Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 11:43 PM EDT

PDB ID	:	1O07
Title	:	Crystal Structure of the complex between Q120L/Y150E mutant of AmpC and a beta-lactam inhibitor (MXG)
Authors	:	Meroueh, S.O.; Minasov, G.; Lee, W.; Shoichet, B.K.; Mobashery, S.
Deposited on	:	2003-02-20
Resolution	:	1.71 Å(reported)

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

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

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

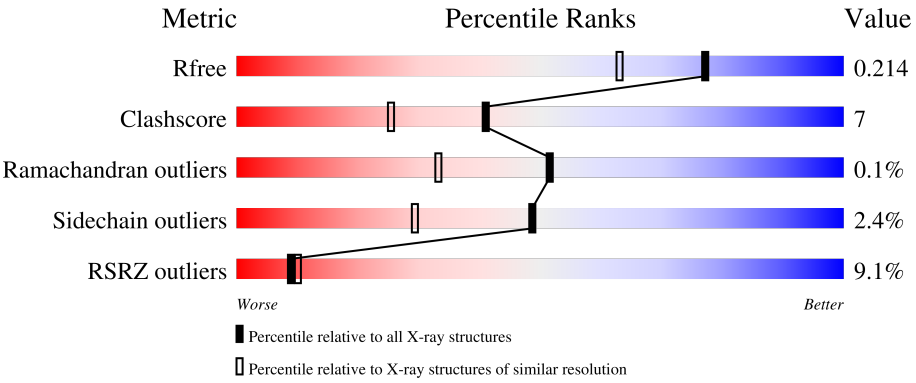
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.71 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	5722 (1.74-1.70)
Clashscore	141614	6152 (1.74-1.70)
Ramachandran outliers	138981	6051 (1.74-1.70)
Sidechain outliers	138945	6051 (1.74-1.70)
RSRZ outliers	127900	5629 (1.74-1.70)

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	358	11% 86% 12%
1	B	358	8% 86% 13%

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
3	MXG	A	400[B]	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7358 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 Beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	45	0
			3152	2014	543	588	7			
1	B	358	Total	C	N	O	S	0	48	0
			3196	2041	555	593	7			

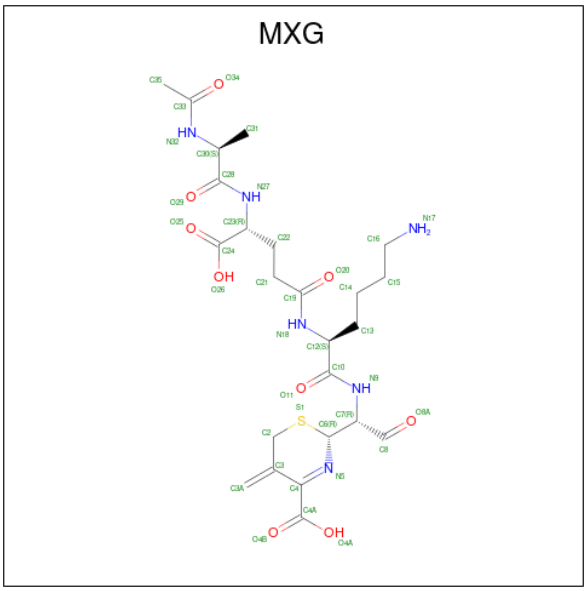
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	LEU	GLN	engineered mutation	UNP P00811
A	150	GLU	TYR	engineered mutation	UNP P00811
B	120	LEU	GLN	engineered mutation	UNP P00811
B	150	GLU	TYR	engineered mutation	UNP P00811

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is 2-(1-{2-[4-(2-ACETYLAMINO-PROPIONYLAMINO)-4-CARBOXY-BUTYRYLAMINO]-6-AMINO-HEXANOYLAMINO}-2-OXO-ETHYL)-5-METHYLENE-5,6-DIHYDRO-2H-[1,3]THIAZINE-4-CARBOXYLIC ACID (three-letter code: MXG) (formula: $C_{24}H_{36}N_6O_9S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 40 24 6 9 1	0	1
3	B	1	Total C N O S 80 48 12 18 2	0	1

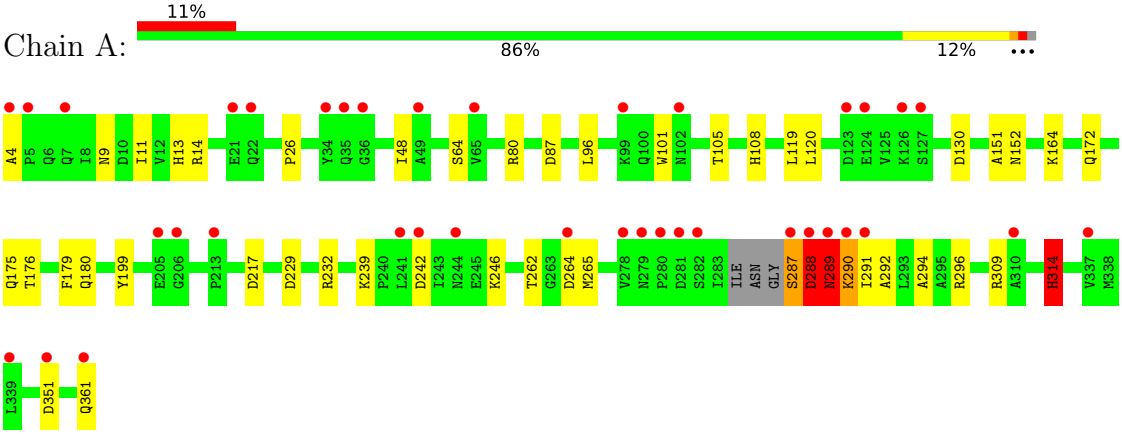
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	398	Total O 436 436	0	62
4	B	408	Total O 452 452	0	68

