Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 03:23 am BST

PDB ID	:	4I73
Title	:	Crystal structure of the Trypanosoma brucei Inosine-Adenosine-Guanosine nucleoside hydrolase in complex with compound UAMC-00312
Authors	:	Giannese, F.; Degano, M.
Deposited on	:	2012-11-30
Resolution	:	2.18 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 following versions of software and data (see references (i)) were used in the production of this report:

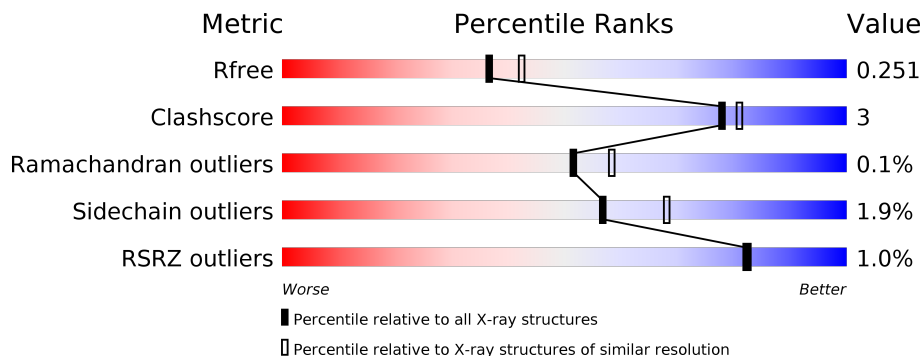|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		1.9%
RSRZ outliers		1.0%

Worse — *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	330	% 92% 6% ••
1	B	330	91% 8% •
1	C	330	2% 89% 7% •
1	D	330	% 93% 6% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10719 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 Inosine-adenosine-guanosine-nucleoside hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2509	1595	419	471	24			
1	B	324	Total	C	N	O	S	0	1	0
			2495	1588	414	469	24			
1	C	318	Total	C	N	O	S	0	0	0
			2434	1551	405	454	24			
1	D	327	Total	C	N	O	S	0	0	0
			2509	1595	419	471	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP Q57ZL6
A	-1	SER	-	EXPRESSION TAG	UNP Q57ZL6
A	0	HIS	-	EXPRESSION TAG	UNP Q57ZL6
B	-2	GLY	-	EXPRESSION TAG	UNP Q57ZL6
B	-1	SER	-	EXPRESSION TAG	UNP Q57ZL6
B	0	HIS	-	EXPRESSION TAG	UNP Q57ZL6
C	-2	GLY	-	EXPRESSION TAG	UNP Q57ZL6
C	-1	SER	-	EXPRESSION TAG	UNP Q57ZL6
C	0	HIS	-	EXPRESSION TAG	UNP Q57ZL6
D	-2	GLY	-	EXPRESSION TAG	UNP Q57ZL6
D	-1	SER	-	EXPRESSION TAG	UNP Q57ZL6
D	0	HIS	-	EXPRESSION TAG	UNP Q57ZL6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

- Molecule 3 is (2R,3R,4S)-2-(hydroxymethyl)-1-[(4-hydroxythieno[3,2-d]pyrimidin-7-yl)methyl]pyrrolidine-3,4-diol (three-letter code: MBY) (formula: $C_{12}H_{15}N_3O_4S$).
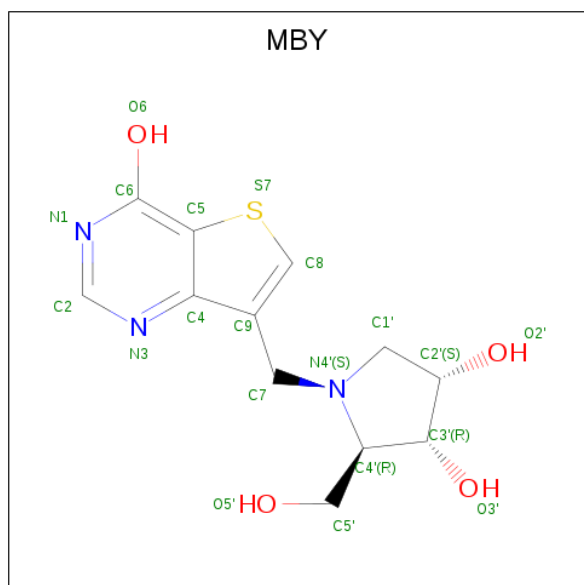
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total C N O S 20 12 3 4 1					0	0
3	B	1	Total C N O S 20 12 3 4 1					0	0
3	C	1	Total C N O S 20 12 3 4 1					0	1
3	D	1	Total C N O S 20 12 3 4 1					0	1

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total Ni 2 2		0	0
4	A	6	Total Ni 6 6		0	0
4	D	3	Total Ni 3 3		0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	6	Total 6	Ni 6	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	200	Total 200	O 200	0	0
5	B	177	Total 178	O 178	0	1
5	C	141	Total 141	O 141	0	0
5	D	152	Total 152	O 152	0	0

