



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:15 PM UTC

PDB ID : 5J5I / pdb_00005j5i
Title : X-Ray Crystal Structure of Acetylcholine Binding Protein (AChBP) in Complex with 4-(2-amino-6-{bis[(pyridin-2-yl)methyl]amino}pyrimidin-4-yl)phenol
Authors : Kaczanowska, K.; Harel, M.; Camacho Hernandez, G.A.; Taylor, P.
Deposited on : 2016-04-02
Resolution : 2.33 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 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

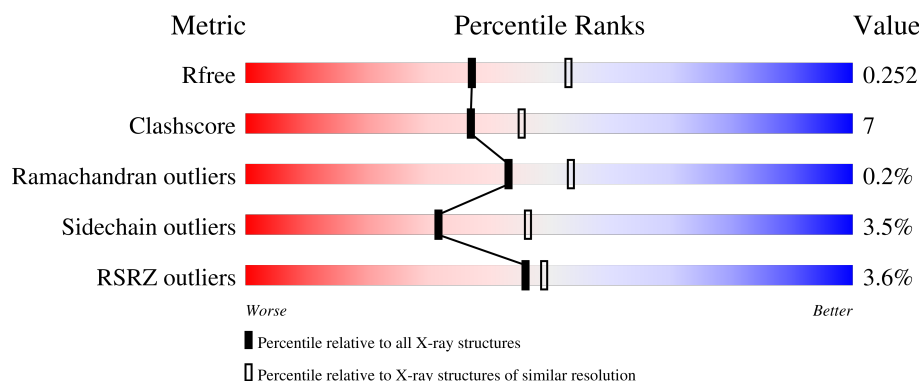
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

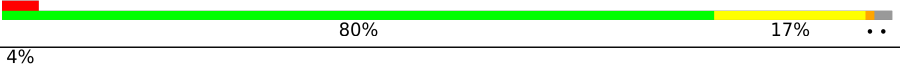
The reported resolution of this entry is 2.33 Å.

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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	A	218	
1	B	218	
1	C	218	
1	D	218	

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Mol	Chain	Length	Quality of chain
1	E	218	% 78% 18% • •
1	F	218	3% 74% 22% • •
1	G	218	6% 77% 20% • •
1	H	218	6% 77% 18% • •
1	I	218	% 82% 14% • •
1	J	218	3% 77% 18% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18123 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	4	0
			1725	1076	293	351	5			
1	B	213	Total	C	N	O	S	0	1	0
			1709	1066	290	348	5			
1	C	213	Total	C	N	O	S	0	0	0
			1706	1064	290	347	5			
1	D	213	Total	C	N	O	S	0	2	0
			1716	1071	290	350	5			
1	E	212	Total	C	N	O	S	0	2	0
			1715	1070	292	348	5			
1	F	212	Total	C	N	O	S	0	0	0
			1702	1062	289	346	5			
1	G	214	Total	C	N	O	S	0	1	0
			1726	1078	294	349	5			
1	H	212	Total	C	N	O	S	0	0	0
			1702	1062	289	346	5			
1	I	212	Total	C	N	O	S	4	2	0
			1710	1068	289	348	5			
1	J	212	Total	C	N	O	S	0	1	0
			1707	1065	289	348	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P58154
A	-6	TYR	-	expression tag	UNP P58154
A	-5	LYS	-	expression tag	UNP P58154
A	-4	ASP	-	expression tag	UNP P58154
A	-3	ASP	-	expression tag	UNP P58154
A	-2	ASP	-	expression tag	UNP P58154
A	-1	ASP	-	expression tag	UNP P58154
A	0	LYS	-	expression tag	UNP P58154
B	-7	ASP	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP P58154
B	-5	LYS	-	expression tag	UNP P58154
B	-4	ASP	-	expression tag	UNP P58154
B	-3	ASP	-	expression tag	UNP P58154
B	-2	ASP	-	expression tag	UNP P58154
B	-1	ASP	-	expression tag	UNP P58154
B	0	LYS	-	expression tag	UNP P58154
C	-7	ASP	-	expression tag	UNP P58154
C	-6	TYR	-	expression tag	UNP P58154
C	-5	LYS	-	expression tag	UNP P58154
C	-4	ASP	-	expression tag	UNP P58154
C	-3	ASP	-	expression tag	UNP P58154
C	-2	ASP	-	expression tag	UNP P58154
C	-1	ASP	-	expression tag	UNP P58154
C	0	LYS	-	expression tag	UNP P58154
D	-7	ASP	-	expression tag	UNP P58154
D	-6	TYR	-	expression tag	UNP P58154
D	-5	LYS	-	expression tag	UNP P58154
D	-4	ASP	-	expression tag	UNP P58154
D	-3	ASP	-	expression tag	UNP P58154
D	-2	ASP	-	expression tag	UNP P58154
D	-1	ASP	-	expression tag	UNP P58154
D	0	LYS	-	expression tag	UNP P58154
E	-7	ASP	-	expression tag	UNP P58154
E	-6	TYR	-	expression tag	UNP P58154
E	-5	LYS	-	expression tag	UNP P58154
E	-4	ASP	-	expression tag	UNP P58154
E	-3	ASP	-	expression tag	UNP P58154
E	-2	ASP	-	expression tag	UNP P58154
E	-1	ASP	-	expression tag	UNP P58154
E	0	LYS	-	expression tag	UNP P58154
F	-7	ASP	-	expression tag	UNP P58154
F	-6	TYR	-	expression tag	UNP P58154
F	-5	LYS	-	expression tag	UNP P58154
F	-4	ASP	-	expression tag	UNP P58154
F	-3	ASP	-	expression tag	UNP P58154
F	-2	ASP	-	expression tag	UNP P58154
F	-1	ASP	-	expression tag	UNP P58154
F	0	LYS	-	expression tag	UNP P58154
G	-7	ASP	-	expression tag	UNP P58154
G	-6	TYR	-	expression tag	UNP P58154
G	-5	LYS	-	expression tag	UNP P58154

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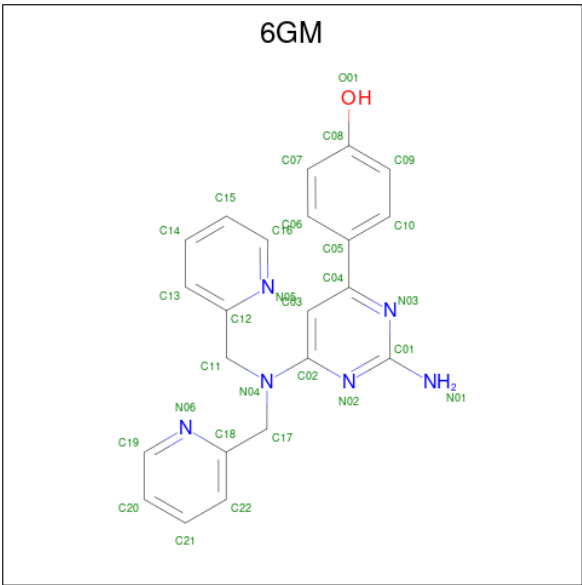
Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ASP	-	expression tag	UNP P58154
G	-3	ASP	-	expression tag	UNP P58154
G	-2	ASP	-	expression tag	UNP P58154
G	-1	ASP	-	expression tag	UNP P58154
G	0	LYS	-	expression tag	UNP P58154
H	-7	ASP	-	expression tag	UNP P58154
H	-6	TYR	-	expression tag	UNP P58154
H	-5	LYS	-	expression tag	UNP P58154
H	-4	ASP	-	expression tag	UNP P58154
H	-3	ASP	-	expression tag	UNP P58154
H	-2	ASP	-	expression tag	UNP P58154
H	-1	ASP	-	expression tag	UNP P58154
H	0	LYS	-	expression tag	UNP P58154
I	-7	ASP	-	expression tag	UNP P58154
I	-6	TYR	-	expression tag	UNP P58154
I	-5	LYS	-	expression tag	UNP P58154
I	-4	ASP	-	expression tag	UNP P58154
I	-3	ASP	-	expression tag	UNP P58154
I	-2	ASP	-	expression tag	UNP P58154
I	-1	ASP	-	expression tag	UNP P58154
I	0	LYS	-	expression tag	UNP P58154
J	-7	ASP	-	expression tag	UNP P58154
J	-6	TYR	-	expression tag	UNP P58154
J	-5	LYS	-	expression tag	UNP P58154
J	-4	ASP	-	expression tag	UNP P58154
J	-3	ASP	-	expression tag	UNP P58154
J	-2	ASP	-	expression tag	UNP P58154
J	-1	ASP	-	expression tag	UNP P58154
J	0	LYS	-	expression tag	UNP P58154

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-(2-amino-6-{bis[(pyridin-2-yl)methyl]amino}pyrimidin-4-yl)phenol (CCD ID: 6GM) (formula: C₂₂H₂₀N₆O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	22	6	1		
3	A	1	Total	C	N	O	0	0
			29	22	6	1		
3	B	1	Total	C	N	O	0	0
			29	22	6	1		
3	C	1	Total	C	N	O	0	0
			29	22	6	1		
3	E	1	Total	C	N	O	0	0
			29	22	6	1		
3	F	1	Total	C	N	O	0	0
			29	22	6	1		
3	F	1	Total	C	N	O	0	0
			29	22	6	1		
3	G	1	Total	C	N	O	0	0
			29	22	6	1		
3	I	1	Total	C	N	O	0	0
			29	22	6	1		
3	I	1	Total	C	N	O	0	0
			29	22	6	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		
4	G	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	H	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	I	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		
4	J	1	Total	O	P	0	0
			5	4	1		

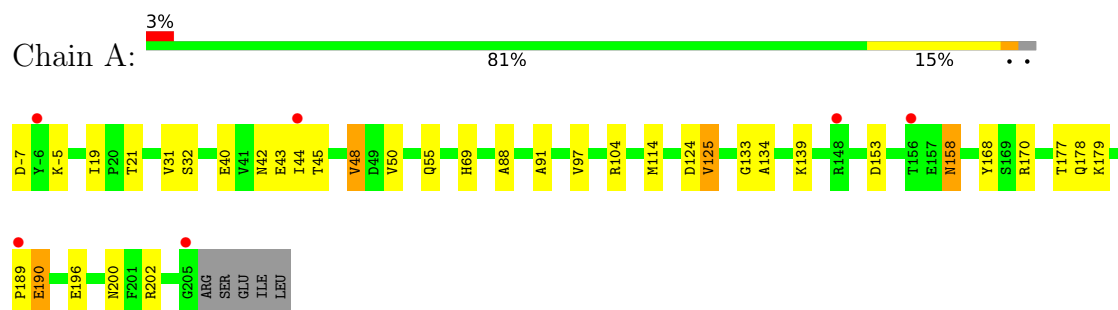
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	54	Total	O	0	0
			54	54		
5	B	45	Total	O	0	0
			45	45		
5	C	49	Total	O	0	0
			49	49		
5	D	55	Total	O	0	0
			55	55		
5	E	68	Total	O	0	0
			68	68		
5	F	38	Total	O	0	0
			38	38		
5	G	30	Total	O	0	0
			30	30		
5	H	34	Total	O	0	0
			34	34		
5	I	45	Total	O	0	0
			45	45		
5	J	52	Total	O	0	0
			52	52		

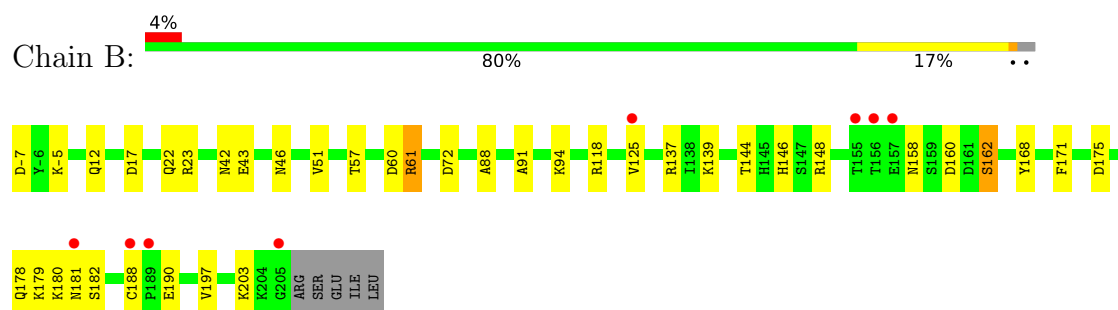
3 Residue-property plots [i](#)

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.

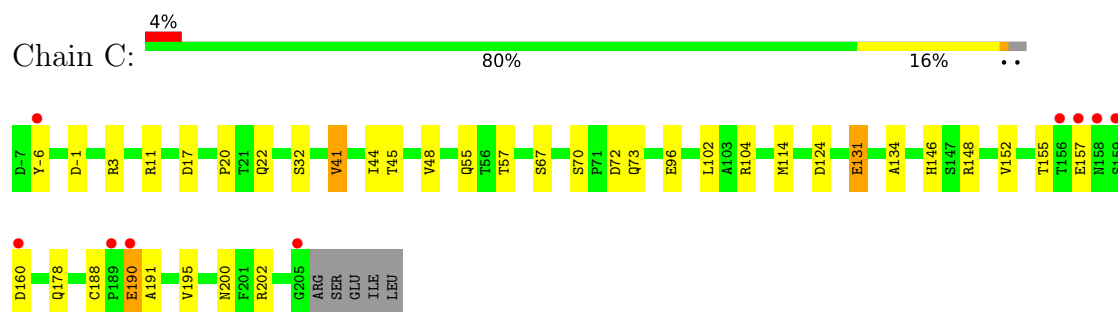
• Molecule 1: Acetylcholine-binding protein



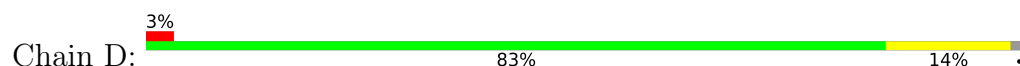
• Molecule 1: Acetylcholine-binding protein

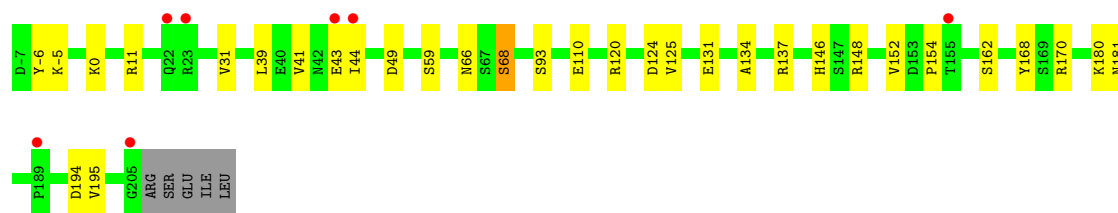


• Molecule 1: Acetylcholine-binding protein

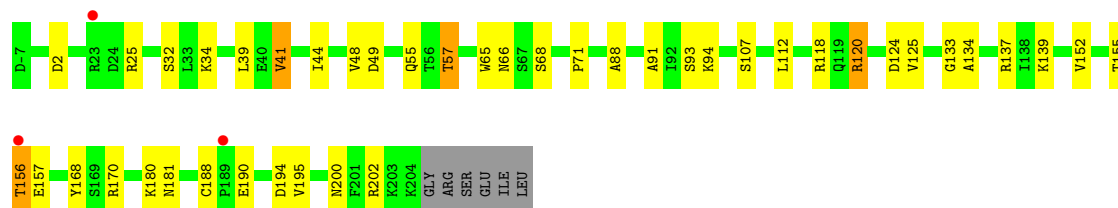
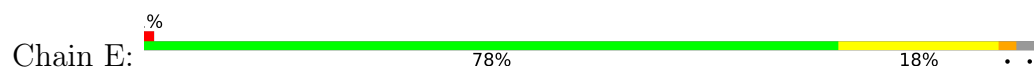


• Molecule 1: Acetylcholine-binding protein

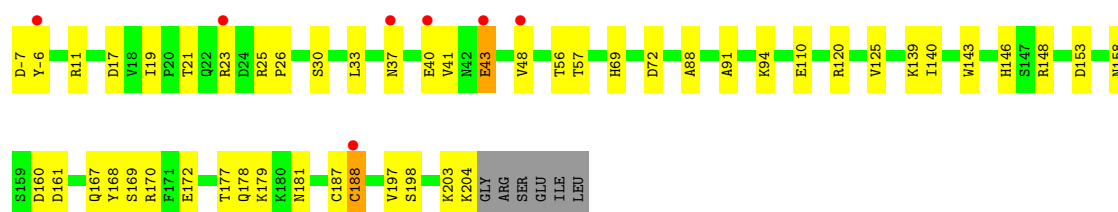
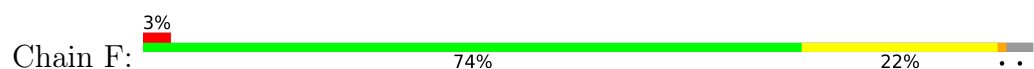




