



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 15, 2024 – 04:10 PM EDT

PDB ID : 1XPO
Title : Structural mechanism of inhibition of the Rho transcription termination factor by the antibiotic bicyclomycin
Authors : Skordalakes, E.; Brogan, A.P.; Park, B.S.; Kohn, H.; Berger, J.M.
Deposited on : 2004-10-09
Resolution : 3.15 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

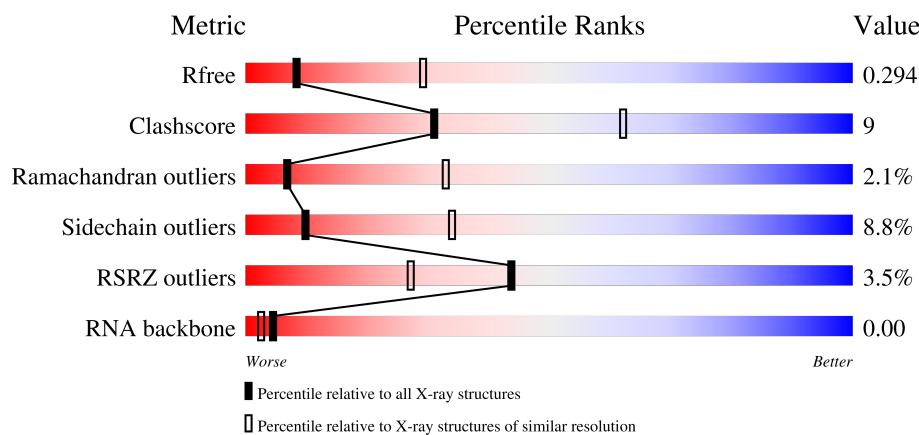
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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

Mol	Chain	Length	Quality of chain
1	G	8	<div> <div>25%</div> <div>12% 12% 75%</div> </div>
1	H	8	<div> <div>12%</div> <div>12% 12% 75%</div> </div>
1	J	8	<div> <div>12%</div> <div>12% 12% 75%</div> </div>
1	K	8	<div> <div>25%</div> <div>12% 12% 75%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	8	
1	M	8	
2	A	419	
2	B	419	
2	C	419	
2	D	419	
2	E	419	
2	F	419	

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	AGS	C	3600	-	-	-	X
4	AGS	E	5600	-	-	X	-
4	AGS	F	6600	-	-	-	X
5	BCM	C	3701	-	-	-	X
5	BCM	D	4701	-	-	-	X
5	BCM	F	6701	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19802 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 RNA chain called 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	M	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	H	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	J	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	K	2	Total	C	N	O	P	0	0	0
			40	18	5	15	2			
1	L	2	Total	C	N	O	P	0	0	0
			37	18	5	13	1			

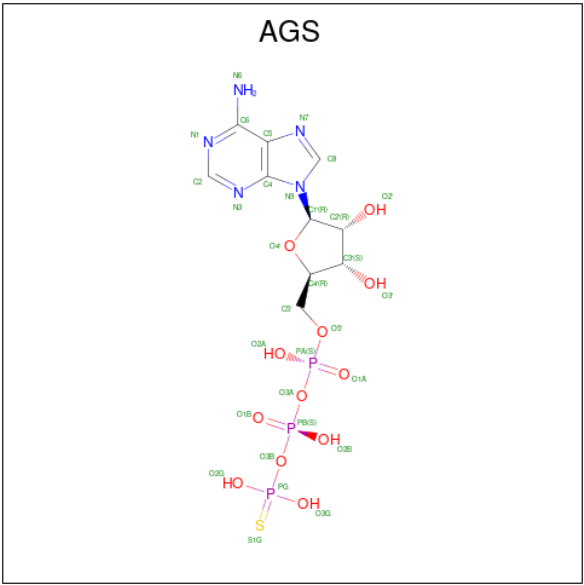
- Molecule 2 is a protein called Rho transcription termination factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	408	Total	C	N	O	S	0	0	0
			3210	2027	564	602	17			
2	B	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	C	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	D	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			
2	E	407	Total	C	N	O	S	0	0	0
			3206	2023	563	603	17			
2	F	408	Total	C	N	O	S	0	0	0
			3213	2028	564	604	17			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



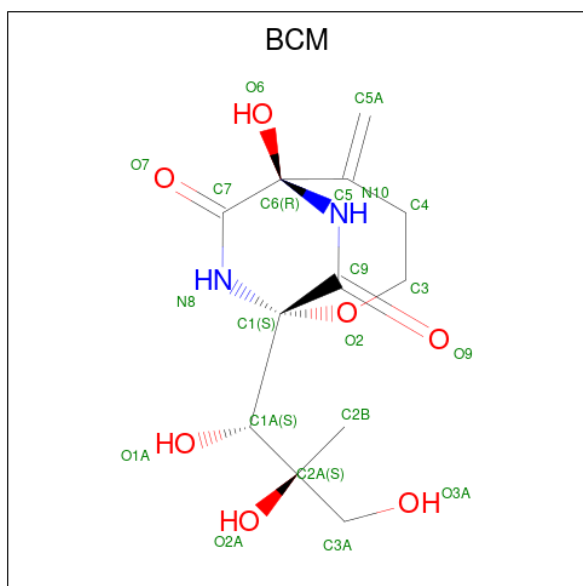
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
4	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 5 is BICYCLOMYCIN (three-letter code: BCM) (formula: $C_{12}H_{18}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			21	12	2	7		
5	C	1	Total	C	N	O	0	0
			21	12	2	7		
5	D	1	Total	C	N	O	0	0
			21	12	2	7		
5	E	1	Total	C	N	O	0	0
			21	12	2	7		
5	F	1	Total	C	N	O	0	0
			21	12	2	7		

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: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'



- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

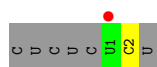


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

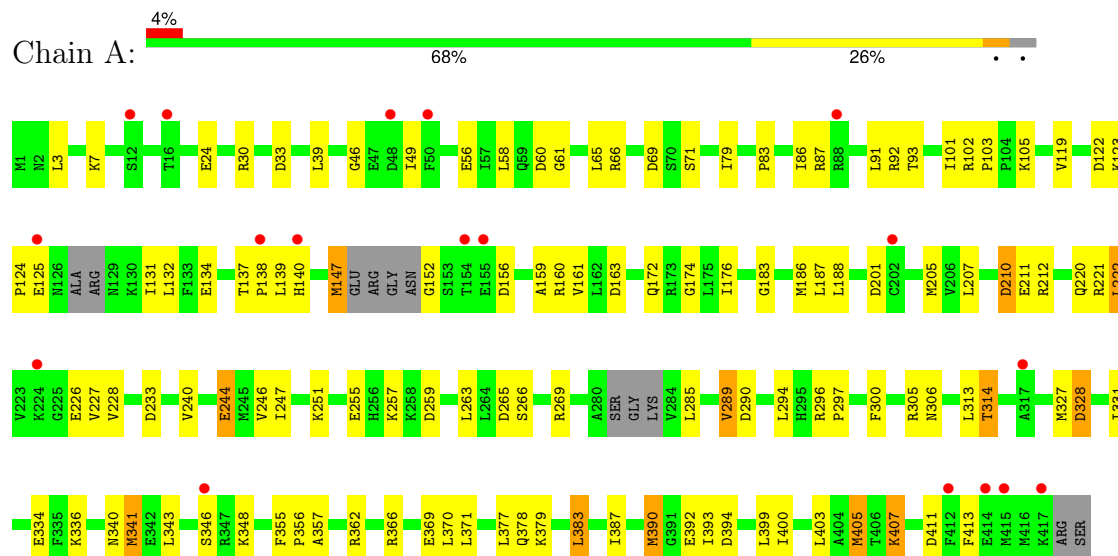


- Molecule 1: 5'-R(*CP*UP*CP*UP*CP*UP*CP*U)-3'

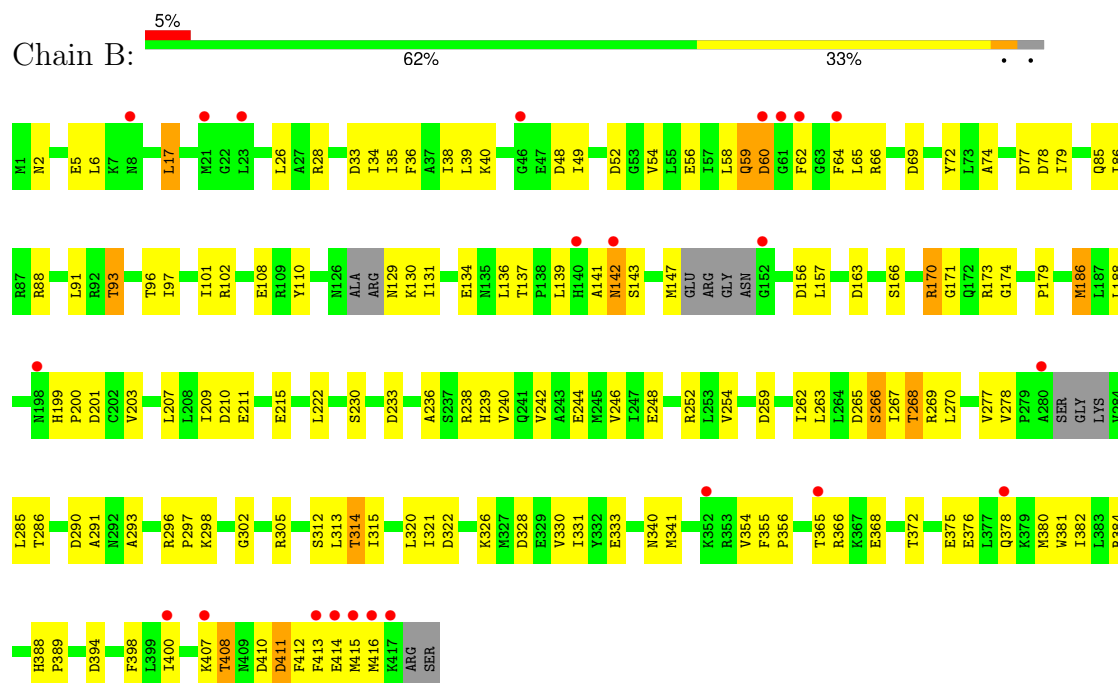




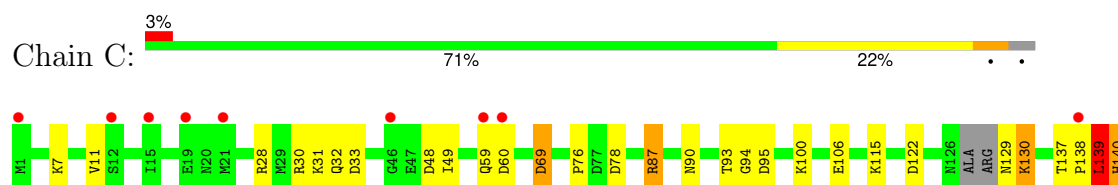
• Molecule 2: Rho transcription termination factor