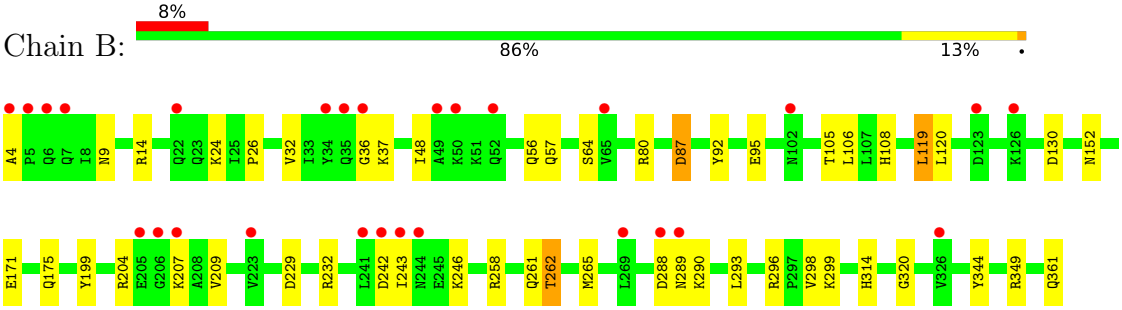
3 Residue-property plots (i)

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: Beta-lactamase



• Molecule 1: Beta-lactamase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	118.81Å 76.30Å 98.13Å 90.00° 116.21° 90.00°	Depositor
Resolution (Å)	24.77 – 1.71 24.74 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.1 (24.77-1.71) 94.9 (24.74-1.71)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.82 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.154 , 0.191 0.188 , 0.214	Depositor DCC
R_{free} test set	4052 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	18.5	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7358	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.41% 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: MXG, K

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	0.81	1/3235 (0.0%)	1.07	24/4405 (0.5%)
1	B	0.76	0/3277	0.99	16/4461 (0.4%)
All	All	0.79	1/6512 (0.0%)	1.03	40/8866 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	SER	C-N	10.61	1.58	1.34

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	SER	CA-C-N	-7.42	100.87	117.20
1	B	242	ASP	CB-CG-OD2	7.29	124.86	118.30
1	B	229	ASP	CB-CG-OD2	7.19	124.77	118.30
1	B	130	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	232[A]	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	232[B]	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	232[A]	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	A	232[B]	ARG	NE-CZ-NH1	-6.84	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	288	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	351	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	242	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	229	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	217	ASP	O-C-N	-5.99	113.11	122.70
1	B	87	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	179	PHE	CB-CG-CD1	5.83	124.88	120.80
1	A	13	HIS	O-C-N	-5.79	113.44	122.70
1	B	232[A]	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	B	232[B]	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	A	264	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	36	GLY	O-C-N	-5.60	113.74	122.70
1	B	204	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	258	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	258	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	130	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	296	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	B	296[A]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	296[B]	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	80	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	80	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	288[A]	ASP	O-C-N	-5.19	114.39	122.70
1	A	288[B]	ASP	O-C-N	-5.19	114.39	122.70
1	A	87	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	80	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	199	TYR	CB-CG-CD2	5.09	124.06	121.00
1	A	289	ASN	O-C-N	5.08	130.83	122.70
1	B	80	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	292	ALA	O-C-N	-5.05	114.61	122.70
1	A	288[A]	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	288[B]	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	199	TYR	CB-CG-CD2	5.02	124.01	121.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	SER	Mainchain
1	A	288[A]	ASP	Peptide
1	A	288[B]	ASP	Peptide
1	A	314	HIS	Mainchain
1	B	32	VAL	Mainchain

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	3152	0	3105	22	0
1	B	3196	0	3161	67	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	40	0	33	4	0
3	B	80	0	64	28	0
4	A	436	0	0	4	0
4	B	452	0	0	11	0
All	All	7358	0	6363	92	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 7.