3 Residue-property plots (i)

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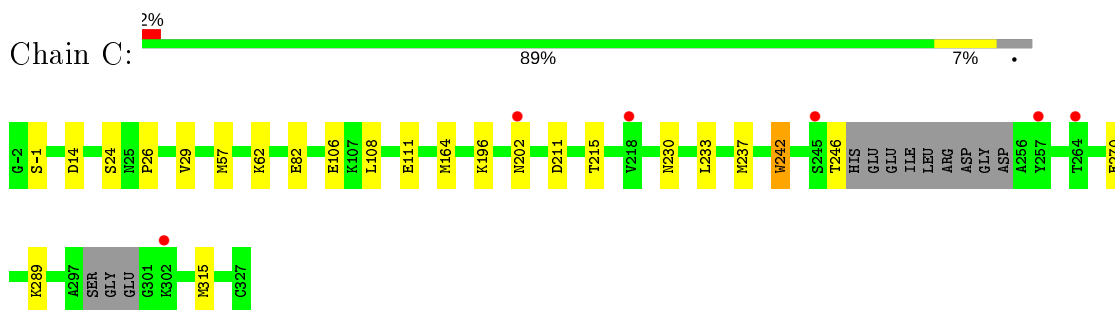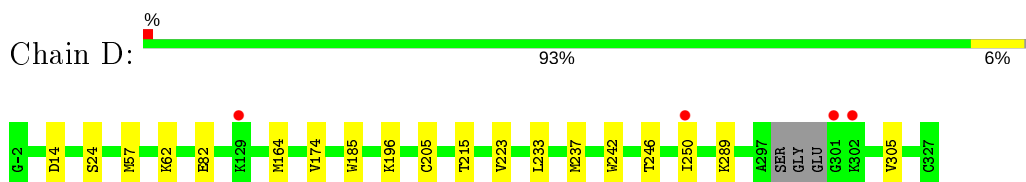
- Molecule 1: Inosine-adenosine-guanosine-nucleoside hydrolase
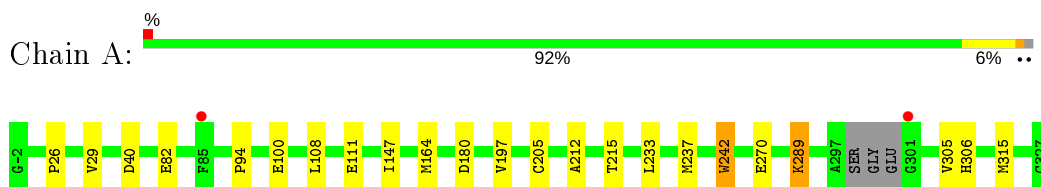
- Molecule 1: Inosine-adenosine-guanosine-nucleoside hydrolase
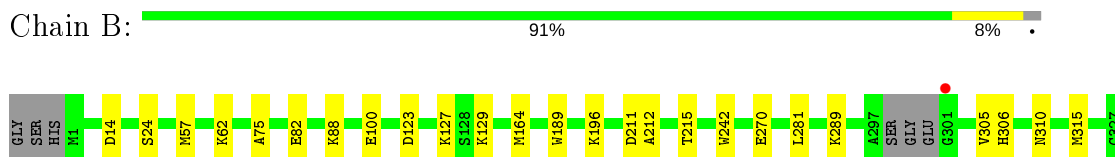
- Molecule 1: Inosine-adenosine-guanosine-nucleoside hydrolase

- Molecule 1: Inosine-adenosine-guanosine-nucleoside hydrolase

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.17Å 131.67Å 71.85Å 90.00° 91.33° 90.00°	Depositor
Resolution (Å)	71.83 – 2.18 47.98 – 2.18	Depositor EDS
% Data completeness (in resolution range)	99.7 (71.83-2.18) 99.7 (47.98-2.18)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 2.18Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.248 0.203 , 0.251	Depositor DCC
R_{free} test set	3089 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 16.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.127 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10719	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3531e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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: NI, CA, MBY

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	0.77	0/2564	0.73	1/3483 (0.0%)
1	B	0.79	0/2552	0.73	1/3467 (0.0%)
1	C	0.84	0/2487	0.74	0/3378
1	D	0.82	0/2564	0.71	0/3483
All	All	0.80	0/10167	0.73	2/13811 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	40	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	123	ASP	CB-CG-OD2	-5.18	113.64	118.30

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	2509	0	2492	20	0
1	B	2495	0	2485	20	3
1	C	2434	0	2428	15	3
1	D	2509	0	2492	12	0
2	A	1	0	0	0	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	20	0	12	0	0
3	B	20	0	12	2	0
3	C	20	0	12	1	0
3	D	20	0	12	1	0
4	A	6	0	0	0	0
4	B	2	0	0	0	0
4	C	6	0	0	0	0
4	D	3	0	0	0	0
5	A	200	0	0	2	0
5	B	178	0	0	4	0
5	C	141	0	0	3	0
5	D	152	0	0	1	0
All	All	10719	0	9945	58	3

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 3.

