



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 24, 2026 – 01:50 am BST

PDB ID : 8PEJ / pdb_00008pej
Title : CjGH35 with a Galactosidase Activity-Based Probe
Authors : Offen, W.A.; Davies, G.J.
Deposited on : 2023-06-14
Resolution : 1.50 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 : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
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

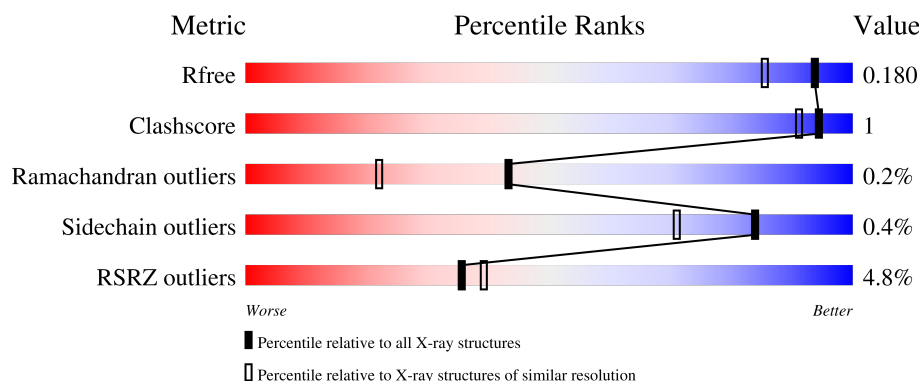
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	550	6% 93% 5%
1	B	550	5% 93% 5%
1	C	550	6% 95% 5%
1	D	550	4% 94% 5%
1	E	550	3% 93% 5%

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Mol	Chain	Length	Quality of chain
1	F	550	4% 94%
1	G	550	5% 91%
1	H	550	6% 92%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 72581 atoms, of which 33577 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	537	Total	C	H	N	O	S	110	7	0
			8365	2721	4118	722	788	16			
1	B	540	Total	C	H	N	O	S	113	6	0
			8419	2735	4143	731	794	16			
1	C	540	Total	C	H	N	O	S	118	8	0
			8451	2747	4159	734	795	16			
1	D	539	Total	C	H	N	O	S	108	10	0
			8471	2752	4174	727	802	16			
1	E	540	Total	C	H	N	O	S	109	11	0
			8509	2762	4199	730	802	16			
1	F	539	Total	C	H	N	O	S	108	12	0
			8558	2772	4225	738	807	16			
1	G	540	Total	C	H	N	O	S	110	14	0
			8574	2779	4226	741	812	16			
1	H	535	Total	C	H	N	O	S	113	12	0
			8488	2755	4187	730	801	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

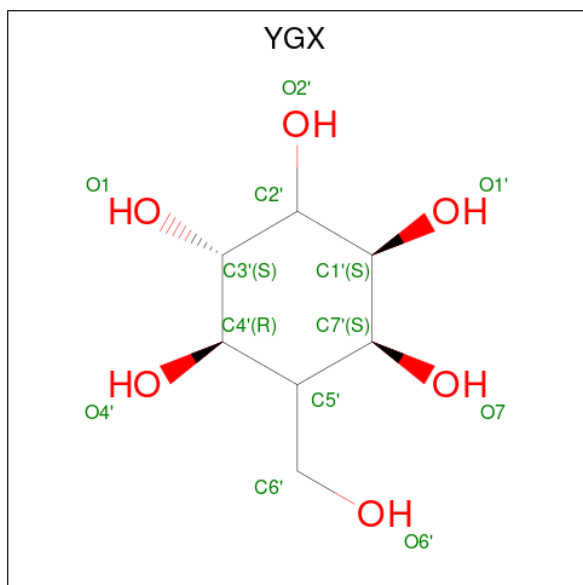
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0
2	B	2	Total Na 2 2	0	0
2	C	4	Total Na 4 4	0	0
2	D	5	Total Na 5 5	0	0
2	E	6	Total Na 6 6	0	0
2	F	4	Total Na 4 4	0	0
2	G	5	Total Na 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	5	Total	Na	0	0
			5	5		

- Molecule 3 is (1S,2S,4S,5R)-6-(hydroxymethyl)cyclohexane-1,2,3,4,5-pentol (CCD ID: YGX) (formula: C₇H₁₄O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	4	0
			25	7	13	5		
3	B	1	Total	C	H	O	4	0
			25	7	13	5		
3	C	1	Total	C	H	O	4	0
			25	7	13	5		
3	D	1	Total	C	H	O	4	0
			25	7	13	5		
3	E	1	Total	C	H	O	4	0
			25	7	13	5		
3	F	1	Total	C	H	O	4	0
			25	7	13	5		
3	G	1	Total	C	H	O	4	0
			25	7	13	5		
3	H	1	Total	C	H	O	4	0
			25	7	13	5		

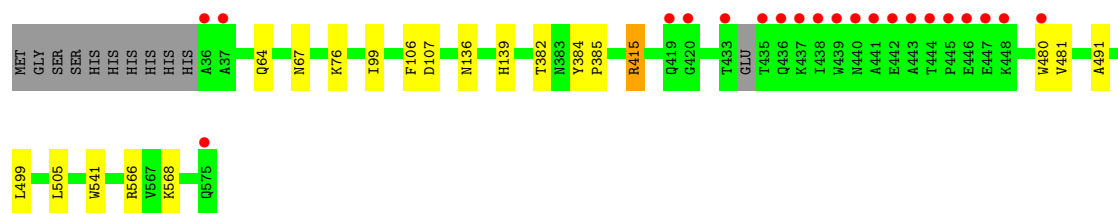
- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	D	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		
4	E	1	Total	C	H	O	0	0
			7	2	3	2		
4	F	1	Total	C	H	O	0	0
			7	2	3	2		
4	F	1	Total	C	H	O	0	0
			7	2	3	2		
4	G	1	Total	C	H	O	0	0
			7	2	3	2		
4	G	1	Total	C	H	O	0	0
			7	2	3	2		
4	G	1	Total	C	H	O	0	0
			7	2	3	2		
4	G	1	Total	C	H	O	0	0
			7	2	3	2		
4	H	1	Total	C	H	O	0	0
			7	2	3	2		
4	H	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 5 is water.

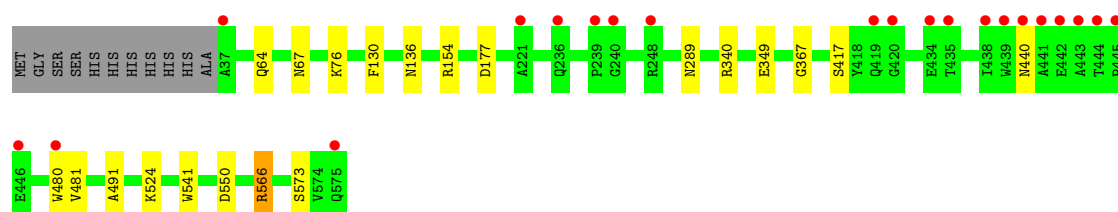
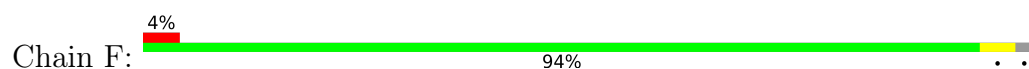
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	468	Total 468	O 468	0	0
5	B	552	Total 552	O 552	0	0
5	C	467	Total 467	O 467	0	0
5	D	590	Total 590	O 590	0	0
5	E	635	Total 635	O 635	0	0
5	F	569	Total 569	O 569	0	0
5	G	635	Total 635	O 635	0	0
5	H	497	Total 497	O 497	0	0



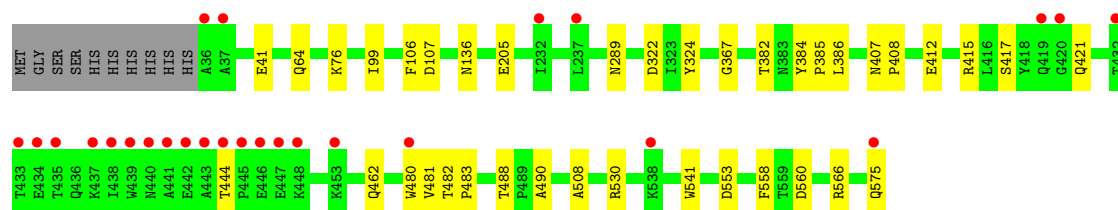
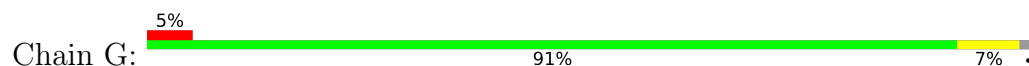
- Molecule 1: Beta-galactosidase, putative, bgl35A