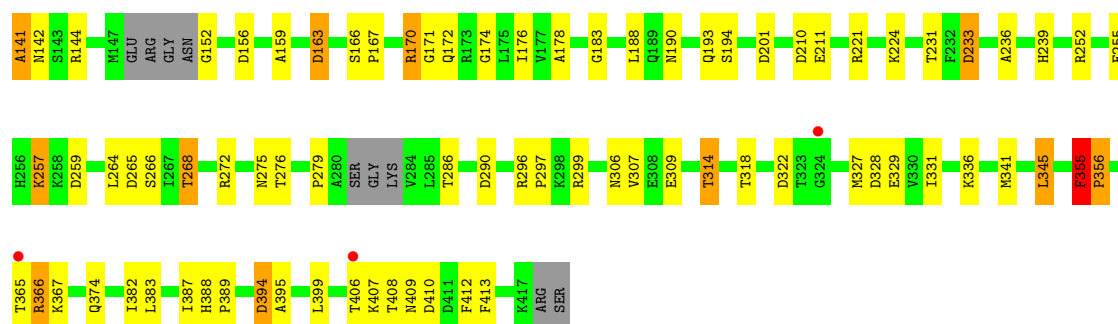


• Molecule 2: Rho transcription termination factor

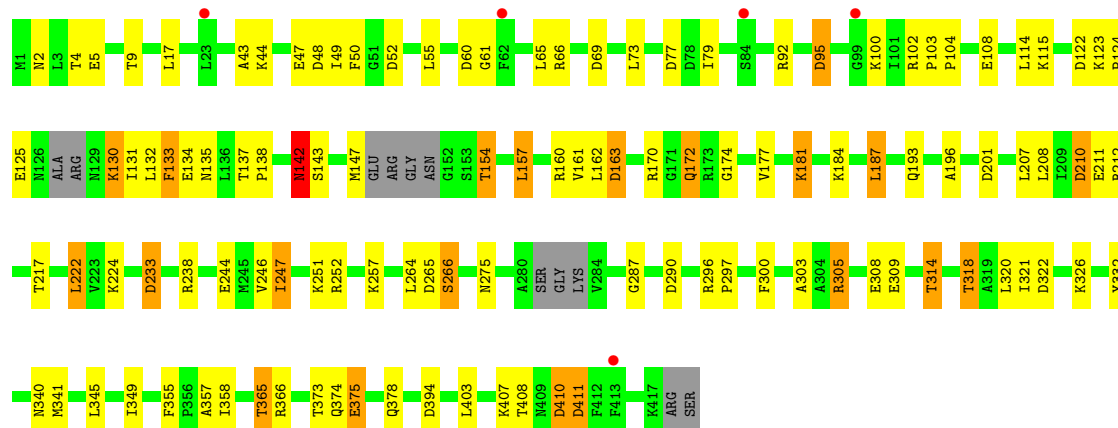


• Molecule 2: Rho transcription termination factor

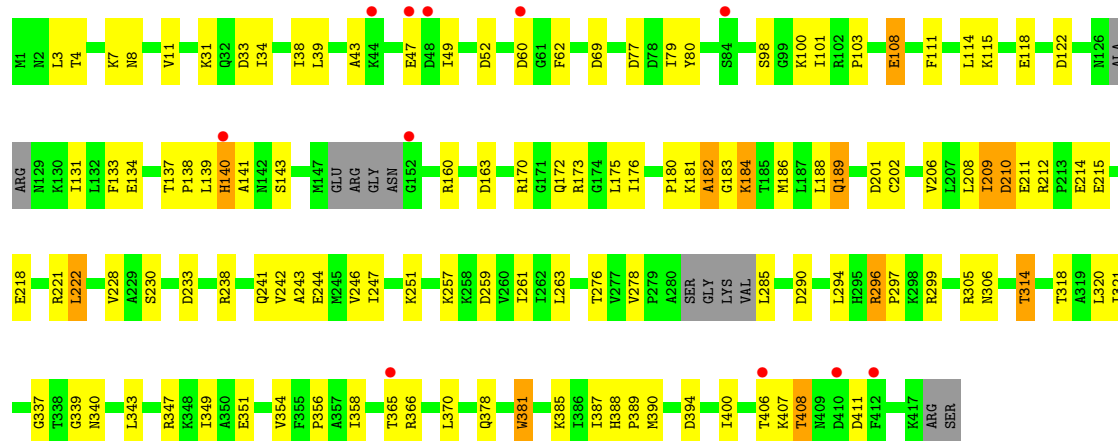




• Molecule 2: Rho transcription termination factor

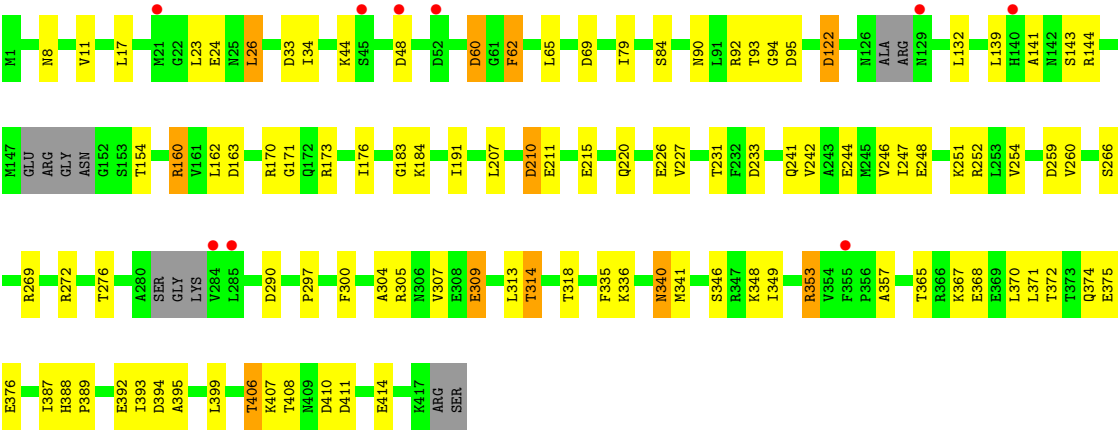


• Molecule 2: Rho transcription termination factor



• Molecule 2: Rho transcription termination factor





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.93Å 111.37Å 161.03Å 90.00° 108.79° 90.00°	Depositor
Resolution (Å)	20.00 – 3.15 28.95 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.6 (20.00-3.15) 68.0 (28.95-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.285 , 0.306 0.276 , 0.294	Depositor DCC
R_{free} test set	2990 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19802	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, BCM

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	G	0.79	0/43	1.10	0/64
1	H	0.76	0/43	0.90	0/64
1	J	0.72	0/43	1.08	0/64
1	K	0.66	0/43	0.93	0/64
1	L	0.77	0/40	1.24	0/60
1	M	0.69	0/43	1.28	0/64
2	A	0.30	0/3256	0.65	13/4383 (0.3%)
2	B	0.31	0/3259	0.65	15/4387 (0.3%)
2	C	0.30	0/3259	0.65	15/4387 (0.3%)
2	D	0.30	0/3259	0.66	15/4387 (0.3%)
2	E	0.30	0/3252	0.64	10/4377 (0.2%)
2	F	0.30	0/3259	0.64	14/4387 (0.3%)
All	All	0.31	0/19799	0.66	82/26688 (0.3%)

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
2	C	0	1

There are no bond length outliers.

The worst 5 of 82 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	69	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	322	ASP	CB-CG-OD2	6.15	123.83	118.30
2	D	77	ASP	CB-CG-OD2	6.09	123.78	118.30
2	E	233	ASP	CB-CG-OD2	6.06	123.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	233	ASP	CB-CG-OD2	5.98	123.68	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	355	PHE	Peptide

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	G	40	0	22	0	0
1	H	40	0	22	0	0
1	J	40	0	22	0	0
1	K	40	0	22	1	0
1	L	37	0	23	0	0
1	M	40	0	22	3	0
2	A	3210	0	3287	57	0
2	B	3213	0	3289	78	0
2	C	3213	0	3289	56	0
2	D	3213	0	3288	59	0
2	E	3206	0	3280	71	0
2	F	3213	0	3289	41	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	2	0
4	C	31	0	12	1	0
4	D	31	0	12	4	0
4	E	31	0	12	12	0
4	F	31	0	12	3	0
5	B	21	0	18	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	21	0	18	4	0
5	D	21	0	18	5	0
5	E	21	0	18	2	0
5	F	21	0	18	7	0
All	All	19802	0	20017	362	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 9.

The worst 5 of 362 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)
2:B:366:ARG:NE	4:C:3600:AGS:S1G	2.30	1.05
2:D:366:ARG:NH2	4:E:5600:AGS:PG	2.33	1.02
2:D:366:ARG:NH1	4:E:5600:AGS:S1G	2.36	0.97
2:D:366:ARG:CZ	4:E:5600:AGS:S1G	2.53	0.96
2:A:140:HIS:CD2	2:A:340:ASN:HD22	1.83	0.95

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	
2	A	400/419 (96%)	328 (82%)	60 (15%)	12 (3%)	4	24
2	B	400/419 (96%)	356 (89%)	37 (9%)	7 (2%)	8	37
2	C	400/419 (96%)	357 (89%)	31 (8%)	12 (3%)	4	24
2	D	400/419 (96%)	343 (86%)	47 (12%)	10 (2%)	5	29
2	E	399/419 (95%)	361 (90%)	32 (8%)	6 (2%)	10	41
2	F	400/419 (96%)	360 (90%)	37 (9%)	3 (1%)	19	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2399/2514 (95%)	2105 (88%)	244 (10%)	50 (2%)	7	33

5 of 50 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	407	LYS
2	B	142	ASN
2	B	408	THR
2	C	140	HIS
2	C	355	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	350/359 (98%)	327 (93%)	23 (7%)	16	47
2	B	351/359 (98%)	322 (92%)	29 (8%)	11	37
2	C	351/359 (98%)	318 (91%)	33 (9%)	8	30
2	D	351/359 (98%)	311 (89%)	40 (11%)	5	23
2	E	350/359 (98%)	321 (92%)	29 (8%)	11	37
2	F	351/359 (98%)	320 (91%)	31 (9%)	10	34
All	All	2104/2154 (98%)	1919 (91%)	185 (9%)	10	34

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	309	GLU
2	E	276	THR
2	D	365	THR
2	E	122	ASP
2	E	321	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	361	ASN
2	F	90	ASN
2	D	374	GLN
2	E	241	GLN
2	F	256	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	G	1/8 (12%)	1 (100%)	0
1	H	1/8 (12%)	1 (100%)	0
1	J	1/8 (12%)	1 (100%)	0
1	K	1/8 (12%)	0	0
1	L	1/8 (12%)	1 (100%)	0
1	M	1/8 (12%)	1 (100%)	0
All	All	6/48 (12%)	5 (83%)	0

