 77%, 9%, •, 13%
1	C	315	%, 91%, 8%, •
1	D	315	91%, 9%

2 Entry composition (i)

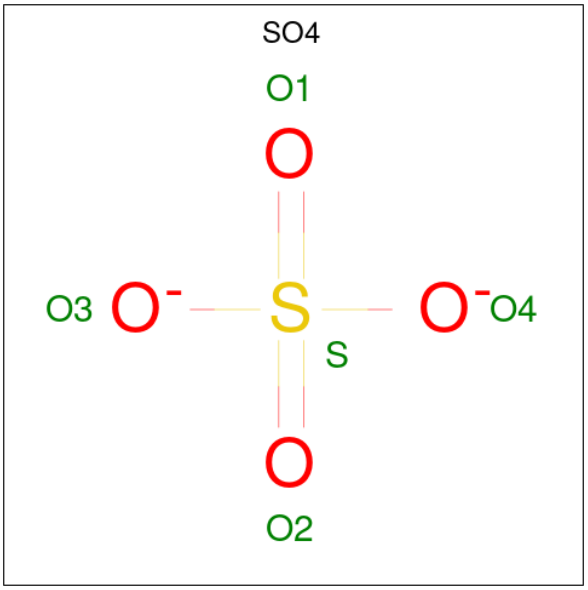
There are 4 unique types of molecules in this entry. The entry contains 9871 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	280	2262	1456	376	420	10	0	0	0
1	B	273	2207	1425	366	407	9	0	0	0
1	C	315	2569	1651	427	480	11	0	0	0
1	D	315	2569	1651	427	480	11	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0

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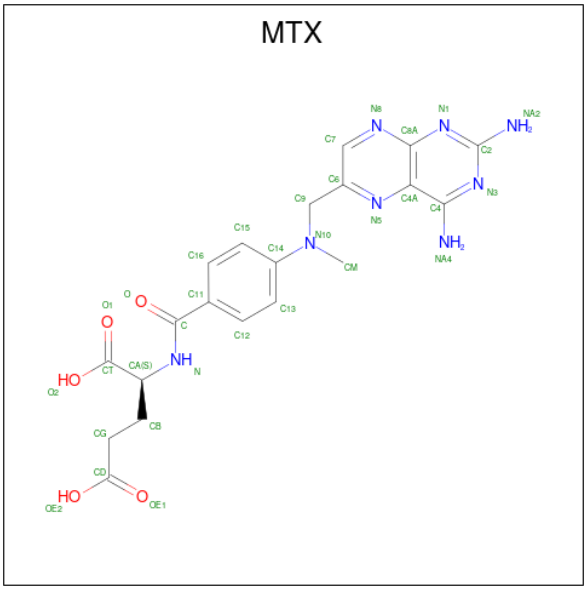
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
2	C	1	5	4	1		0	0
			Total	O	S			
2	D	1	5	4	1		0	0

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: $C_{20}H_{22}N_8O_5$).



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

- Molecule 4 is water.

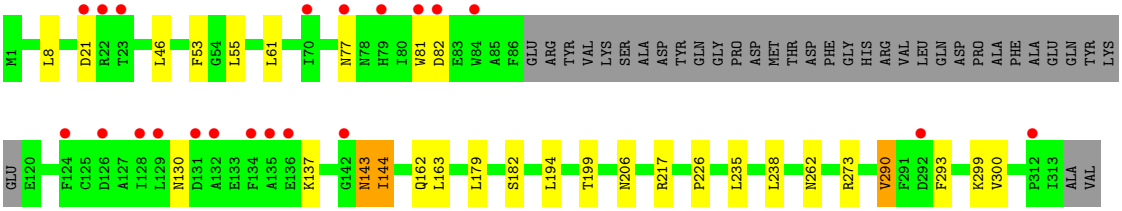
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	35	35	35	0	0
			Total	O		
4	B	42	42	42	0	0
			Total	O		
4	C	51	51	51	0	0
			Total	O		
4	D	50	50	50	0	0

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.