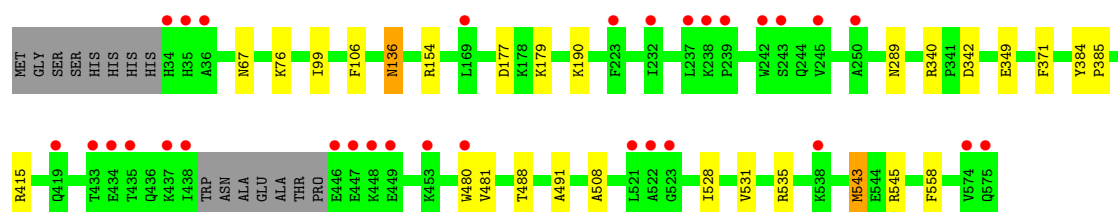
- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



- Molecule 1: Beta-galactosidase, putative, bgl35A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.32Å 116.21Å 116.40Å 90.24° 89.89° 90.09°	Depositor
Resolution (Å)	82.54 – 1.50 82.54 – 1.50	Depositor EDS
% Data completeness (in resolution range)	96.3 (82.54-1.50) 94.4 (82.54-1.50)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0411, REFMAC 5.8.0411	Depositor
R, R_{free}	0.157 , 0.181 0.156 , 0.180	Depositor DCC
R_{free} test set	40271 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for h,-l,k 0.008 for h,l,-k 0.009 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,-l,-k 0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	72581	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.75% 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: YGX, NA, ACT

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	0.71	1/4363 (0.0%)	1.03	5/5945 (0.1%)
1	B	0.72	1/4393 (0.0%)	1.04	4/5986 (0.1%)
1	C	0.70	0/4408	1.05	1/6007 (0.0%)
1	D	0.80	1/4413 (0.0%)	1.08	3/6013 (0.0%)
1	E	0.80	1/4433 (0.0%)	1.09	3/6039 (0.0%)
1	F	0.78	1/4447 (0.0%)	1.10	7/6052 (0.1%)
1	G	0.83	1/4462 (0.0%)	1.10	8/6076 (0.1%)
1	H	0.72	1/4418 (0.0%)	1.03	8/6017 (0.1%)
All	All	0.76	7/35337 (0.0%)	1.06	39/48135 (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	A	0	4
1	D	0	1
1	E	0	3
1	F	0	2
1	G	0	1
1	H	0	3
All	All	0	14

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	349	GLU	CD-OE2	7.43	1.39	1.25
1	H	349	GLU	CD-OE2	6.14	1.37	1.25
1	G	490	ALA	CA-CB	-5.39	1.44	1.53
1	F	349	GLU	CD-OE2	5.34	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	GLU	CD-OE2	5.31	1.35	1.25

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	289	ASN	CA-CB-CG	8.43	121.03	112.60
1	H	543	MET	CG-SD-CE	-7.10	85.29	100.90
1	A	340	ARG	O-C-N	-6.96	117.25	121.71
1	E	130	PHE	CA-CB-CG	6.91	120.71	113.80
1	F	67	ASN	CA-CB-CG	6.67	119.27	112.60

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ARG	Sidechain
1	A	191[A]	ARG	Sidechain
1	A	415[A]	ARG	Sidechain
1	A	530	ARG	Sidechain
1	D	415	ARG	Sidechain

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	4247	4118	4058	10	0
1	B	4276	4143	4087	17	0
1	C	4292	4159	4091	8	0
1	D	4297	4174	4122	9	0
1	E	4310	4199	4146	14	0
1	F	4333	4225	4169	5	0
1	G	4348	4226	4166	17	0
1	H	4301	4187	4133	9	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	6	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	12	13	0	0	0
3	B	12	13	0	0	0
3	C	12	13	0	0	0
3	D	12	13	0	0	0
3	E	12	13	0	0	0
3	F	12	13	0	0	0
3	G	12	13	0	0	0
3	H	12	13	0	0	0
4	A	4	3	3	0	0
4	D	12	9	9	0	0
4	E	8	6	6	0	0
4	F	8	6	6	0	0
4	G	16	12	12	0	0
4	H	8	6	6	0	0
5	A	468	0	0	3	0
5	B	552	0	0	5	0
5	C	467	0	0	2	0
5	D	590	0	0	5	2
5	E	635	0	0	5	1
5	F	569	0	0	1	4
5	G	635	0	0	6	3
5	H	497	0	0	3	0
All	All	39004	33577	33014	88	5

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 1.

The worst 5 of 88 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:E:326[B]:ARG:NH1	5:E:701:HOH:O	2.12	0.80
1:C:457:SER:O	5:C:701:HOH:O	2.02	0.76
1:E:76:LYS:HE2	5:E:947:HOH:O	1.92	0.69
1:G:41:GLU:OE2	5:G:702:HOH:O	2.10	0.68
1:D:76:LYS:HE2	5:D:740:HOH:O	1.93	0.67

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:943:HOH:O	5:G:704:HOH:O[1_565]	2.07	0.13
5:F:997:HOH:O	5:G:1163:HOH:O[1_565]	2.07	0.13
5:D:1210:HOH:O	5:G:1305:HOH:O[1_565]	2.10	0.10
5:D:906:HOH:O	5:F:704:HOH:O[1_554]	2.16	0.04
5:E:1235:HOH:O	5:F:1249:HOH:O[1_554]	2.16	0.04

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	540/550 (98%)	519 (96%)	20 (4%)	1 (0%)	43	22
1	B	542/550 (98%)	520 (96%)	20 (4%)	2 (0%)	30	12
1	C	544/550 (99%)	524 (96%)	19 (4%)	1 (0%)	43	22
1	D	545/550 (99%)	526 (96%)	18 (3%)	1 (0%)	43	22
1	E	549/550 (100%)	529 (96%)	19 (4%)	1 (0%)	43	22
1	F	549/550 (100%)	527 (96%)	20 (4%)	2 (0%)	30	12
1	G	552/550 (100%)	534 (97%)	18 (3%)	0	100	100
1	H	543/550 (99%)	524 (96%)	18 (3%)	1 (0%)	43	22
All	All	4364/4400 (99%)	4203 (96%)	152 (4%)	9 (0%)	43	22

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	522	ALA
1	D	491	ALA
1	A	491	ALA
1	B	491	ALA
1	E	491	ALA

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	431/461 (94%)	430 (100%)	1 (0%)	87	77
1	B	436/461 (95%)	435 (100%)	1 (0%)	87	77
1	C	436/461 (95%)	435 (100%)	1 (0%)	87	77
1	D	441/461 (96%)	439 (100%)	2 (0%)	81	66
1	E	442/461 (96%)	441 (100%)	1 (0%)	87	77
1	F	445/461 (96%)	444 (100%)	1 (0%)	87	77
1	G	445/461 (96%)	440 (99%)	5 (1%)	65	41
1	H	443/461 (96%)	441 (100%)	2 (0%)	81	66
All	All	3519/3688 (95%)	3505 (100%)	14 (0%)	84	71

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	136	ASN
1	G	382	THR
1	H	190	LYS
1	G	444	THR
1	H	136	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	105	GLN
1	H	64	GLN
1	E	45	ASN
1	H	354	GLN
1	G	354	GLN

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](#)