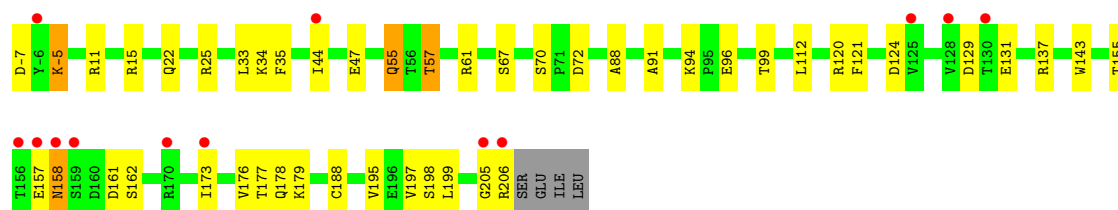
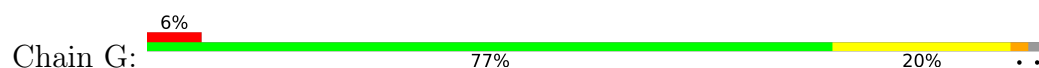
• Molecule 1: Acetylcholine-binding protein



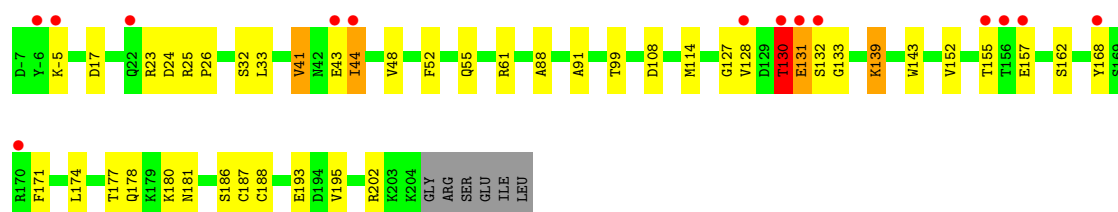
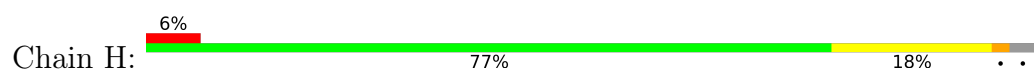
• Molecule 1: Acetylcholine-binding protein



• Molecule 1: Acetylcholine-binding protein

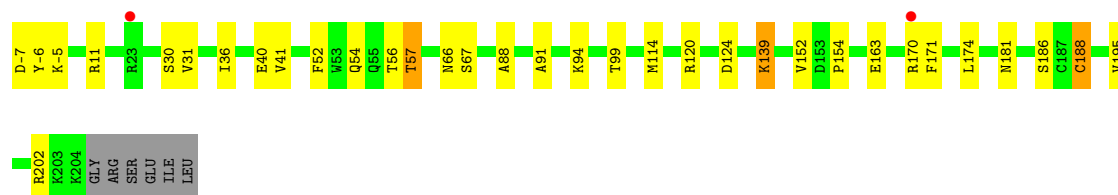


• Molecule 1: Acetylcholine-binding protein



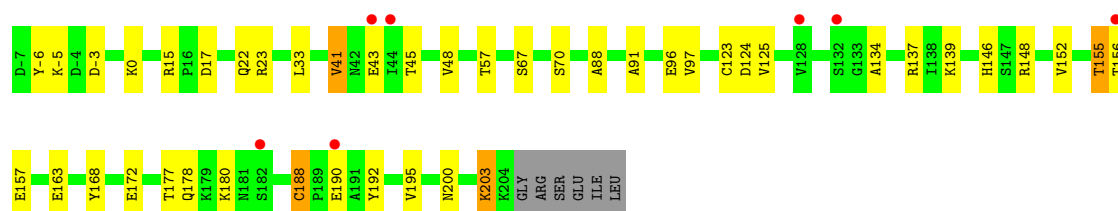
- Molecule 1: Acetylcholine-binding protein

Chain I:  82% 14% ..



- Molecule 1: Acetylcholine-binding protein

Chain J:  77% 18% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.14Å 127.01Å 122.12Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	43.57 – 2.33 43.57 – 2.33	Depositor EDS
% Data completeness (in resolution range)	97.8 (43.57-2.33) 97.8 (43.57-2.33)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.32Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.250 0.194 , 0.252	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18123	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: 6GM, NAG, PO4

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	0.55	0/1771	0.84	3/2414 (0.1%)
1	B	0.53	0/1749	0.84	2/2385 (0.1%)
1	C	0.53	0/1743	0.83	1/2377 (0.0%)
1	D	0.55	0/1759	0.83	0/2399
1	E	0.56	0/1758	0.81	2/2398 (0.1%)
1	F	0.52	0/1739	0.79	0/2372
1	G	0.46	0/1767	0.84	6/2409 (0.2%)
1	H	0.53	0/1739	0.85	2/2372 (0.1%)
1	I	0.52	0/1753	0.85	2/2392 (0.1%)
1	J	0.52	0/1747	0.78	2/2383 (0.1%)
All	All	0.53	0/17525	0.83	20/23901 (0.1%)

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	B	0	1
1	H	0	1
All	All	0	2

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	188	CYS	CA-C-N	7.85	127.92	119.28
1	I	188	CYS	C-N-CA	7.85	127.92	119.28
1	H	131	GLU	N-CA-C	7.53	126.85	110.80
1	B	188	CYS	CA-C-N	6.99	126.81	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	CYS	C-N-CA	6.99	126.81	119.05
1	G	94	LYS	CA-C-N	-5.83	113.94	119.76
1	G	94	LYS	C-N-CA	-5.83	113.94	119.76
1	A	153	ASP	CA-C-N	5.76	125.69	119.76
1	A	153	ASP	C-N-CA	5.76	125.69	119.76
1	E	188	CYS	CA-C-N	5.74	125.27	119.19
1	E	188	CYS	C-N-CA	5.74	125.27	119.19
1	C	160	ASP	N-CA-C	-5.72	106.17	114.12
1	G	188	CYS	CA-C-N	5.70	125.80	119.87
1	G	188	CYS	C-N-CA	5.70	125.80	119.87
1	H	130	THR	N-CA-C	-5.43	101.38	109.96
1	J	188	CYS	CA-C-N	5.27	124.96	119.64
1	J	188	CYS	C-N-CA	5.27	124.96	119.64
1	G	15	ARG	CA-C-N	5.22	124.89	119.56
1	G	15	ARG	C-N-CA	5.22	124.89	119.56
1	A	158	ASN	N-CA-C	5.03	116.60	108.26

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	180	LYS	Peptide
1	H	130	THR	Peptide

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	1725	0	1648	23	0
1	B	1709	0	1640	29	0
1	C	1706	0	1634	22	0
1	D	1716	0	1648	22	0
1	E	1715	0	1648	31	1
1	F	1702	0	1632	34	0
1	G	1726	0	1657	30	0
1	H	1702	0	1632	33	0
1	I	1710	0	1645	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1707	0	1638	26	1
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
2	E	14	0	13	1	0
2	F	14	0	13	1	0
2	G	14	0	13	1	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
3	A	58	0	0	0	0
3	B	29	0	0	0	0
3	C	29	0	0	0	0
3	E	29	0	0	1	0
3	F	58	0	0	3	0
3	G	29	0	0	0	0
3	I	58	0	0	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	20	0	0	0	0
4	E	10	0	0	0	0
4	F	15	0	0	1	0
4	G	5	0	0	1	0
4	H	15	0	0	0	0
4	I	10	0	0	0	0
4	J	10	0	0	0	0
5	A	54	0	0	0	1
5	B	45	0	0	0	0
5	C	49	0	0	1	0
5	D	55	0	0	0	1
5	E	68	0	0	2	0
5	F	38	0	0	0	0
5	G	30	0	0	0	0
5	H	34	0	0	1	0
5	I	45	0	0	1	0
5	J	52	0	0	1	0
All	All	18123	0	16552	243	2