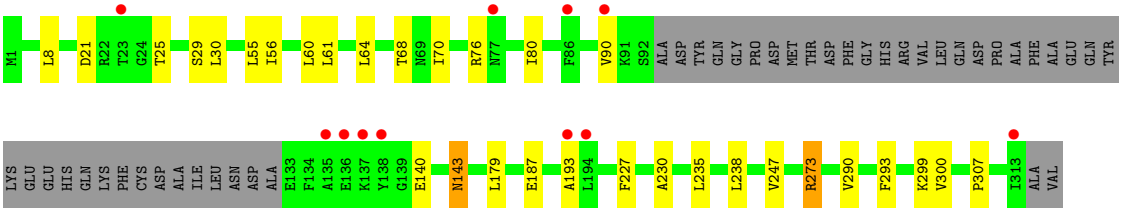
• Molecule 1: Thymidylate synthase

Chain A:



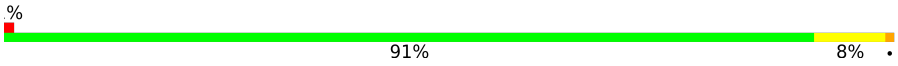
• Molecule 1: Thymidylate synthase

Chain B:



• Molecule 1: Thymidylate synthase

Chain C:



• Molecule 1: Thymidylate synthase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.23Å 94.14Å 96.29Å 90.00° 94.14° 90.00°	Depositor
Resolution (Å)	96.04 – 2.50 67.23 – 2.50	Depositor EDS
% Data completeness (in resolution range)	78.4 (96.04-2.50) 78.4 (67.23-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.47 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.200 , 0.273 0.204 , 0.274	Depositor DCC
R_{free} test set	1731 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	15.7	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 30.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9871	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.92% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MTX, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.60	0/2323	0.81	0/3150
1	B	0.61	0/2267	0.81	1/3073 (0.0%)
1	C	0.62	0/2641	0.81	2/3579 (0.1%)
1	D	0.66	0/2641	0.81	0/3579
All	All	0.62	0/9872	0.81	3/13381 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	217	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	217	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	76	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	2262	0	2169	9	0
1	B	2207	0	2128	5	0
1	C	2569	0	2463	8	0
1	D	2569	0	2463	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	C	33	0	20	0	0
3	D	33	0	20	2	0
4	A	35	0	0	2	0
4	B	42	0	0	0	0
4	C	51	0	0	1	0
4	D	50	0	0	2	0
All	All	9871	0	9263	30	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.

All (30) 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:D:77:ASN:HB3	4:D:550:HOH:O	1.87	0.73
1:D:22:ARG:HH12	1:D:315:VAL:HG21	1.58	0.68
1:B:56:ILE:HD13	1:B:230:ALA:HB3	1.79	0.63
1:C:78:ASN:OD1	1:C:80:ILE:HG12	2.00	0.61
1:C:265:GLU:OE2	1:D:265:GLU:OE2	2.20	0.59
1:A:290:VAL:HG12	4:A:534:HOH:O	2.01	0.59
1:A:130:ASN:ND2	4:A:501:HOH:O	2.38	0.56
1:B:187:GLU:HG3	1:C:154:THR:HG22	1.89	0.54
1:C:21:ASP:OD2	1:C:23:THR:OG1	2.15	0.52
3:D:402:MTX:H91	4:D:524:HOH:O	2.08	0.52
1:A:46:LEU:HD22	1:A:226:PRO:HB3	1.92	0.50
1:A:162:GLN:HE22	1:A:182:SER:H	1.59	0.50
1:D:78:ASN:OD1	1:D:80:ILE:HG12	2.13	0.49
1:D:56:ILE:HD13	1:D:230:ALA:HB3	1.95	0.48
1:B:68:THR:HG23	1:B:140:GLU:OE1	2.14	0.47
1:D:45:LEU:HD22	1:D:51:VAL:HB	1.96	0.47
1:B:290:VAL:O	1:B:293:PHE:HB2	2.16	0.46
1:A:162:GLN:NE2	1:A:182:SER:H	2.15	0.44
1:C:179:LEU:HB2	4:C:521:HOH:O	2.17	0.44
1:D:56:ILE:HD13	1:D:230:ALA:CB	2.48	0.44
1:B:273:ARG:NH2	1:B:307:PRO:O	2.50	0.43
1:D:46:LEU:HD22	1:D:226:PRO:HB3	2.00	0.43
1:C:214:LEU:HD22	1:C:232:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ASN:O	1:A:144:ILE:HG23	2.19	0.42
1:D:220:ASP:OD2	3:D:402:MTX:N3	2.52	0.42
1:C:145:TYR:OH	1:C:197:CYS:N	2.50	0.42
1:A:199:THR:HG21	1:A:217:ARG:HB3	2.01	0.41
1:C:39:LEU:HB2	1:C:247:VAL:HG13	2.03	0.41
1:A:290:VAL:HA	1:A:293:PHE:CD1	2.56	0.41
1:A:53:PHE:CD2	1:A:300:VAL:HG23	2.55	0.41