All (58) 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:127:LYS:HG3	5:B:628:HOH:O	1.39	1.17
1:D:215:THR:HG21	5:D:642:HOH:O	1.50	1.11
1:B:24:SER:HB3	1:B:57:MET:HE1	1.67	0.75
1:C:106:GLU:HG3	5:C:619:HOH:O	1.89	0.72
1:C:14:ASP:OD2	3:C:402[A]:MBY:H13	1.93	0.68
1:C:215:THR:O	1:C:215:THR:HG22	1.95	0.66
1:C:215:THR:O	1:C:215:THR:CG2	2.44	0.65
1:C:24:SER:HB3	1:C:57:MET:HE1	1.78	0.65
1:A:289:LYS:HD2	1:B:127:LYS:HZ1	1.62	0.64
1:A:289:LYS:CD	1:B:127:LYS:HZ1	2.11	0.64
1:C:106:GLU:HG2	5:C:591:HOH:O	1.98	0.63
1:A:289:LYS:CE	1:B:127:LYS:NZ	2.63	0.61
1:A:289:LYS:HE3	1:B:127:LYS:NZ	2.17	0.59
1:A:289:LYS:CE	1:B:127:LYS:HZ1	2.17	0.58
1:D:14:ASP:OD2	3:D:402[A]:MBY:H13	2.04	0.57
1:C:242:TRP:O	1:C:246:THR:HG23	2.06	0.56
1:A:180:ASP:HB3	1:B:127:LYS:HE3	1.87	0.56
1:A:289:LYS:HE3	1:B:127:LYS:HZ2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:THR:O	1:D:215:THR:CG2	2.56	0.53
1:B:270:GLU:HB3	1:B:315:MET:HE1	1.92	0.51
1:B:88:LYS:HE2	1:D:250:ILE:HD12	1.93	0.51
1:B:82:GLU:H	1:B:82:GLU:CD	2.14	0.51
1:A:100:GLU:OE1	5:A:510:HOH:O	2.19	0.50
1:D:215:THR:O	1:D:215:THR:HG22	2.13	0.49
1:A:94:PRO:HB2	1:C:230:ASN:OD1	2.12	0.48
1:C:233:LEU:O	1:C:237:MET:HG3	2.13	0.48
1:A:215:THR:CG2	1:A:215:THR:O	2.61	0.48
1:C:26:PRO:HA	1:C:29:VAL:O	2.14	0.48
1:D:24:SER:HB3	1:D:57:MET:HE1	1.96	0.48
1:C:82:GLU:H	1:C:82:GLU:CD	2.17	0.47
1:B:75:ALA:HB2	1:B:189:TRP:CE2	2.51	0.46
1:A:270:GLU:HB3	1:A:315:MET:HE1	1.98	0.45
1:D:82:GLU:CD	1:D:82:GLU:H	2.19	0.45
1:D:223:VAL:HG21	1:D:246:THR:CG2	2.46	0.45
1:A:215:THR:HG22	1:A:215:THR:O	2.17	0.45
1:B:306:HIS:HE1	5:B:619:HOH:O	1.99	0.44
1:B:281:LEU:HD11	1:B:305:VAL:HG21	1.99	0.44
1:C:270:GLU:HB3	1:C:315:MET:HE1	1.98	0.44
1:C:215:THR:HG21	5:C:575:HOH:O	2.19	0.43
1:B:88:LYS:HE2	1:D:250:ILE:CD1	2.49	0.43
1:C:242:TRP:CE3	1:C:242:TRP:HA	2.53	0.43
1:B:129:LYS:NZ	5:B:651:HOH:O	2.26	0.43
1:B:14:ASP:OD2	3:B:402:MBY:H13	2.19	0.43
1:A:108:LEU:O	1:A:111:GLU:HG2	2.19	0.42
1:A:233:LEU:O	1:A:237:MET:HG3	2.20	0.42
1:A:306:HIS:HE1	5:A:526:HOH:O	2.02	0.42
1:A:147:ILE:HD12	1:A:197:VAL:HG22	2.02	0.42
1:A:212:ALA:O	1:A:215:THR:HB	2.20	0.42
1:B:100:GLU:HB2	5:B:513:HOH:O	2.19	0.42
3:B:402:MBY:H3	3:B:402:MBY:O5'	2.20	0.42
1:A:26:PRO:HA	1:A:29:VAL:O	2.19	0.41
1:A:242:TRP:CE3	1:A:242:TRP:HA	2.56	0.41
1:D:205:CYS:HB2	1:D:305:VAL:HG12	2.03	0.41
1:B:212:ALA:O	1:B:215:THR:HB	2.22	0.40
1:A:205:CYS:HB2	1:A:305:VAL:HG12	2.04	0.40
1:C:108:LEU:O	1:C:111:GLU:HG2	2.22	0.40
1:D:233:LEU:O	1:D:237:MET:HG3	2.22	0.40
1:D:174:VAL:HG22	1:D:185:TRP:CD1	2.57	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:ASN:ND2	1:C:202:ASN:OD1[2_456]	1.42	0.78
1:B:310:ASN:CG	1:C:202:ASN:OD1[2_456]	1.75	0.45
1:B:310:ASN:ND2	1:C:202:ASN:CG[2_456]	2.07	0.13

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	323/330 (98%)	315 (98%)	8 (2%)	0	100	100
1	B	321/330 (97%)	316 (98%)	5 (2%)	0	100	100
1	C	312/330 (94%)	304 (97%)	7 (2%)	1 (0%)	41	43
1	D	323/330 (98%)	315 (98%)	8 (2%)	0	100	100
All	All	1279/1320 (97%)	1250 (98%)	28 (2%)	1 (0%)	51	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	-1	SER

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	276/278 (99%)	272 (99%)	4 (1%)	67	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	275/278 (99%)	269 (98%)	6 (2%)	52	62
1	C	268/278 (96%)	262 (98%)	6 (2%)	52	62
1	D	276/278 (99%)	271 (98%)	5 (2%)	59	70
All	All	1095/1112 (98%)	1074 (98%)	21 (2%)	57	68

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	A	164	MET
1	A	242	TRP
1	A	289	LYS
1	B	62	LYS
1	B	164	MET
1	B	196	LYS
1	B	211	ASP
1	B	242	TRP
1	B	289	LYS
1	C	62	LYS
1	C	164	MET
1	C	196	LYS
1	C	211	ASP
1	C	242	TRP
1	C	289	LYS
1	D	62	LYS
1	D	164	MET
1	D	196	LYS
1	D	242	TRP
1	D	289	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	B	77	ASN
1	B	306	HIS
1	C	77	ASN
1	C	314	GLN
1	C	317	HIS
1	D	77	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 25 ligands modelled in this entry, 21 are monoatomic - leaving 4 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	MBY	C	402[A]	2	19,22,22	2.22	4 (21%)	19,32,32	2.63	7 (36%)
3	MBY	A	402	2	19,22,22	1.50	4 (21%)	19,32,32	2.93	5 (26%)
3	MBY	D	402[A]	2	19,22,22	1.96	3 (15%)	19,32,32	2.35	6 (31%)
3	MBY	B	402	2	19,22,22	1.80	3 (15%)	19,32,32	2.19	5 (26%)