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 (243) 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:F:25:ARG:HD3	1:F:26:PRO:HD2	1.42	0.99
1:G:158:ASN:HD21	1:G:177:THR:HG22	1.29	0.95
1:H:130:THR:C	1:H:131:GLU:HG2	2.00	0.85
1:I:94:LYS:HE3	1:J:96:GLU:HG3	1.59	0.84
1:D:43:GLU:O	1:E:170:ARG:NH2	2.13	0.82
1:F:168:TYR:OH	1:J:137:ARG:NH2	2.13	0.81
1:H:139:LYS:NZ	1:H:181:ASN:OD1	2.13	0.80
1:C:96:GLU:OE1	5:C:401:HOH:O	2.01	0.79
1:E:57:THR:OG1	3:E:302:6GM:O01	2.01	0.77
1:A:32:SER:HA	1:A:178:GLN:HE22	1.50	0.76
1:F:57:THR:OG1	3:F:303:6GM:O01	2.04	0.75
1:H:130:THR:HG22	1:H:131:GLU:N	2.03	0.74
1:H:131:GLU:HG3	1:H:133:GLY:H	1.53	0.73
1:E:137:ARG:NH1	5:E:402:HOH:O	2.19	0.73
1:B:-5:LYS:NZ	2:F:301:NAG:O6	2.23	0.70
1:H:41:VAL:HG22	1:H:48:VAL:HG12	1.71	0.70
1:F:69:HIS:ND1	4:F:306:PO4:O2	2.25	0.69
1:F:167:GLN:CD	1:F:167:GLN:H	2.01	0.68
1:E:190:GLU:OE1	5:E:401:HOH:O	2.12	0.65
1:I:139:LYS:NZ	1:I:181:ASN:HD22	1.95	0.65
1:H:131:GLU:HG3	1:H:133:GLY:N	2.11	0.65
1:F:11:ARG:NH2	1:J:17:ASP:OD2	2.24	0.63
1:A:139:LYS:HG2	1:A:196:GLU:HG2	1.79	0.63
1:D:137:ARG:HG2	1:D:137:ARG:HH11	1.63	0.62
1:D:43:GLU:HG3	1:D:125:VAL:HG13	1.81	0.62
1:H:61:ARG:NH1	1:H:108:ASP:O	2.25	0.62
1:F:41:VAL:HG22	1:F:48:VAL:HG23	1.81	0.62
1:E:181:ASN:HB3	1:E:194:ASP:OD1	1.99	0.62
1:H:43:GLU:HG3	1:H:44:ILE:HG13	1.81	0.62
1:H:186:SER:OG	1:I:163:GLU:OE2	2.15	0.61
1:H:152:VAL:HG12	1:H:195:VAL:HG23	1.83	0.60
1:I:40:GLU:HA	1:I:170:ARG:HH21	1.66	0.60
1:B:190:GLU:H	1:B:190:GLU:CD	2.10	0.60
1:H:33:LEU:H	1:H:178:GLN:HE22	1.50	0.60
1:B:160:ASP:OD1	1:B:162:SER:OG	2.20	0.59
1:E:152:VAL:CG1	1:E:195:VAL:HG23	2.32	0.59
1:C:152:VAL:HG12	1:C:195:VAL:HG23	1.84	0.59
1:F:40:GLU:OE1	1:F:120:ARG:NH1	2.36	0.59
1:B:17:ASP:OD2	1:C:11:ARG:NH2	2.28	0.58
1:D:146:HIS:CE1	1:D:148:ARG:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ASP:OD2	1:G:11:ARG:NH2	2.30	0.58
1:F:88:ALA:HB3	1:F:91:ALA:HB2	1.83	0.58
1:G:177:THR:OG1	1:G:198:SER:HB2	2.03	0.58
1:I:88:ALA:HB3	1:I:91:ALA:HB2	1.85	0.58
1:F:172:GLU:HG3	1:F:204:LYS:HG2	1.84	0.58
1:E:155:THR:HG23	1:E:156:THR:O	2.04	0.58
1:F:33:LEU:HD11	1:F:140:ILE:HD11	1.86	0.58
1:J:152:VAL:HG12	1:J:195:VAL:HG23	1.86	0.58
1:G:124:ASP:HB2	1:H:168:TYR:CE1	2.38	0.57
1:C:131:GLU:O	1:C:202:ARG:NH1	2.36	0.57
1:A:179:LYS:HG3	1:A:196:GLU:HB2	1.87	0.57
1:G:178:GLN:HG2	1:G:197:VAL:HG22	1.86	0.57
1:I:120:ARG:HG3	1:I:120:ARG:HH11	1.69	0.57
1:H:127:GLY:HA2	1:H:131:GLU:OE2	2.05	0.57
1:C:146:HIS:CE1	1:C:148:ARG:HB3	2.39	0.56
1:I:154:PRO:HB3	1:I:195:VAL:HG13	1.87	0.56
1:C:-6:TYR:HE1	1:C:72:ASP:HB2	1.69	0.56
1:G:173:ILE:HD12	1:G:199:LEU:HD11	1.87	0.55
1:G:-5:LYS:NZ	4:G:303:PO4:O4	2.36	0.55
1:H:180:LYS:HE3	1:H:193:GLU:OE1	2.06	0.55
1:A:19:ILE:HG13	1:A:21:THR:HG23	1.88	0.55
1:J:41:VAL:HG13	1:J:48:VAL:HG12	1.87	0.55
3:F:302:6GM:O01	1:G:57:THR:OG1	2.25	0.55
1:F:37:ASN:ND2	1:F:169:SER:HB2	2.21	0.55
1:I:124:ASP:HB2	1:J:168:TYR:CE1	2.42	0.55
1:D:146:HIS:HE1	1:D:148:ARG:HB2	1.72	0.54
1:B:22:GLN:NE2	1:B:60:ASP:HA	2.22	0.54
1:B:43:GLU:HA	1:B:125:VAL:CG2	2.38	0.54
1:G:34:LYS:HG2	1:G:55:GLN:HE21	1.73	0.54
1:H:143:TRP:CZ2	1:I:99:THR:HG21	2.43	0.54
1:F:139:LYS:NZ	1:F:181:ASN:ND2	2.55	0.53
1:J:157:GLU:O	1:J:177:THR:HA	2.09	0.53
1:I:174:LEU:HD21	1:I:202:ARG:HG2	1.89	0.53
1:D:154:PRO:HB3	1:D:195:VAL:HG22	1.91	0.53
1:H:174:LEU:HD11	1:H:202:ARG:HD3	1.91	0.53
1:B:158:ASN:ND2	1:B:175:ASP:OD1	2.41	0.53
1:C:190:GLU:OE1	1:C:191:ALA:N	2.42	0.53
1:H:32:SER:HB2	1:H:155:THR:HG22	1.90	0.53
1:I:66:ASN:OD1	1:I:66:ASN:C	2.53	0.52
1:I:186:SER:OG	1:J:163:GLU:OE2	2.26	0.52
1:A:133:GLY:HA2	1:A:202:ARG:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB3	1:A:91:ALA:HB2	1.92	0.51
1:B:146:HIS:CE1	1:B:148:ARG:HB2	2.46	0.51
1:D:-6:TYR:CZ	1:D:-5:LYS:HE3	2.45	0.51
1:G:35:PHE:N	1:G:161:ASP:OD2	2.39	0.51
1:C:41:VAL:HG22	1:C:48:VAL:HG12	1.93	0.51
1:F:178:GLN:HG2	1:F:197:VAL:HG22	1.93	0.51
1:D:152:VAL:CG1	1:D:195:VAL:HG23	2.40	0.51
1:I:31:VAL:HB	1:I:195:VAL:HG21	1.92	0.51
1:D:59:SER:HB2	1:D:110[B]:GLU:OE2	2.11	0.51
1:H:32:SER:HB2	1:H:155:THR:CG2	2.41	0.51
1:J:0:LYS:NZ	5:J:402:HOH:O	2.35	0.50
1:C:17:ASP:OD2	1:D:11:ARG:NH2	2.38	0.50
1:A:44:ILE:HG13	1:A:45:THR:HG23	1.93	0.50
1:E:152:VAL:HG12	1:E:195:VAL:HG23	1.94	0.50
1:B:88:ALA:HB3	1:B:91:ALA:HB2	1.93	0.50
2:D:301:NAG:H82	2:D:301:NAG:O3	2.12	0.50
1:J:146:HIS:CE1	1:J:148:ARG:HB3	2.47	0.50
1:F:168:TYR:CE1	1:J:124:ASP:HB2	2.47	0.50
1:E:49:ASP:OD2	1:E:118:ARG:NH2	2.40	0.49
1:F:19:ILE:HG13	1:F:21:THR:HG23	1.94	0.49
1:I:139:LYS:HZ1	1:I:181:ASN:HD22	1.59	0.49
1:H:157:GLU:O	1:H:177:THR:HA	2.13	0.49
1:I:94:LYS:HE2	1:J:97:VAL:O	2.13	0.49
1:F:94:LYS:HE3	1:G:96:GLU:HG3	1.95	0.49
1:J:134:ALA:O	1:J:200:ASN:HA	2.12	0.49
1:G:-7:ASP:N	1:G:72:ASP:OD1	2.46	0.49
1:D:154:PRO:HG3	1:D:180:LYS:N	2.28	0.48
1:D:66:ASN:OD1	1:D:68:SER:OG	2.29	0.48
1:A:69:HIS:HB3	2:G:301:NAG:H81	1.95	0.48
1:F:-6:TYR:HE1	1:F:72:ASP:HB2	1.78	0.48
1:F:139:LYS:HZ2	1:F:181:ASN:ND2	2.12	0.48
1:F:170:ARG:HD2	1:J:45:THR:HA	1.96	0.48
1:I:66:ASN:OD1	1:I:67:SER:N	2.47	0.48
1:B:144:THR:HG21	1:C:102:LEU:HB2	1.96	0.48
1:C:20:PRO:HA	1:D:0:LYS:HE3	1.94	0.48
1:F:172:GLU:HG2	1:F:204:LYS:HE2	1.95	0.47
1:D:124:ASP:HB2	1:E:168:TYR:CE1	2.49	0.47
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.49	0.47
1:E:88:ALA:HB3	1:E:91:ALA:HB2	1.96	0.47
1:H:61:ARG:NH2	5:H:401:HOH:O	2.36	0.47
1:H:130:THR:CG2	1:H:131:GLU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:23:ARG:HA	1:H:23:ARG:HD3	1.66	0.47
1:A:-7:ASP:OD1	1:A:-5:LYS:HD2	2.15	0.47
1:F:168:TYR:HH	1:J:137:ARG:HH21	1.52	0.47
1:H:130:THR:HB	1:H:131:GLU:OE2	2.14	0.47
1:I:-6:TYR:OH	1:I:-5:LYS:NZ	2.48	0.47
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.80	0.47
1:E:32:SER:HB3	1:E:55:GLN:HB2	1.96	0.47
1:I:30:SER:HB2	1:I:57[B]:THR:HG22	1.96	0.47
1:F:143:TRP:CZ2	1:G:99:THR:HG21	2.50	0.46
1:G:88:ALA:HB3	1:G:91:ALA:HB2	1.97	0.46
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.51	0.46
1:F:23:ARG:O	1:F:23:ARG:HG3	2.16	0.46
1:G:129:ASP:C	1:G:206:ARG:HD2	2.40	0.46
1:G:47:GLU:HA	1:G:121:PHE:O	2.16	0.46
1:H:33:LEU:HD22	1:H:52:PHE:CD1	2.51	0.46
3:I:303:6GM:O01	1:J:57:THR:HG23	2.15	0.46
1:G:47:GLU:OE1	1:G:120:ARG:NH2	2.47	0.46
1:B:43:GLU:HA	1:B:125:VAL:HG21	1.98	0.46
1:C:146:HIS:HB2	1:C:190:GLU:OE1	2.16	0.46
1:E:41:VAL:HG22	1:E:48:VAL:HG12	1.97	0.46
1:A:48:VAL:HG13	1:A:50:VAL:HG13	1.96	0.46
1:G:22:GLN:HE22	1:G:61:ARG:NE	2.14	0.46
1:G:178:GLN:HG3	1:G:197:VAL:HG13	1.98	0.46
1:D:39:LEU:HB2	1:D:49:ASP:HB3	1.98	0.45
1:F:146:HIS:CE1	1:F:148:ARG:HB2	2.52	0.45
1:I:40:GLU:HA	1:I:170:ARG:NH2	2.29	0.45
1:E:125:VAL:HG12	1:E:125:VAL:O	2.17	0.45
1:H:88:ALA:HB3	1:H:91:ALA:HB2	1.99	0.45
1:F:30:SER:HA	1:F:153:ASP:O	2.16	0.45
1:F:43:GLU:OE2	1:F:125:VAL:HG12	2.16	0.45
1:A:170[B]:ARG:HD3	1:E:44:ILE:HG22	1.98	0.45
1:G:176:VAL:HA	1:G:198:SER:O	2.17	0.45
1:E:66:ASN:C	1:E:66:ASN:OD1	2.59	0.45
1:H:25:ARG:HG3	1:H:26:PRO:HD2	1.99	0.44
1:B:51:VAL:HG22	1:B:118:ARG:HB2	1.98	0.44
1:A:97:VAL:O	1:E:94:LYS:HE3	2.18	0.44
1:G:158:ASN:HD21	1:G:177:THR:CG2	2.16	0.44
1:A:43:GLU:HG3	1:A:125:VAL:CG1	2.48	0.44
1:I:36:ILE:HG12	1:I:52:PHE:HA	2.00	0.44
1:H:17:ASP:OD2	1:I:11:ARG:NH2	2.35	0.44
1:B:22:GLN:NE2	1:B:61:ARG:H	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:GLU:HA	1:B:125:VAL:HG23	2.00	0.43
1:J:203:LYS:HE3	1:J:203:LYS:HB2	1.64	0.43
1:E:93:SER:HB3	1:E:120[B]:ARG:HB2	2.00	0.43
1:F:160:ASP:OD1	1:F:161:ASP:N	2.51	0.43
1:E:155:THR:OG1	1:E:156:THR:N	2.51	0.43
1:I:-7:ASP:N	1:I:67:SER:O	2.48	0.43
1:E:39:LEU:HD12	1:E:118:ARG:CZ	2.49	0.43
1:F:57:THR:HG21	1:F:110:GLU:OE2	2.18	0.43
3:F:302:6GM:C10	1:G:55:GLN:OE1	2.66	0.43
1:G:34:LYS:CG	1:G:55:GLN:HE21	2.30	0.43
1:B:137:ARG:HA	1:B:197:VAL:O	2.18	0.43
1:I:170:ARG:HE	1:I:171:PHE:HE1	1.64	0.43
1:A:104:ARG:HA	1:A:104:ARG:HD2	1.89	0.43
1:E:133:GLY:HA2	1:E:202:ARG:HB3	2.01	0.43
1:H:143:TRP:CE2	1:I:99:THR:HG21	2.54	0.43
1:D:125:VAL:HA	1:D:134:ALA:HB1	2.00	0.43
1:E:134:ALA:O	1:E:200:ASN:HA	2.18	0.43
1:J:155:THR:HB	1:J:156:THR:H	1.69	0.43
1:D:49:ASP:OD1	1:D:120:ARG:HG2	2.19	0.42
1:G:158:ASN:ND2	1:G:177:THR:HG22	2.13	0.42
1:B:12:GLN:OE1	1:J:15:ARG:NH1	2.52	0.42
1:B:139:LYS:NZ	1:B:181:ASN:HD21	2.17	0.42
1:C:55:GLN:HG2	1:C:114:MET:SD	2.59	0.42
1:E:152:VAL:HG11	1:E:195:VAL:HG23	2.00	0.42
1:F:143:TRP:CE2	1:G:99:THR:HG21	2.54	0.42
1:B:181:ASN:HB2	1:B:182:SER:H	1.51	0.42
1:C:73:GLN:HB2	1:C:104:ARG:NH2	2.34	0.42
1:D:93:SER:HB3	1:D:120:ARG:HB2	2.00	0.42
1:D:181:ASN:HB3	1:D:194:ASP:OD1	2.19	0.42
1:I:120:ARG:NH1	5:I:405:HOH:O	2.52	0.42
1:B:160:ASP:CG	1:B:162:SER:HG	2.25	0.42
1:F:-7:ASP:H2	1:F:72:ASP:CG	2.26	0.42
1:F:187:CYS:SG	1:F:188:CYS:N	2.93	0.42
1:A:43:GLU:HG3	1:A:125:VAL:HG12	2.01	0.42
1:J:67:SER:HA	1:J:70:SER:OG	2.18	0.42
1:J:88:ALA:HB3	1:J:91:ALA:HB2	2.00	0.42
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.55	0.42
1:B:171:PHE:CE2	1:B:203:LYS:HG2	2.54	0.42
1:A:55:GLN:HG2	1:A:114:MET:SD	2.60	0.42
1:A:158:ASN:OD1	1:A:177:THR:HG22	2.19	0.42
1:B:-7:ASP:N	1:B:72:ASP:OD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ASP:HB3	1:E:71:PRO:HD2	2.02	0.42
1:G:143:TRP:CZ2	1:H:99:THR:HG21	2.54	0.42
1:C:32:SER:HB2	1:C:155:THR:HB	2.02	0.42
1:C:45:THR:HA	1:D:170:ARG:HG3	2.01	0.42
1:H:32:SER:HB3	1:H:55:GLN:HE21	1.84	0.42
1:B:46:ASN:OD1	1:B:125:VAL:HG22	2.20	0.42
1:C:148:ARG:NH2	1:D:-5:LYS:HA	2.34	0.42
1:G:143:TRP:HZ2	1:H:114:MET:O	2.03	0.42
1:J:146:HIS:HB3	1:J:192:TYR:CE2	2.55	0.42
1:E:57:THR:HG23	1:E:112:LEU:HG	2.02	0.41
1:G:176:VAL:HG22	1:G:199:LEU:HD12	2.02	0.41
1:C:134:ALA:O	1:C:200:ASN:HA	2.20	0.41
1:E:93:SER:HB3	1:E:120[A]:ARG:HB2	2.02	0.41
1:B:42:ASN:O	1:B:125:VAL:HG21	2.20	0.41
1:H:128:VAL:HG21	1:H:171:PHE:HE2	1.84	0.41
1:C:67:SER:HA	1:C:70:SER:OG	2.20	0.41
1:H:187:CYS:SG	1:H:188:CYS:N	2.93	0.41
1:J:22:GLN:C	1:J:23:ARG:HG3	2.45	0.41
1:J:88:ALA:HA	1:J:139:LYS:O	2.19	0.41
1:J:123:CYS:O	1:J:125:VAL:HG23	2.20	0.41
1:A:190:GLU:H	1:A:190:GLU:HG2	1.43	0.41
1:B:94:LYS:HE3	1:C:96:GLU:HG2	2.03	0.41
1:E:139:LYS:HE2	1:E:194:ASP:OD2	2.20	0.41
1:E:34:LYS:NZ	1:E:157:GLU:OE2	2.45	0.41
1:I:54:GLN:O	1:I:114:MET:HA	2.20	0.41
1:I:120:ARG:HG3	1:I:120:ARG:NH1	2.35	0.41
1:J:33:LEU:H	1:J:178:GLN:HE22	1.69	0.41
1:B:139:LYS:CE	1:B:181:ASN:HD21	2.34	0.41
1:F:177:THR:OG1	1:F:198:SER:HB2	2.21	0.41
1:E:68:SER:HB2	2:E:301:NAG:H82	2.03	0.40
1:G:33:LEU:H	1:G:178:GLN:NE2	2.18	0.40
1:G:67:SER:HA	1:G:70:SER:OG	2.21	0.40
1:A:42:ASN:OD1	1:A:44:ILE:HG12	2.21	0.40
1:C:-1:ASP:O	1:C:3:ARG:HG3	2.20	0.40
1:E:65:TRP:CZ3	1:E:107:SER:HA	2.56	0.40
1:B:178:GLN:HG2	1:B:197:VAL:HG22	2.03	0.40
1:A:134:ALA:O	1:A:200:ASN:HA	2.22	0.40
1:B:46:ASN:HA	1:B:125:VAL:HG22	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:THR:OG1	1:J:-6:TYR:OH[1_455]	1.93	0.27
5:A:416:HOH:O	5:D:402:HOH:O[2_947]	2.06	0.14

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	214/218 (98%)	211 (99%)	2 (1%)	1 (0%)	24	30
1	B	212/218 (97%)	209 (99%)	3 (1%)	0	100	100
1	C	211/218 (97%)	206 (98%)	5 (2%)	0	100	100
1	D	213/218 (98%)	210 (99%)	3 (1%)	0	100	100
1	E	212/218 (97%)	208 (98%)	3 (1%)	1 (0%)	24	30
1	F	210/218 (96%)	206 (98%)	4 (2%)	0	100	100
1	G	213/218 (98%)	205 (96%)	6 (3%)	2 (1%)	14	16
1	H	210/218 (96%)	205 (98%)	5 (2%)	0	100	100
1	I	212/218 (97%)	209 (99%)	3 (1%)	0	100	100
1	J	210/218 (96%)	209 (100%)	0	1 (0%)	24	30
All	All	2117/2180 (97%)	2078 (98%)	34 (2%)	5 (0%)	43	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	205	GLY
1	E	156	THR
1	G	155	THR
1	A	189	PRO
1	J	155	THR

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	
1	A	202/204 (99%)	197 (98%)	5 (2%)	42	59
1	B	200/204 (98%)	196 (98%)	4 (2%)	48	66
1	C	199/204 (98%)	190 (96%)	9 (4%)	24	36
1	D	201/204 (98%)	195 (97%)	6 (3%)	36	52
1	E	201/204 (98%)	195 (97%)	6 (3%)	36	52
1	F	199/204 (98%)	193 (97%)	6 (3%)	36	52
1	G	201/204 (98%)	188 (94%)	13 (6%)	15	21
1	H	199/204 (98%)	192 (96%)	7 (4%)	32	46
1	I	201/204 (98%)	194 (96%)	7 (4%)	32	46
1	J	200/204 (98%)	191 (96%)	9 (4%)	24	36
All	All	2003/2040 (98%)	1931 (96%)	72 (4%)	32	45

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	40	GLU
1	A	48	VAL
1	A	125	VAL
1	A	190	GLU
1	B	57	THR
1	B	61	ARG
1	B	162	SER
1	B	179	LYS
1	C	22	GLN
1	C	41	VAL
1	C	44	ILE
1	C	57	THR
1	C	131	GLU
1	C	157	GLU
1	C	178	GLN

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Mol	Chain	Res	Type
1	C	188	CYS
1	C	190	GLU
1	D	31	VAL
1	D	41	VAL
1	D	44	ILE
1	D	68	SER
1	D	131	GLU
1	D	162	SER
1	E	25	ARG
1	E	41	VAL
1	E	57	THR
1	E	120[A]	ARG
1	E	120[B]	ARG
1	E	180	LYS
1	F	43	GLU
1	F	56	THR
1	F	158	ASN
1	F	179	LYS
1	F	188	CYS
1	F	203	LYS
1	G	-5	LYS
1	G	25	ARG
1	G	44	ILE
1	G	55	GLN
1	G	57	THR
1	G	112	LEU
1	G	131	GLU
1	G	137	ARG
1	G	157	GLU
1	G	158	ASN
1	G	162	SER
1	G	179	LYS
1	G	195	VAL
1	H	-5	LYS
1	H	24	ASP
1	H	41	VAL
1	H	44	ILE
1	H	132	SER
1	H	139	LYS
1	H	162	SER
1	I	41	VAL
1	I	56	THR

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Mol	Chain	Res	Type
1	I	57[A]	THR
1	I	57[B]	THR
1	I	139	LYS
1	I	152	VAL
1	I	188	CYS
1	J	-5	LYS
1	J	-3	ASP
1	J	41	VAL
1	J	43	GLU
1	J	172	GLU
1	J	180	LYS
1	J	188	CYS
1	J	190	GLU
1	J	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	181	ASN
1	A	200	ASN
1	B	181	ASN
1	B	200	ASN
1	C	181	ASN
1	D	22	GLN
1	E	12	GLN
1	E	54	GLN
1	E	146	HIS
1	F	37	ASN
1	F	119	GLN
1	F	181	ASN
1	G	146	HIS
1	G	158	ASN
1	H	200	ASN
1	I	119	GLN
1	I	181	ASN
1	J	37	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