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	276/315 (88%)	256 (93%)	18 (6%)	2 (1%)	22	39
1	B	269/315 (85%)	253 (94%)	13 (5%)	3 (1%)	14	26
1	C	313/315 (99%)	297 (95%)	16 (5%)	0	100	100
1	D	313/315 (99%)	302 (96%)	10 (3%)	1 (0%)	41	61
All	All	1171/1260 (93%)	1108 (95%)	57 (5%)	6 (0%)	29	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	ILE
1	B	90	VAL
1	D	145	TYR
1	A	77	ASN
1	B	143	ASN
1	B	193	ALA

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	240/273 (88%)	222 (92%)	18 (8%)	13	26
1	B	234/273 (86%)	214 (92%)	20 (8%)	10	21
1	C	273/273 (100%)	257 (94%)	16 (6%)	19	37
1	D	273/273 (100%)	258 (94%)	15 (6%)	21	41
All	All	1020/1092 (93%)	951 (93%)	69 (7%)	16	30

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	21	ASP
1	A	55	LEU
1	A	61	LEU
1	A	81	TRP
1	A	82	ASP
1	A	137	LYS
1	A	143	ASN
1	A	163	LEU
1	A	179	LEU
1	A	194	LEU
1	A	206	ASN
1	A	235	LEU
1	A	238	LEU
1	A	262	ASN
1	A	273	ARG
1	A	290	VAL
1	A	299	LYS
1	B	8	LEU
1	B	21	ASP
1	B	25	THR
1	B	29	SER
1	B	30	LEU
1	B	55	LEU

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	61	LEU
1	B	64	LEU
1	B	70	ILE
1	B	80	ILE
1	B	143	ASN
1	B	179	LEU
1	B	227	PHE
1	B	235	LEU
1	B	238	LEU
1	B	247	VAL
1	B	273	ARG
1	B	299	LYS
1	B	300	VAL
1	C	1	MET
1	C	29	SER
1	C	60	LEU
1	C	61	LEU
1	C	122	GLN
1	C	129	LEU
1	C	162	GLN
1	C	163	LEU
1	C	173	ASN
1	C	179	LEU
1	C	231	SER
1	C	235	LEU
1	C	238	LEU
1	C	247	VAL
1	C	280	THR
1	C	301	GLU
1	D	45	LEU
1	D	60	LEU
1	D	61	LEU
1	D	65	LYS
1	D	101	THR
1	D	102	ASP
1	D	129	LEU
1	D	163	LEU
1	D	179	LEU
1	D	198	HIS
1	D	206	ASN
1	D	238	LEU