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	MBY	C	402[A]	2	-	2/5/22/22	0/3/3/3
3	MBY	A	402	2	-	2/5/22/22	0/3/3/3
3	MBY	D	402[A]	2	-	2/5/22/22	0/3/3/3
3	MBY	B	402	2	-	2/5/22/22	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402[A]	MBY	C8-C9	6.65	1.41	1.37
3	D	402[A]	MBY	C8-C9	6.03	1.40	1.37
3	B	402	MBY	C8-C9	5.78	1.40	1.37
3	C	402[A]	MBY	C8-S7	5.52	1.78	1.70
3	A	402	MBY	C8-C9	3.83	1.39	1.37
3	D	402[A]	MBY	C8-S7	3.67	1.75	1.70
3	A	402	MBY	C4'-N4'	2.81	1.50	1.47
3	B	402	MBY	C1'-C2'	-2.41	1.48	1.52
3	D	402[A]	MBY	C1'-C2'	-2.27	1.48	1.52
3	B	402	MBY	C4-N3	-2.24	1.34	1.37
3	C	402[A]	MBY	C4-N3	-2.23	1.34	1.37
3	A	402	MBY	C4-N3	-2.19	1.34	1.37
3	C	402[A]	MBY	C1'-C2'	-2.15	1.48	1.52
3	A	402	MBY	C1'-C2'	-2.09	1.49	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	MBY	C2-N3-C4	9.39	122.12	114.81
3	C	402[A]	MBY	C2-N3-C4	7.37	120.55	114.81
3	D	402[A]	MBY	C2-N3-C4	6.30	119.72	114.81
3	B	402	MBY	C2-N3-C4	5.87	119.38	114.81
3	A	402	MBY	N3-C2-N1	-4.81	121.16	128.68
3	C	402[A]	MBY	C5-C4-N3	-4.36	119.82	124.96
3	A	402	MBY	C7-N4'-C4'	4.05	119.10	113.52
3	C	402[A]	MBY	N3-C2-N1	-3.85	122.65	128.68
3	D	402[A]	MBY	C5-C4-N3	-3.62	120.69	124.96
3	B	402	MBY	N3-C2-N1	-3.60	123.05	128.68
3	A	402	MBY	C5-C4-N3	-3.59	120.73	124.96
3	D	402[A]	MBY	N3-C2-N1	-3.57	123.10	128.68
3	B	402	MBY	C5-C4-N3	-3.43	120.91	124.96
3	C	402[A]	MBY	C7-N4'-C4'	3.42	118.23	113.52
3	B	402	MBY	C7-N4'-C4'	3.22	117.95	113.52
3	D	402[A]	MBY	C8-S7-C5	2.90	94.71	91.24
3	B	402	MBY	C8-S7-C5	2.87	94.67	91.24
3	D	402[A]	MBY	C7-N4'-C4'	2.53	117.00	113.52
3	C	402[A]	MBY	O2'-C2'-C1'	-2.37	105.35	110.94
3	A	402	MBY	C7-N4'-C1'	2.35	116.32	113.16
3	D	402[A]	MBY	O2'-C2'-C3'	2.27	115.56	111.27
3	C	402[A]	MBY	O5'-C5'-C4'	2.15	116.02	111.42
3	C	402[A]	MBY	O3'-C3'-C2'	-2.02	107.18	112.04