41 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	301	1	14,14,15	0.68	0	17,19,21	0.61	0
4	PO4	F	306	-	4,4,4	0.86	0	6,6,6	0.41	0
2	NAG	E	301	1	14,14,15	1.02	1 (7%)	17,19,21	1.28	1 (5%)
2	NAG	H	301	1	14,14,15	0.26	0	17,19,21	0.66	0
4	PO4	E	303	-	4,4,4	0.92	0	6,6,6	0.54	0
2	NAG	A	301	1	14,14,15	0.52	0	17,19,21	0.48	0
4	PO4	H	304	-	4,4,4	0.88	0	6,6,6	0.53	0
4	PO4	D	303	-	4,4,4	1.00	0	6,6,6	0.76	0
4	PO4	I	305	-	4,4,4	0.93	0	6,6,6	0.45	0
4	PO4	E	304	-	4,4,4	0.86	0	6,6,6	0.49	0
2	NAG	G	301	1	14,14,15	0.27	0	17,19,21	0.61	0
4	PO4	F	305	-	4,4,4	0.97	0	6,6,6	0.33	0
4	PO4	J	303	-	4,4,4	0.99	0	6,6,6	0.46	0
3	6GM	I	303	-	32,32,32	2.16	5 (15%)	42,43,43	2.12	10 (23%)
4	PO4	H	303	-	4,4,4	0.85	0	6,6,6	0.76	0
2	NAG	I	301	1	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
4	PO4	F	304	-	4,4,4	1.09	0	6,6,6	0.60	0
4	PO4	G	303	-	4,4,4	0.93	0	6,6,6	0.44	0
3	6GM	B	302	-	32,32,32	2.04	5 (15%)	42,43,43	2.19	13 (30%)
2	NAG	F	301	1	14,14,15	0.25	0	17,19,21	0.61	0
4	PO4	B	303	-	4,4,4	0.80	0	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6GM	I	302	-	32,32,32	2.22	5 (15%)	42,43,43	2.09	13 (30%)
4	PO4	D	304	-	4,4,4	0.82	0	6,6,6	0.62	0
3	6GM	C	302	-	32,32,32	2.12	5 (15%)	42,43,43	2.21	10 (23%)
3	6GM	E	302	-	32,32,32	1.99	6 (18%)	42,43,43	2.13	16 (38%)
3	6GM	G	302	-	32,32,32	2.10	6 (18%)	42,43,43	2.08	13 (30%)
3	6GM	A	303	-	32,32,32	2.15	6 (18%)	42,43,43	2.04	12 (28%)
4	PO4	J	302	-	4,4,4	0.97	0	6,6,6	0.72	0
4	PO4	H	302	-	4,4,4	0.70	0	6,6,6	0.66	0
4	PO4	C	303	-	4,4,4	0.92	0	6,6,6	0.62	0
2	NAG	J	301	1	14,14,15	0.26	0	17,19,21	0.67	0
4	PO4	A	304	-	4,4,4	0.90	0	6,6,6	0.68	0
3	6GM	F	303	-	32,32,32	2.16	5 (15%)	42,43,43	2.21	11 (26%)
3	6GM	A	302	-	32,32,32	2.15	5 (15%)	42,43,43	2.07	11 (26%)
3	6GM	F	302	-	32,32,32	2.08	5 (15%)	42,43,43	2.10	10 (23%)
4	PO4	D	302	-	4,4,4	0.76	0	6,6,6	0.81	0
2	NAG	B	301	1	14,14,15	0.18	0	17,19,21	0.58	0
4	PO4	I	304	-	4,4,4	0.85	0	6,6,6	0.56	0
4	PO4	D	305	-	4,4,4	0.92	0	6,6,6	0.49	0
4	PO4	C	304	-	4,4,4	0.90	0	6,6,6	0.48	0
2	NAG	C	301	1	14,14,15	0.84	1 (7%)	17,19,21	1.26	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	301	1	-	4/6/23/26	0/1/1/1
2	NAG	E	301	1	-	2/6/23/26	0/1/1/1
2	NAG	H	301	1	-	3/6/23/26	0/1/1/1
2	NAG	A	301	1	-	4/6/23/26	0/1/1/1
2	NAG	G	301	1	-	3/6/23/26	0/1/1/1
3	6GM	I	303	-	-	0/16/16/16	0/4/4/4
2	NAG	I	301	1	-	4/6/23/26	0/1/1/1
3	6GM	B	302	-	-	0/16/16/16	0/4/4/4
2	NAG	F	301	1	-	4/6/23/26	0/1/1/1
3	6GM	I	302	-	-	1/16/16/16	0/4/4/4
3	6GM	C	302	-	-	0/16/16/16	0/4/4/4
3	6GM	E	302	-	-	0/16/16/16	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	6GM	G	302	-	-	0/16/16/16	0/4/4/4
3	6GM	A	303	-	-	0/16/16/16	0/4/4/4
2	NAG	J	301	1	-	1/6/23/26	0/1/1/1
3	6GM	F	303	-	-	0/16/16/16	0/4/4/4
3	6GM	A	302	-	-	0/16/16/16	0/4/4/4
3	6GM	F	302	-	-	4/16/16/16	0/4/4/4
2	NAG	B	301	1	-	2/6/23/26	0/1/1/1
2	NAG	C	301	1	-	2/6/23/26	0/1/1/1

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	302	6GM	C17-C18	-7.01	1.39	1.51
3	A	302	6GM	C17-C18	-6.79	1.39	1.51
3	I	302	6GM	C11-C12	-6.78	1.39	1.51
3	I	303	6GM	C17-C18	-6.77	1.39	1.51
3	F	303	6GM	C11-C12	-6.71	1.39	1.51
3	C	302	6GM	C11-C12	-6.59	1.40	1.51
3	A	303	6GM	C11-C12	-6.41	1.40	1.51
3	A	303	6GM	C17-C18	-6.41	1.40	1.51
3	I	303	6GM	C11-C12	-6.39	1.40	1.51
3	F	303	6GM	C05-C04	-6.31	1.39	1.49
3	C	302	6GM	C17-C18	-6.26	1.40	1.51
3	G	302	6GM	C11-C12	-6.16	1.40	1.51
3	F	302	6GM	C05-C04	-6.15	1.39	1.49
3	I	303	6GM	C05-C04	-6.12	1.39	1.49
3	B	302	6GM	C17-C18	-6.08	1.40	1.51
3	B	302	6GM	C05-C04	-6.06	1.39	1.49
3	E	302	6GM	C17-C18	-6.05	1.41	1.51
3	G	302	6GM	C17-C18	-6.05	1.41	1.51
3	A	302	6GM	C11-C12	-6.03	1.41	1.51
3	G	302	6GM	C05-C04	-6.03	1.39	1.49
3	C	302	6GM	C05-C04	-6.01	1.39	1.49
3	F	302	6GM	C17-C18	-5.96	1.41	1.51
3	I	302	6GM	C05-C04	-5.94	1.39	1.49
3	F	302	6GM	C11-C12	-5.94	1.41	1.51
3	A	302	6GM	C05-C04	-5.92	1.39	1.49
3	F	303	6GM	C17-C18	-5.91	1.41	1.51
3	A	303	6GM	C05-C04	-5.73	1.40	1.49
3	E	302	6GM	C11-C12	-5.63	1.41	1.51
3	E	302	6GM	C05-C04	-5.61	1.40	1.49
3	B	302	6GM	C11-C12	-5.60	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	NAG	C1-C2	3.59	1.57	1.52
3	G	302	6GM	C16-N05	3.24	1.41	1.34
3	A	303	6GM	C19-N06	3.18	1.41	1.34
3	A	302	6GM	C16-N05	3.17	1.41	1.34
3	A	303	6GM	C16-N05	3.16	1.41	1.34
3	F	302	6GM	C19-N06	3.03	1.41	1.34
3	E	302	6GM	C16-N05	3.02	1.40	1.34
3	I	302	6GM	C16-N05	3.00	1.40	1.34
3	C	302	6GM	C19-N06	2.99	1.40	1.34
3	B	302	6GM	C16-N05	2.98	1.40	1.34
3	F	302	6GM	C16-N05	2.95	1.40	1.34
3	I	303	6GM	C19-N06	2.90	1.40	1.34
2	C	301	NAG	O5-C1	2.82	1.48	1.43
3	F	303	6GM	C19-N06	2.75	1.40	1.34
3	F	303	6GM	C16-N05	2.73	1.40	1.34
3	B	302	6GM	C19-N06	2.71	1.40	1.34
3	G	302	6GM	C19-N06	2.65	1.40	1.34
3	A	302	6GM	C19-N06	2.64	1.40	1.34
3	I	302	6GM	C19-N06	2.59	1.40	1.34
3	C	302	6GM	C16-N05	2.58	1.40	1.34
3	I	303	6GM	C16-N05	2.58	1.40	1.34
3	E	302	6GM	C19-N06	2.48	1.39	1.34
3	A	303	6GM	C02-N04	-2.12	1.32	1.37
3	G	302	6GM	C02-N04	-2.09	1.33	1.37
3	E	302	6GM	C17-N04	2.07	1.49	1.46

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	6GM	C04-N03-C01	8.44	121.35	116.35
3	I	303	6GM	C04-N03-C01	8.40	121.32	116.35
3	B	302	6GM	C04-N03-C01	8.14	121.17	116.35
3	F	302	6GM	C04-N03-C01	7.96	121.06	116.35
3	I	302	6GM	C04-N03-C01	7.45	120.76	116.35
3	A	303	6GM	C04-N03-C01	7.42	120.74	116.35
3	G	302	6GM	C04-N03-C01	7.33	120.69	116.35
3	A	302	6GM	C04-N03-C01	7.28	120.66	116.35
3	F	303	6GM	C04-N03-C01	7.21	120.62	116.35
3	F	303	6GM	C01-N02-C02	6.87	122.07	116.61
3	E	302	6GM	C04-N03-C01	6.55	120.23	116.35
3	E	302	6GM	C01-N02-C02	6.30	121.62	116.61
3	C	302	6GM	C01-N02-C02	5.98	121.37	116.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	6GM	C01-N02-C02	5.91	121.31	116.61
3	I	303	6GM	C01-N02-C02	5.90	121.31	116.61
3	G	302	6GM	C01-N02-C02	5.61	121.07	116.61
3	I	302	6GM	C01-N02-C02	5.50	120.98	116.61
3	F	302	6GM	C01-N02-C02	5.29	120.82	116.61
3	A	302	6GM	C01-N02-C02	5.11	120.67	116.61
2	C	301	NAG	C1-O5-C5	4.70	118.48	112.19
3	A	303	6GM	C01-N02-C02	4.59	120.26	116.61
2	E	301	NAG	C1-O5-C5	4.36	118.03	112.19
3	C	302	6GM	N02-C01-N03	-3.68	119.84	125.48
3	I	303	6GM	N02-C01-N03	-3.65	119.89	125.48
3	F	303	6GM	N02-C01-N03	-3.65	119.89	125.48
3	B	302	6GM	N02-C01-N03	-3.62	119.94	125.48
3	E	302	6GM	C19-N06-C18	3.61	122.48	117.41
3	F	303	6GM	C16-N05-C12	3.31	122.05	117.41
3	F	302	6GM	N02-C01-N03	-3.30	120.43	125.48
3	G	302	6GM	N02-C01-N03	-3.16	120.64	125.48
3	G	302	6GM	C16-N05-C12	3.16	121.84	117.41
3	A	302	6GM	N02-C01-N03	-3.15	120.65	125.48
3	A	302	6GM	C05-C04-N03	3.14	120.58	116.04
3	C	302	6GM	C16-N05-C12	3.11	121.78	117.41
3	A	303	6GM	C05-C04-N03	3.07	120.48	116.04
3	E	302	6GM	C16-N05-C12	3.03	121.67	117.41
3	I	302	6GM	N02-C01-N03	-3.02	120.86	125.48
3	E	302	6GM	N02-C01-N03	-3.01	120.86	125.48
3	A	303	6GM	C15-C16-N05	-2.96	118.73	123.42
3	A	303	6GM	N02-C01-N03	-2.92	121.01	125.48
3	F	303	6GM	C15-C16-N05	-2.91	118.81	123.42
3	F	303	6GM	N01-C01-N03	2.87	121.53	117.22
3	F	303	6GM	C05-C04-N03	2.87	120.19	116.04
3	C	302	6GM	C15-C16-N05	-2.85	118.91	123.42
3	I	302	6GM	C19-N06-C18	2.83	121.38	117.41
3	C	302	6GM	C05-C04-N03	2.81	120.10	116.04
3	G	302	6GM	C19-N06-C18	2.80	121.33	117.41
3	I	302	6GM	C16-N05-C12	2.80	121.33	117.41
3	B	302	6GM	C16-N05-C12	2.79	121.32	117.41
3	G	302	6GM	C15-C16-N05	-2.74	119.09	123.42
3	A	303	6GM	C19-N06-C18	2.69	121.18	117.41
3	I	303	6GM	N01-C01-N02	2.65	121.19	117.22
3	A	303	6GM	C20-C19-N06	-2.64	119.24	123.42
3	F	302	6GM	N02-C02-N04	2.64	119.89	116.56
3	A	303	6GM	C16-N05-C12	2.63	121.09	117.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	303	6GM	C12-C11-N04	-2.61	110.57	114.14
3	E	302	6GM	C20-C19-N06	-2.59	119.32	123.42
3	E	302	6GM	C17-C18-N06	2.58	122.09	116.19
3	F	302	6GM	C17-C18-N06	2.57	122.07	116.19
3	B	302	6GM	C17-C18-N06	2.54	122.02	116.19
3	I	303	6GM	C16-N05-C12	2.53	120.95	117.41
3	G	302	6GM	C17-C18-N06	2.52	121.95	116.19
3	C	302	6GM	C17-C18-N06	2.51	121.92	116.19
3	B	302	6GM	C05-C04-N03	2.48	119.62	116.04
3	A	302	6GM	C15-C16-N05	-2.47	119.52	123.42
3	A	303	6GM	C03-C04-N03	-2.46	119.49	122.34
3	I	303	6GM	C17-C18-N06	2.44	121.78	116.19
3	I	302	6GM	C20-C19-N06	-2.43	119.58	123.42
3	B	302	6GM	C20-C19-N06	-2.42	119.59	123.42
3	E	302	6GM	C03-C02-N02	-2.40	118.71	123.34
3	I	302	6GM	C03-C04-N03	-2.40	119.56	122.34
3	B	302	6GM	C19-N06-C18	2.39	120.76	117.41
3	E	302	6GM	N02-C02-N04	2.38	119.57	116.56
3	A	302	6GM	C16-N05-C12	2.38	120.75	117.41
3	A	302	6GM	C11-C12-N05	2.38	121.63	116.19
3	A	303	6GM	C17-C18-N06	2.37	121.62	116.19
3	F	303	6GM	C17-C18-N06	2.34	121.55	116.19
3	G	302	6GM	N01-C01-N03	2.34	120.73	117.22
2	I	301	NAG	C1-O5-C5	-2.34	109.05	112.19
3	E	302	6GM	C22-C18-N06	-2.33	118.87	122.22
3	I	302	6GM	C15-C16-N05	-2.33	119.73	123.42
3	C	302	6GM	C19-N06-C18	2.32	120.66	117.41
3	A	302	6GM	C17-C18-N06	2.30	121.47	116.19
3	E	302	6GM	C05-C04-N03	2.30	119.36	116.04
3	I	303	6GM	C19-N06-C18	2.29	120.62	117.41
3	F	302	6GM	C03-C04-N03	-2.28	119.69	122.34
3	G	302	6GM	C20-C19-N06	-2.27	119.82	123.42
3	I	302	6GM	C05-C04-N03	2.26	119.31	116.04
3	G	302	6GM	C11-C12-N05	2.26	121.36	116.19
3	I	303	6GM	C15-C16-N05	-2.24	119.87	123.42
3	F	303	6GM	C20-C19-N06	-2.24	119.88	123.42
3	A	302	6GM	N02-C02-N04	2.23	119.38	116.56
3	F	303	6GM	C19-N06-C18	2.23	120.54	117.41
3	A	302	6GM	C03-C04-N03	-2.22	119.76	122.34
3	C	302	6GM	N01-C01-N03	2.19	120.51	117.22
3	F	302	6GM	C10-C05-C04	-2.18	117.84	121.28
3	A	302	6GM	C20-C19-N06	-2.17	119.98	123.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	6GM	C13-C12-N05	-2.17	119.09	122.22
3	I	302	6GM	C03-C02-N02	-2.17	119.16	123.34
3	I	302	6GM	C17-C18-N06	2.17	121.15	116.19
3	I	303	6GM	C11-C12-N05	2.17	121.15	116.19
3	A	303	6GM	C11-C12-N05	2.15	121.11	116.19
3	E	302	6GM	C15-C16-N05	-2.14	120.03	123.42
3	E	302	6GM	C03-C04-N03	-2.14	119.86	122.34
3	E	302	6GM	N01-C01-N02	2.13	120.42	117.22
3	I	303	6GM	C20-C19-N06	-2.13	120.05	123.42
3	G	302	6GM	C13-C12-N05	-2.11	119.18	122.22
3	E	302	6GM	C13-C12-N05	-2.11	119.18	122.22
3	C	302	6GM	C20-C19-N06	-2.11	120.08	123.42
3	F	302	6GM	C11-C12-N05	2.09	120.97	116.19
3	B	302	6GM	C11-C12-N05	2.09	120.97	116.19
3	F	302	6GM	C19-N06-C18	2.08	120.33	117.41
3	F	302	6GM	C16-N05-C12	2.08	120.33	117.41
3	E	302	6GM	C11-C12-N05	2.08	120.94	116.19
3	B	302	6GM	N02-C02-N04	2.07	119.18	116.56
3	I	302	6GM	C11-C12-N05	2.06	120.91	116.19
3	A	303	6GM	C11-N04-C02	2.06	123.72	120.97
3	I	302	6GM	C07-C06-C05	-2.06	118.48	121.12
3	B	302	6GM	C03-C04-N03	-2.05	119.96	122.34
3	G	302	6GM	C22-C18-N06	-2.02	119.31	122.22
3	G	302	6GM	C03-C04-N03	-2.01	120.00	122.34
3	B	302	6GM	C15-C16-N05	-2.00	120.25	123.42