Of 57 ligands modelled in this entry, 35 are monoatomic - leaving 22 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	YGX	B	602	1	12,12,13	0.60	0	14,17,19	0.79	1 (7%)
3	YGX	F	604	1	12,12,13	1.04	1 (8%)	14,17,19	0.78	0
3	YGX	D	605	1	12,12,13	0.72	0	14,17,19	0.81	0
4	ACT	F	606	-	3,3,3	0.92	0	3,3,3	0.74	0
4	ACT	E	606	-	3,3,3	0.76	0	3,3,3	1.05	0
4	ACT	H	603	-	3,3,3	0.94	0	3,3,3	1.03	0
3	YGX	G	603	1	12,12,13	0.56	0	14,17,19	0.83	0
3	YGX	A	602	1	12,12,13	0.55	0	14,17,19	0.88	0
4	ACT	A	603	-	3,3,3	0.92	0	3,3,3	0.78	0
4	ACT	F	605	-	3,3,3	1.06	0	3,3,3	0.80	0
4	ACT	H	604	-	3,3,3	1.21	0	3,3,3	1.03	0
4	ACT	D	606	-	3,3,3	0.80	0	3,3,3	0.99	0
4	ACT	G	605	-	3,3,3	0.73	0	3,3,3	0.99	0
4	ACT	D	607	-	3,3,3	1.08	0	3,3,3	0.88	0
3	YGX	E	604	1	12,12,13	0.72	0	14,17,19	0.90	0
4	ACT	E	605	-	3,3,3	1.16	0	3,3,3	0.60	0
4	ACT	G	606	-	3,3,3	1.37	0	3,3,3	0.38	0
3	YGX	H	602	1	12,12,13	0.64	0	14,17,19	0.96	1 (7%)
4	ACT	G	607	-	3,3,3	0.94	0	3,3,3	1.02	0
4	ACT	G	604	-	3,3,3	1.09	0	3,3,3	0.59	0
4	ACT	D	604	-	3,3,3	0.92	0	3,3,3	1.22	0
3	YGX	C	603	1	12,12,13	0.47	0	14,17,19	1.13	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	YGX	A	602	1	-	0/2/22/26	0/1/1/1
3	YGX	B	602	1	-	0/2/22/26	0/1/1/1
3	YGX	F	604	1	-	0/2/22/26	0/1/1/1
3	YGX	H	602	1	-	0/2/22/26	0/1/1/1
3	YGX	D	605	1	-	0/2/22/26	0/1/1/1
3	YGX	C	603	1	-	0/2/22/26	0/1/1/1
3	YGX	G	603	1	-	0/2/22/26	0/1/1/1
3	YGX	E	604	1	-	0/2/22/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	604	YGX	C3'-C2'	-2.32	1.48	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	602	YGX	C3'-C2'-C1'	-2.57	106.95	110.69
3	C	603	YGX	C3'-C2'-C1'	-2.24	107.42	110.69
3	B	602	YGX	O1'-C1'-C2'	2.11	114.04	109.99

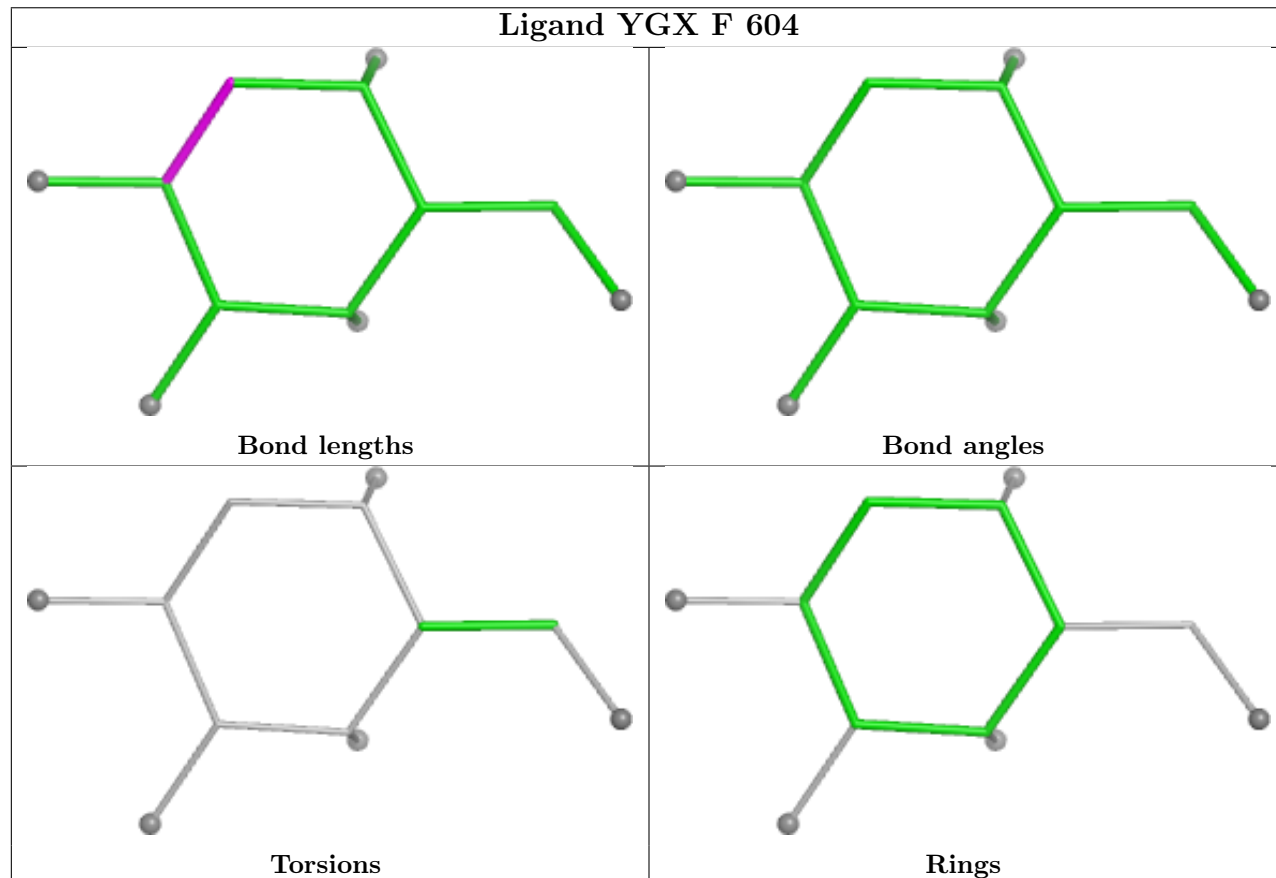
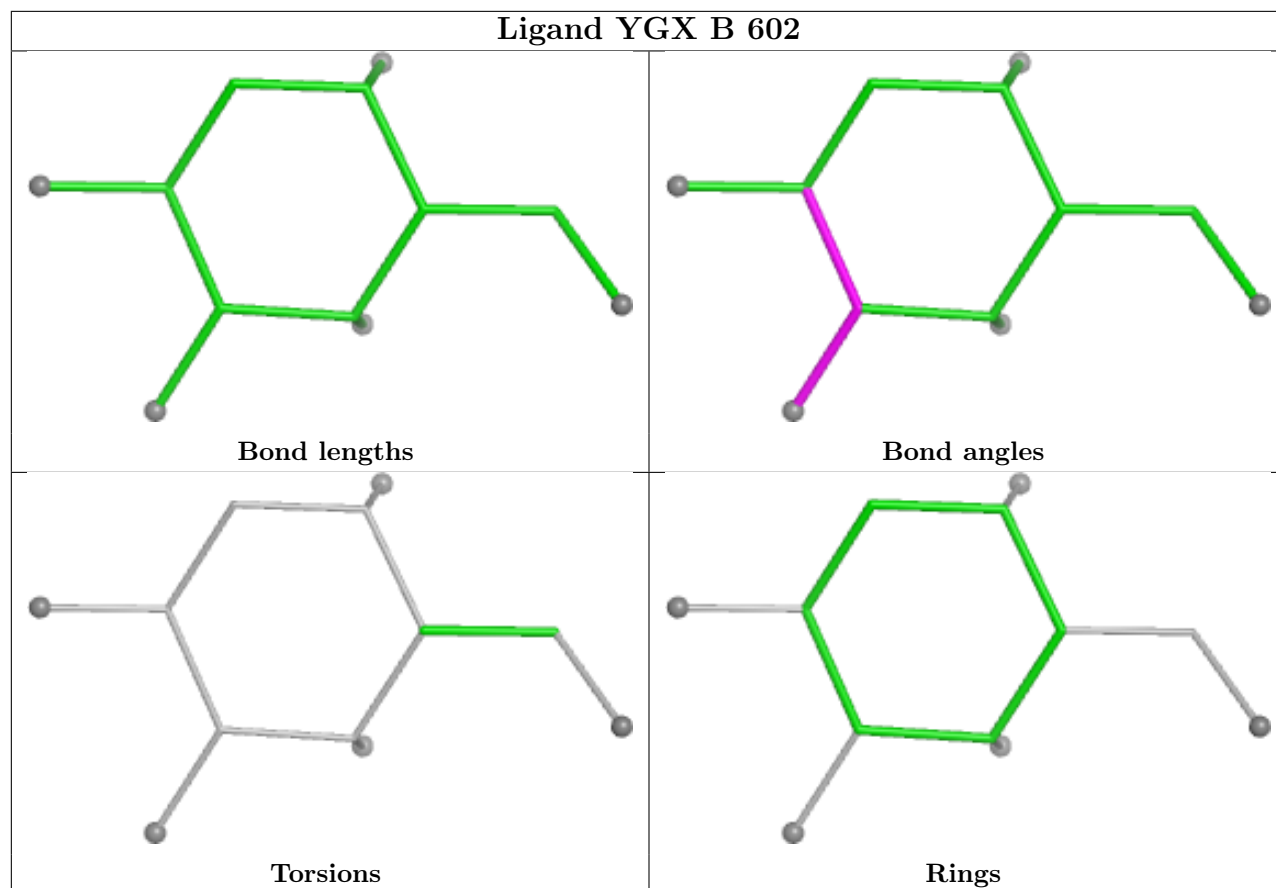
There are no chirality outliers.