There are no chirality outliers.
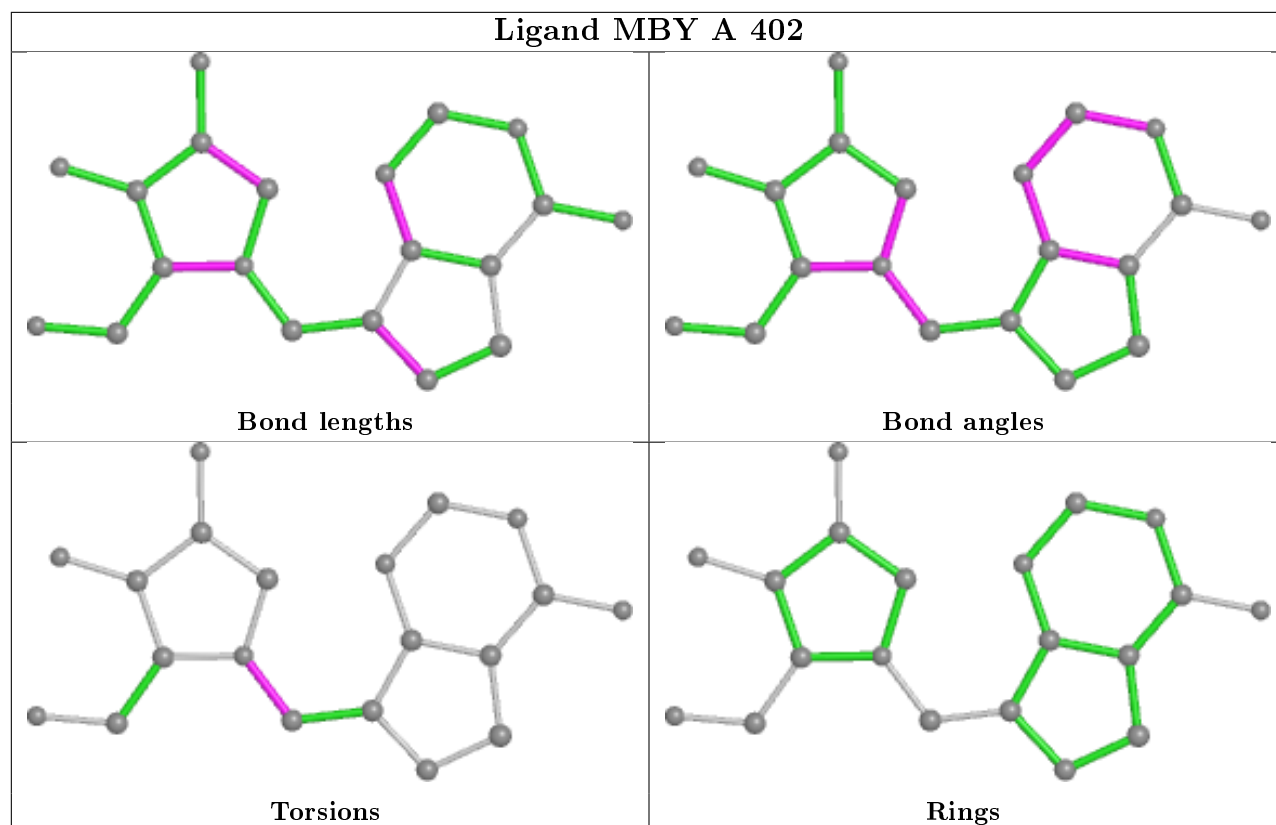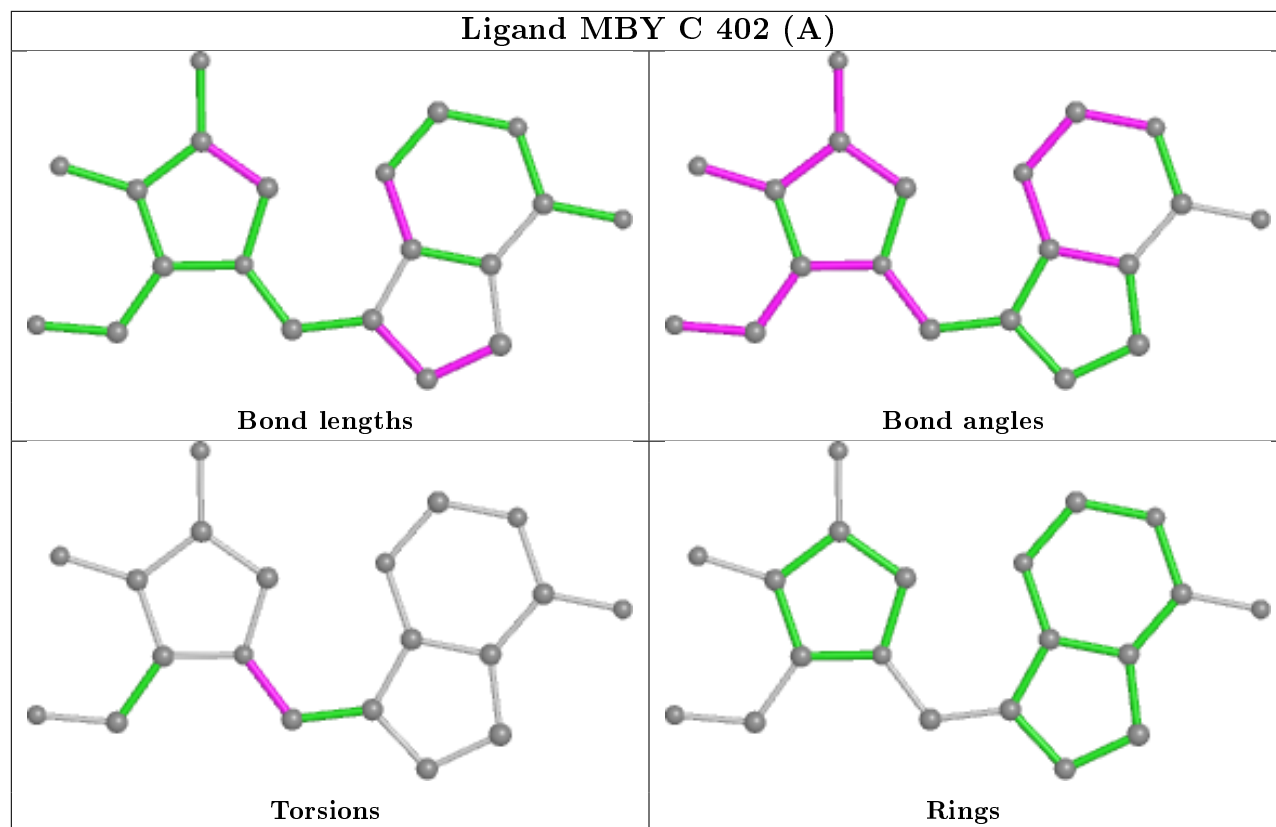
All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402[A]	MBY	C9-C7-N4'-C1'
3	A	402	MBY	C9-C7-N4'-C1'
3	D	402[A]	MBY	C9-C7-N4'-C1'
3	B	402	MBY	C9-C7-N4'-C1'
3	C	402[A]	MBY	C9-C7-N4'-C4'
3	A	402	MBY	C9-C7-N4'-C4'
3	D	402[A]	MBY	C9-C7-N4'-C4'
3	B	402	MBY	C9-C7-N4'-C4'

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402[A]	MBY	1	0
3	D	402[A]	MBY	1	0
3	B	402	MBY	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 MBY C 402 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand MBY A 402

Bond lengths

Bond angles

Torsions

Rings

Ligand MBY D 402 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand MBY B 402