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	301	NAG	O5-C5-C6-O6
2	A	301	NAG	O5-C5-C6-O6
2	H	301	NAG	O5-C5-C6-O6
2	I	301	NAG	O5-C5-C6-O6
2	F	301	NAG	C4-C5-C6-O6
2	B	301	NAG	O5-C5-C6-O6
2	H	301	NAG	C4-C5-C6-O6
2	A	301	NAG	C4-C5-C6-O6
2	I	301	NAG	C4-C5-C6-O6
2	G	301	NAG	C4-C5-C6-O6
2	B	301	NAG	C4-C5-C6-O6
2	F	301	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	301	NAG	C8-C7-N2-C2
2	A	301	NAG	O7-C7-N2-C2
2	C	301	NAG	C8-C7-N2-C2
2	C	301	NAG	O7-C7-N2-C2
2	D	301	NAG	C8-C7-N2-C2
2	D	301	NAG	O7-C7-N2-C2
2	E	301	NAG	C8-C7-N2-C2
2	E	301	NAG	O7-C7-N2-C2
2	D	301	NAG	C4-C5-C6-O6
2	H	301	NAG	C3-C2-N2-C7
2	D	301	NAG	O5-C5-C6-O6
2	F	301	NAG	C1-C2-N2-C7
2	I	301	NAG	C1-C2-N2-C7
2	J	301	NAG	C4-C5-C6-O6
2	I	301	NAG	C3-C2-N2-C7
3	F	302	6GM	N03-C04-C05-C10
3	F	302	6GM	N03-C04-C05-C06
2	F	301	NAG	C3-C2-N2-C7
2	G	301	NAG	C3-C2-N2-C7
3	F	302	6GM	C03-C04-C05-C10
3	F	302	6GM	C03-C04-C05-C06
3	I	302	6GM	N03-C04-C05-C10

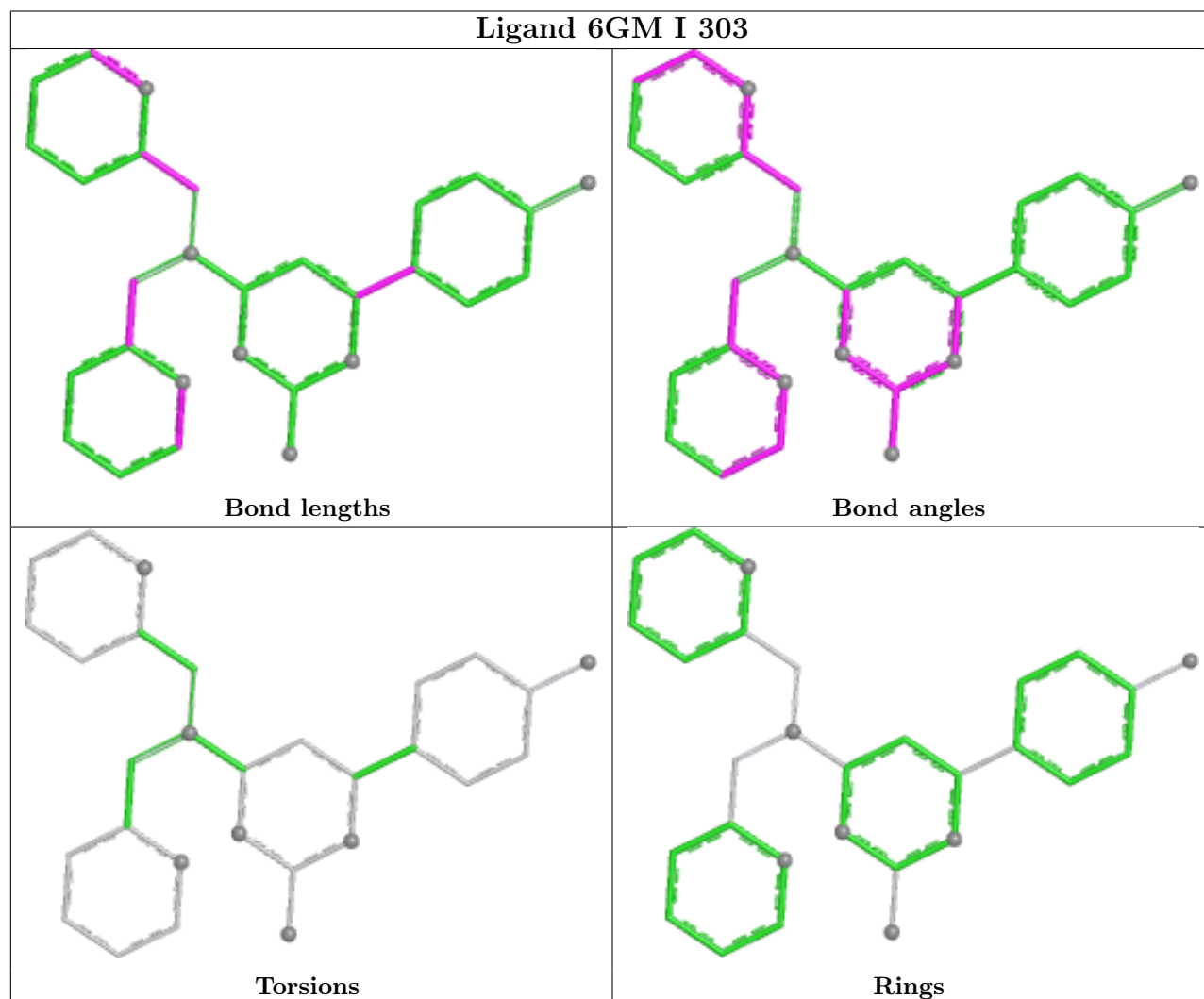
There are no ring outliers.

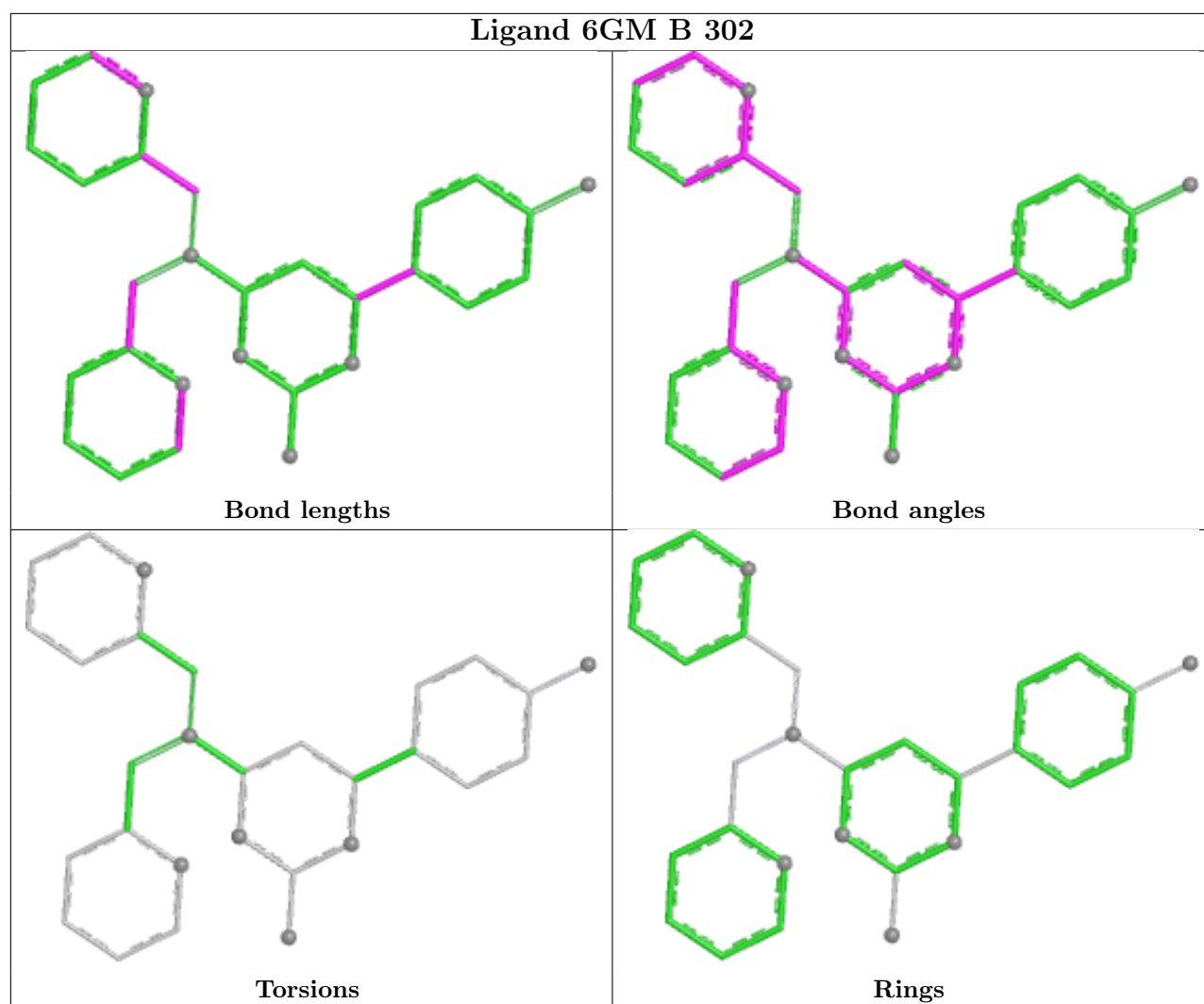
10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	NAG	1	0
4	F	306	PO4	1	0
2	E	301	NAG	1	0
2	G	301	NAG	1	0
3	I	303	6GM	1	0
4	G	303	PO4	1	0
2	F	301	NAG	1	0
3	E	302	6GM	1	0
3	F	303	6GM	1	0
3	F	302	6GM	2	0

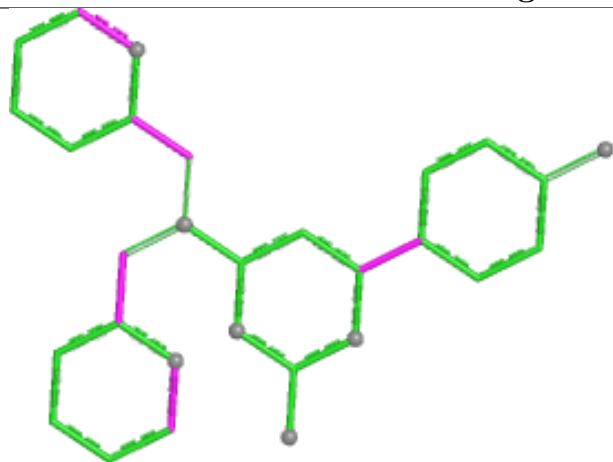
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