All (92) 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:B:209[B]:VAL:HG11	3:B:400[B]:MXG:C35	1.49	1.39
1:B:209[B]:VAL:CG1	3:B:400[B]:MXG:H352	1.68	1.22
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:HC22	1.19	1.17
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:C2	1.81	1.10
1:B:289[B]:ASN:HB3	1:B:293[B]:LEU:HD23	1.37	1.03
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:HC21	1.49	0.93
1:B:119[B]:LEU:HD22	1:B:120[B]:LEU:CD1	2.05	0.87
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:HC22	2.05	0.86
1:B:14[B]:ARG:HD3	4:B:800[B]:HOH:O	1.76	0.84
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:C2	2.07	0.84
1:A:119[B]:LEU:HD21	3:A:400[B]:MXG:S1	2.18	0.84
1:B:293[B]:LEU:HB3	3:B:400[B]:MXG:HC32	1.63	0.81
1:B:289[B]:ASN:HB3	1:B:293[B]:LEU:CD2	2.11	0.79
3:B:400[B]:MXG:H151	4:B:807[B]:HOH:O	1.83	0.79
1:B:209[B]:VAL:HG11	3:B:400[B]:MXG:H352	0.81	0.78
1:A:4[B]:ALA:HB1	1:A:9[B]:ASN:HD21	1.52	0.75
1:B:119[B]:LEU:HD22	1:B:120[B]:LEU:HD12	1.68	0.74
1:B:57[B]:GLN:HB3	4:B:783:HOH:O	1.87	0.74
1:B:209[B]:VAL:CG1	3:B:400[B]:MXG:C35	2.46	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293[A]:LEU:CD1	3:B:400[A]:MXG:HC21	2.19	0.72
1:A:180[A]:GLN:NE2	4:A:583[A]:HOH:O	2.24	0.71
1:B:290[A]:LYS:NZ	4:B:789:HOH:O	2.24	0.71
1:B:289[B]:ASN:O	1:B:293[B]:LEU:HG	1.94	0.68
1:A:119[B]:LEU:CD2	3:A:400[B]:MXG:S1	2.82	0.68
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:C2	2.66	0.67
1:B:289[B]:ASN:CB	1:B:293[B]:LEU:HD23	2.20	0.66
1:B:37[B]:LYS:NZ	4:B:699[B]:HOH:O	2.29	0.66
1:B:64[A]:SER:N	3:B:400[A]:MXG:O8A	2.29	0.66
1:A:4[B]:ALA:HB1	1:A:9[B]:ASN:ND2	2.11	0.66
1:A:11[B]:ILE:HD11	4:A:761[B]:HOH:O	1.96	0.64
1:A:289:ASN:O	1:A:290:LYS:HG2	1.97	0.64
1:B:262[A]:THR:HG23	1:B:265[A]:MET:SD	2.38	0.63
1:A:4[B]:ALA:CB	1:A:9[B]:ASN:HD21	2.12	0.63
1:A:262[A]:THR:O	1:A:265[A]:MET:HG3	2.02	0.60
1:A:175[A]:GLN:O	1:A:180[A]:GLN:HG2	2.02	0.59
1:B:207[B]:LYS:O	1:B:209[B]:VAL:HG23	2.02	0.59
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:HE2	2.22	0.59
1:B:119[B]:LEU:HD23	3:B:400[B]:MXG:S1	2.43	0.58
1:A:11[B]:ILE:HG12	1:A:14[B]:ARG:NH1	2.19	0.57
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C3	2.34	0.57
1:A:119[B]:LEU:O	1:A:152[B]:ASN:HB2	2.05	0.57
1:B:119[B]:LEU:CD2	3:B:400[B]:MXG:S1	2.93	0.57
1:B:293[B]:LEU:HB3	3:B:400[B]:MXG:C3A	2.33	0.57
3:A:400[B]:MXG:H142	4:A:797[B]:HOH:O	2.04	0.56
1:A:314:HIS:CD2	1:A:314:HIS:C	2.78	0.56
1:B:262[A]:THR:CG2	1:B:265[A]:MET:SD	2.93	0.56
1:B:57[B]:GLN:CB	4:B:783:HOH:O	2.49	0.56
1:B:261[B]:GLN:OE1	1:B:299[B]:LYS:HE2	2.07	0.54
1:B:119[B]:LEU:CD2	1:B:120[B]:LEU:HD12	2.37	0.53
1:A:291:ILE:HG21	1:A:294:ALA:HB2	1.91	0.53
1:B:289[B]:ASN:O	1:B:293[B]:LEU:CG	2.56	0.53
1:B:289[B]:ASN:O	1:B:293[B]:LEU:CD2	2.57	0.52
1:B:293[A]:LEU:CD1	3:B:400[A]:MXG:C2	2.84	0.51
1:B:293[A]:LEU:HD21	3:B:400[A]:MXG:HC21	1.87	0.50
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:CE	2.80	0.49
1:B:14[B]:ARG:CD	4:B:800[B]:HOH:O	2.45	0.49
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C4	2.42	0.49
1:B:293[A]:LEU:HD11	3:B:400[A]:MXG:C3	2.42	0.49
1:B:289[B]:ASN:O	1:B:293[B]:LEU:HD23	2.12	0.49
3:B:400[A]:MXG:H353	4:B:806[A]:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:400[B]:MXG:H312	3:A:400[B]:MXG:H23	1.95	0.48
1:B:207[B]:LYS:HG2	1:B:209[B]:VAL:HG22	1.95	0.48
1:B:92:TYR:CE2	1:B:106:LEU:HD11	2.48	0.47
1:A:172[A]:GLN:HE21	1:A:176:THR:HG23	1.79	0.47
1:B:171[A]:GLU:HG2	1:B:175[A]:GLN:NE2	2.30	0.46
1:B:243[B]:ILE:HD11	4:B:756:HOH:O	2.15	0.46
1:B:105:THR:H	1:B:108:HIS:HD2	1.62	0.46
1:B:56[B]:GLN:HG2	1:B:57[B]:GLN:HG3	1.98	0.46
1:A:120:LEU:CD2	1:A:152[B]:ASN:HD22	2.30	0.45
1:A:26:PRO:HB3	1:A:48:ILE:HD11	1.97	0.45
1:B:87:ASP:OD2	1:B:92:TYR:OH	2.32	0.45
1:B:57[B]:GLN:CG	4:B:783:HOH:O	2.64	0.45
1:B:243[B]:ILE:CD1	4:B:756:HOH:O	2.64	0.45
1:B:262[B]:THR:HG22	1:B:298:VAL:HG12	1.99	0.45
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:S1	2.58	0.44
1:B:4:ALA:HB3	1:B:9:ASN:ND2	2.33	0.44
1:B:171[A]:GLU:O	1:B:175[A]:GLN:HG3	2.17	0.44
1:B:293[A]:LEU:CD2	3:B:400[A]:MXG:HC21	2.46	0.44
1:B:289[B]:ASN:C	1:B:293[B]:LEU:HD23	2.37	0.43
1:A:309[B]:ARG:HD3	1:B:246[B]:LYS:NZ	2.34	0.43
1:B:262[B]:THR:CG2	1:B:298:VAL:HG12	2.49	0.43
1:B:152[B]:ASN:ND2	3:B:400[B]:MXG:O11	2.42	0.42
1:A:119[A]:LEU:HA	1:A:151:ALA:HA	2.02	0.42
1:B:26:PRO:HB3	1:B:48:ILE:HD11	2.01	0.42
1:B:320:GLY:HA3	3:B:400[B]:MXG:H32	1.86	0.41
1:A:4[B]:ALA:HB2	4:A:589:HOH:O	2.19	0.41
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.55	0.41
1:B:261[B]:GLN:CD	1:B:299[B]:LYS:NZ	2.74	0.41
1:A:105:THR:H	1:A:108:HIS:HD2	1.68	0.41
1:B:119[B]:LEU:HD21	3:B:400[B]:MXG:C2	2.51	0.40
1:B:261[B]:GLN:OE1	1:B:299[B]:LYS:CE	2.68	0.40
1:A:96[A]:LEU:HD21	1:A:101:TRP:CD2	2.57	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	395/358 (110%)	381 (96%)	14 (4%)	0	100 100
1	B	404/358 (113%)	396 (98%)	6 (2%)	2 (0%)	29 13
All	All	799/716 (112%)	777 (97%)	20 (2%)	2 (0%)	51 24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	119[A]	LEU
1	B	119[B]	LEU