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Mol	Chain	Res	Type
1	D	247	VAL
1	D	299	LYS
1	D	300	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	143	ASN
1	A	148	GLN
1	A	162	GLN
1	A	258	HIS
1	A	270	GLN
1	C	121	HIS
1	C	173	ASN
1	C	228	ASN
1	C	268	GLN
1	C	270	GLN
1	D	121	HIS
1	D	151	HIS
1	D	228	ASN
1	D	258	HIS
1	D	261	GLN
1	D	268	GLN
1	D	270	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	MTX	C	402	-	35,35,35	2.23	7 (20%)	46,49,49	4.11	21 (45%)
2	SO4	B	401	-	4,4,4	0.29	0	6,6,6	0.32	0
2	SO4	C	401	-	4,4,4	0.51	0	6,6,6	0.37	0
2	SO4	A	401	-	4,4,4	0.28	0	6,6,6	0.32	0
3	MTX	D	402	-	35,35,35	2.09	6 (17%)	46,49,49	3.07	20 (43%)
2	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.37	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	MTX	C	402	-	-	8/25/25/25	0/3/3/3
3	MTX	D	402	-	-	6/25/25/25	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	MTX	O-C	8.65	1.40	1.23
3	C	402	MTX	O-C	8.51	1.40	1.23
3	D	402	MTX	C7-N8	5.06	1.40	1.31
3	C	402	MTX	C7-N8	5.02	1.39	1.31
3	C	402	MTX	C9-C6	-3.41	1.45	1.51
3	C	402	MTX	CA-N	2.77	1.51	1.45
3	D	402	MTX	C8A-N8	2.68	1.40	1.37
3	D	402	MTX	C9-C6	-2.60	1.47	1.51
3	C	402	MTX	C8A-N8	2.54	1.40	1.37
3	D	402	MTX	C4-N3	2.47	1.38	1.33
3	C	402	MTX	C14-N10	2.40	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	MTX	C9-N10	2.30	1.51	1.46
3	D	402	MTX	C14-N10	2.28	1.45	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	MTX	C6-C9-N10	-12.16	92.75	113.60
3	C	402	MTX	N8-C8A-N1	9.02	126.12	115.82
3	D	402	MTX	C6-C9-N10	-8.96	98.24	113.60
3	C	402	MTX	C9-C6-N5	-8.90	102.69	116.96
3	C	402	MTX	C4-C4A-N5	-8.86	113.50	120.33
3	C	402	MTX	C6-C7-N8	-8.85	114.45	123.13
3	D	402	MTX	C6-C7-N8	-6.54	116.72	123.13
3	D	402	MTX	N8-C8A-N1	6.43	123.16	115.82
3	C	402	MTX	CM-N10-C14	-6.28	108.73	119.57
3	D	402	MTX	C4-C4A-N5	-6.18	115.57	120.33
3	C	402	MTX	C9-C6-C7	5.97	132.02	121.60
3	C	402	MTX	C7-C6-N5	5.53	124.45	120.85
3	D	402	MTX	C4A-C4-N3	-5.39	117.47	121.01
3	C	402	MTX	C11-C-N	5.14	126.92	117.06
3	D	402	MTX	C9-C6-N5	-5.02	108.91	116.96
3	C	402	MTX	C7-N8-C8A	4.58	121.29	116.69
3	C	402	MTX	C4A-C8A-N1	-4.53	114.37	121.71
3	D	402	MTX	C7-C6-N5	4.26	123.63	120.85
3	C	402	MTX	C2-N1-C8A	4.16	120.11	115.36
3	C	402	MTX	O-C-N	-3.99	115.11	122.45
3	D	402	MTX	N1-C2-N3	-3.99	121.91	127.22
3	D	402	MTX	C15-C14-N10	-3.86	116.07	121.62
3	D	402	MTX	C2-N1-C8A	3.74	119.62	115.36
3	C	402	MTX	O2-CT-O1	-3.69	115.72	124.09
3	C	402	MTX	C4A-C4-N3	-3.66	118.61	121.01
3	D	402	MTX	CM-N10-C14	-3.50	113.53	119.57
3	C	402	MTX	N1-C2-N3	-3.44	122.63	127.22
3	D	402	MTX	O2-CT-O1	-3.43	116.31	124.09
3	D	402	MTX	C9-C6-C7	3.24	127.25	121.60
3	D	402	MTX	C4A-C8A-N1	-2.95	116.93	121.71
3	D	402	MTX	C7-N8-C8A	2.91	119.61	116.69
3	D	402	MTX	C13-C14-N10	2.90	125.78	121.62
3	D	402	MTX	OE2-CD-OE1	-2.89	116.11	123.30
3	C	402	MTX	NA2-C2-N1	2.84	122.42	117.79
3	C	402	MTX	CT-CA-N	2.53	116.54	110.55
3	D	402	MTX	O2-CT-CA	2.47	121.60	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	402	MTX	OE2-CD-CG	2.46	121.94	114.03
3	C	402	MTX	NA4-C4-N3	2.29	123.30	117.07
3	C	402	MTX	CG-CB-CA	2.22	117.31	113.16
3	D	402	MTX	NA4-C4-N3	2.11	122.80	117.07
3	C	402	MTX	O2-CT-CA	2.06	120.26	113.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	MTX	C15-C14-N10-CM
3	D	402	MTX	C13-C14-N10-CM
3	D	402	MTX	C15-C14-N10-CM
3	C	402	MTX	C13-C14-N10-CM
3	C	402	MTX	C13-C14-N10-C9
3	C	402	MTX	C15-C14-N10-C9
3	D	402	MTX	C13-C14-N10-C9
3	D	402	MTX	C15-C14-N10-C9
3	C	402	MTX	N-CA-CB-CG
3	C	402	MTX	OE1-CD-CG-CB
3	D	402	MTX	OE2-CD-CG-CB
3	C	402	MTX	OE2-CD-CG-CB
3	D	402	MTX	OE1-CD-CG-CB
3	C	402	MTX	CT-CA-CB-CG

