



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 11:17 AM UTC

PDB ID : 1JYV / pdb_00001jyv
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH ONPG
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.75 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 : 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

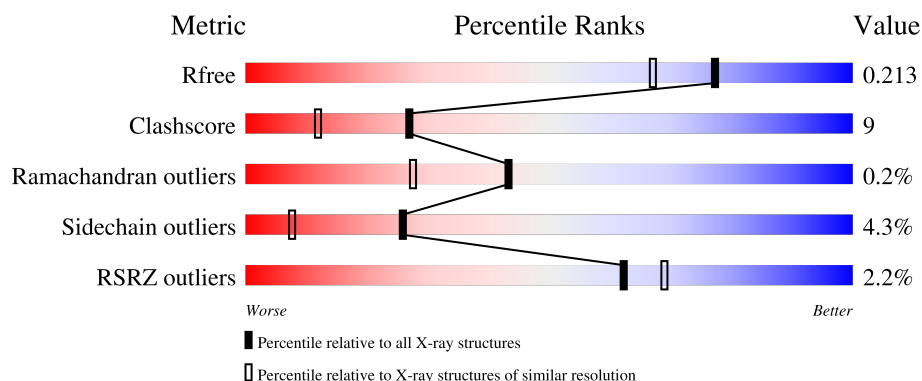
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	1023	
1	B	1023	
1	C	1023	
1	D	1023	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	8412	-	-	X	-
5	DMS	C	8415	-	X	-	-
5	DMS	D	8703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? P00722
A	8	PRO	ALA	cloning artifact	? P00722
A	537	GLN	GLU	engineered mutation	? P00722
B	1	GLY	THR	cloning artifact	? P00722
B	2	SER	MET	cloning artifact	? P00722
B	3	HIS	ILE	cloning artifact	? P00722
B	4	MET	THR	cloning artifact	? P00722
B	5	LEU	ASP	cloning artifact	? P00722
B	6	GLU	SER	cloning artifact	? P00722
B	7	ASP	LEU	cloning artifact	? P00722
B	8	PRO	ALA	cloning artifact	? P00722
B	537	GLN	GLU	engineered mutation	? P00722
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	537	GLN	GLU	engineered mutation	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact	? P00722
D	5	LEU	ASP	cloning artifact	? P00722
D	6	GLU	SER	cloning artifact	? P00722
D	7	ASP	LEU	cloning artifact	? P00722
D	8	PRO	ALA	cloning artifact	? P00722
D	537	GLN	GLU	engineered mutation	? P00722

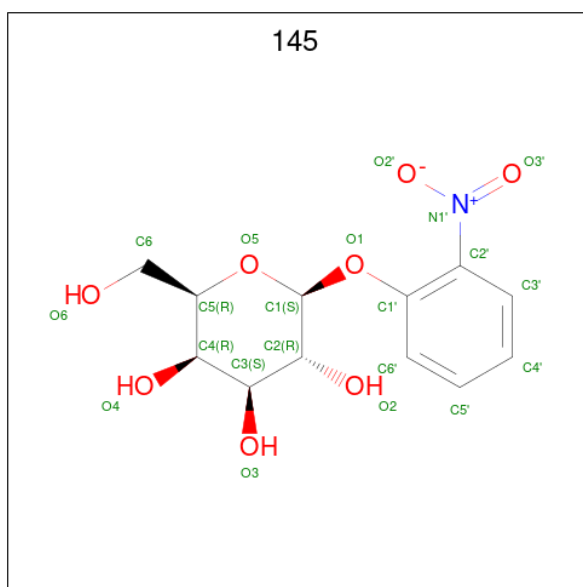
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	5	Total Mg 5 5	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is 2-nitrophenyl beta-D-galactopyranoside (CCD ID: 145) (formula: C₁₂H₁₅NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	12	1	8		
4	A	1	Total	C	N	O	0	0
			21	12	1	8		
4	B	1	Total	C	N	O	0	0
			21	12	1	8		
4	B	1	Total	C	N	O	0	0
			21	12	1	8		
4	C	1	Total	C	N	O	0	0
			21	12	1	8		
4	C	1	Total	C	N	O	0	0
			21	12	1	8		
4	D	1	Total	C	N	O	0	0
			21	12	1	8		
4	D	1	Total	C	N	O	0	0
			21	12	1	8		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0