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	334/292 (114%)	321 (96%)	13 (4%)	32 12
1	B	339/292 (116%)	332 (98%)	7 (2%)	53 35
All	All	673/584 (115%)	653 (97%)	20 (3%)	49 21

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64[A]	SER
1	A	64[B]	SER
1	A	164[A]	LYS
1	A	164[B]	LYS
1	A	239	LYS
1	A	246[A]	LYS
1	A	246[B]	LYS
1	A	288[A]	ASP
1	A	288[B]	ASP
1	A	289	ASN

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Mol	Chain	Res	Type
1	A	290	LYS
1	A	314	HIS
1	A	361	GLN
1	B	24	LYS
1	B	95[A]	GLU
1	B	95[B]	GLU
1	B	262[A]	THR
1	B	262[B]	THR
1	B	314	HIS
1	B	361	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	102	ASN
1	A	108	HIS
1	A	137	ASN
1	A	249	GLN
1	A	361	GLN
1	B	9	ASN
1	B	108	HIS
1	B	137	ASN
1	B	172	GLN
1	B	249	GLN
1	B	253	GLN
1	B	358	ASN
1	B	361	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)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MXG	B	400[A]	-	30,40,40	1.07	3 (10%)	32,53,53	3.46	13 (40%)
3	MXG	B	400[B]	-	30,40,40	1.13	3 (10%)	32,53,53	2.90	10 (31%)
3	MXG	A	400[B]	-	30,40,40	0.77	2 (6%)	32,53,53	2.02	7 (21%)

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	MXG	B	400[A]	-	-	16/34/61/61	0/0/1/1
3	MXG	B	400[B]	-	-	15/34/61/61	0/0/1/1
3	MXG	A	400[B]	-	-	18/34/61/61	0/0/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	400[A]	MXG	C4A-C4	-3.59	1.46	1.52
3	B	400[B]	MXG	C4A-C4	-3.25	1.47	1.52
3	A	400[B]	MXG	C4A-C4	-3.03	1.47	1.52
3	B	400[A]	MXG	C2-S1	-2.46	1.76	1.82
3	B	400[A]	MXG	C22-C23	2.41	1.56	1.53
3	B	400[B]	MXG	C4-N5	-2.22	1.26	1.28
3	B	400[B]	MXG	C2-S1	-2.15	1.77	1.82
3	A	400[B]	MXG	C2-S1	-2.14	1.77	1.82

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400[A]	MXG	C23-N27-C28	12.09	141.32	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	400[B]	MXG	C23-N27-C28	9.46	137.37	123.19
3	B	400[B]	MXG	C7-N9-C10	7.72	131.55	123.12
3	A	400[B]	MXG	C22-C23-N27	-6.46	100.80	110.19
3	B	400[A]	MXG	C7-N9-C10	6.33	130.03	123.12
3	B	400[A]	MXG	C12-N18-C19	6.31	137.87	121.65
3	B	400[A]	MXG	C13-C12-N18	-5.56	99.64	110.88
3	A	400[B]	MXG	C23-N27-C28	4.90	130.53	123.19
3	B	400[B]	MXG	C22-C23-N27	-4.83	103.16	110.19
3	B	400[B]	MXG	C30-C28-N27	4.59	127.44	116.75
3	B	400[A]	MXG	C30-C28-N27	4.54	127.33	116.75
3	B	400[A]	MXG	C22-C23-N27	-4.24	104.02	110.19
3	A	400[B]	MXG	C7-N9-C10	3.97	127.45	123.12
3	B	400[A]	MXG	C2-S1-C6	3.94	102.19	94.47
3	B	400[A]	MXG	C21-C19-N18	-3.89	109.08	115.83
3	B	400[A]	MXG	C10-C12-N18	3.46	120.56	111.16
3	B	400[A]	MXG	O29-C28-N27	-3.41	116.61	122.93
3	B	400[B]	MXG	C12-N18-C19	3.36	130.29	121.65
3	B	400[B]	MXG	C21-C22-C23	3.34	121.69	113.41
3	A	400[B]	MXG	C30-C28-N27	3.17	124.12	116.75
3	B	400[B]	MXG	O20-C19-C21	-3.12	116.31	122.02
3	B	400[B]	MXG	O29-C28-C30	-2.85	114.20	120.52
3	B	400[A]	MXG	C13-C12-C10	2.82	116.78	110.20
3	A	400[B]	MXG	C12-N18-C19	2.59	128.30	121.65
3	B	400[A]	MXG	O20-C19-N18	2.56	127.27	122.95
3	A	400[B]	MXG	C31-C30-C28	2.50	114.89	110.14
3	B	400[B]	MXG	O29-C28-N27	-2.47	118.35	122.93
3	A	400[B]	MXG	O20-C19-C21	-2.37	117.69	122.02
3	B	400[B]	MXG	C30-N32-C33	2.13	124.75	121.54
3	B	400[A]	MXG	O29-C28-C30	-2.02	116.04	120.52