There are no ring outliers.

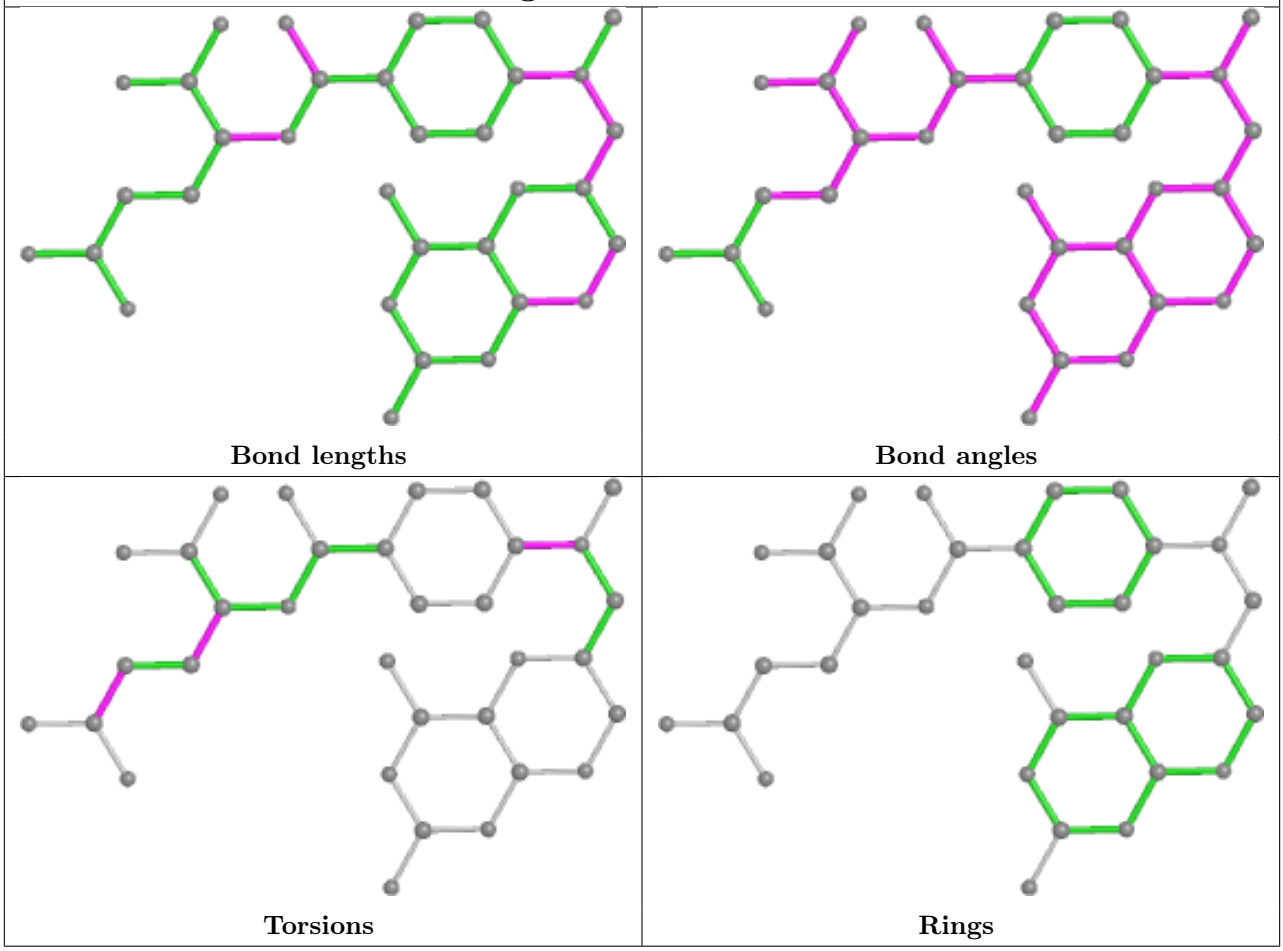
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	MTX	2	0