All (5) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	G	2	C
1	M	2	C
1	H	2	C
1	J	2	C
1	L	2	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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
5	BCM	B	2701	3	14,22,22	1.16	1 (7%)	11,36,36	2.08	1 (9%)
5	BCM	D	4701	-	14,22,22	1.17	1 (7%)	11,36,36	2.09	2 (18%)
4	AGS	C	3600	3	28,33,33	2.23	7 (25%)	31,52,52	1.49	5 (16%)
4	AGS	B	2600	3	28,33,33	2.28	7 (25%)	31,52,52	1.49	4 (12%)
4	AGS	F	6600	3	28,33,33	2.28	7 (25%)	31,52,52	1.48	4 (12%)
4	AGS	A	1600	3	28,33,33	2.33	7 (25%)	31,52,52	1.48	4 (12%)
5	BCM	C	3701	3	14,22,22	1.14	1 (7%)	11,36,36	2.02	1 (9%)
5	BCM	F	6701	-	14,22,22	1.16	1 (7%)	11,36,36	2.00	1 (9%)
4	AGS	E	5600	3,2	28,33,33	2.41	7 (25%)	31,52,52	1.53	4 (12%)
5	BCM	E	5701	3	14,22,22	1.12	1 (7%)	11,36,36	2.11	2 (18%)
4	AGS	D	4600	3	28,33,33	2.33	6 (21%)	31,52,52	1.48	4 (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
5	BCM	B	2701	3	-	6/10/50/50	0/1/2/2
5	BCM	D	4701	-	-	4/10/50/50	0/1/2/2
4	AGS	C	3600	3	-	4/17/38/38	0/3/3/3
4	AGS	B	2600	3	-	2/17/38/38	0/3/3/3
4	AGS	F	6600	3	-	5/17/38/38	0/3/3/3
4	AGS	A	1600	3	-	3/17/38/38	0/3/3/3
5	BCM	C	3701	3	-	4/10/50/50	0/1/2/2
5	BCM	F	6701	-	-	6/10/50/50	0/1/2/2
4	AGS	E	5600	3,2	-	5/17/38/38	0/3/3/3
5	BCM	E	5701	3	-	7/10/50/50	0/1/2/2
4	AGS	D	4600	3	-	7/17/38/38	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	5600	AGS	PG-S1G	8.30	2.08	1.90
4	A	1600	AGS	PG-S1G	7.63	2.07	1.90
4	D	4600	AGS	PG-S1G	7.63	2.07	1.90
4	B	2600	AGS	PG-S1G	7.30	2.06	1.90
4	F	6600	AGS	PG-S1G	7.23	2.06	1.90

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2701	BCM	C7-C6-N10	6.12	117.69	109.66
5	E	5701	BCM	C7-C6-N10	6.12	117.69	109.66
5	D	4701	BCM	C7-C6-N10	6.02	117.56	109.66
5	F	6701	BCM	C7-C6-N10	5.95	117.46	109.66
5	C	3701	BCM	C7-C6-N10	5.91	117.41	109.66

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

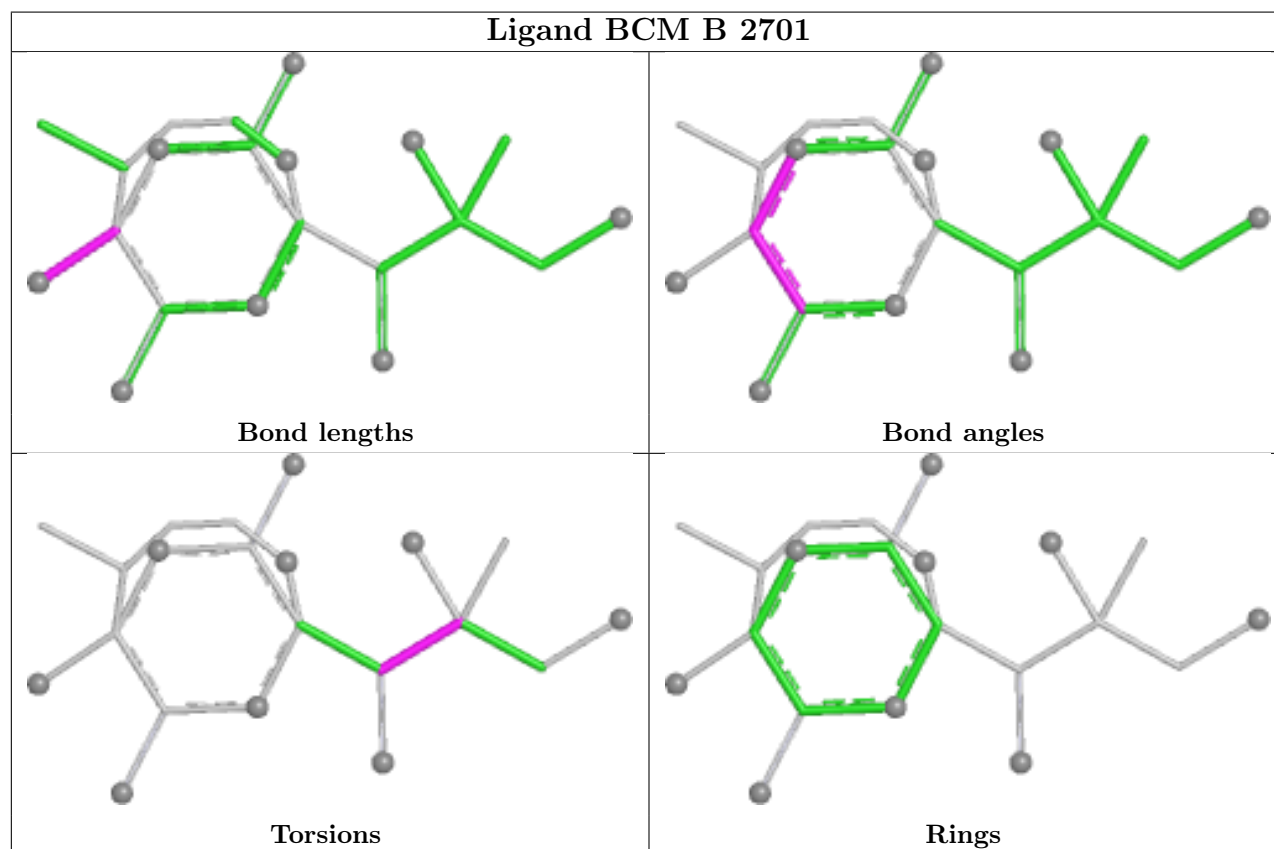
Mol	Chain	Res	Type	Atoms
4	C	3600	AGS	C5'-O5'-PA-O3A
4	D	4600	AGS	C5'-O5'-PA-O2A
4	E	5600	AGS	C5'-O5'-PA-O2A
4	E	5600	AGS	C5'-O5'-PA-O3A
4	F	6600	AGS	C5'-O5'-PA-O3A

There are no ring outliers.

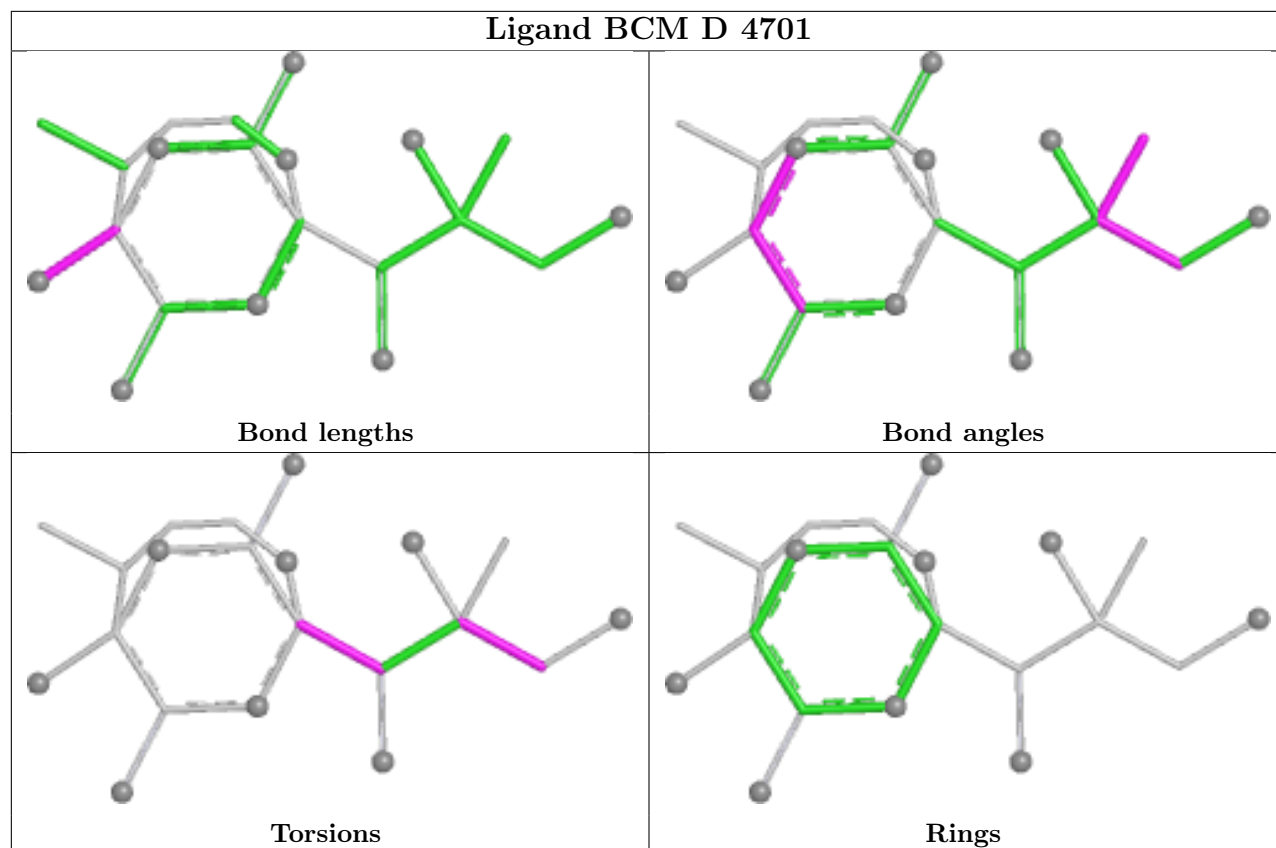
11 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2701	BCM	4	0
5	D	4701	BCM	5	0
4	C	3600	AGS	1	0
4	B	2600	AGS	2	0
4	F	6600	AGS	3	0
4	A	1600	AGS	1	0
5	C	3701	BCM	4	0
5	F	6701	BCM	7	0
4	E	5600	AGS	12	0
5	E	5701	BCM	2	0
4	D	4600	AGS	4	0

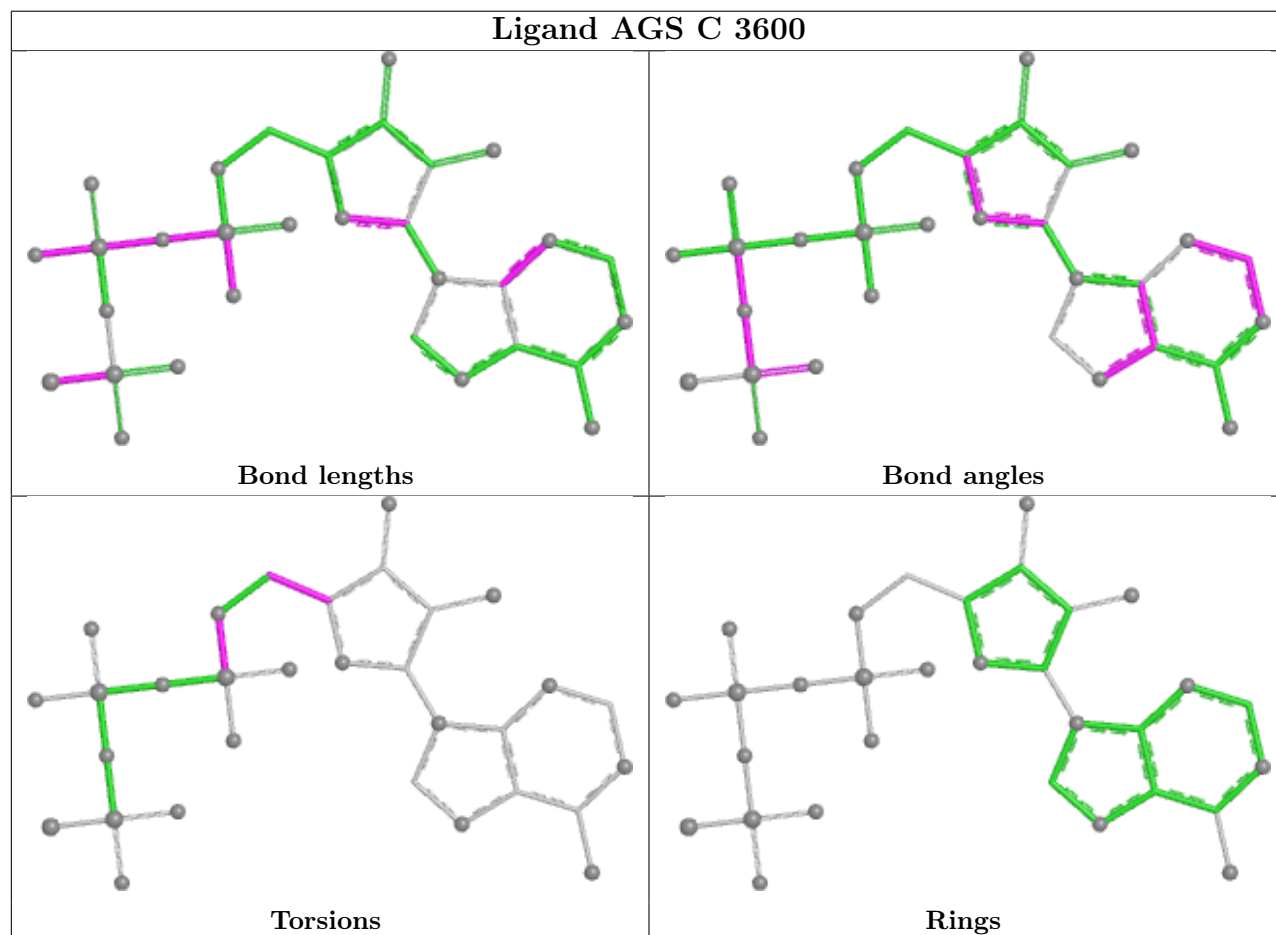
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