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	400[A]	MXG	C24-C23-N27-C28
3	B	400[A]	MXG	C10-C12-N18-C19
3	B	400[A]	MXG	C8-C7-N9-C10
3	A	400[B]	MXG	N18-C12-C13-C14
3	B	400[A]	MXG	O11-C10-C12-C13
3	B	400[A]	MXG	N9-C10-C12-C13
3	A	400[B]	MXG	C10-C12-C13-C14
3	B	400[B]	MXG	O11-C10-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	400[B]	MXG	O29-C28-N27-C23
3	B	400[A]	MXG	O29-C28-N27-C23
3	B	400[B]	MXG	O29-C28-N27-C23
3	B	400[A]	MXG	C12-C13-C14-C15
3	B	400[B]	MXG	C30-C28-N27-C23
3	B	400[B]	MXG	N9-C10-C12-C13
3	A	400[B]	MXG	C30-C28-N27-C23
3	B	400[A]	MXG	C30-C28-N27-C23
3	B	400[A]	MXG	C19-C21-C22-C23
3	B	400[B]	MXG	N27-C28-C30-C31
3	B	400[B]	MXG	O29-C28-C30-C31
3	A	400[B]	MXG	O20-C19-C21-C22
3	B	400[B]	MXG	N27-C28-C30-N32
3	B	400[B]	MXG	O29-C28-C30-N32
3	A	400[B]	MXG	O29-C28-C30-C31
3	A	400[B]	MXG	N18-C19-C21-C22
3	A	400[B]	MXG	C14-C15-C16-N17
3	B	400[A]	MXG	O20-C19-C21-C22
3	B	400[B]	MXG	C13-C12-N18-C19
3	A	400[B]	MXG	O29-C28-C30-N32
3	A	400[B]	MXG	N27-C28-C30-N32
3	B	400[A]	MXG	N18-C19-C21-C22
3	B	400[A]	MXG	O29-C28-C30-N32
3	B	400[B]	MXG	O20-C19-C21-C22
3	A	400[B]	MXG	O11-C10-C12-N18
3	A	400[B]	MXG	C13-C12-N18-C19
3	B	400[A]	MXG	N27-C28-C30-N32
3	A	400[B]	MXG	C13-C14-C15-C16
3	A	400[B]	MXG	O11-C10-C12-C13
3	A	400[B]	MXG	N27-C28-C30-C31
3	B	400[B]	MXG	N18-C19-C21-C22
3	B	400[B]	MXG	C12-C13-C14-C15
3	A	400[B]	MXG	N9-C10-C12-N18
3	B	400[B]	MXG	N9-C10-C12-N18
3	B	400[B]	MXG	O11-C10-C12-N18
3	B	400[A]	MXG	C21-C22-C23-N27
3	A	400[B]	MXG	C28-C30-N32-C33
3	B	400[A]	MXG	O29-C28-C30-C31
3	B	400[B]	MXG	C14-C15-C16-N17
3	B	400[A]	MXG	C28-C30-N32-C33
3	A	400[B]	MXG	N9-C10-C12-C13

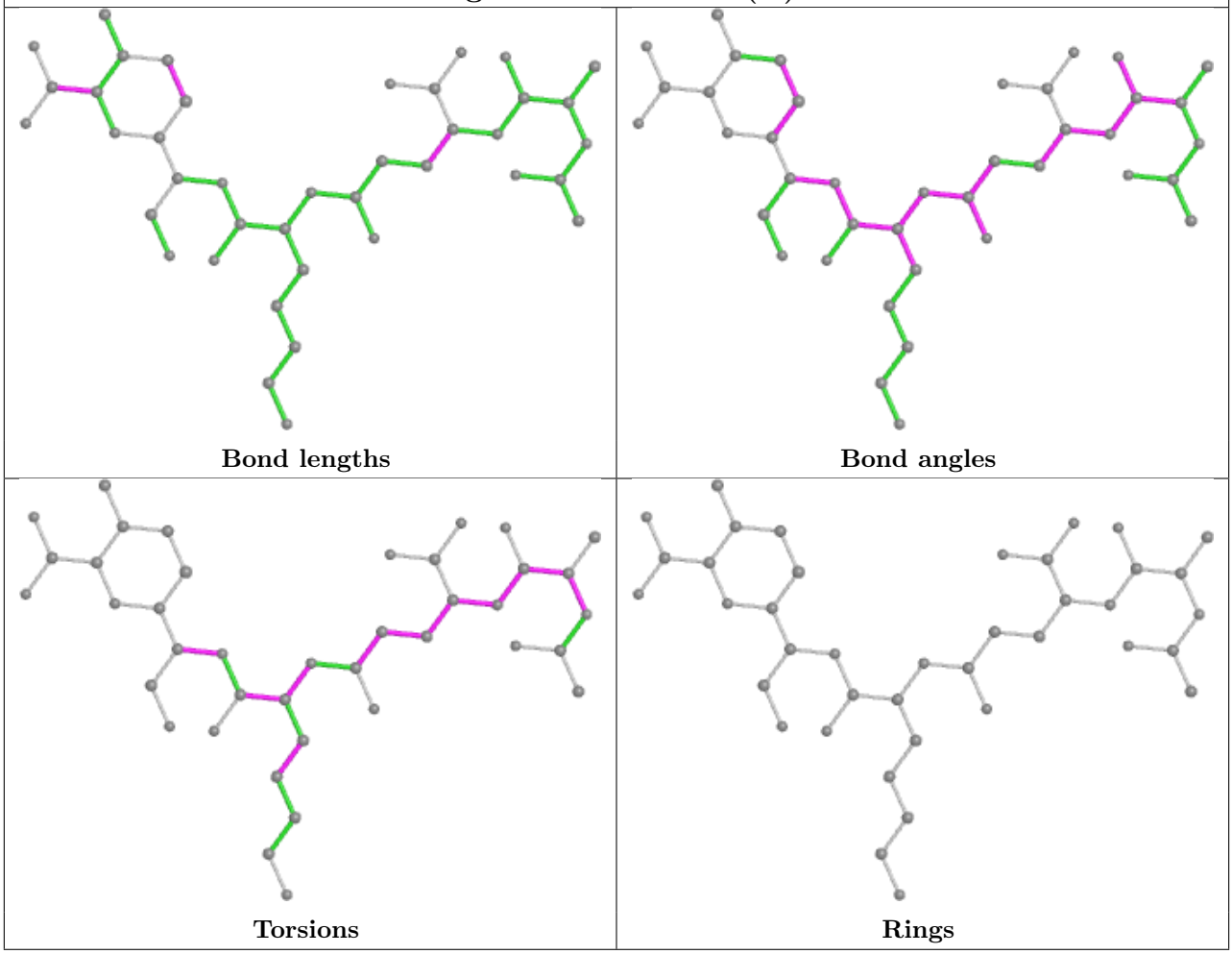
There are no ring outliers.