Bond lengths

Bond angles

Torsions

Rings
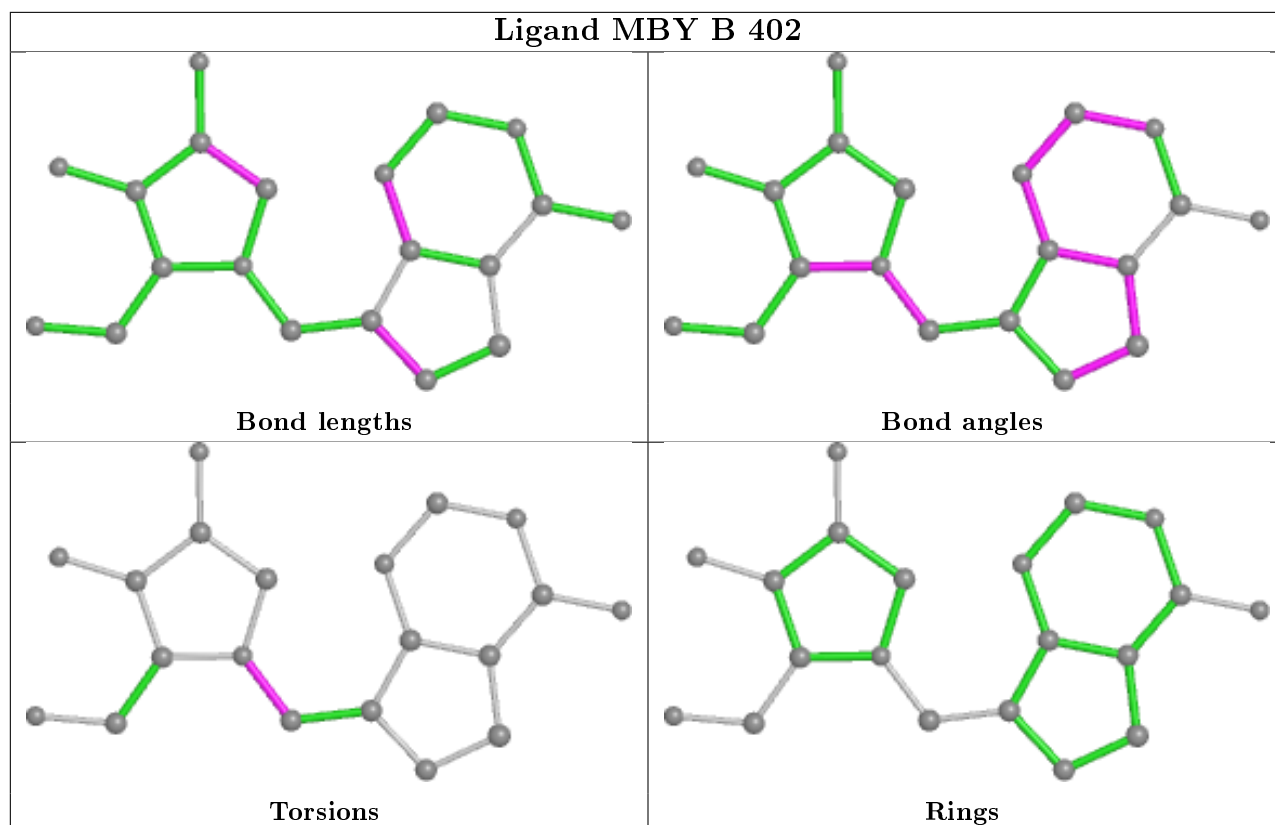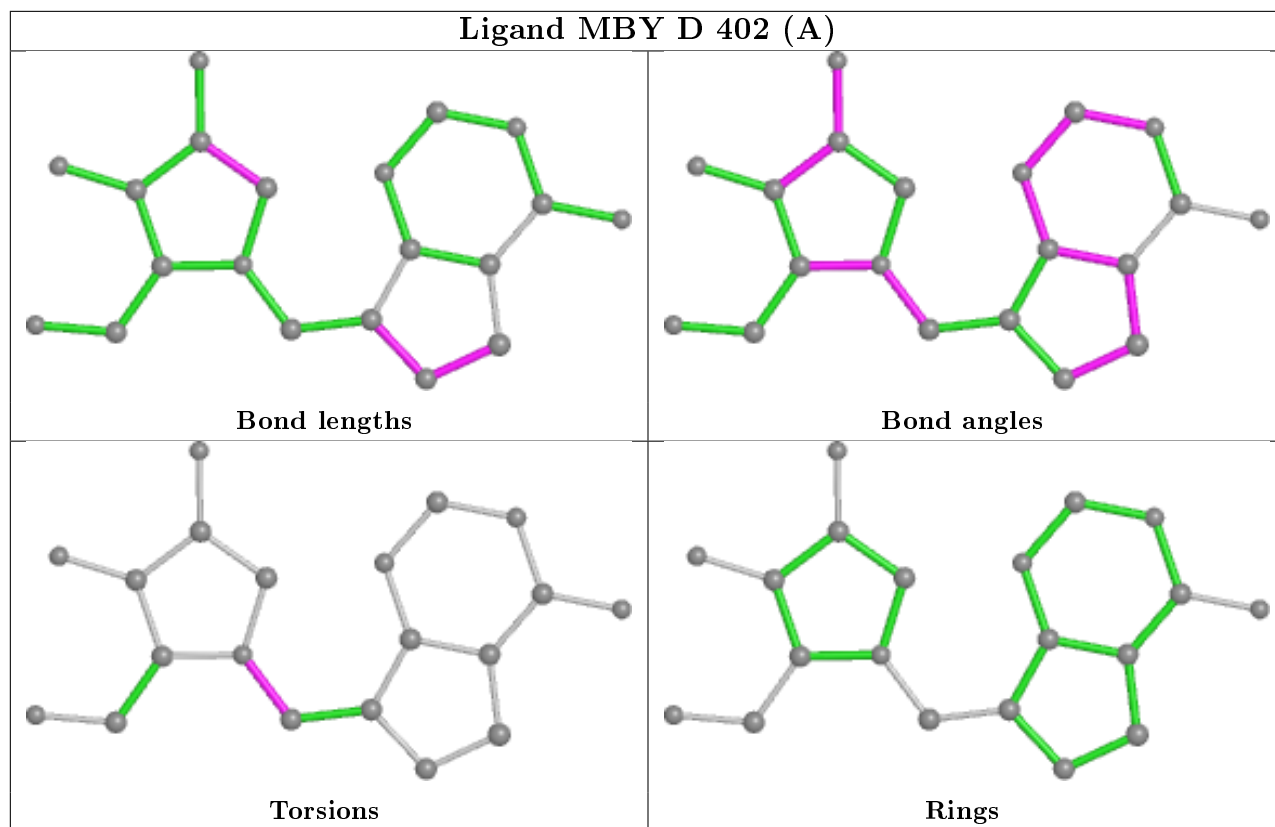
5.7 Other polymers (i)