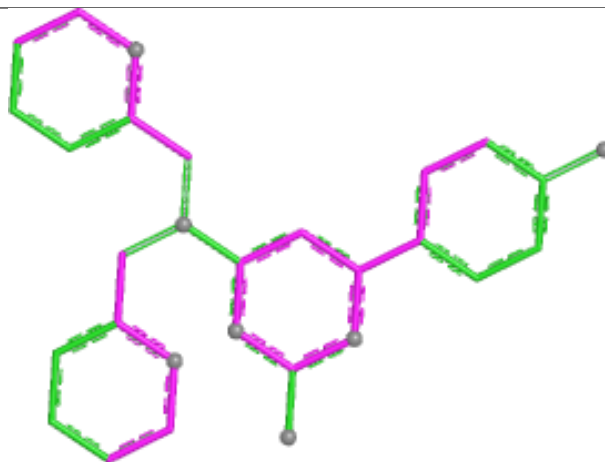




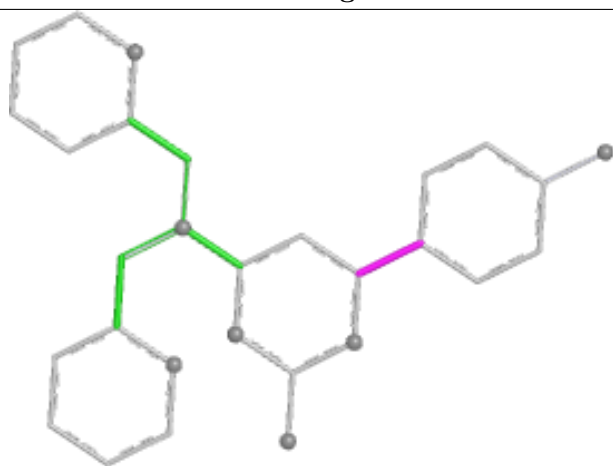
Ligand 6GM I 302



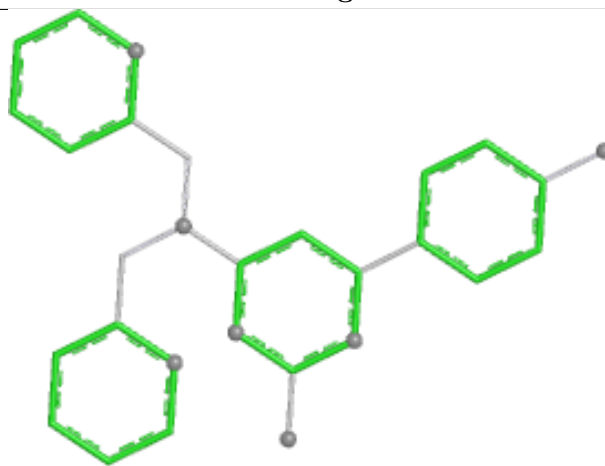
Bond lengths



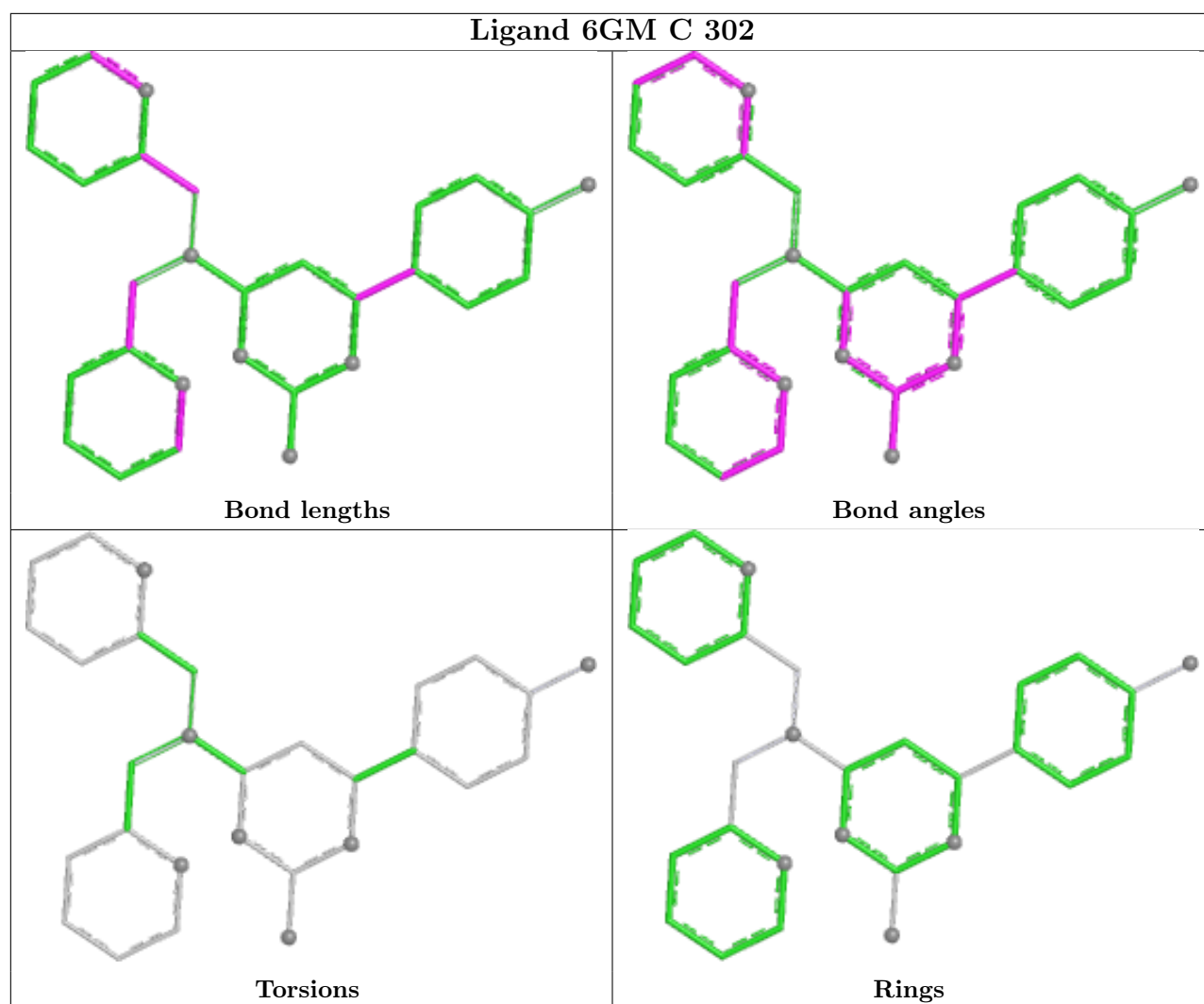
Bond angles



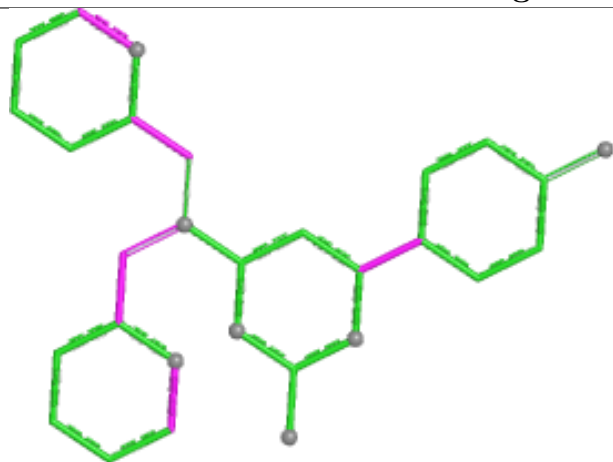
Torsions



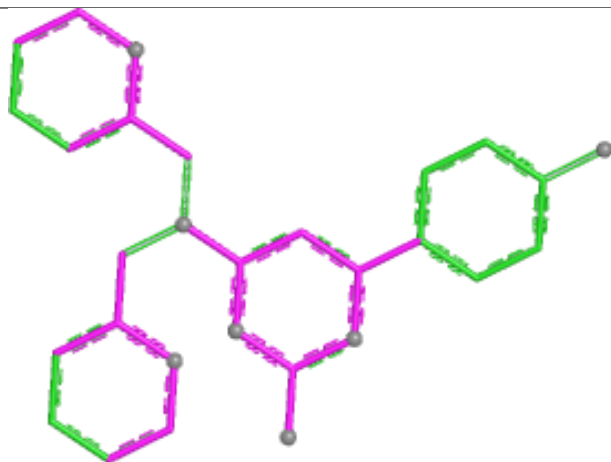
Rings



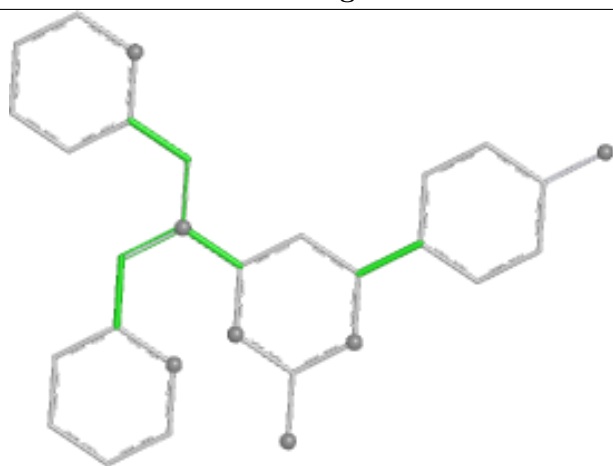
Ligand 6GM E 302



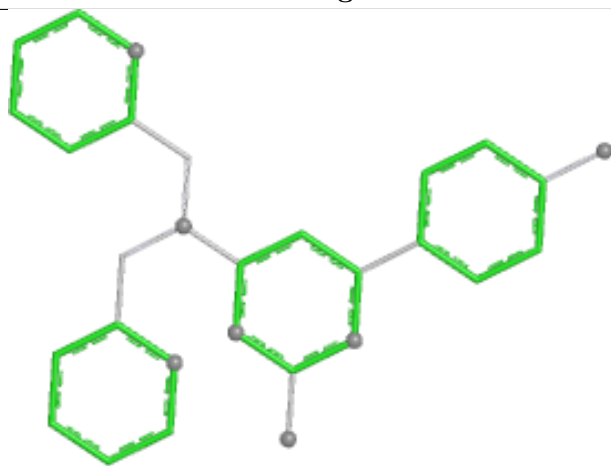
Bond lengths



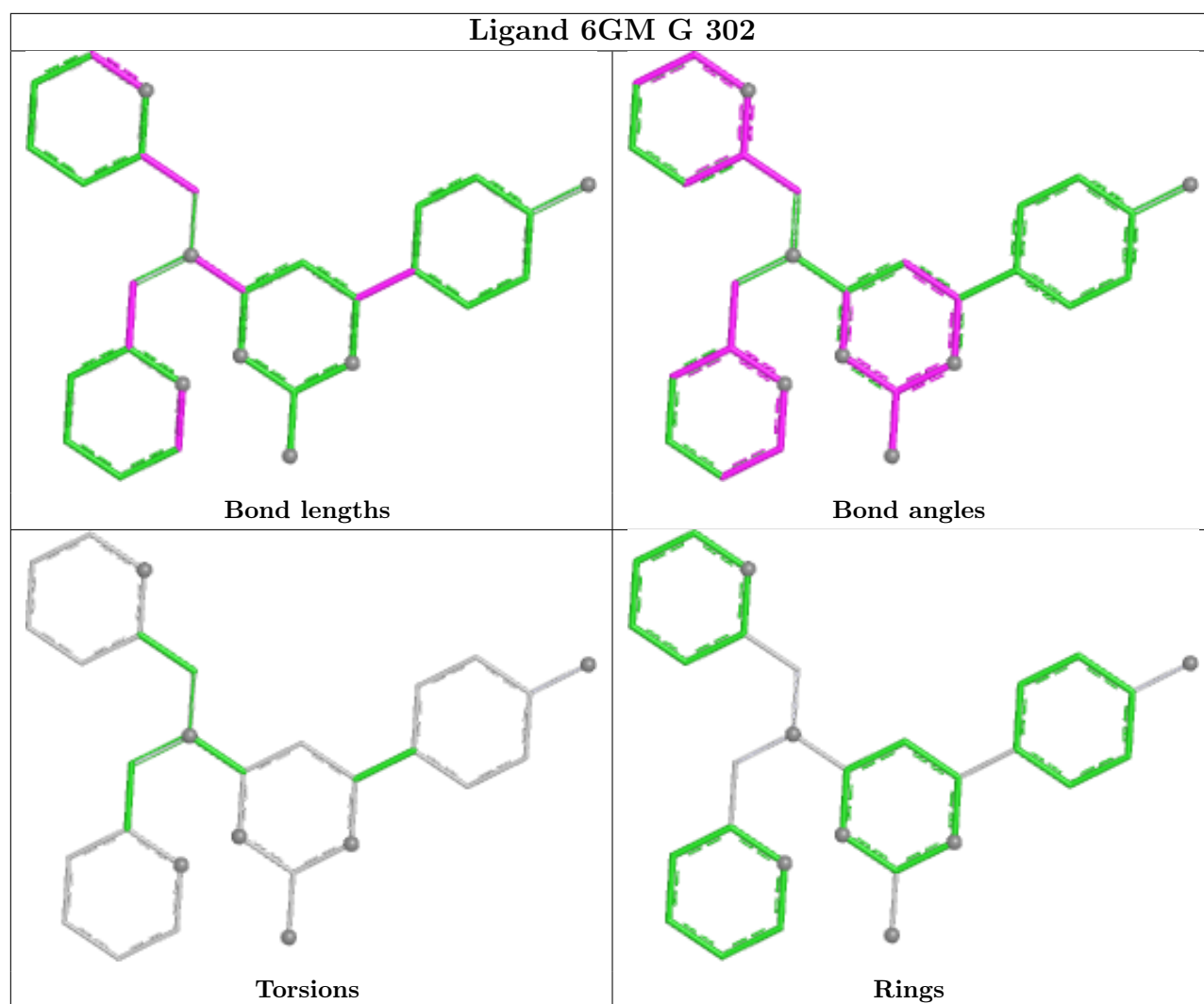
Bond angles

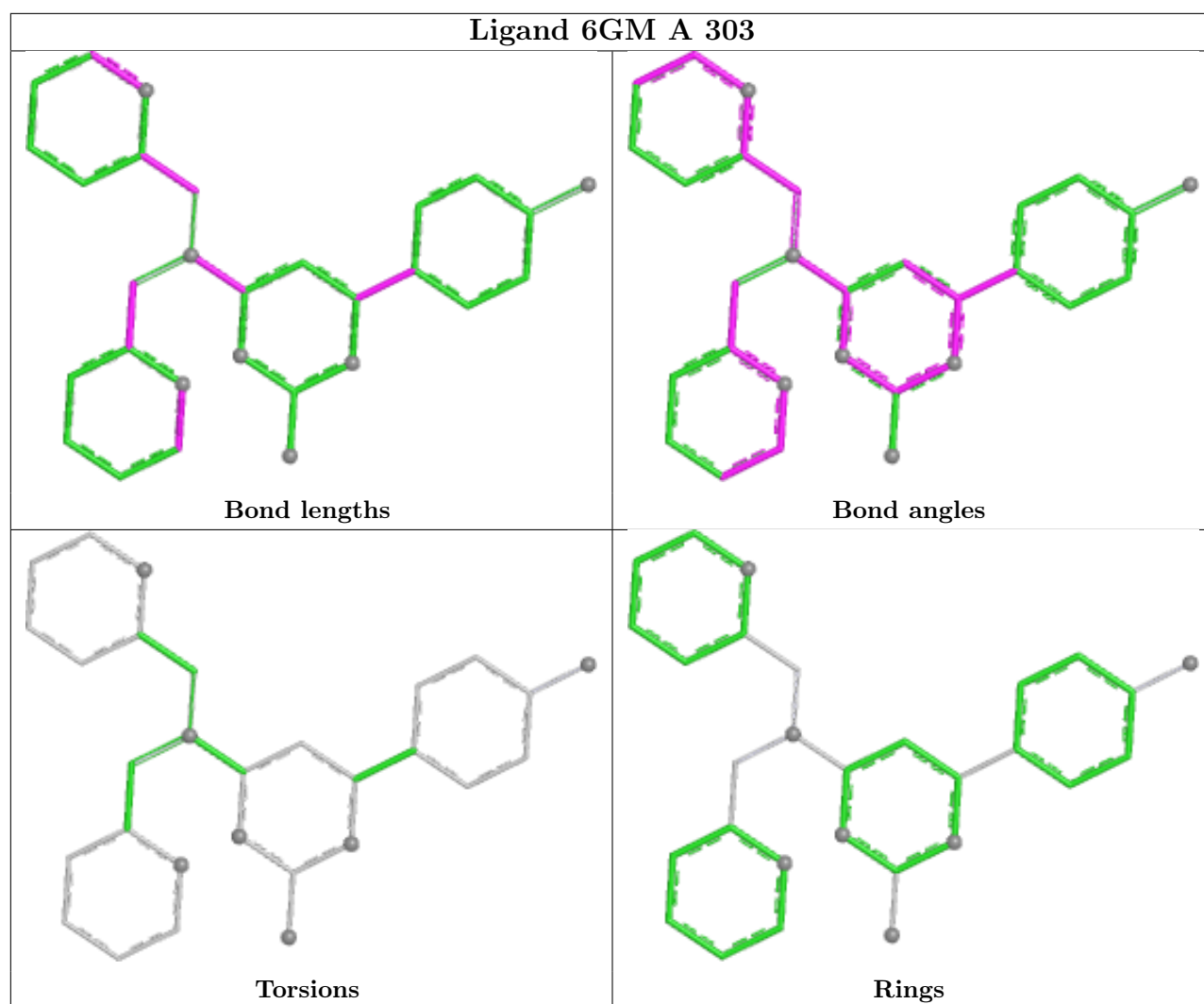


Torsions

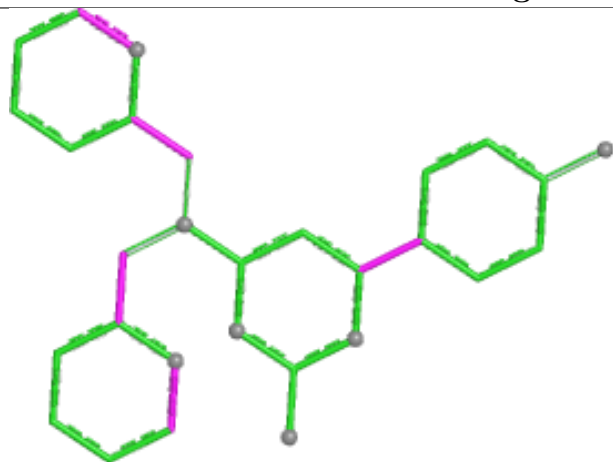


Rings

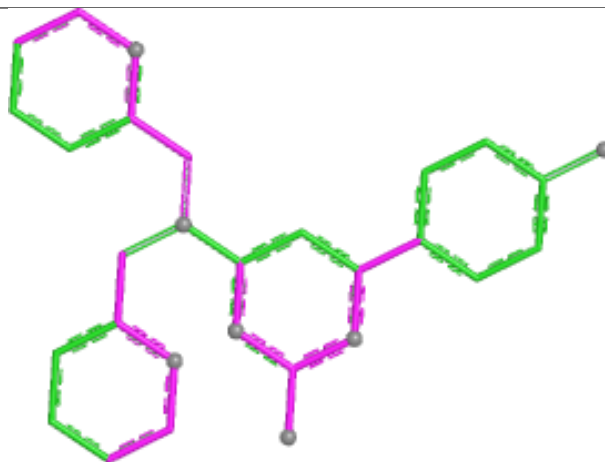




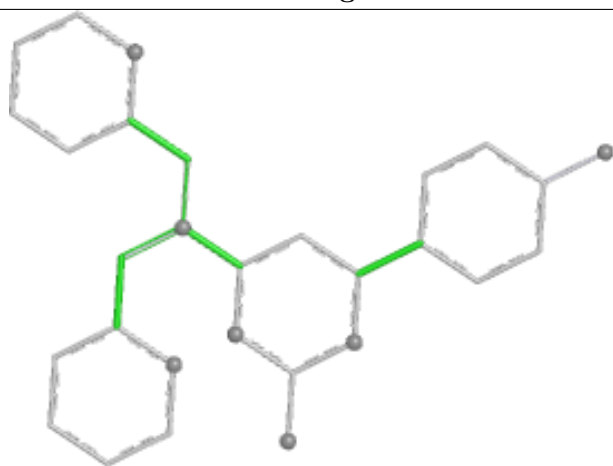
Ligand 6GM F 303



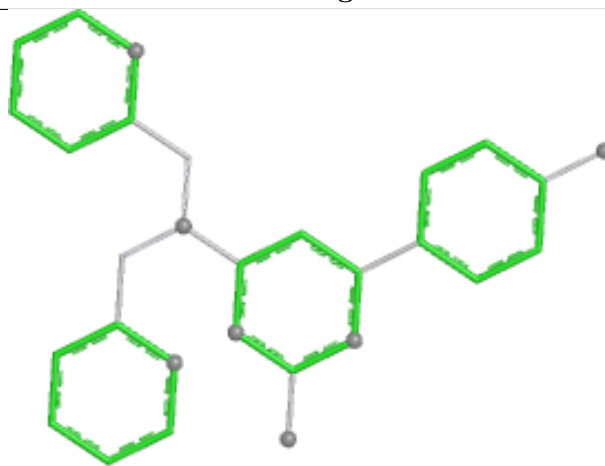
Bond lengths



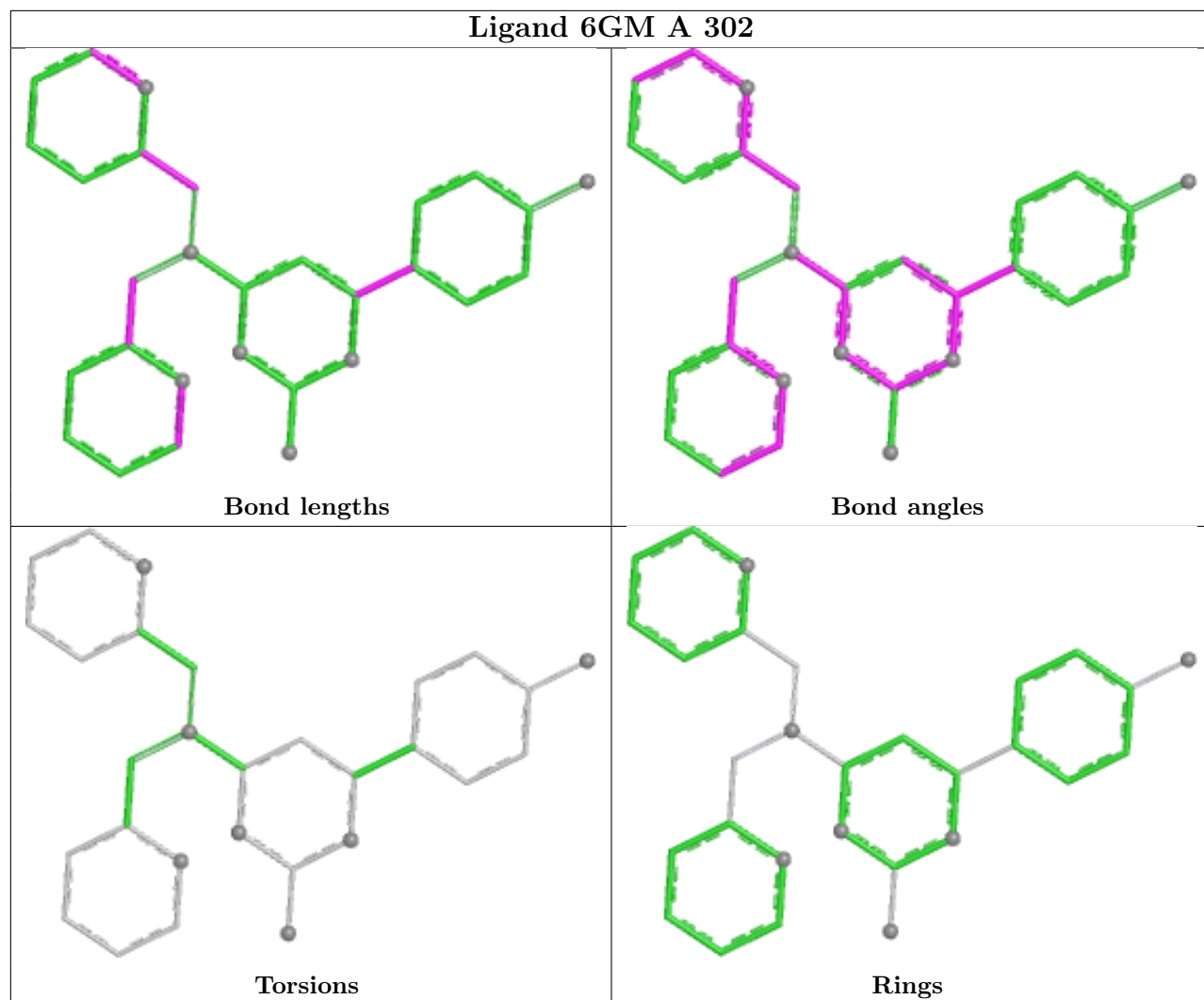
Bond angles

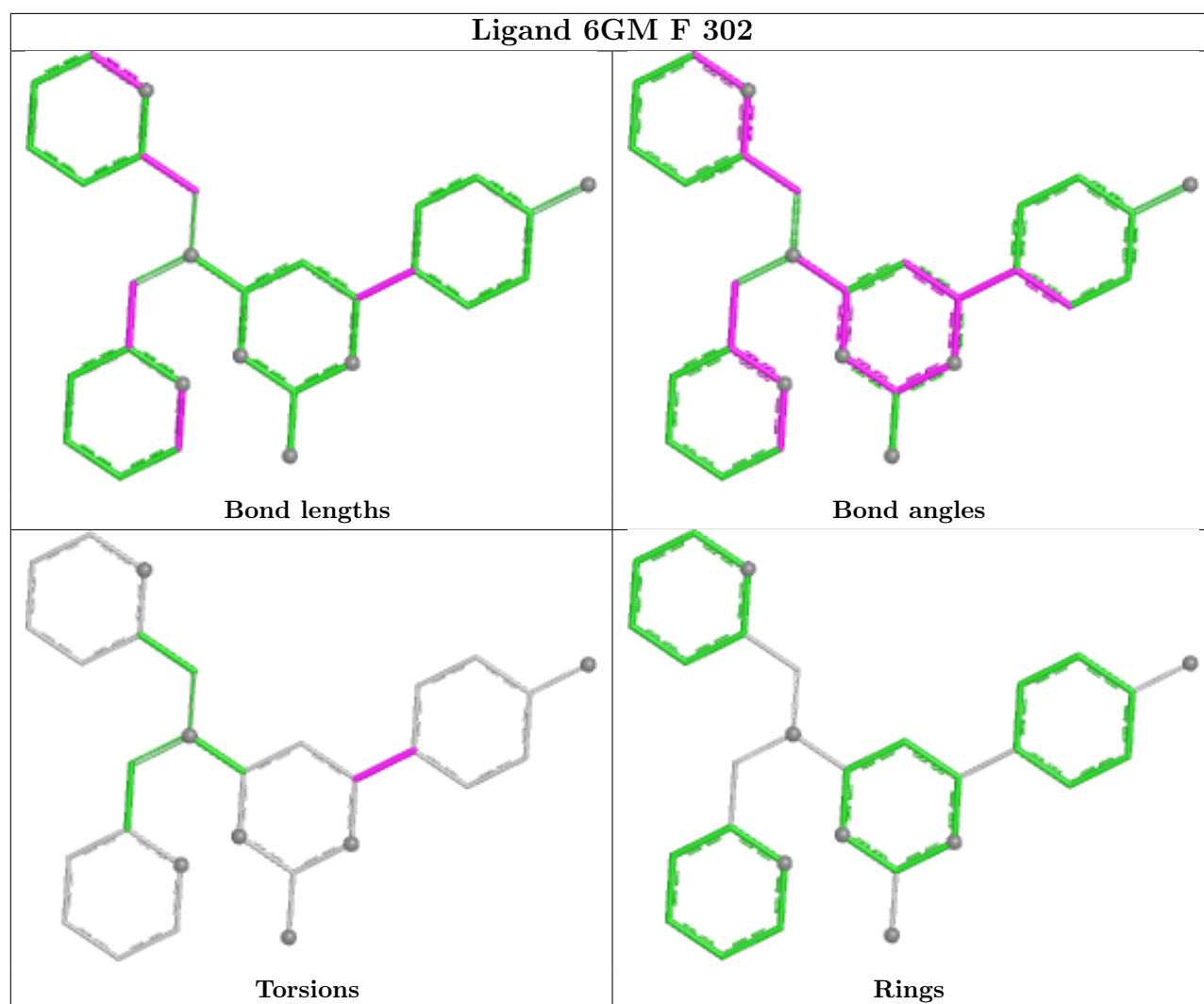


Torsions



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	213/218 (97%)	0.05	6 (2%) 55 57	21, 35, 54, 75	3 (1%)
1	B	213/218 (97%)	0.24	8 (3%) 44 47	23, 39, 64, 83	1 (0%)
1	C	213/218 (97%)	0.19	9 (4%) 40 43	24, 37, 63, 72	0
1	D	213/218 (97%)	0.03	7 (3%) 49 52	19, 34, 57, 76	2 (0%)
1	E	212/218 (97%)	-0.19	3 (1%) 73 75	19, 30, 51, 72	2 (0%)
1	F	212/218 (97%)	0.33	7 (3%) 49 52	27, 42, 63, 78	0
1	G	214/218 (98%)	0.54	13 (6%) 27 30	26, 47, 72, 84	1 (0%)
1	H	212/218 (97%)	0.39	14 (6%) 24 27	26, 42, 69, 80	0
1	I	212/218 (97%)	0.10	2 (0%) 81 82	18, 38, 55, 72	2 (0%)
1	J	212/218 (97%)	0.22	7 (3%) 49 52	22, 39, 63, 73	1 (0%)
All	All	2126/2180 (97%)	0.19	76 (3%) 46 49	18, 38, 63, 84	12 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	-6[A]	TYR	7.1
1	E	156	THR	6.7
1	H	130	THR	5.9
1	B	156	THR	5.0
1	D	44	ILE	4.9
1	F	-6	TYR	4.2
1	G	205	GLY	4.1
1	A	-6	TYR	3.9
1	A	189	PRO	3.9
1	G	156	THR	3.9
1	C	-6	TYR	3.8
1	C	158	ASN	3.6
1	J	156	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	132	SER	3.5
1	C	205	GLY	3.5
1	B	205	GLY	3.4
1	G	128	VAL	3.3
1	G	125	VAL	3.3
1	H	170	ARG	3.2
1	D	205	GLY	3.2
1	H	156	THR	3.0
1	G	157	GLU	3.0
1	A	156	THR	2.9
1	G	158	ASN	2.9
1	C	159	SER	2.9
1	G	170	ARG	2.8
1	H	44	ILE	2.8
1	H	-6	TYR	2.7
1	C	160	ASP	2.7
1	F	43	GLU	2.7
1	H	131	GLU	2.7
1	G	159	SER	2.6
1	B	188	CYS	2.6
1	F	48	VAL	2.6
1	G	206	ARG	2.6
1	F	23	ARG	2.5
1	J	128	VAL	2.5
1	J	190	GLU	2.5
1	B	181	ASN	2.4
1	D	22	GLN	2.4
1	C	189	PRO	2.4
1	J	132	SER	2.4
1	D	23	ARG	2.4
1	G	44	ILE	2.4
1	B	157	GLU	2.4