3 monomers are involved in 32 short contacts:

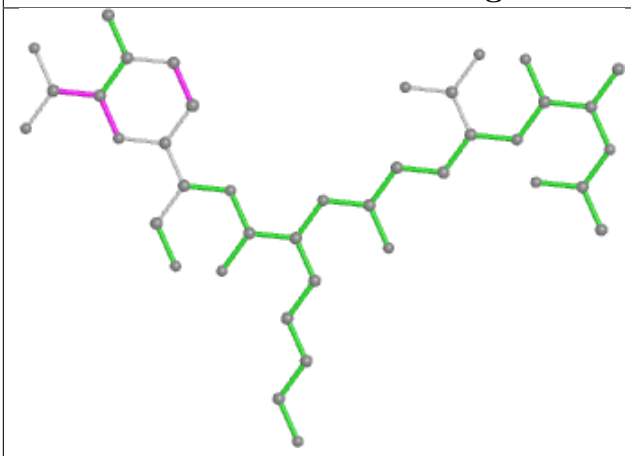
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	400[A]	MXG	13	0
3	B	400[B]	MXG	15	0
3	A	400[B]	MXG	4	0

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.

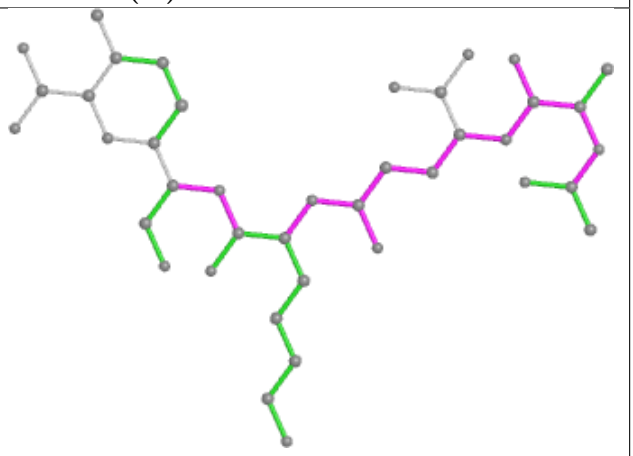
Ligand MXG B 400 (A)



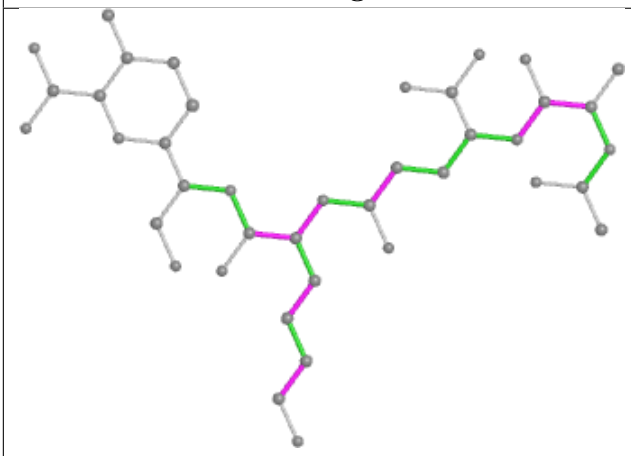
Ligand MXG B 400 (B)



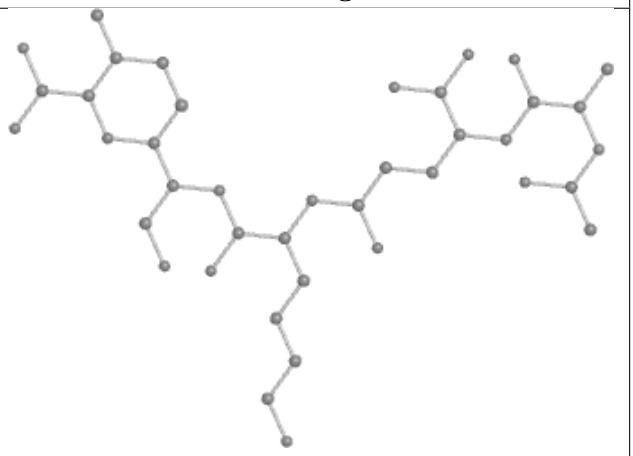
Bond lengths



Bond angles

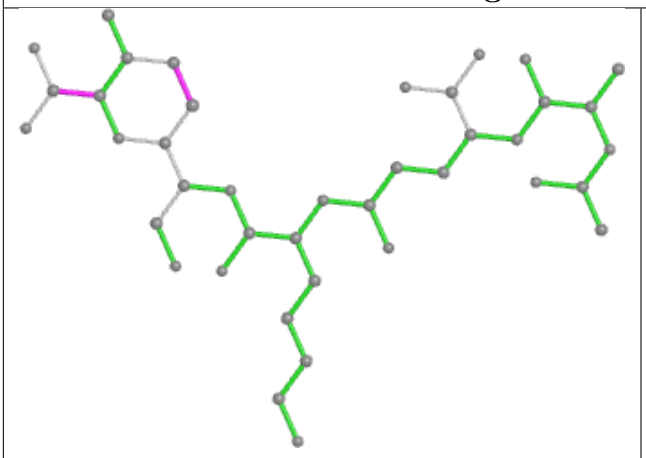


Torsions

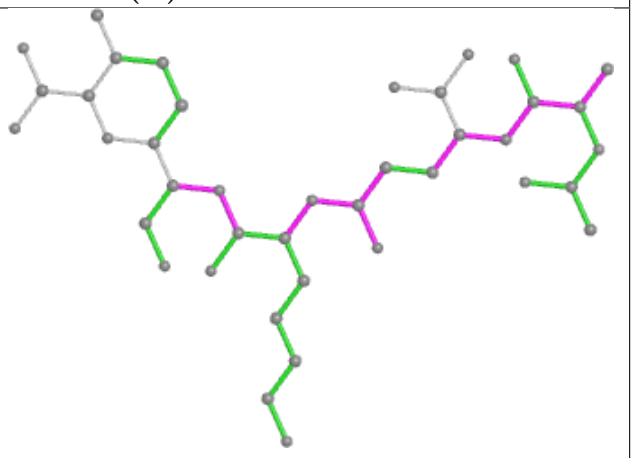


Rings

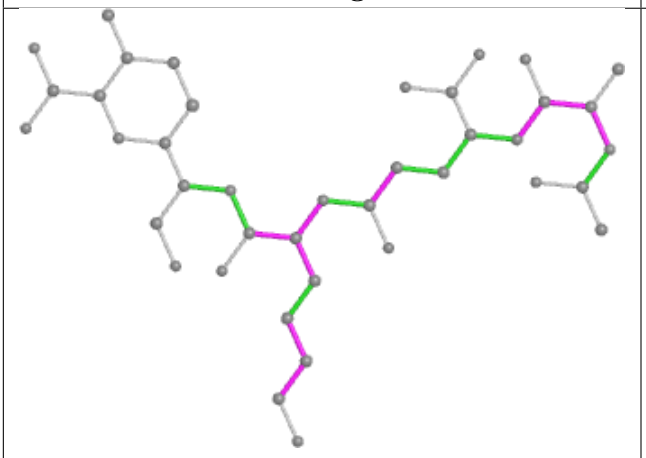
Ligand MXG A 400 (B)