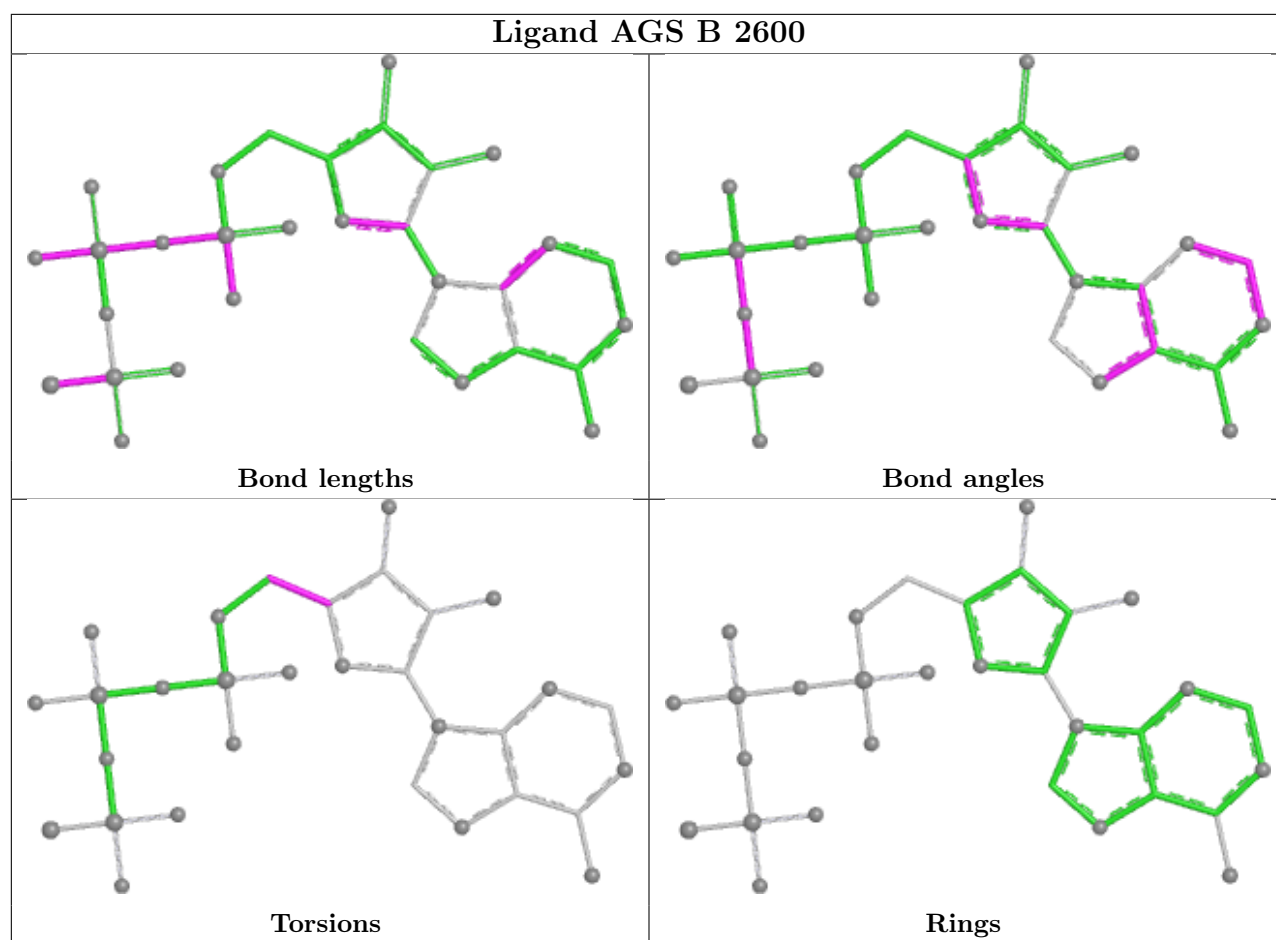


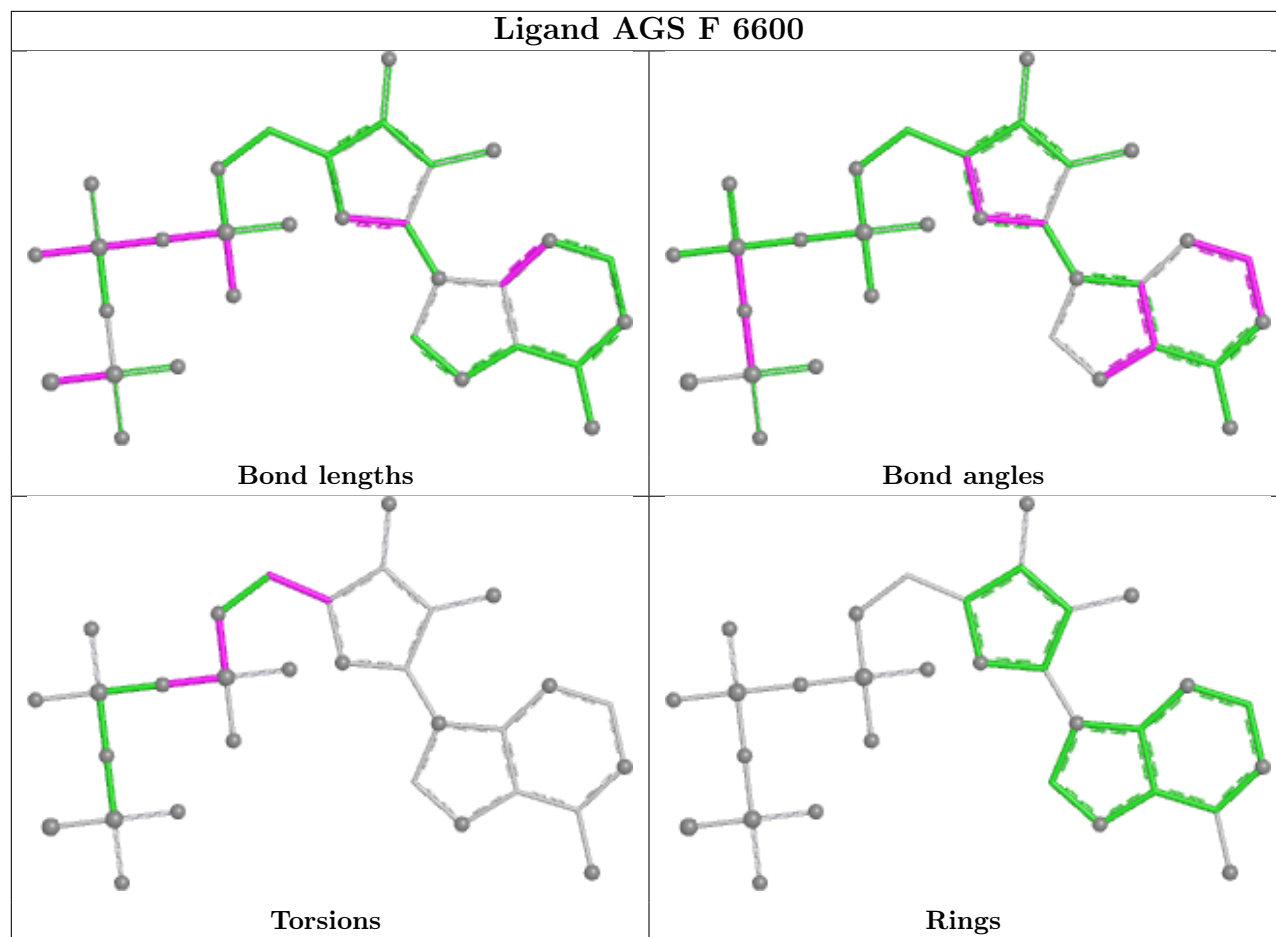
Ligand BCM D 4701

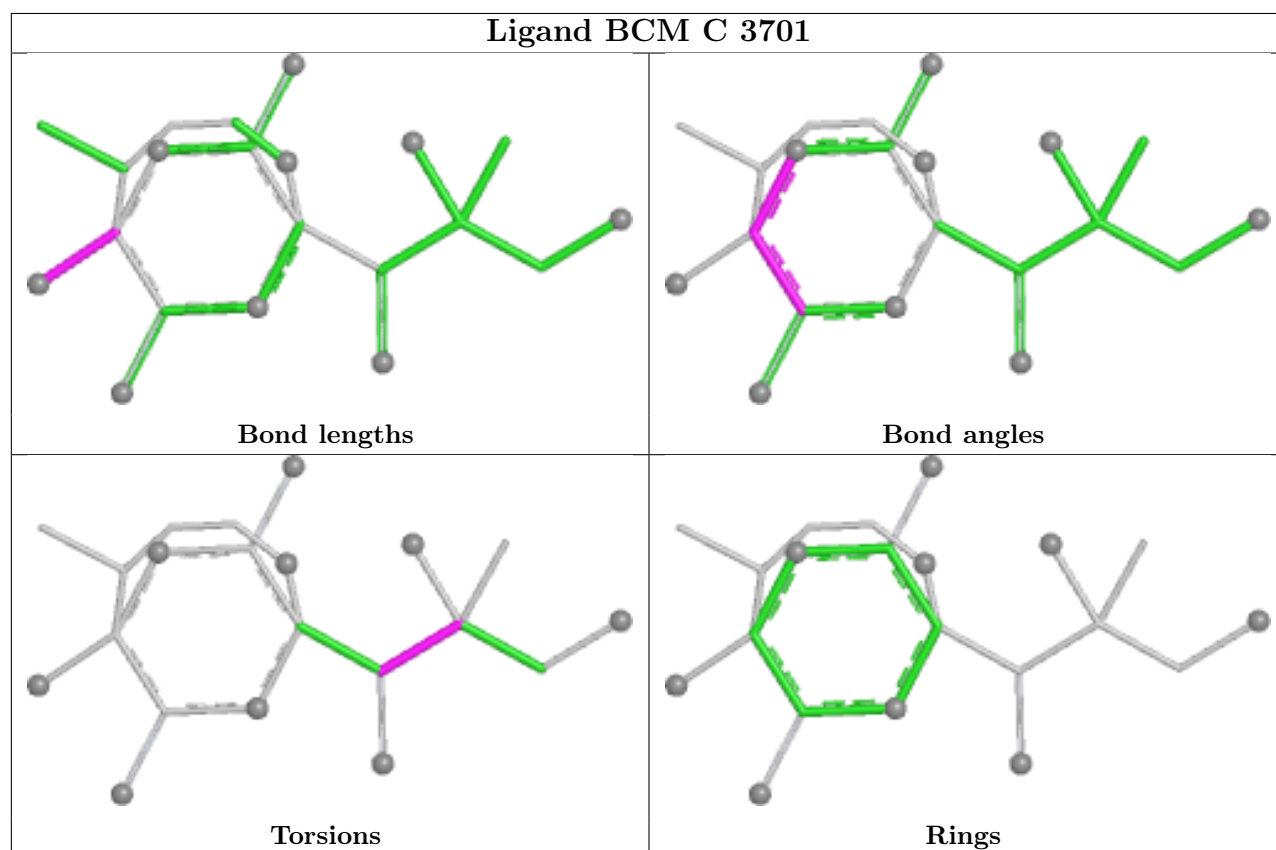
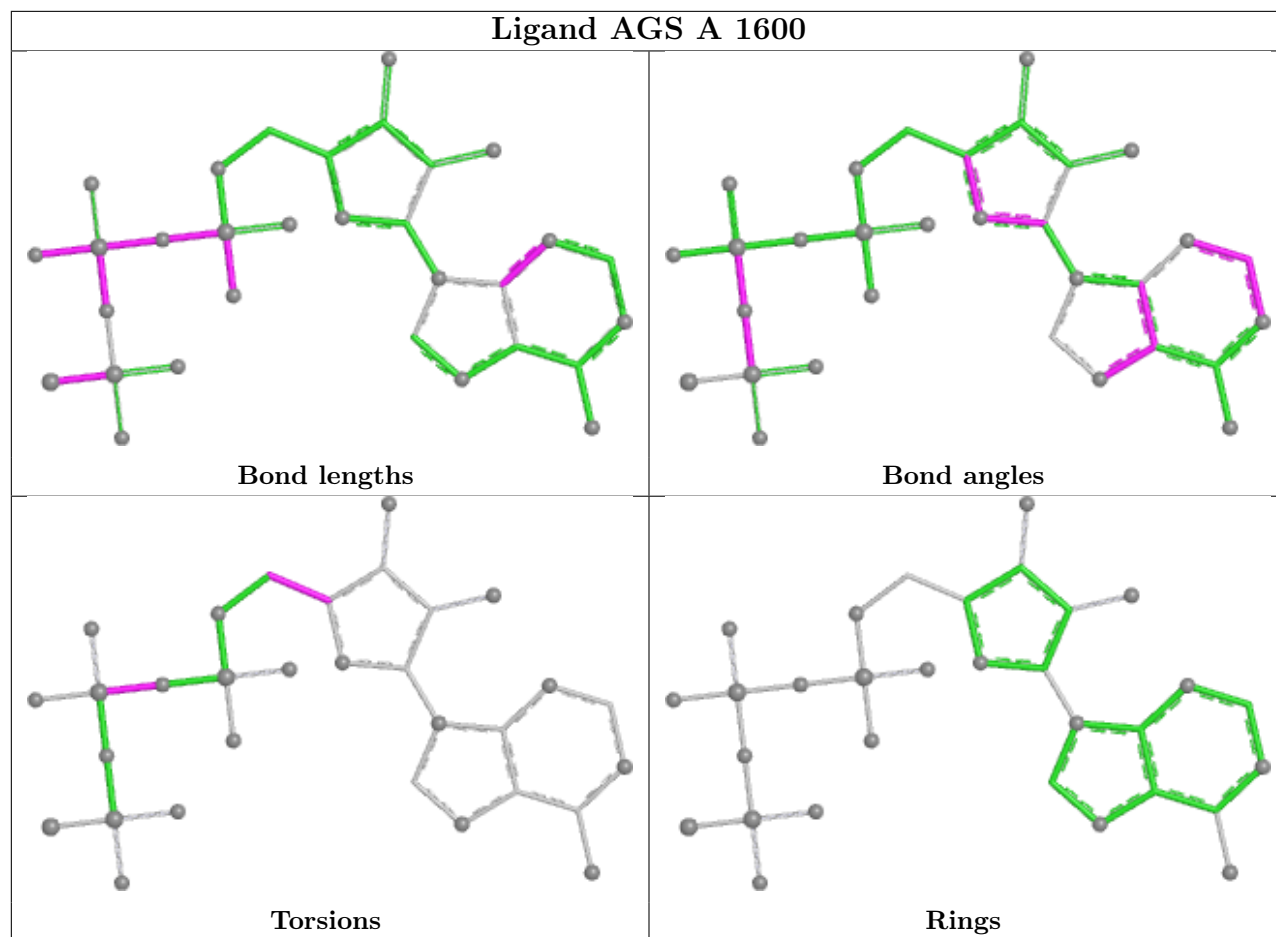