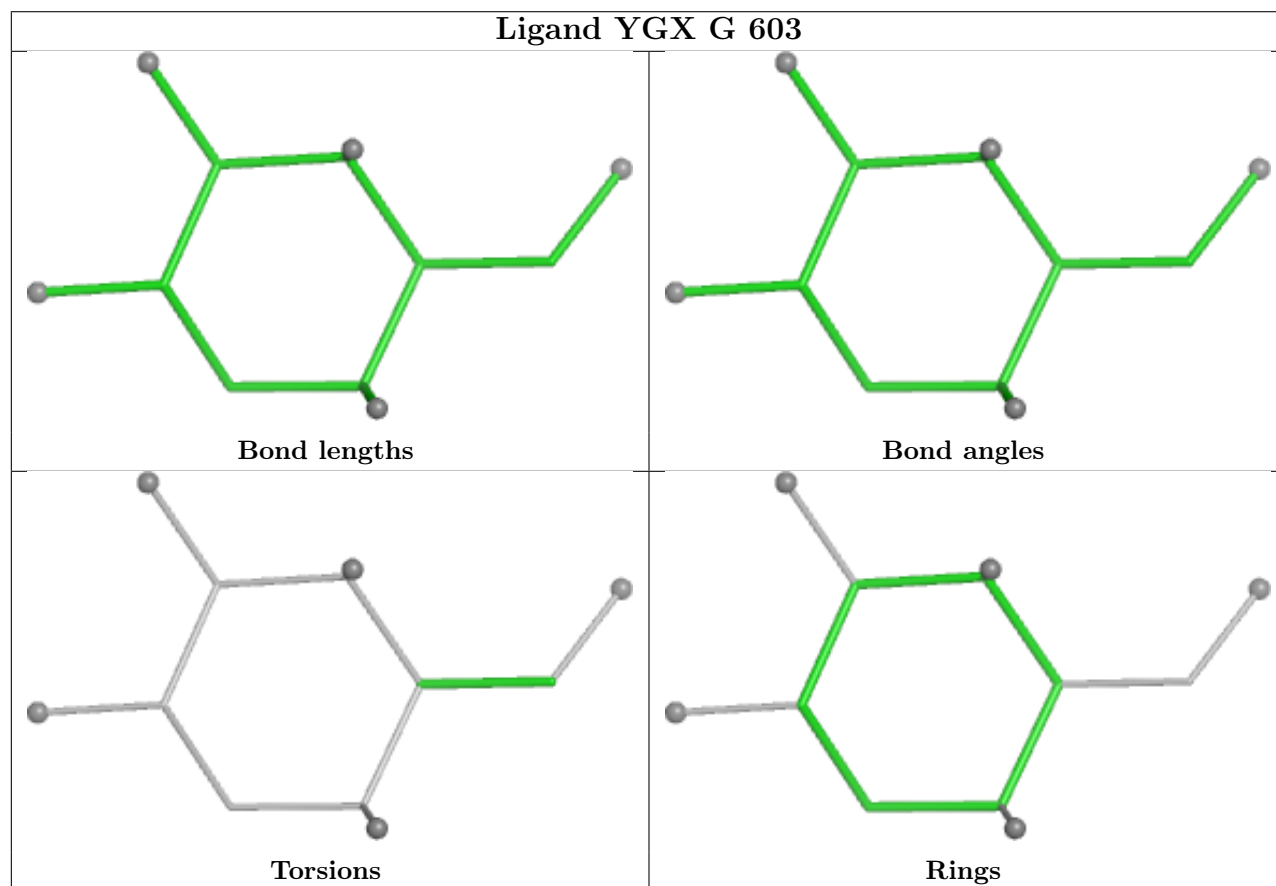
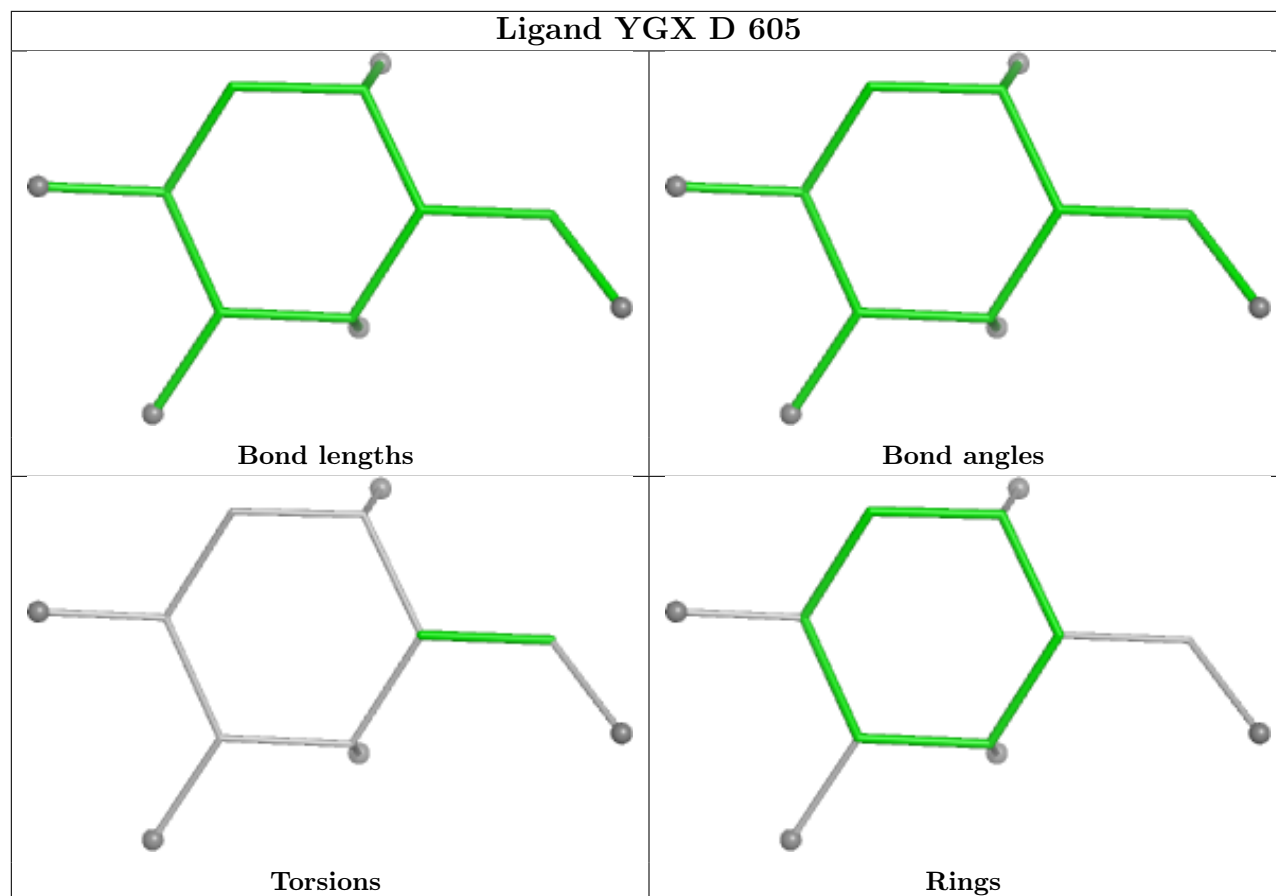
There are no torsion outliers.