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, 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	327/330 (99%)	-0.31	2 (0%)	89	89	12, 22, 34, 56	0
1	B	324/330 (98%)	-0.31	1 (0%)	94	94	12, 22, 33, 56	0
1	C	318/330 (96%)	-0.20	6 (1%)	66	67	13, 22, 34, 56	0
1	D	327/330 (99%)	-0.22	4 (1%)	79	79	12, 22, 34, 56	0
All	All	1296/1320 (98%)	-0.26	13 (1%)	82	82	12, 22, 34, 56	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	4.3
1	A	85	PHE	4.0
1	C	302	LYS	3.2
1	C	257	TYR	3.2
1	C	245	SER	3.0
1	D	250	ILE	2.9
1	D	129	LYS	2.9
1	B	301	GLY	2.6
1	C	202	ASN	2.5
1	D	301	GLY	2.5
1	C	218	VAL	2.4
1	D	302	LYS	2.3
1	C	264	THR	2.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MBY	C	402[A]	20/20	0.93	0.18	14,17,22,23	20
3	MBY	A	402	20/20	0.95	0.10	14,18,23,24	0
3	MBY	D	402[A]	20/20	0.95	0.12	15,17,23,23	20
4	NI	C	405	1/1	0.96	0.47	23,23,23,23	1
4	NI	B	404	1/1	0.96	0.06	85,85,85,85	0
4	NI	C	407	1/1	0.96	0.07	83,83,83,83	0
4	NI	A	408	1/1	0.97	0.26	35,35,35,35	1
4	NI	C	406[B]	1/1	0.97	0.15	29,29,29,29	1
4	NI	C	403	1/1	0.97	0.26	36,36,36,36	1
3	MBY	B	402	20/20	0.97	0.09	14,18,22,23	0
4	NI	C	404	1/1	0.98	0.07	51,51,51,51	0
4	NI	C	408	1/1	0.98	0.20	36,36,36,36	1
4	NI	A	407	1/1	0.98	0.18	35,35,35,35	1
2	CA	D	401	1/1	0.99	0.06	14,14,14,14	0
4	NI	A	403	1/1	0.99	0.07	26,26,26,26	0
4	NI	A	404	1/1	0.99	0.07	29,29,29,29	0