1	G	130	THR	2.3
1	C	157	GLU	2.3
1	H	155	THR	2.3
1	J	43	GLU	2.3
1	H	-5	LYS	2.2
1	H	43	GLU	2.2
1	A	44	ILE	2.2
1	J	44	ILE	2.2
1	C	190	GLU	2.2
1	F	40	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	22	GLN	2.2
1	J	182	SER	2.2
1	H	157	GLU	2.2
1	D	155	THR	2.2
1	E	23	ARG	2.1
1	A	205	GLY	2.1
1	B	155	THR	2.1
1	A	148	ARG	2.1
1	E	189	PRO	2.1
1	C	156	THR	2.1
1	B	125	VAL	2.1
1	I	170	ARG	2.1
1	F	188	CYS	2.1
1	B	189	PRO	2.1
1	F	37	ASN	2.0
1	D	189	PRO	2.0
1	H	168	TYR	2.0
1	H	128	VAL	2.0
1	I	23	ARG	2.0
1	D	43	GLU	2.0
1	G	173	ILE	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	B	301	14/15	0.54	0.19	67,73,80,88	0
2	NAG	I	301	14/15	0.62	0.18	72,80,88,90	0

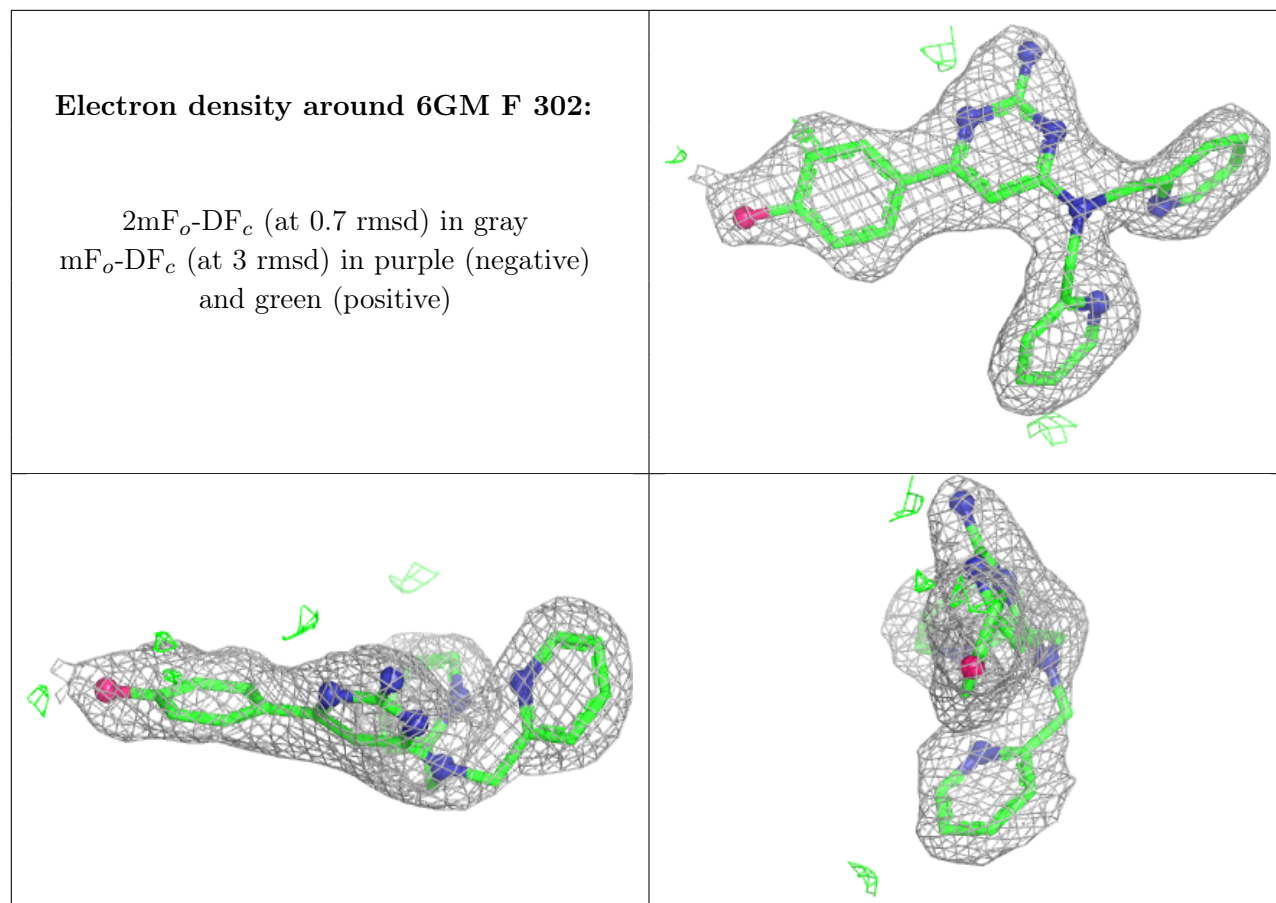
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	H	301	14/15	0.64	0.19	50,62,69,77	0
2	NAG	E	301	14/15	0.64	0.18	63,74,78,83	0
2	NAG	F	301	14/15	0.66	0.17	57,64,69,72	0
2	NAG	D	301	14/15	0.67	0.18	63,70,85,86	0
2	NAG	G	301	14/15	0.67	0.20	63,75,81,81	0
2	NAG	A	301	14/15	0.68	0.17	57,70,75,78	0
2	NAG	C	301	14/15	0.70	0.18	50,60,68,68	0
4	PO4	G	303	5/5	0.71	0.13	69,74,76,84	0
4	PO4	F	306	5/5	0.73	0.14	68,71,78,90	0
4	PO4	D	304	5/5	0.77	0.14	63,67,73,85	0
4	PO4	C	304	5/5	0.81	0.10	66,71,80,85	0
4	PO4	D	305	5/5	0.85	0.16	61,64,72,75	0
4	PO4	E	303	5/5	0.86	0.15	64,66,79,81	0
4	PO4	H	304	5/5	0.87	0.13	54,67,79,84	0
4	PO4	E	304	5/5	0.88	0.12	55,64,73,80	0
3	6GM	F	302	29/29	0.90	0.10	35,52,58,59	0
4	PO4	J	303	5/5	0.90	0.15	45,52,60,61	0
4	PO4	I	305	5/5	0.91	0.11	57,64,77,79	0
3	6GM	F	303	29/29	0.93	0.08	30,38,42,43	0
3	6GM	G	302	29/29	0.93	0.09	34,43,46,48	0
4	PO4	I	304	5/5	0.93	0.13	55,61,66,71	0
3	6GM	A	302	29/29	0.93	0.09	27,39,43,44	0
2	NAG	J	301	14/15	0.93	0.08	26,33,46,47	0
3	6GM	B	302	29/29	0.94	0.08	32,39,44,47	0
3	6GM	I	302	29/29	0.95	0.07	29,34,40,41	0
3	6GM	C	302	29/29	0.95	0.08	28,33,38,40	0
3	6GM	A	303	29/29	0.95	0.07	27,32,37,38	0
3	6GM	I	303	29/29	0.96	0.06	28,35,39,40	0
3	6GM	E	302	29/29	0.96	0.06	21,25,29,31	0
4	PO4	F	305	5/5	0.98	0.06	21,26,28,30	0
4	PO4	B	303	5/5	0.99	0.05	26,27,30,30	0
4	PO4	C	303	5/5	0.99	0.04	21,23,25,26	0
4	PO4	H	302	5/5	0.99	0.05	23,27,30,31	0
4	PO4	H	303	5/5	0.99	0.06	26,27,31,32	0
4	PO4	A	304	5/5	0.99	0.06	23,25,26,26	0
4	PO4	D	302	5/5	0.99	0.04	21,21,23,24	0
4	PO4	F	304	5/5	0.99	0.04	26,27,28,31	0
4	PO4	J	302	5/5	0.99	0.04	23,25,27,27	0
4	PO4	D	303	5/5	0.99	0.04	21,22,24,25	0