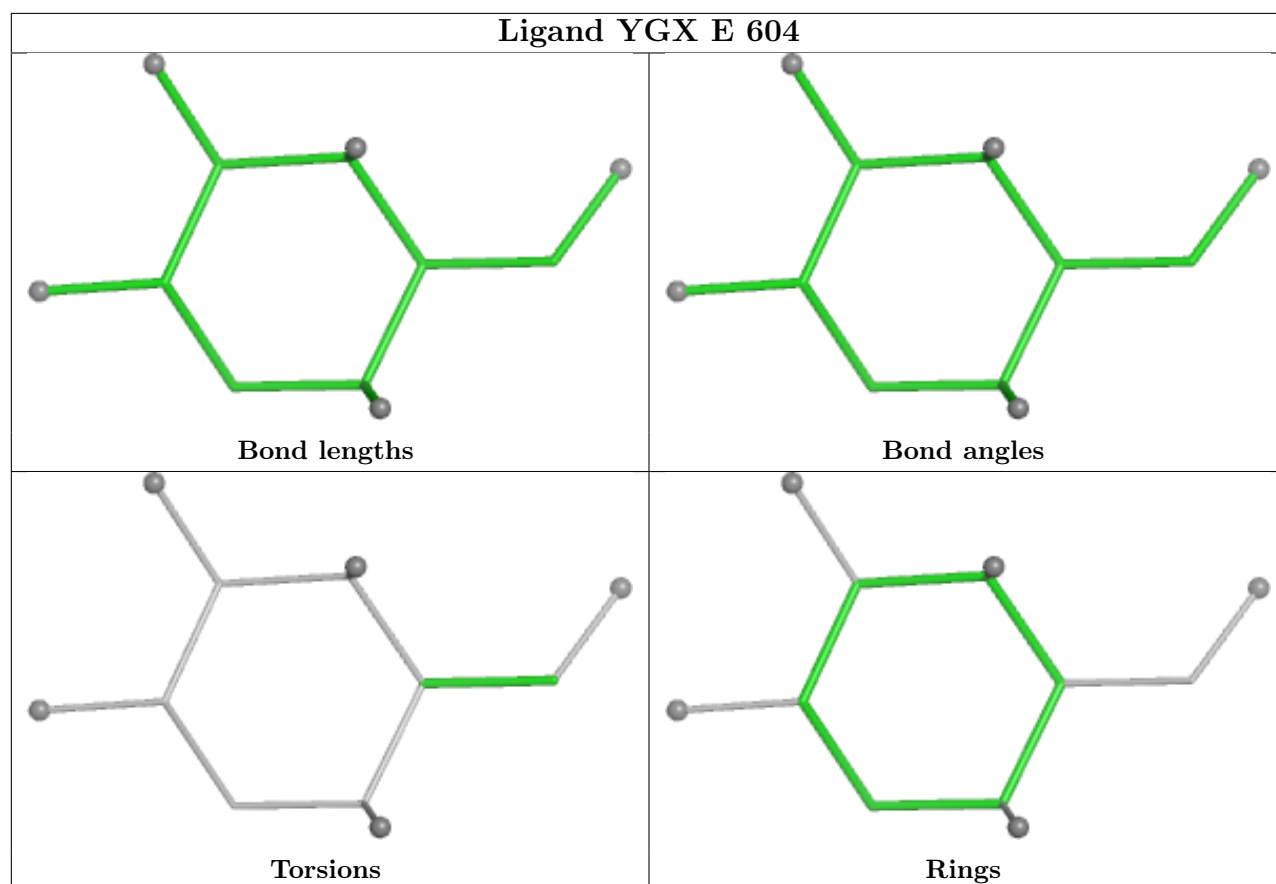
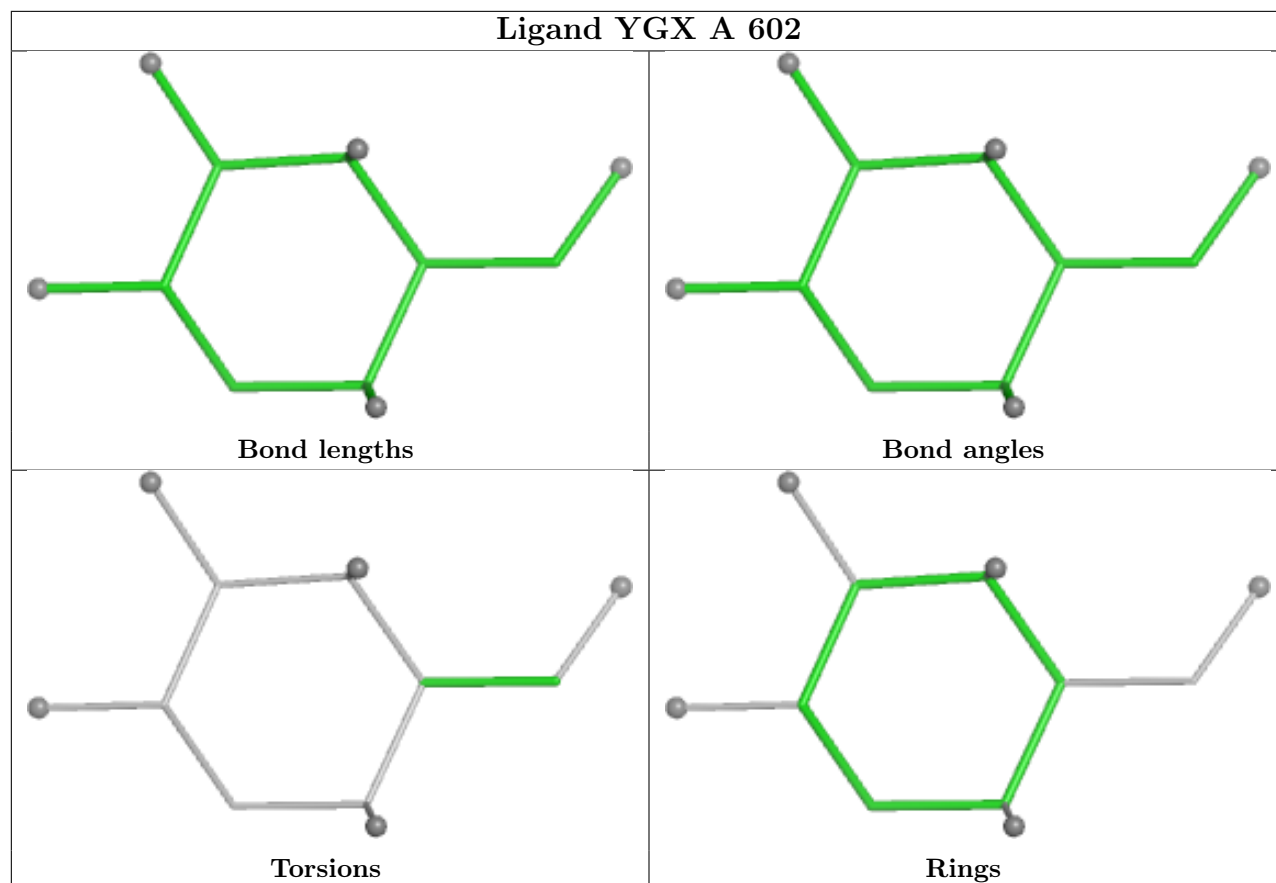
There are no ring outliers.