Ligand AGS C 3600

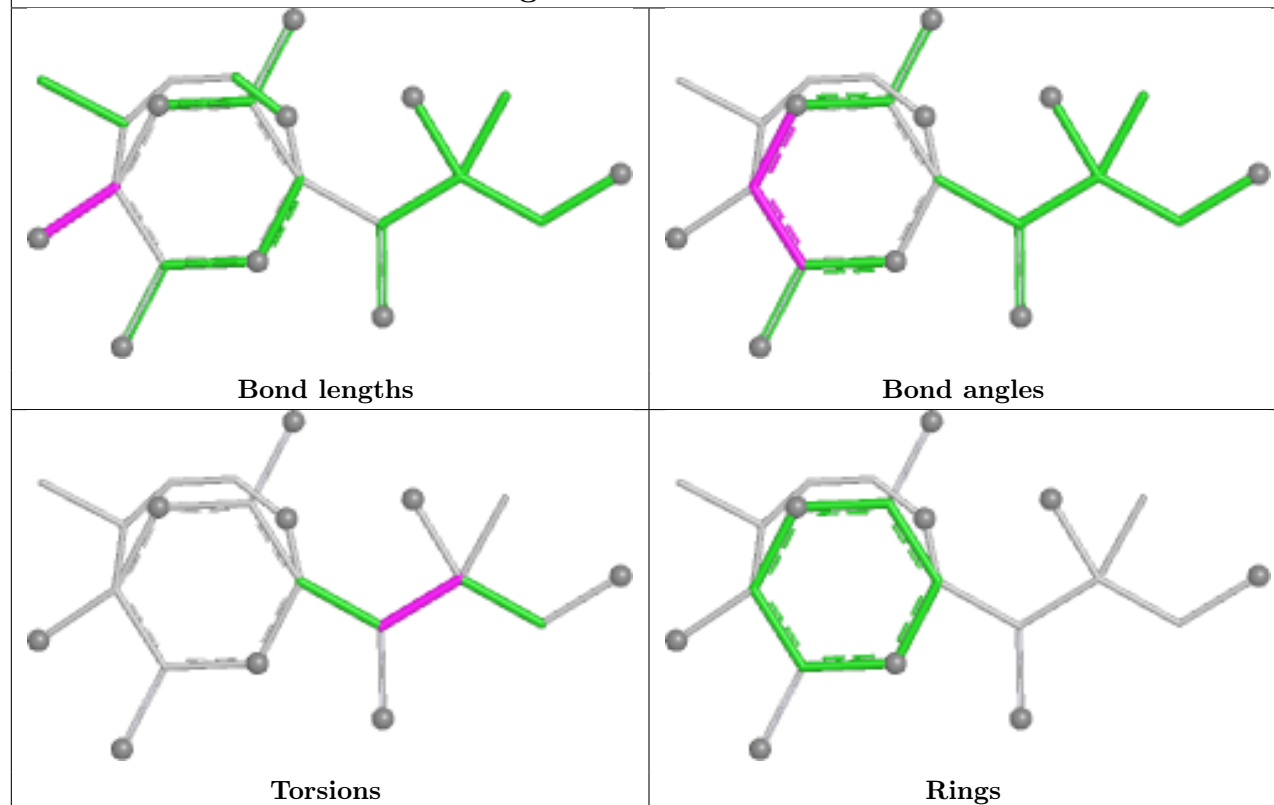




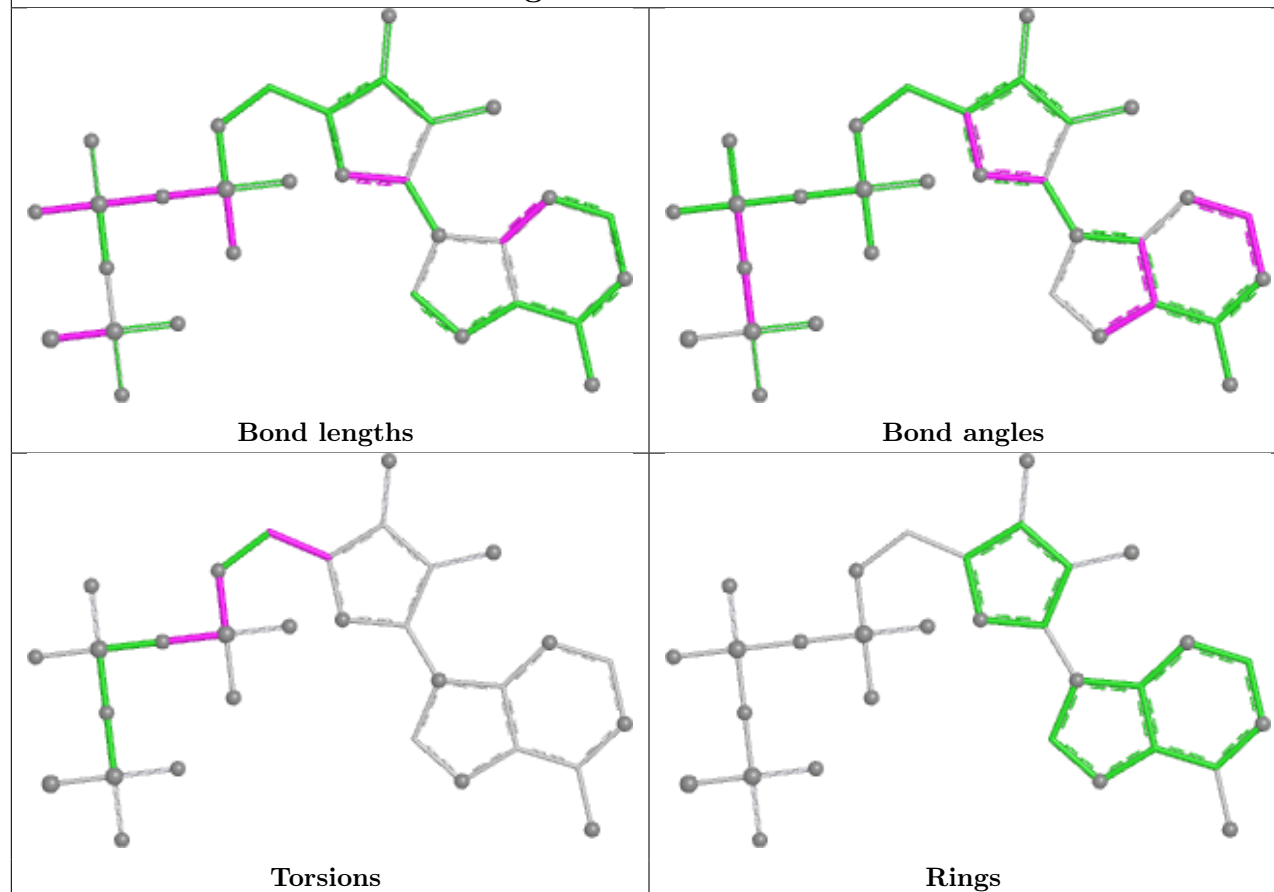




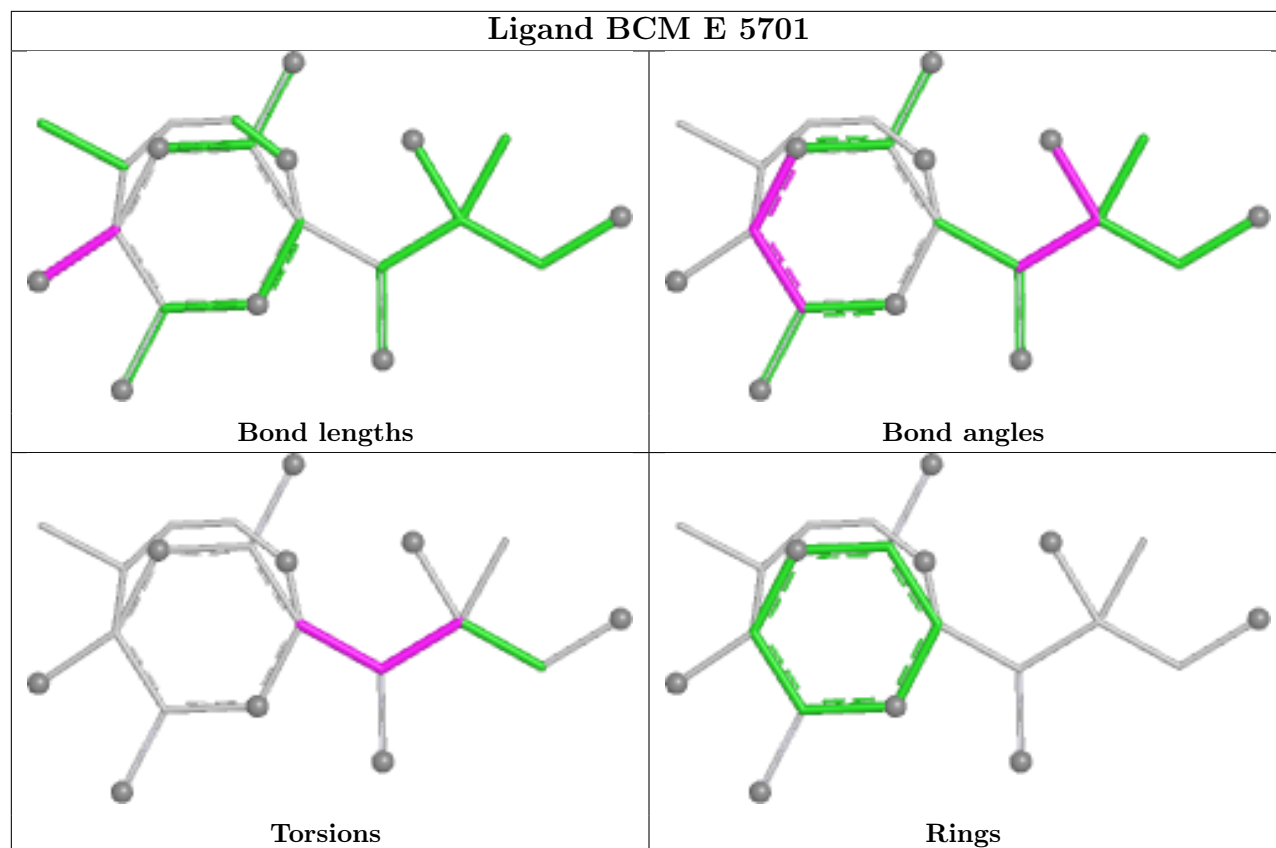
Ligand BCM F 6701



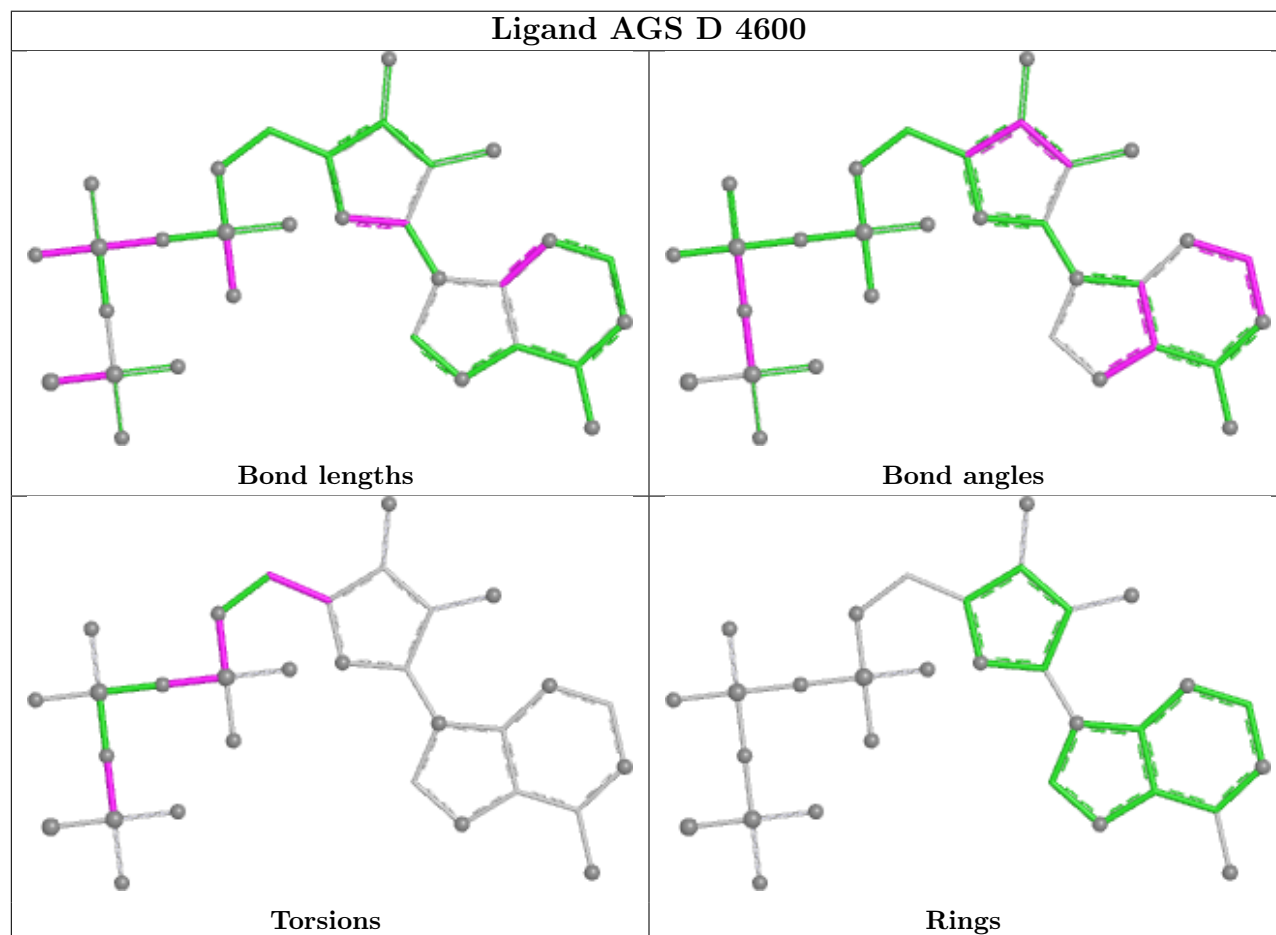
Ligand AGS E 5600



Ligand BCM E 5701



Ligand AGS D 4600



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	G	2/8 (25%)	7.68	2 (100%) 0 0	143, 143, 143, 143	0
1	H	2/8 (25%)	2.88	1 (50%) 0 0	143, 143, 143, 143	0
1	J	2/8 (25%)	2.03	1 (50%) 0 0	143, 143, 143, 143	0
1	K	2/8 (25%)	2.84	2 (100%) 0 0	143, 143, 143, 143	0
1	L	2/8 (25%)	2.84	1 (50%) 0 0	143, 143, 143, 143	0
1	M	2/8 (25%)	5.39	2 (100%) 0 0	143, 143, 143, 143	0
2	A	408/419 (97%)	0.25	18 (4%) 34 20	64, 96, 139, 140	0
2	B	408/419 (97%)	0.21	23 (5%) 24 12	56, 92, 125, 139	0
2	C	408/419 (97%)	0.07	12 (2%) 51 35	46, 68, 120, 124	0
2	D	408/419 (97%)	0.10	5 (1%) 79 68	52, 79, 114, 138	0
2	E	407/419 (97%)	0.10	11 (2%) 54 38	53, 80, 122, 139	0
2	F	408/419 (97%)	0.13	9 (2%) 62 47	60, 88, 128, 138	0
All	All	2459/2562 (95%)	0.16	87 (3%) 44 27	46, 85, 137, 143	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	2	C	7.8
1	G	1	U	7.6
1	M	2	C	6.7
2	C	138	PRO	6.5
2	B	415	MET	5.3