4	NI	B	403	1/1	0.99	0.07	38,38,38,38	0
4	NI	D	405[B]	1/1	0.99	0.14	13,13,13,13	1
4	NI	D	403	1/1	0.99	0.09	52,52,52,52	0
4	NI	A	406	1/1	0.99	0.04	36,36,36,36	0
4	NI	A	405	1/1	0.99	0.06	30,30,30,30	0
2	CA	A	401	1/1	0.99	0.11	14,14,14,14	0
2	CA	B	401	1/1	0.99	0.08	14,14,14,14	0
2	CA	C	401	1/1	1.00	0.03	16,16,16,16	0
4	NI	D	404	1/1	1.00	0.08	31,31,31,31	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 MBY C 402 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
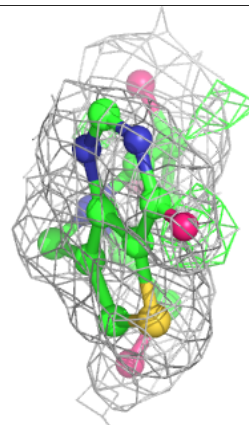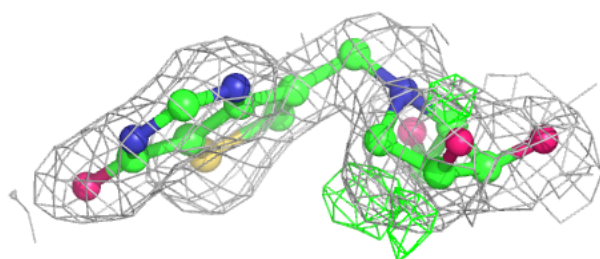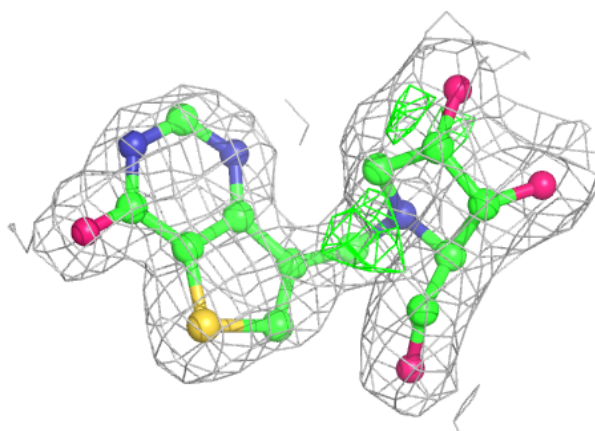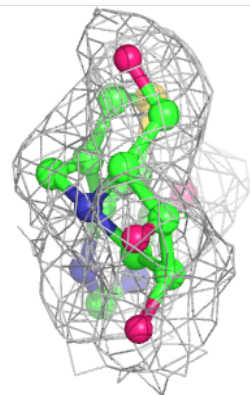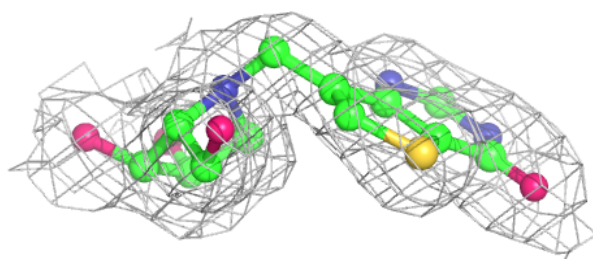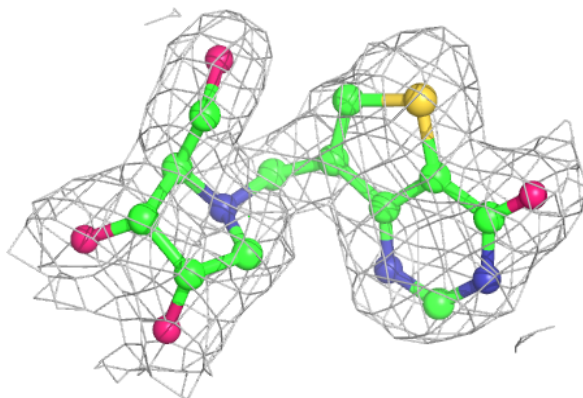and green (positive)
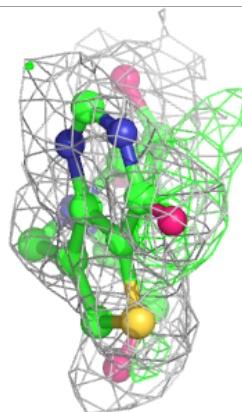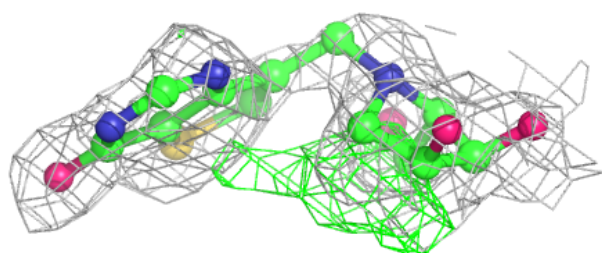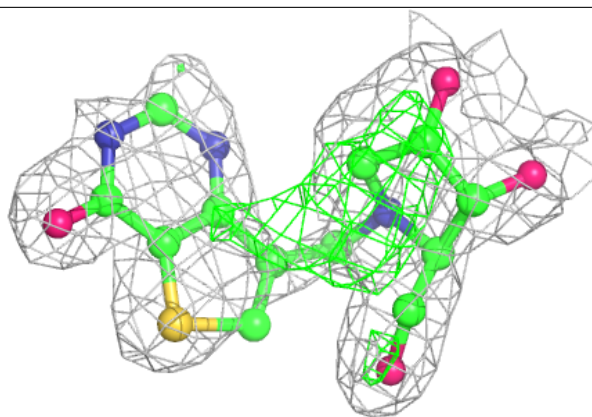
Electron density around MBY A 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
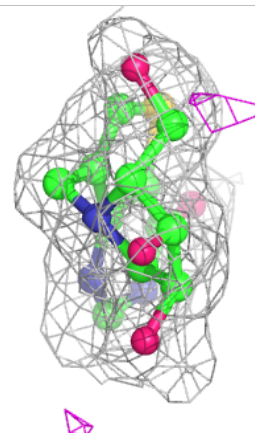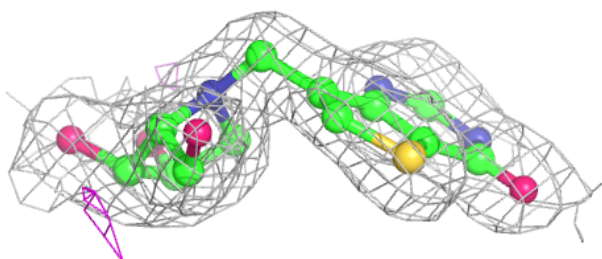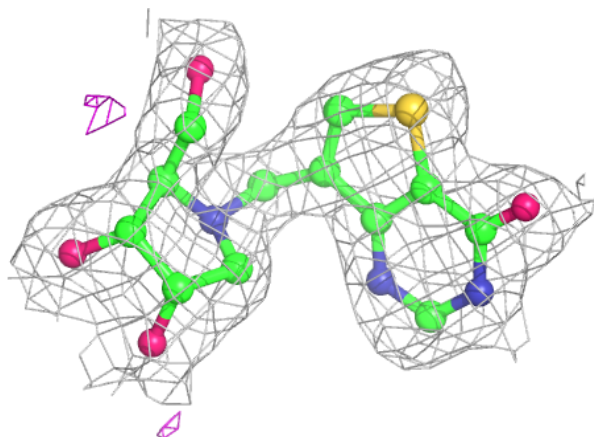
Electron density around MBY D 402 (A):

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

Electron density around MBY B 402:

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

6.5 Other polymers (i)

There are no such residues in this entry.