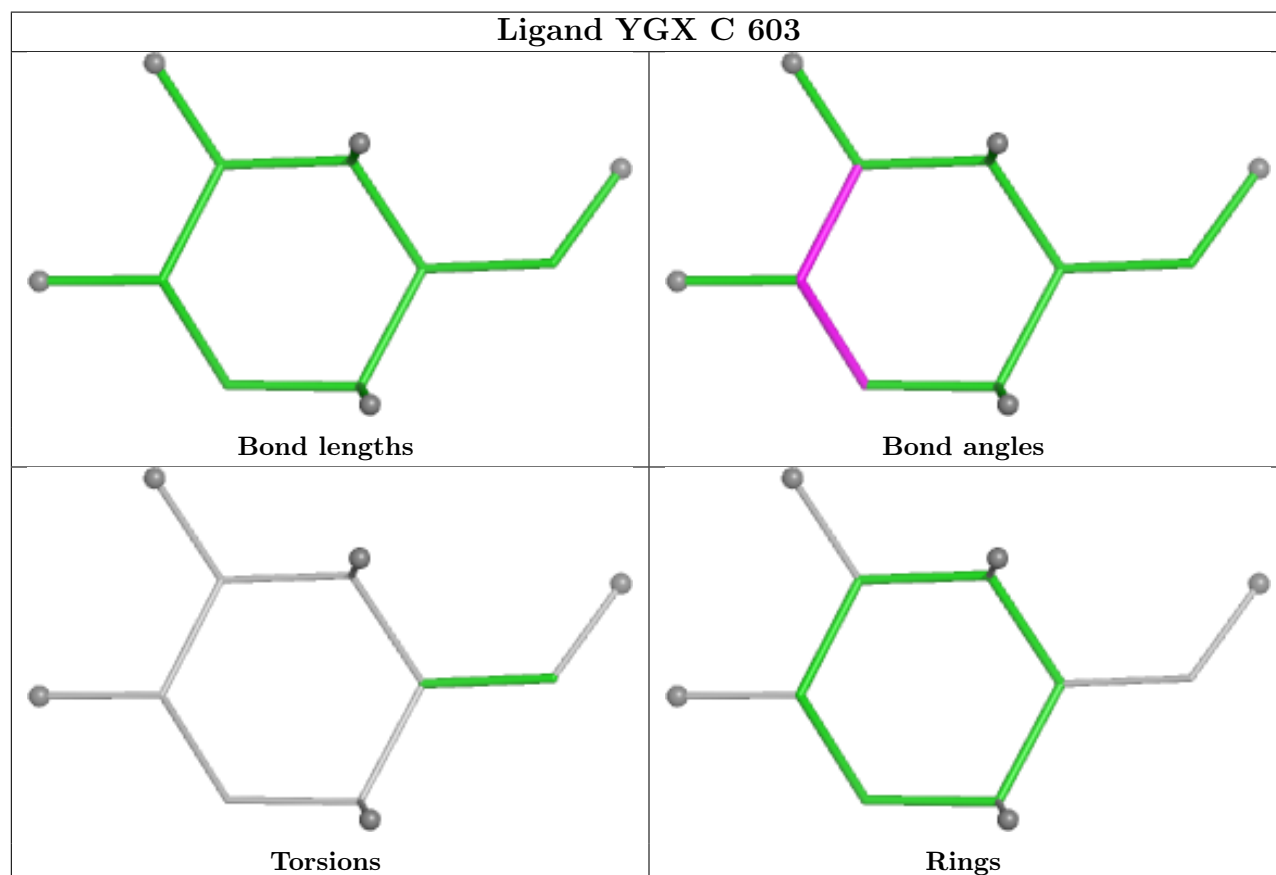
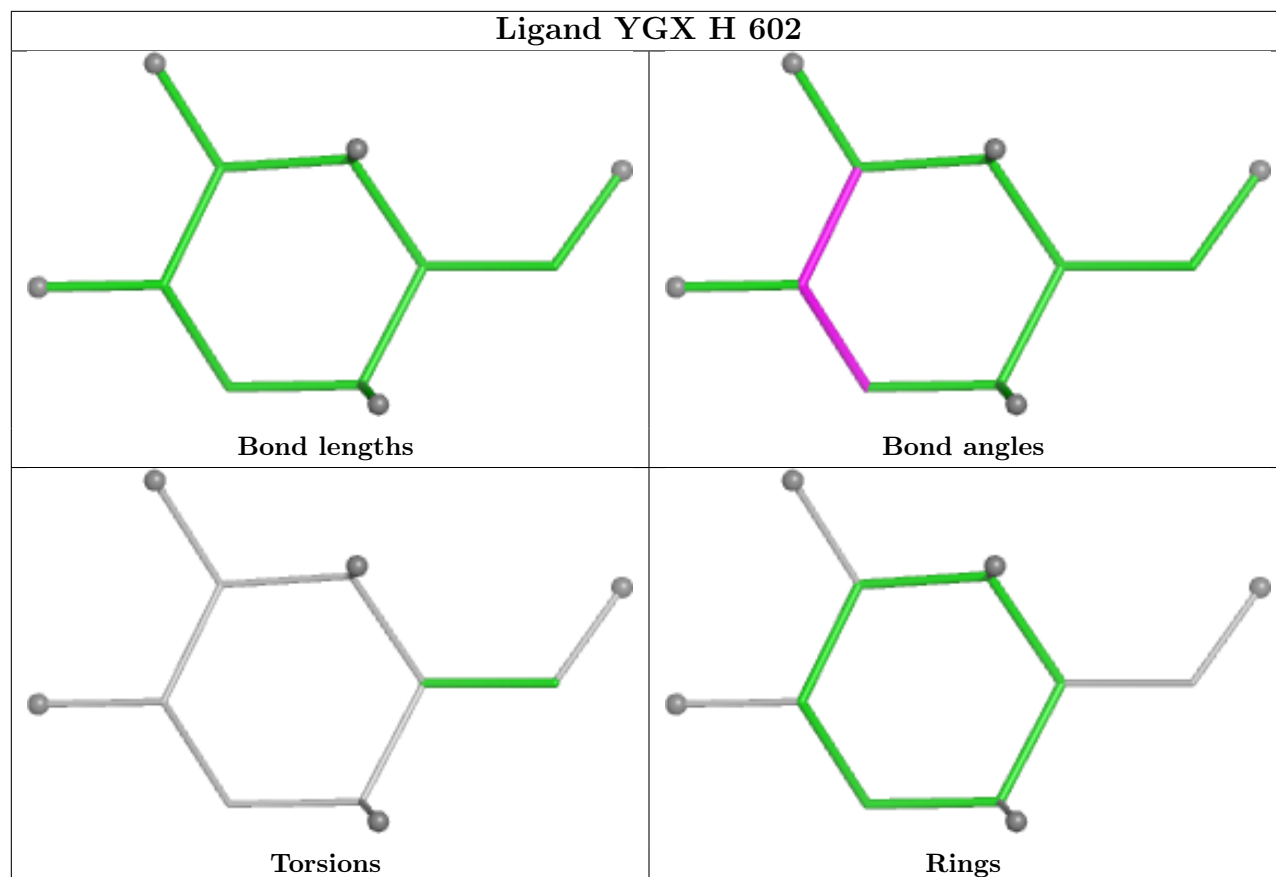
No monomer is involved in short contacts.

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	537/550 (97%)	0.26	33 (6%)	27	29	9, 24, 38, 59	48 (8%)
1	B	540/550 (98%)	-0.04	26 (4%)	35	39	11, 22, 35, 51	40 (7%)
1	C	540/550 (98%)	0.24	31 (5%)	29	32	10, 24, 37, 62	42 (7%)
1	D	539/550 (98%)	-0.13	21 (3%)	43	47	8, 20, 34, 55	42 (7%)
1	E	540/550 (98%)	-0.17	17 (3%)	51	55	8, 20, 32, 49	43 (7%)
1	F	539/550 (98%)	-0.03	21 (3%)	43	47	8, 21, 36, 49	47 (8%)
1	G	540/550 (98%)	-0.11	26 (4%)	35	39	7, 19, 33, 47	45 (8%)
1	H	535/550 (97%)	0.11	31 (5%)	29	31	9, 23, 36, 59	56 (10%)
All	All	4310/4400 (97%)	0.02	206 (4%)	35	39	7, 22, 36, 62	363 (8%)

The worst 5 of 206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	439	TRP	15.0
1	E	439	TRP	14.9
1	A	438	ILE	14.3
1	G	445	PRO	13.6
1	A	439	TRP	13.5

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 ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ACT	D	606	4/4	0.81	0.18	40,40,44,44	7
4	ACT	G	606	4/4	0.84	0.16	30,32,35,36	7
4	ACT	F	606	4/4	0.88	0.16	28,28,29,29	7
4	ACT	G	605	4/4	0.88	0.21	34,34,35,36	7
4	ACT	D	607	4/4	0.88	0.15	30,39,39,40	7
4	ACT	H	603	4/4	0.88	0.15	37,44,44,44	7
4	ACT	E	605	4/4	0.89	0.23	23,24,25,26	7
4	ACT	E	606	4/4	0.89	0.20	29,34,34,34	7
4	ACT	A	603	4/4	0.89	0.14	27,33,33,34	7
2	NA	E	608	1/1	0.90	0.15	39,39,39,39	0
4	ACT	H	604	4/4	0.91	0.11	27,31,32,34	7
4	ACT	G	607	4/4	0.92	0.12	33,34,34,35	7
4	ACT	G	604	4/4	0.93	0.17	20,23,24,24	7
4	ACT	F	605	4/4	0.93	0.11	28,33,34,35	7
2	NA	H	601	1/1	0.94	0.09	34,34,34,34	0
2	NA	C	602	1/1	0.94	0.10	38,38,38,38	0
4	ACT	D	604	4/4	0.94	0.09	29,33,34,38	0
2	NA	C	601	1/1	0.95	0.07	45,45,45,45	0
2	NA	E	607	1/1	0.95	0.09	28,28,28,28	0
2	NA	H	608	1/1	0.96	0.07	39,39,39,39	0
2	NA	D	601	1/1	0.96	0.06	22,22,22,22	0
2	NA	F	607	1/1	0.96	0.11	26,26,26,26	0
2	NA	A	606	1/1	0.96	0.11	32,32,32,32	0
2	NA	H	607	1/1	0.96	0.07	30,30,30,30	1
2	NA	A	604	1/1	0.97	0.08	27,27,27,27	0
2	NA	C	605	1/1	0.97	0.06	30,30,30,30	0
2	NA	A	605	1/1	0.97	0.11	34,34,34,34	0
2	NA	D	609	1/1	0.97	0.07	28,28,28,28	0
2	NA	G	608	1/1	0.98	0.06	25,25,25,25	0
2	NA	D	602	1/1	0.98	0.06	24,24,24,24	0
2	NA	H	605	1/1	0.98	0.14	27,27,27,27	0
2	NA	H	606	1/1	0.98	0.07	31,31,31,31	0
2	NA	E	601	1/1	0.98	0.08	22,22,22,22	0
2	NA	F	602	1/1	0.98	0.05	25,25,25,25	0
3	YGX	A	602	12/13	0.98	0.04	17,18,21,21	4
3	YGX	B	602	12/13	0.98	0.04	16,17,20,21	4
3	YGX	C	603	12/13	0.98	0.04	17,19,21,25	4