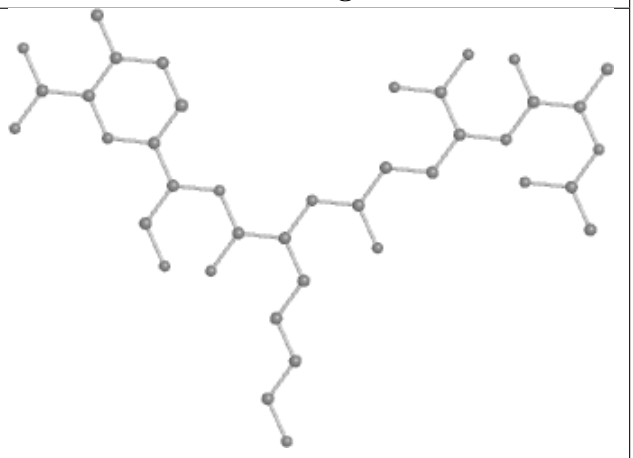
Bond lengths



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	355/358 (99%)	0.54	38 (10%) 6 6	4, 10, 26, 58	0
1	B	358/358 (100%)	0.36	27 (7%) 14 16	5, 10, 23, 30	0
All	All	713/716 (99%)	0.45	65 (9%) 9 10	4, 10, 23, 58	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	289	ASN	9.7
1	A	287	SER	6.5
1	A	279	ASN	6.1
1	A	288[A]	ASP	6.1
1	A	290	LYS	5.9
1	A	4[A]	ALA	5.1
1	B	244	ASN	5.1
1	B	4	ALA	4.7
1	A	126	LYS	4.6
1	A	281	ASP	4.5
1	A	244	ASN	4.2
1	B	206	GLY	4.0
1	B	49	ALA	3.9
1	B	6	GLN	3.8
1	A	22	GLN	3.8
1	A	242	ASP	3.6
1	A	34	TYR	3.6
1	B	242	ASP	3.5
1	B	289[A]	ASN	3.3
1	B	205[A]	GLU	3.3
1	B	207[A]	LYS	3.2
1	A	278	VAL	3.2
1	B	126	LYS	3.2
1	A	35	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	102	ASN	3.0
1	A	36	GLY	3.0
1	A	282	SER	3.0
1	B	7	GLN	3.0
1	A	123	ASP	3.0
1	A	241	LEU	2.8
1	B	288	ASP	2.7
1	B	35	GLN	2.7
1	A	124[A]	GLU	2.7
1	B	241	LEU	2.7
1	A	205[A]	GLU	2.6
1	A	206	GLY	2.6
1	A	65	VAL	2.6
1	B	5	PRO	2.6
1	B	36	GLY	2.6
1	A	49	ALA	2.6
1	A	337	VAL	2.6
1	B	269	LEU	2.5
1	B	326	VAL	2.5
1	B	52[A]	GLN	2.4
1	A	264	ASP	2.4
1	B	50	LYS	2.4
1	A	213[A]	PRO	2.4
1	A	127	SER	2.4
1	B	34	TYR	2.3
1	B	223	VAL	2.3
1	A	339	LEU	2.3
1	A	21[A]	GLU	2.3
1	B	65	VAL	2.3
1	A	310	ALA	2.3
1	A	361	GLN	2.3
1	A	99	LYS	2.3
1	B	123	ASP	2.2
1	A	7	GLN	2.2
1	B	22[A]	GLN	2.2
1	B	102[A]	ASN	2.2
1	A	351	ASP	2.2
1	A	291	ILE	2.1
1	A	280	PRO	2.1
1	B	243[A]	ILE	2.1
1	A	5	PRO	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)

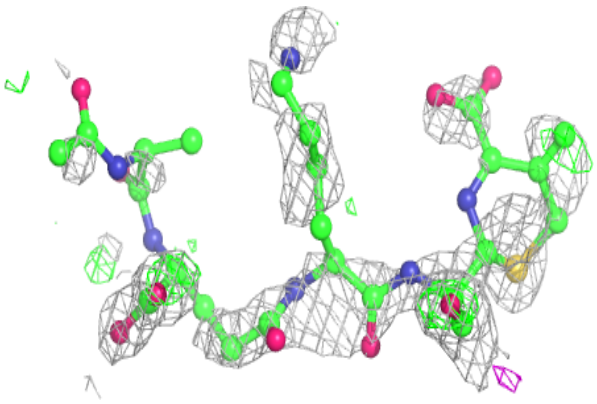
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

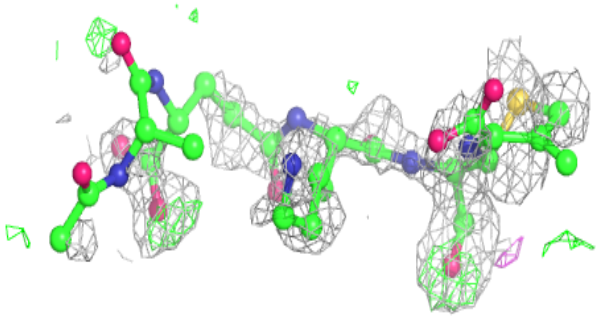
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MXG	A	400[B]	40/40	0.54	0.44	14,41,48,49	40
3	MXG	B	400[A]	40/40	0.66	0.33	29,46,54,55	40
3	MXG	B	400[B]	40/40	0.66	0.33	17,44,50,52	40
2	K	A	2	1/1	0.84	0.11	42,42,42,42	0
2	K	B	1	1/1	0.89	0.11	40,40,40,40	0