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

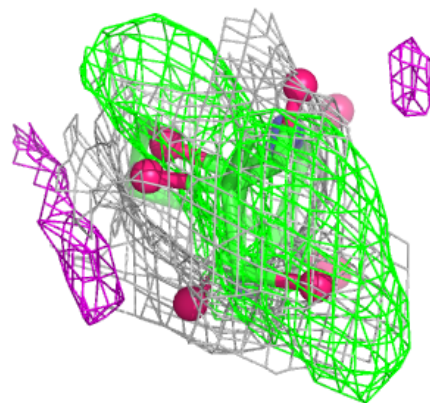
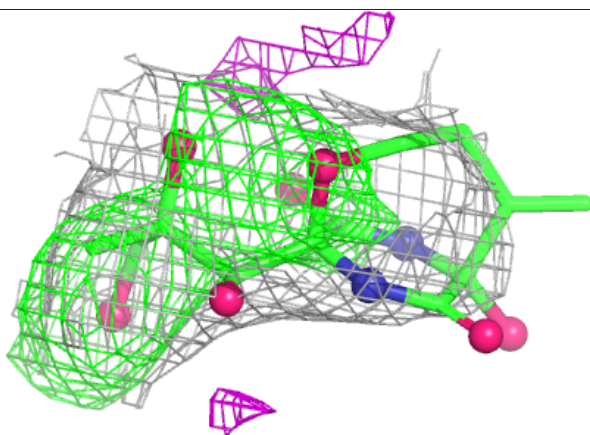
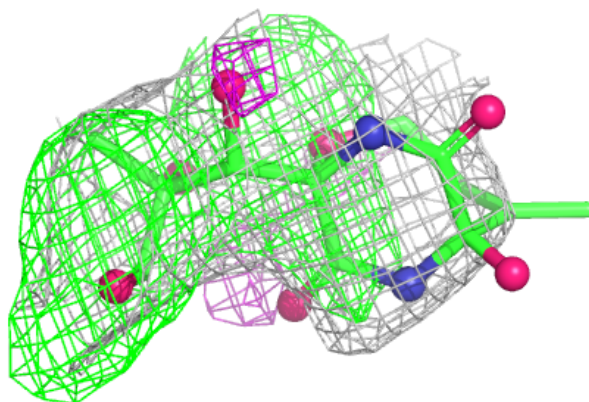
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	3601	1/1	0.46	0.37	89,89,89,89	0
5	BCM	F	6701	21/21	0.58	0.59	78,78,79,79	0
4	AGS	C	3600	31/31	0.69	0.41	93,95,104,104	0
3	MG	A	1601	1/1	0.72	0.20	89,89,89,89	0
3	MG	E	5601	1/1	0.72	0.32	82,82,82,82	0
5	BCM	D	4701	21/21	0.77	0.48	77,77,77,77	0
5	BCM	C	3701	21/21	0.77	0.40	77,77,77,77	0
4	AGS	B	2600	31/31	0.78	0.33	93,96,104,104	0
4	AGS	F	6600	31/31	0.79	0.42	92,95,104,104	0
5	BCM	E	5701	21/21	0.80	0.46	86,86,86,86	0
5	BCM	B	2701	21/21	0.81	0.26	76,76,76,76	0
4	AGS	A	1600	31/31	0.83	0.22	93,95,104,104	0
4	AGS	D	4600	31/31	0.84	0.30	93,95,103,104	0
4	AGS	E	5600	31/31	0.86	0.23	93,95,104,104	0
3	MG	F	6601	1/1	0.88	0.18	69,69,69,69	0
3	MG	B	2601	1/1	0.93	0.61	85,85,85,85	0
3	MG	D	4601	1/1	0.94	0.51	70,70,70,70	0

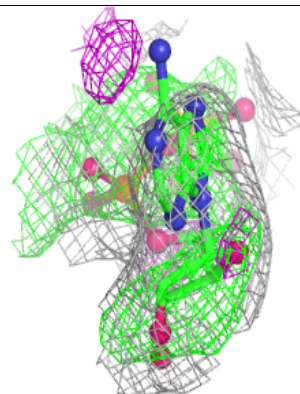
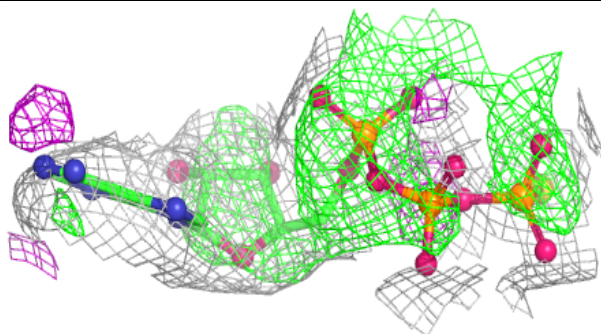
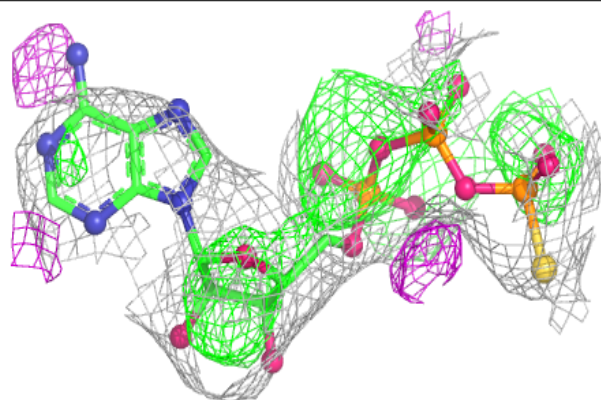
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BCM F 6701:

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

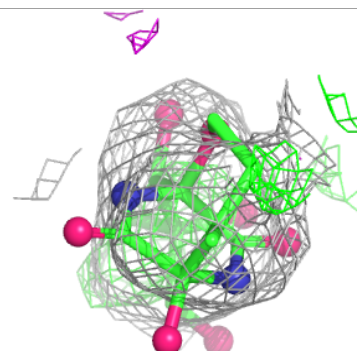
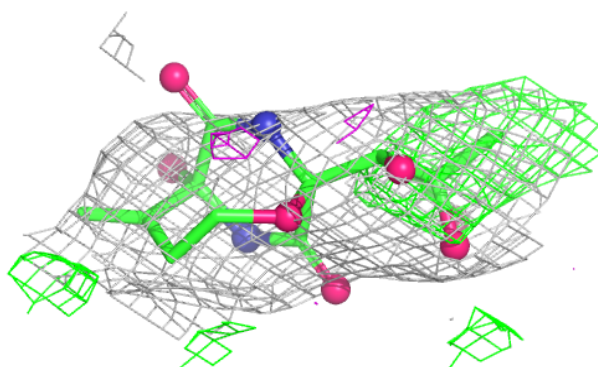
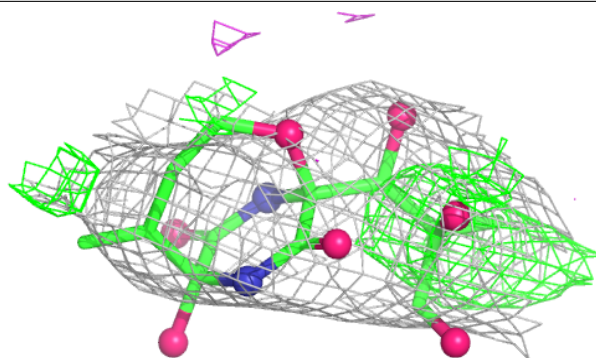
**Electron density around AGS C 3600:**

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

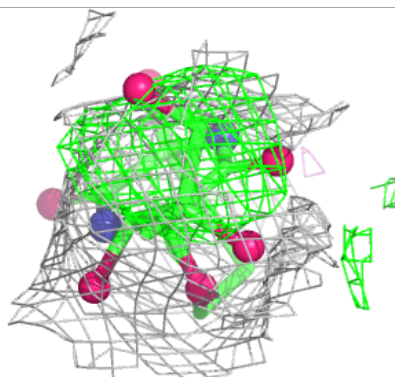
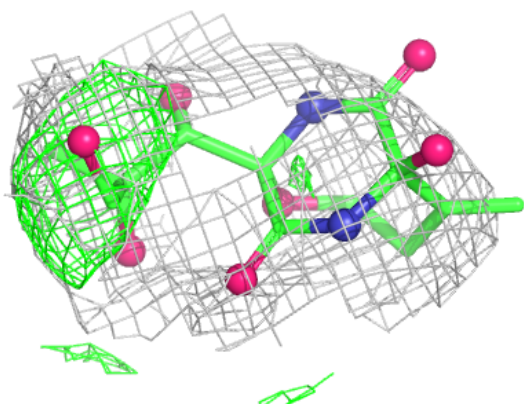
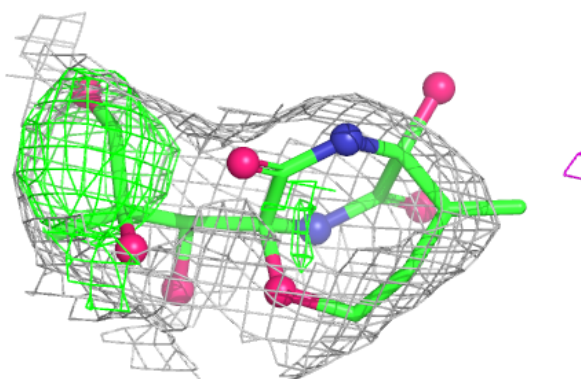


Electron density around BCM D 4701:

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

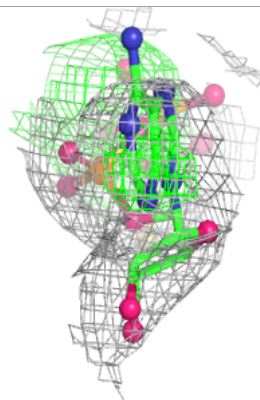
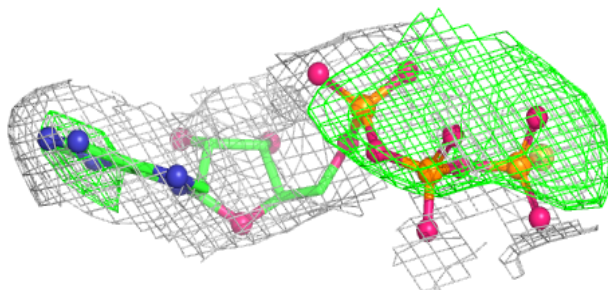
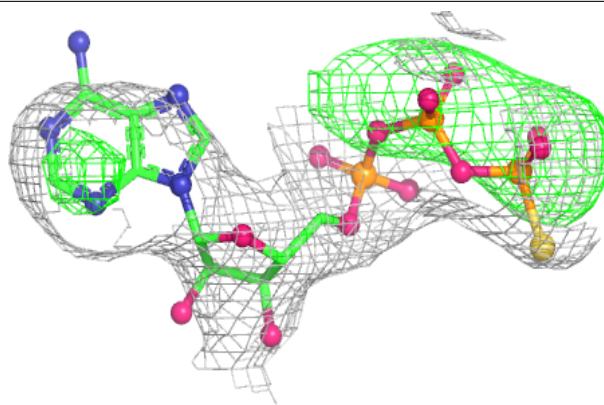
**Electron density around BCM C 3701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

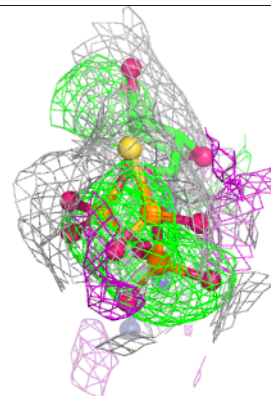
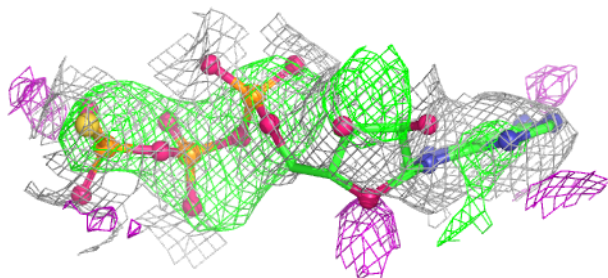
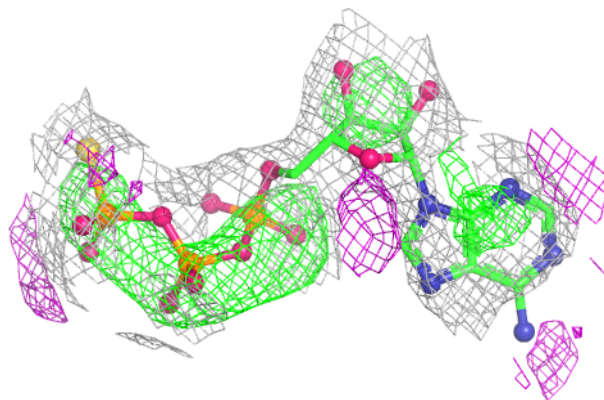


Electron density around AGS B 2600:

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

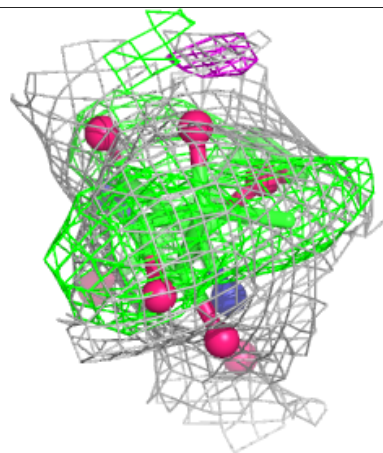
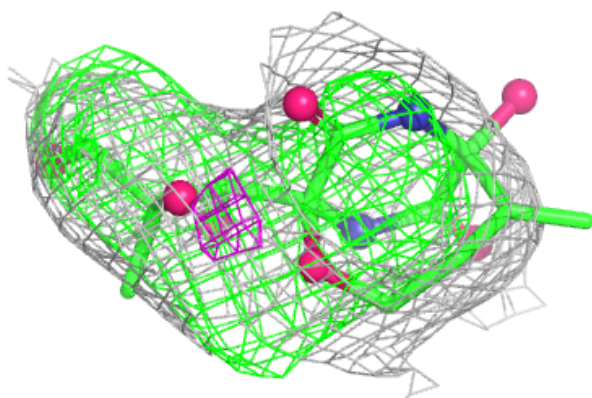
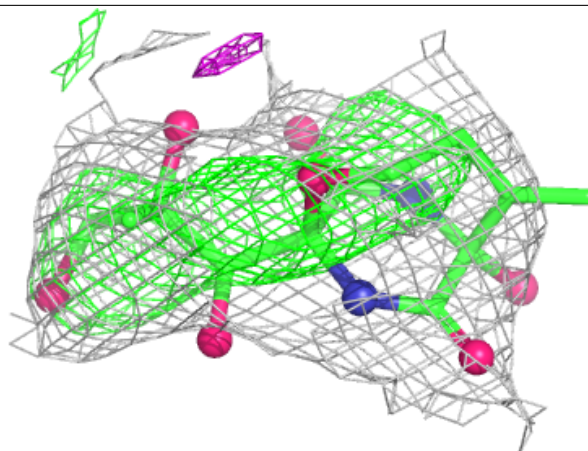
**Electron density around AGS F 6600:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



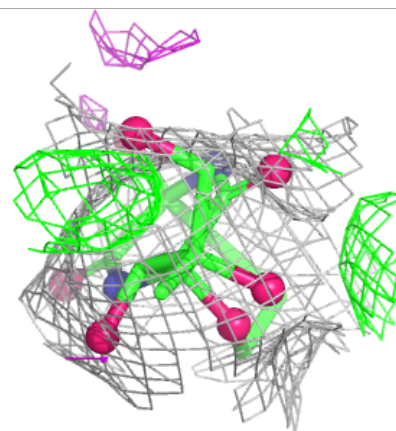
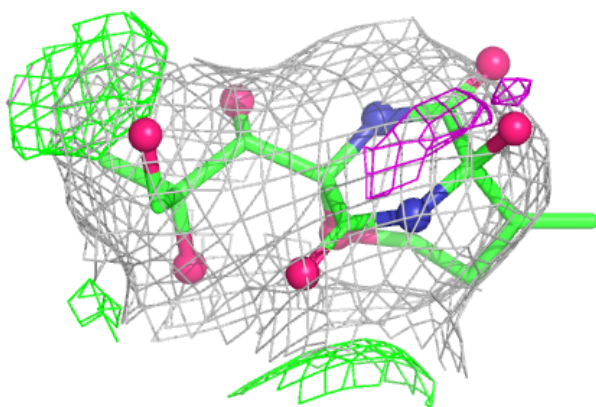
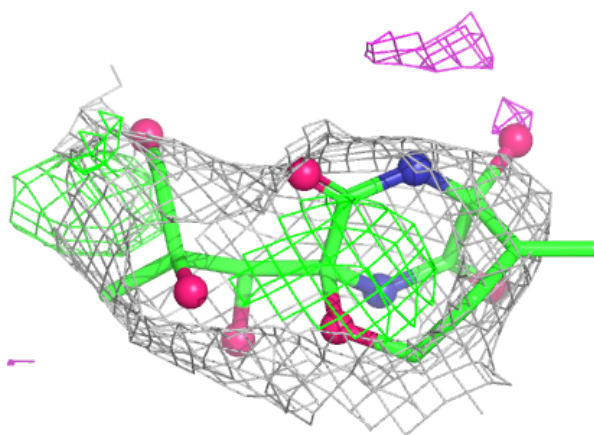
Electron density around BCM E 5701:

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



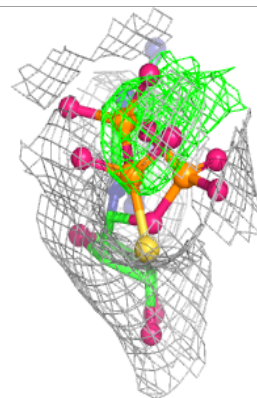
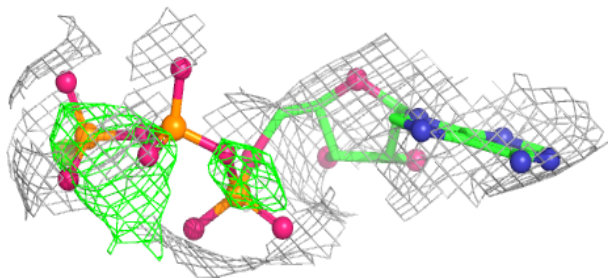
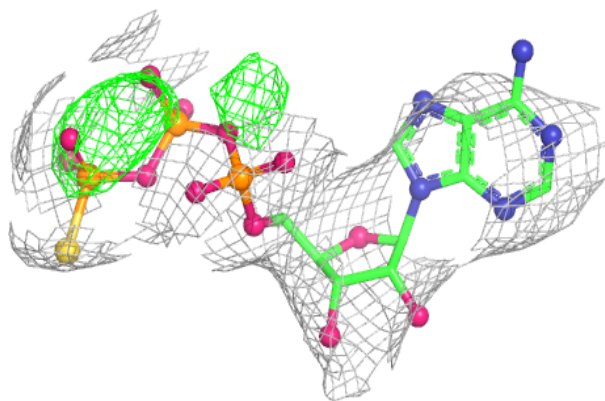
Electron density around BCM B 2701:

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

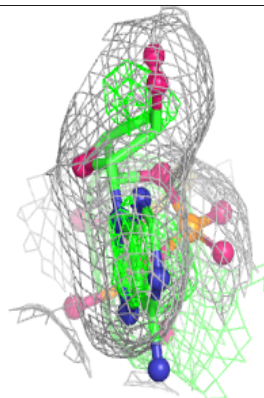
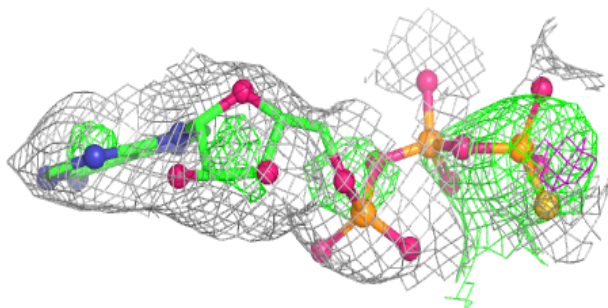
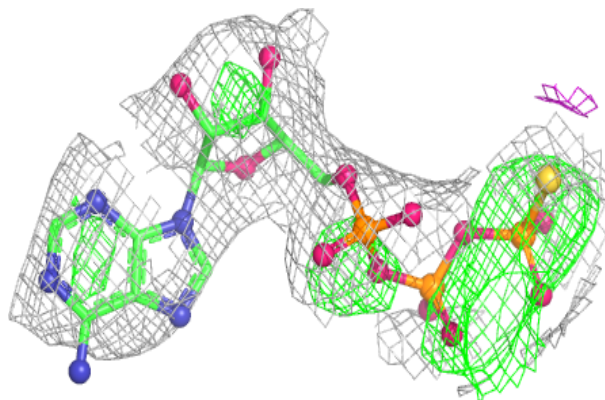


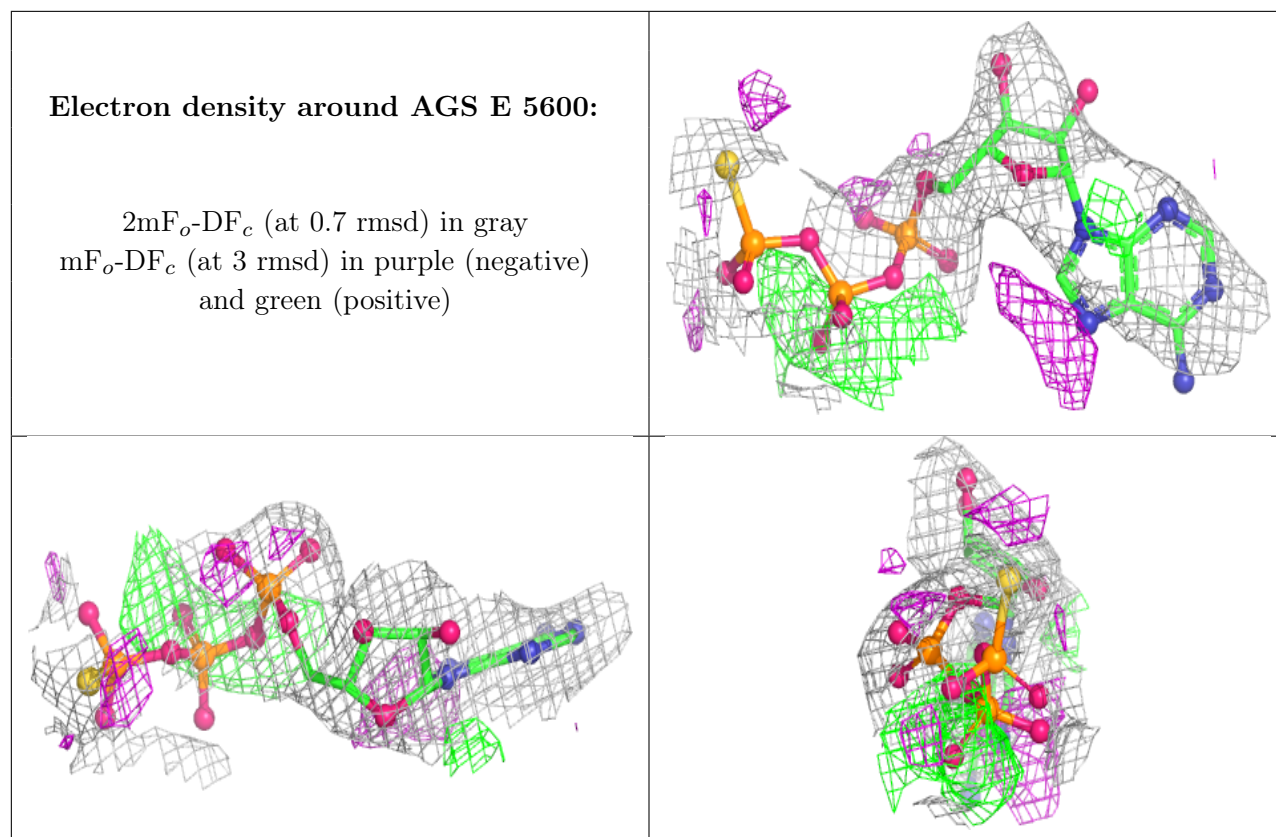
Electron density around AGS A 1600:

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

**Electron density around AGS D 4600:**

$2mF_o-DF_c$ (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.