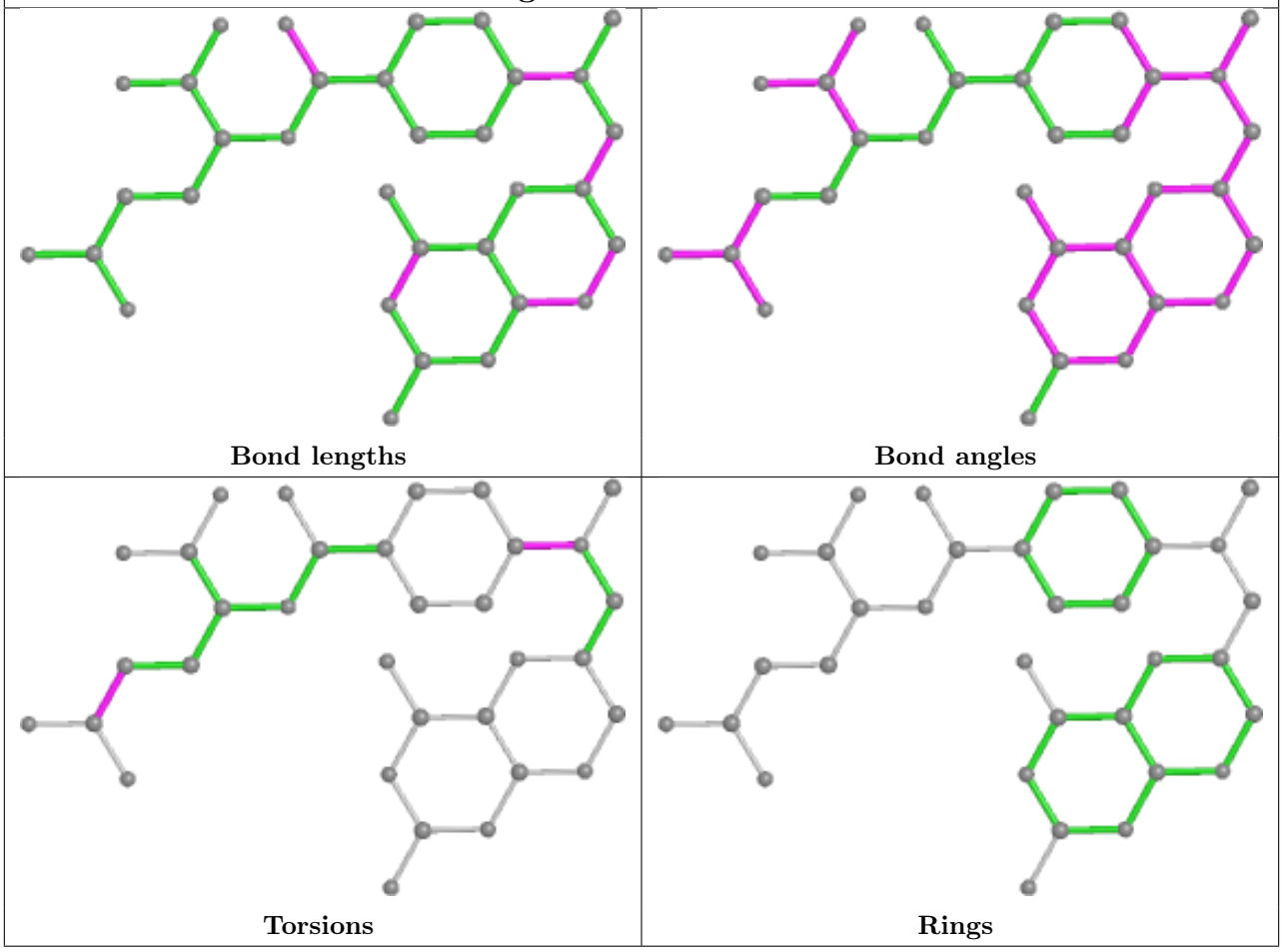
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 MTX C 402