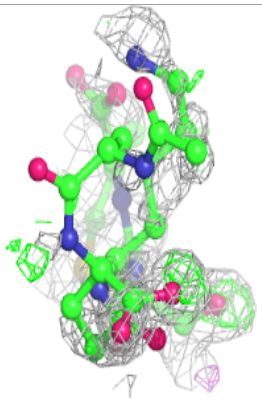
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MXG A 400 (B):

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

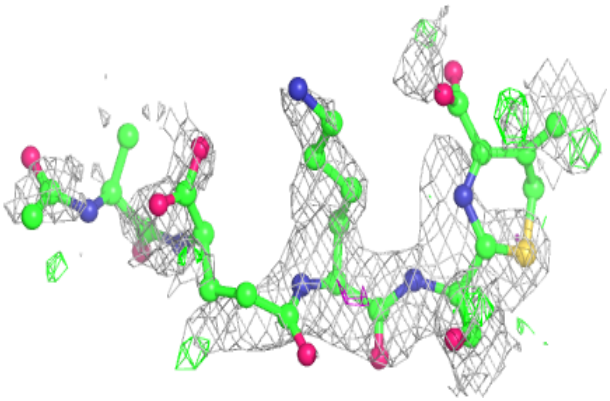


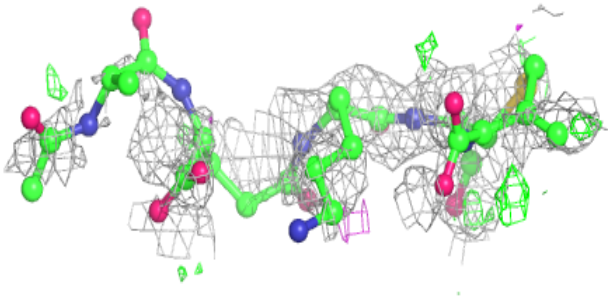


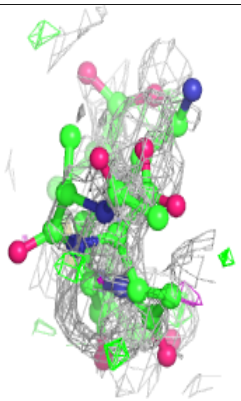


Electron density around MXG B 400 (A):

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

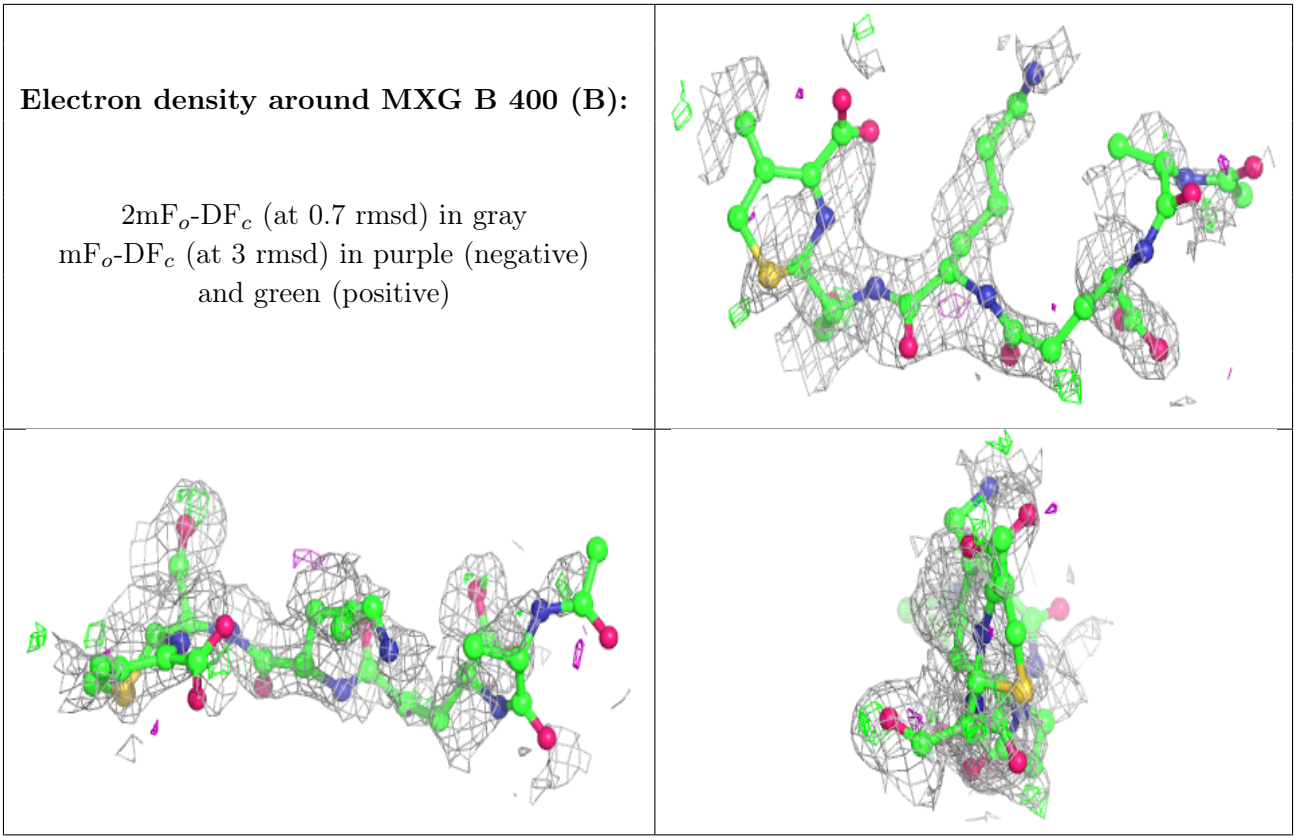






Electron density around MXG B 400 (B):

$2mF_o$-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.