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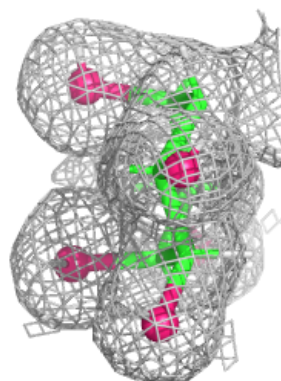
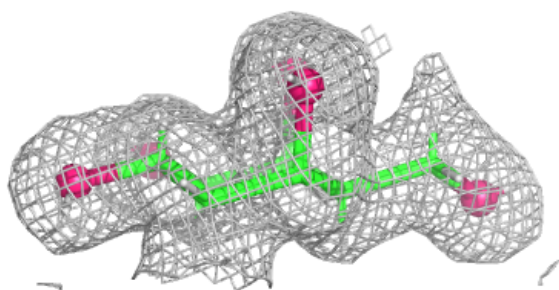
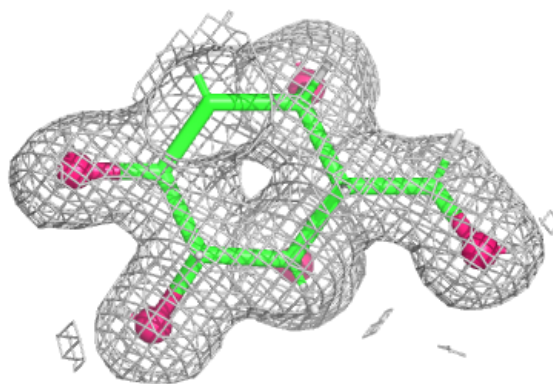
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	YGX	E	604	12/13	0.98	0.04	14,15,17,18	4
3	YGX	F	604	12/13	0.98	0.04	14,16,17,18	4
3	YGX	G	603	12/13	0.98	0.04	14,15,16,17	4
2	NA	E	602	1/1	0.98	0.04	20,20,20,20	0
2	NA	G	602	1/1	0.99	0.05	20,20,20,20	0
3	YGX	H	602	12/13	0.99	0.03	17,18,20,20	4
2	NA	B	603	1/1	0.99	0.07	27,27,27,27	0
2	NA	G	609	1/1	0.99	0.04	24,24,24,24	0
2	NA	G	610	1/1	0.99	0.06	25,25,25,25	0
2	NA	A	601	1/1	0.99	0.05	29,29,29,29	0
2	NA	E	603	1/1	0.99	0.03	22,22,22,22	0
2	NA	B	601	1/1	0.99	0.05	31,31,31,31	0
2	NA	D	603	1/1	0.99	0.03	20,20,20,20	0
2	NA	E	609	1/1	0.99	0.14	23,23,23,23	0
2	NA	F	601	1/1	0.99	0.08	23,23,23,23	0
2	NA	D	608	1/1	0.99	0.07	24,24,24,24	0
2	NA	F	603	1/1	0.99	0.03	20,20,20,20	0
3	YGX	D	605	12/13	0.99	0.04	16,16,18,19	4
2	NA	C	604	1/1	0.99	0.09	28,28,28,28	0
2	NA	G	601	1/1	0.99	0.12	24,24,24,24	0

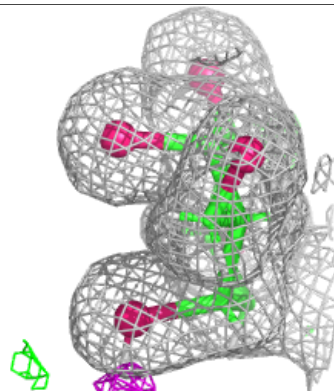
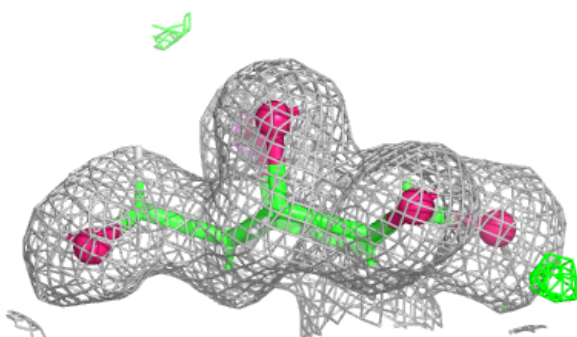
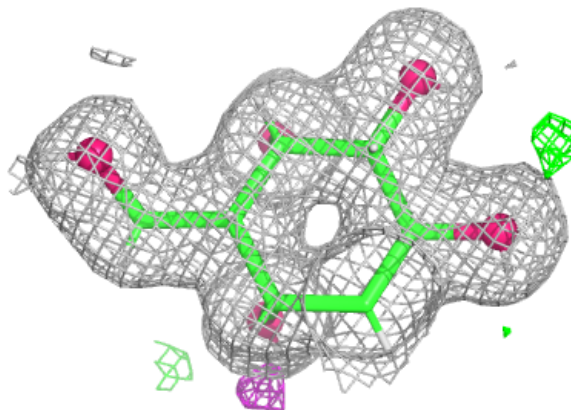
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around YGX A 602:

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

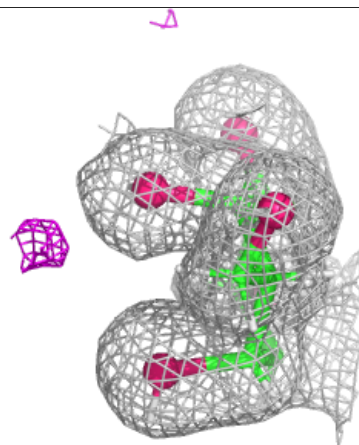
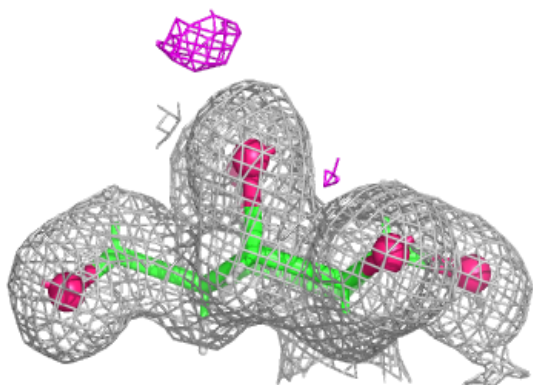
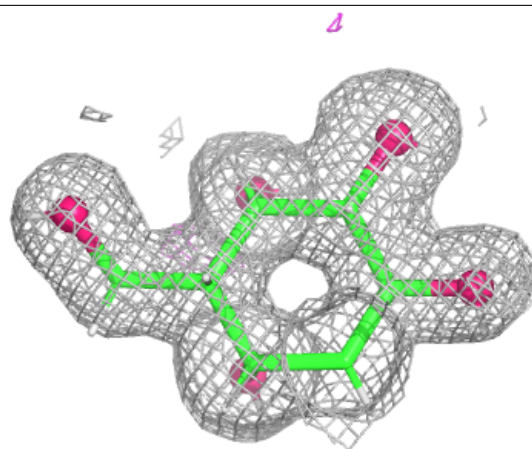
**Electron density around YGX B 602:**