Ligand MTX D 402



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	280/315 (88%)	0.34	21 (7%)	14	14	7, 18, 58, 67	0
1	B	273/315 (86%)	0.11	11 (4%)	38	41	6, 15, 42, 66	0
1	C	315/315 (100%)	-0.13	2 (0%)	89	90	5, 10, 28, 38	0
1	D	315/315 (100%)	-0.15	0	100	100	4, 11, 27, 41	0
All	All	1183/1260 (93%)	0.03	34 (2%)	51	55	4, 13, 41, 67	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	5.9
1	A	135	ALA	4.9
1	A	132	ALA	4.9
1	A	142	GLY	3.6
1	B	135	ALA	3.6
1	A	126	ASP	3.4
1	A	23	THR	3.4
1	B	86	PHE	3.2
1	B	194	LEU	3.0
1	A	134	PHE	2.9
1	A	22	ARG	2.9
1	A	84	TRP	2.8
1	B	77	ASN	2.8
1	A	82	ASP	2.8
1	A	136	GLU	2.7
1	A	128	ILE	2.7
1	B	138	TYR	2.6
1	C	112	ALA	2.5
1	A	124	PHE	2.5
1	B	90	VAL	2.4
1	B	23	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	136	GLU	2.4
1	A	131	ASP	2.4
1	B	313	ILE	2.3
1	A	70	ILE	2.3
1	A	79	HIS	2.2
1	A	81	TRP	2.2
1	A	77	ASN	2.2
1	A	292	ASP	2.1
1	A	21	ASP	2.1
1	C	97	GLY	2.1
1	A	312	PRO	2.1
1	B	193	ALA	2.0
1	B	137	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