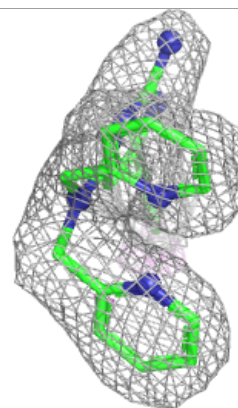
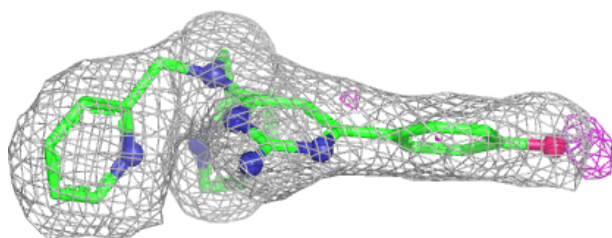
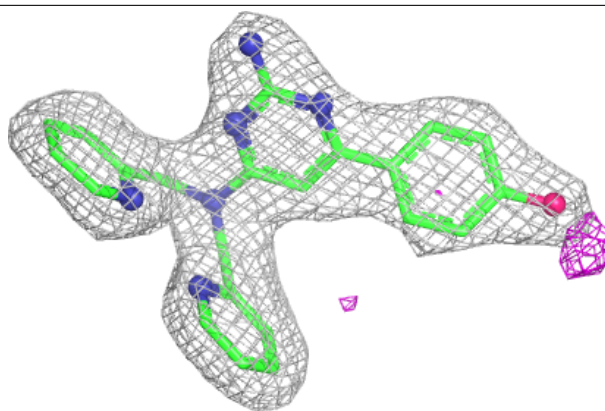
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

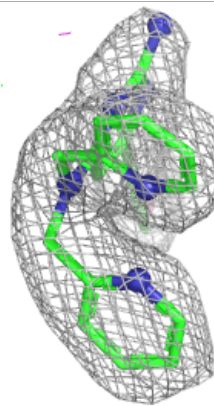
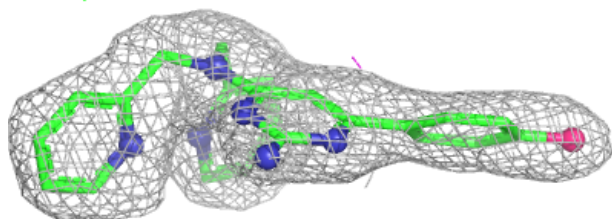
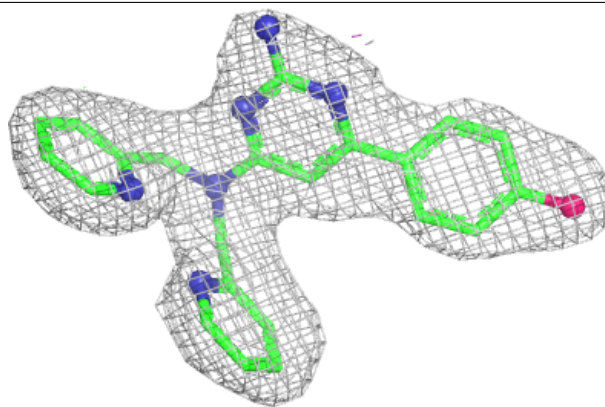


Electron density around 6GM F 303:

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

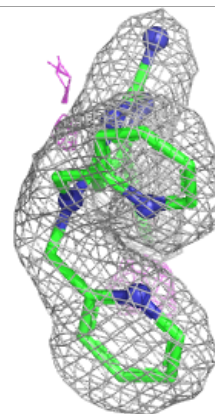
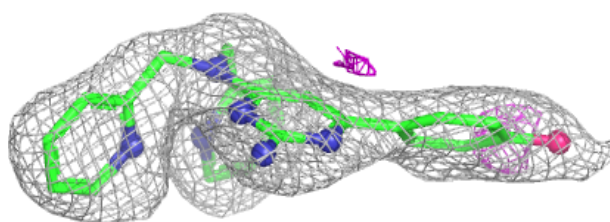
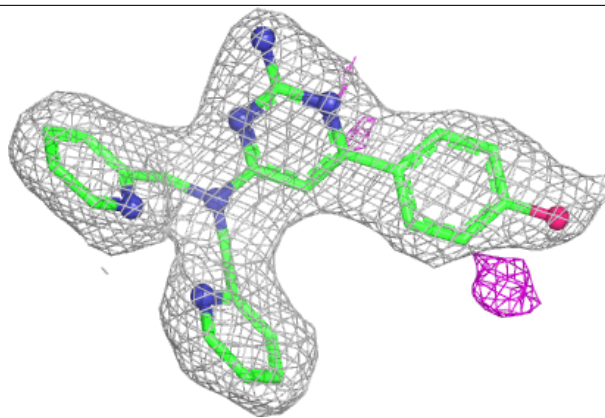
**Electron density around 6GM G 302:**

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



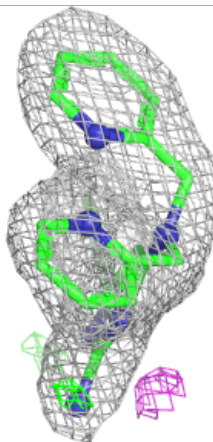
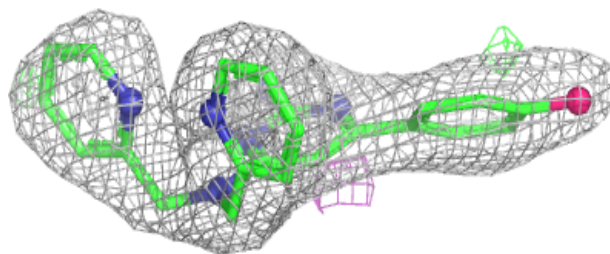
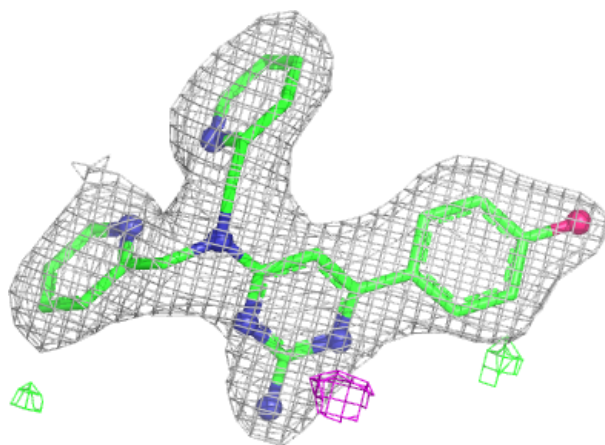
Electron density around 6GM A 302:

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



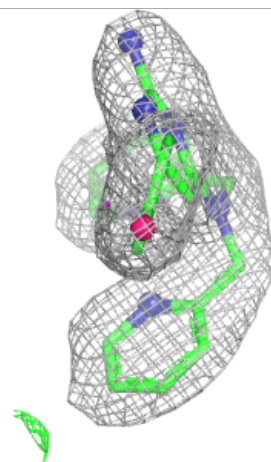
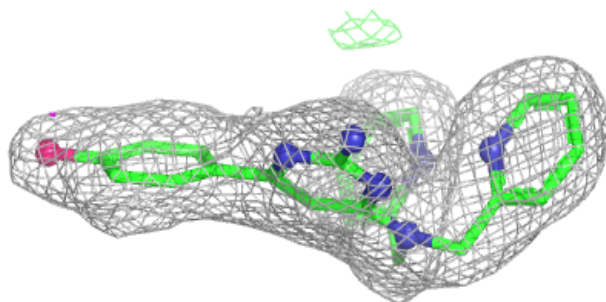
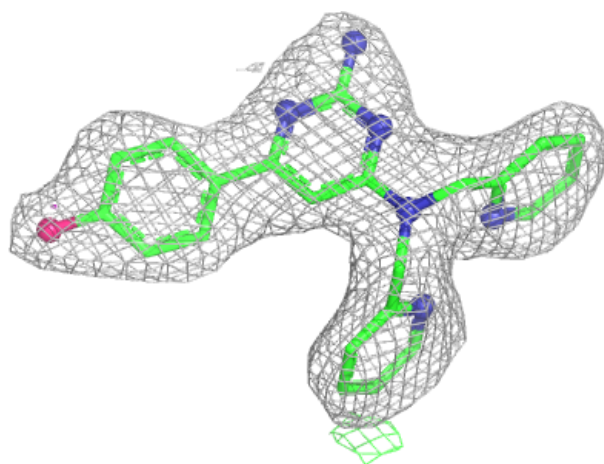
Electron density around 6GM B 302:

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



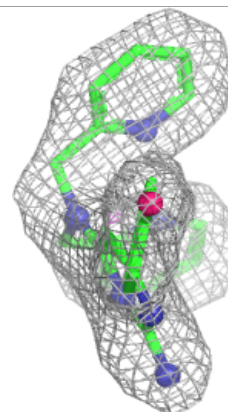
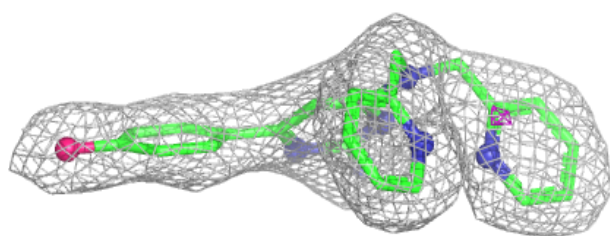
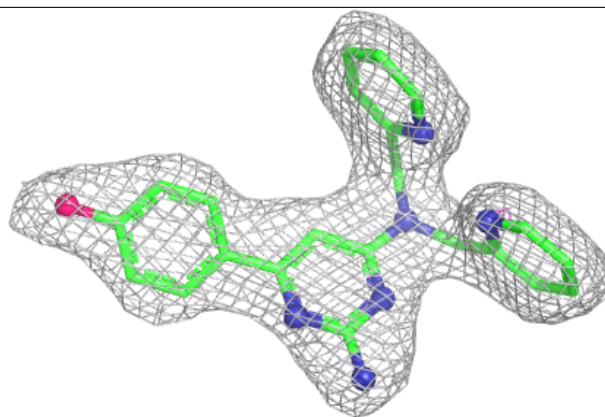
Electron density around 6GM I 302:

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

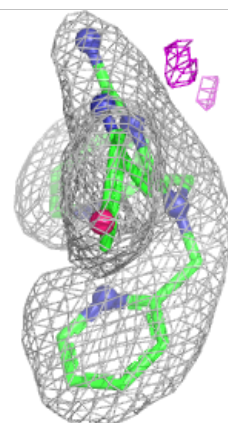
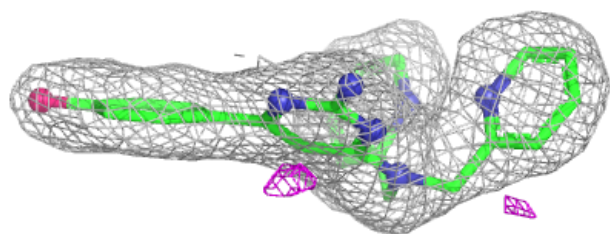
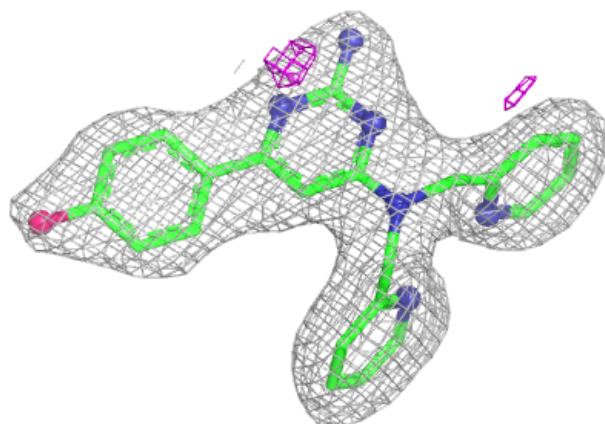


Electron density around 6GM C 302:

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

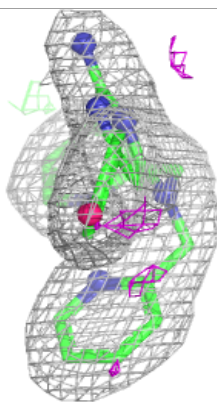
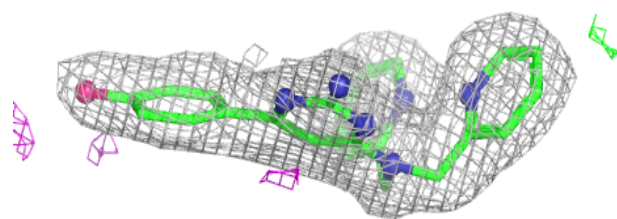
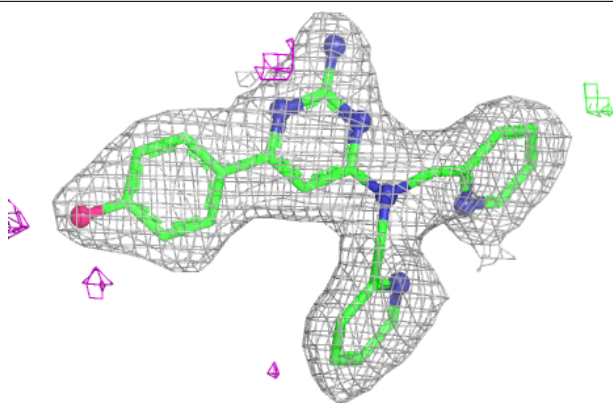
**Electron density around 6GM A 303:**

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

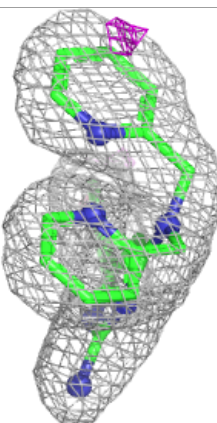
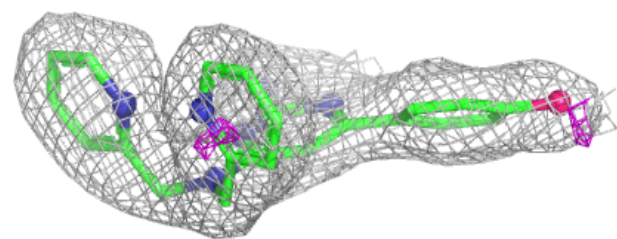
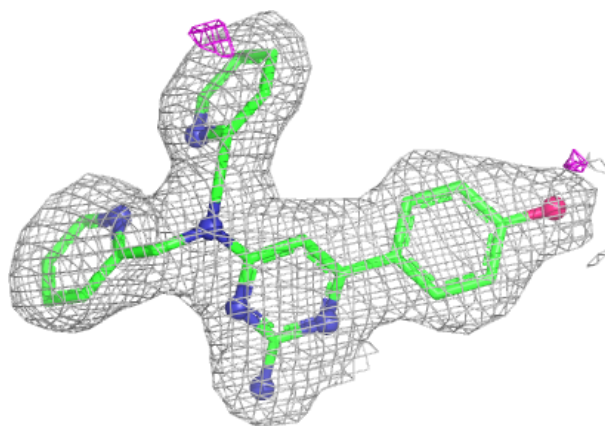


Electron density around 6GM I 303:

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

**Electron density around 6GM E 302:**

$2mF_o-DF_c$ (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.