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



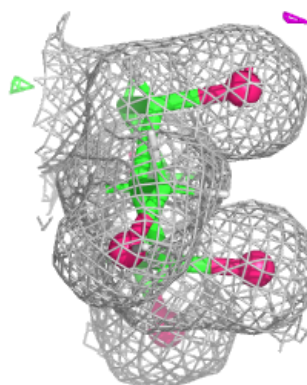
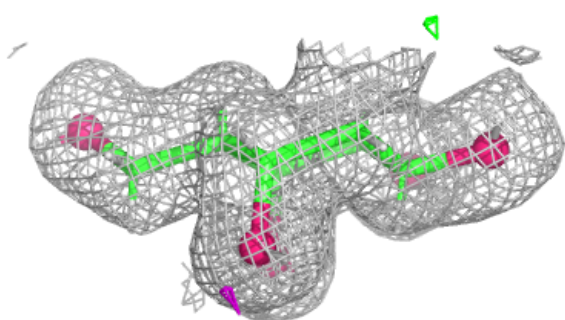
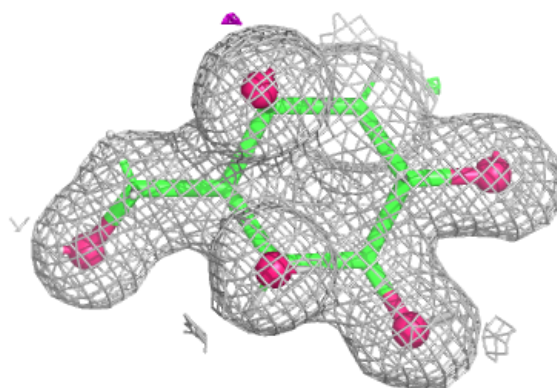
Electron density around YGX C 603:

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and green (positive)

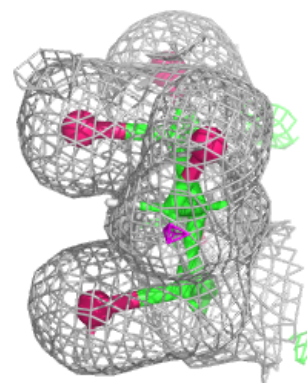
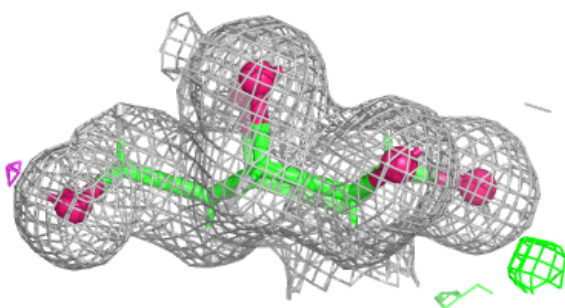
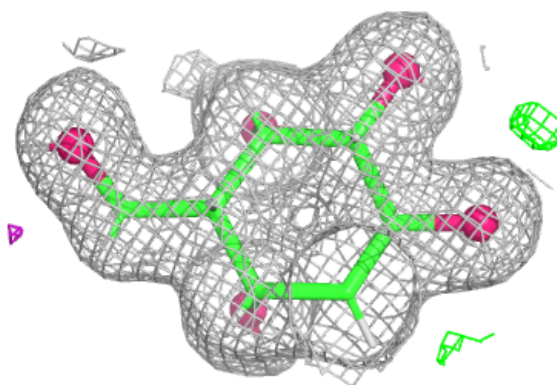


Electron density around YGX E 604:

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

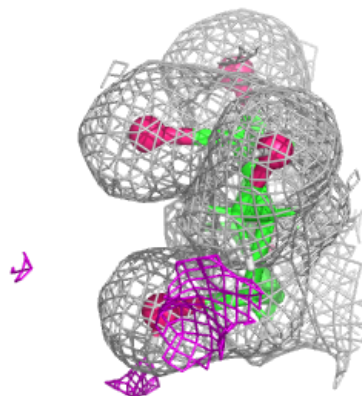
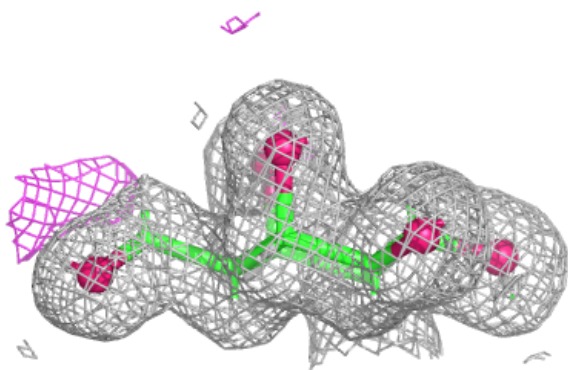
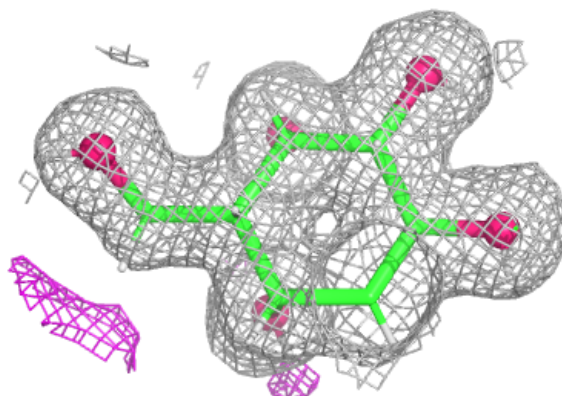
**Electron density around YGX F 604:**

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

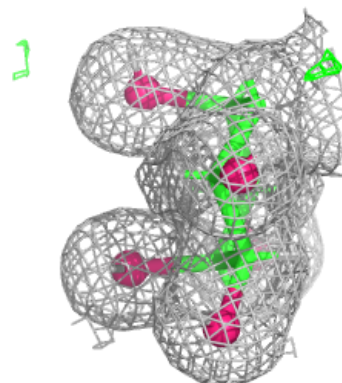
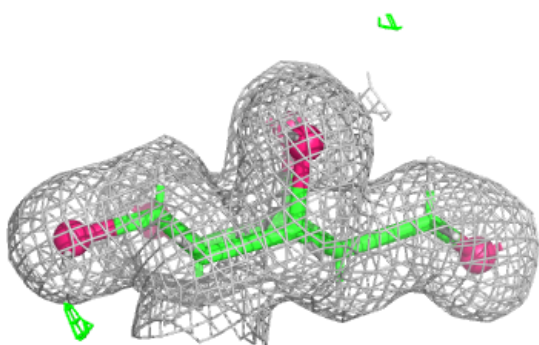
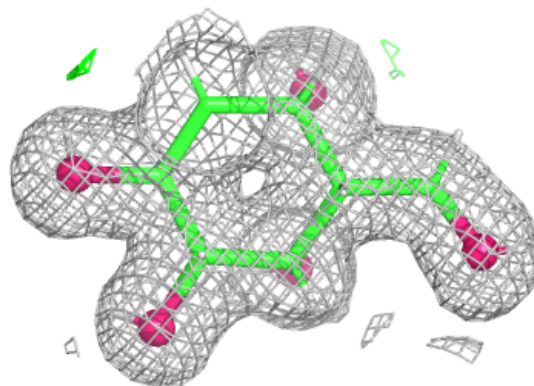


Electron density around YGX G 603:

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

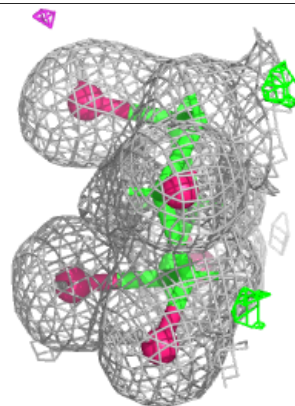
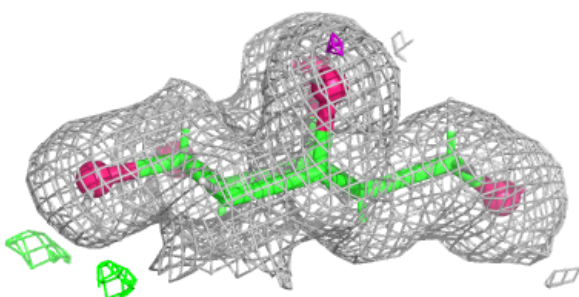
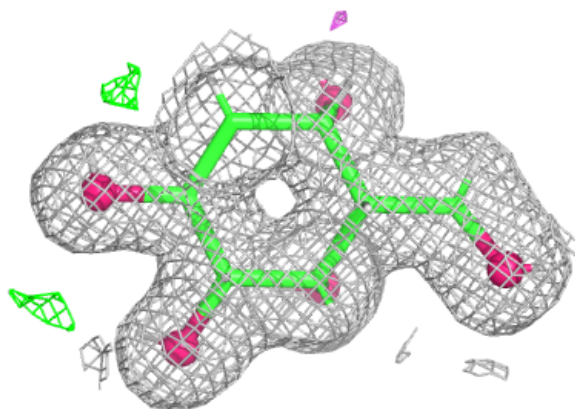
**Electron density around YGX H 602:**

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



Electron density around YGX D 605:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.