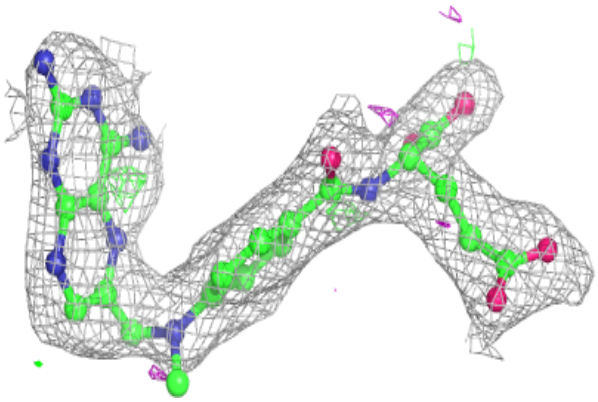
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

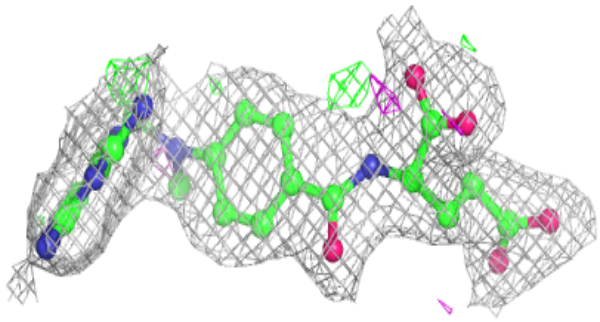
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MTX	D	402	33/33	0.86	0.18	15,21,33,33	0
3	MTX	C	402	33/33	0.90	0.20	11,12,13,14	0
2	SO4	A	401	5/5	0.93	0.24	4,4,4,4	5
2	SO4	B	401	5/5	0.93	0.28	12,12,12,12	5
2	SO4	C	401	5/5	0.98	0.16	12,12,12,12	0
2	SO4	D	401	5/5	0.98	0.13	12,12,12,12	0

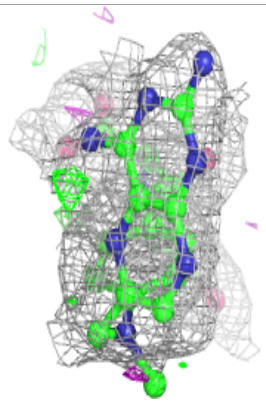
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MTX D 402:

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

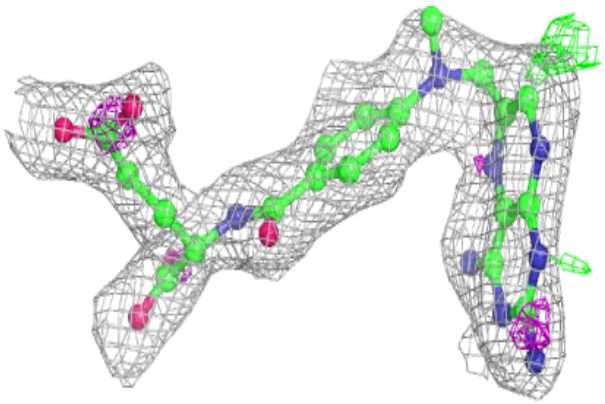


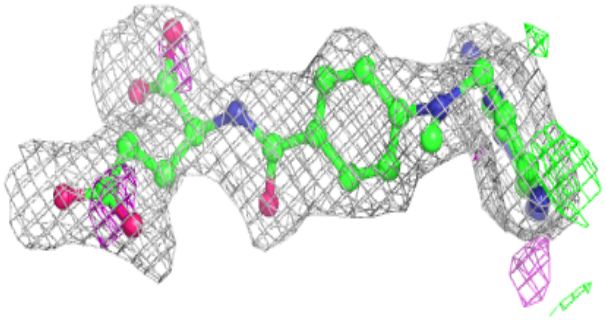


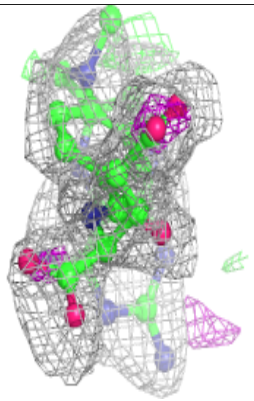


Electron density around MTX C 402:

$2mF_o$-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.