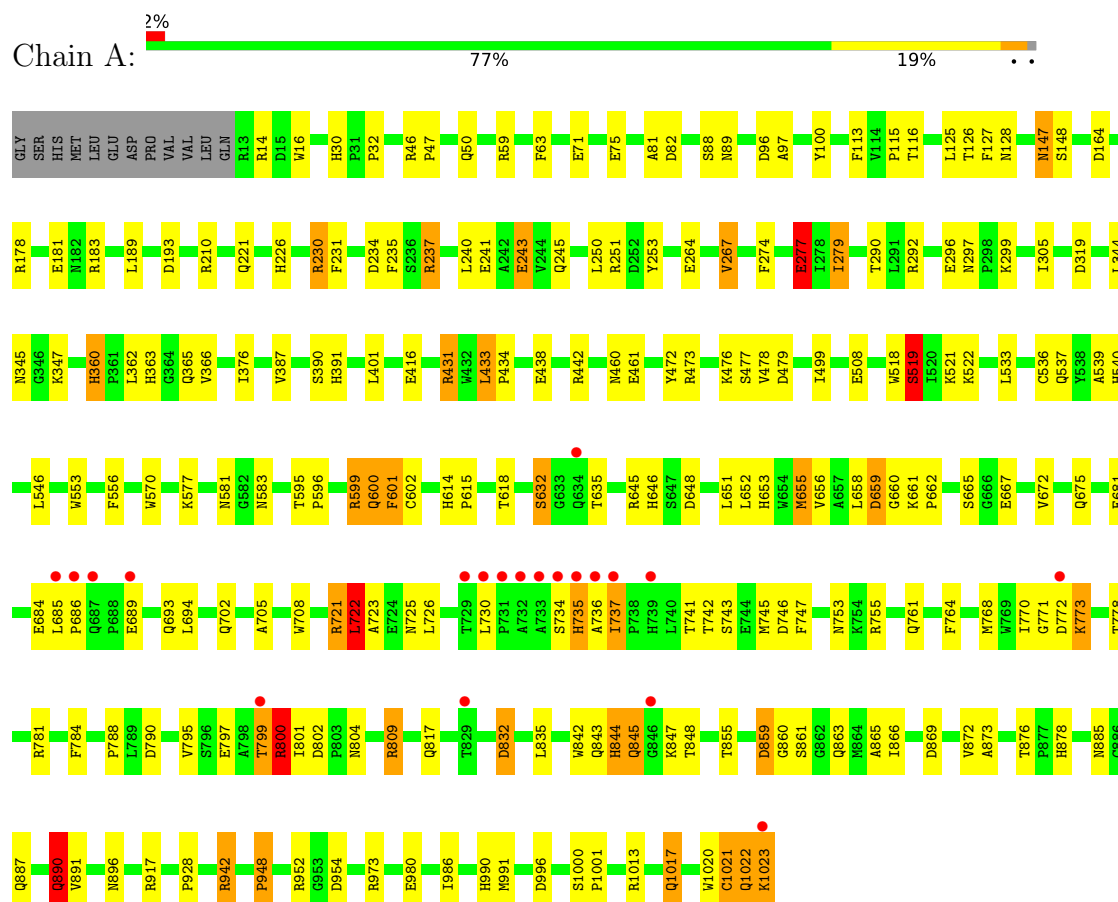
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1060	Total O 1060 1060	0	0
6	B	1013	Total O 1013 1013	0	0
6	C	987	Total O 987 987	0	0
6	D	1021	Total O 1021 1021	0	0

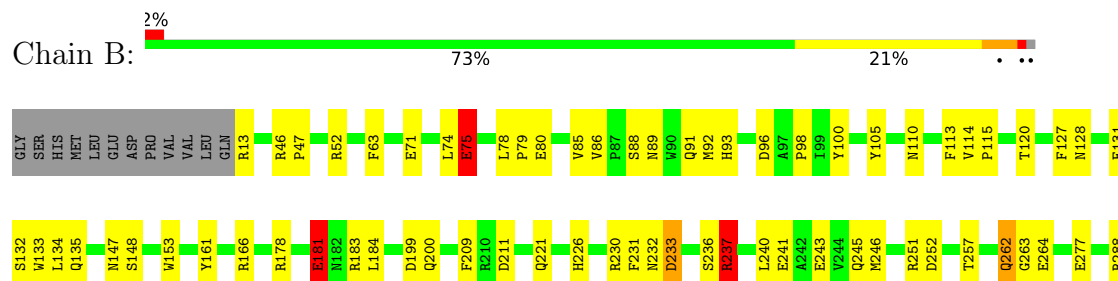
3 Residue-property plots

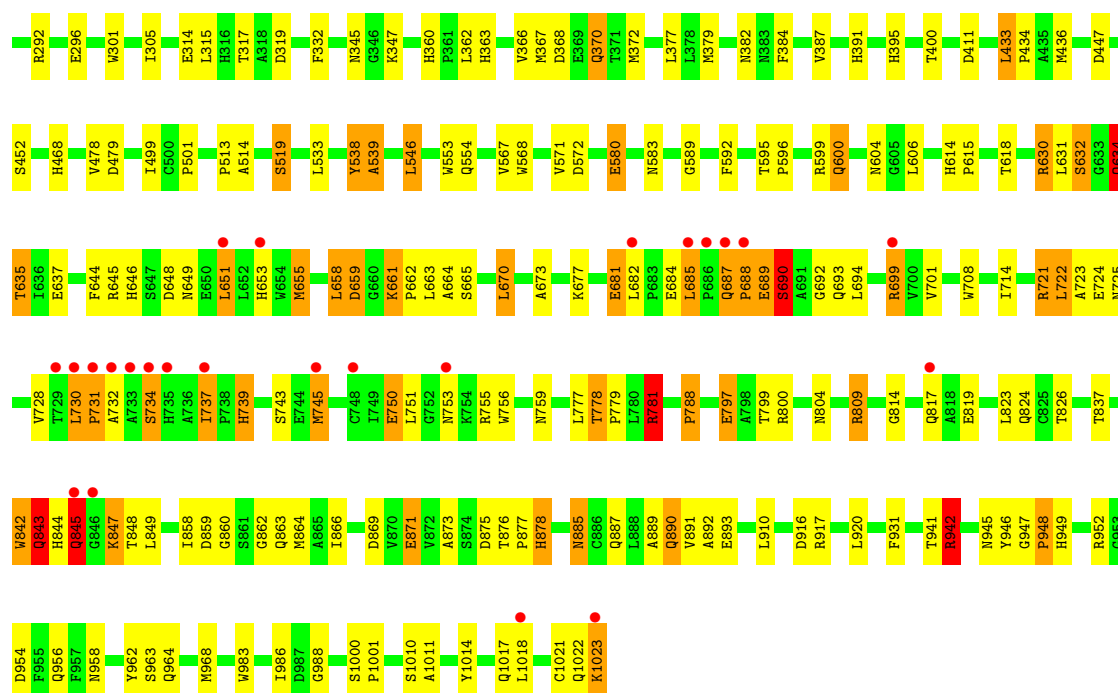
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-Galactosidase

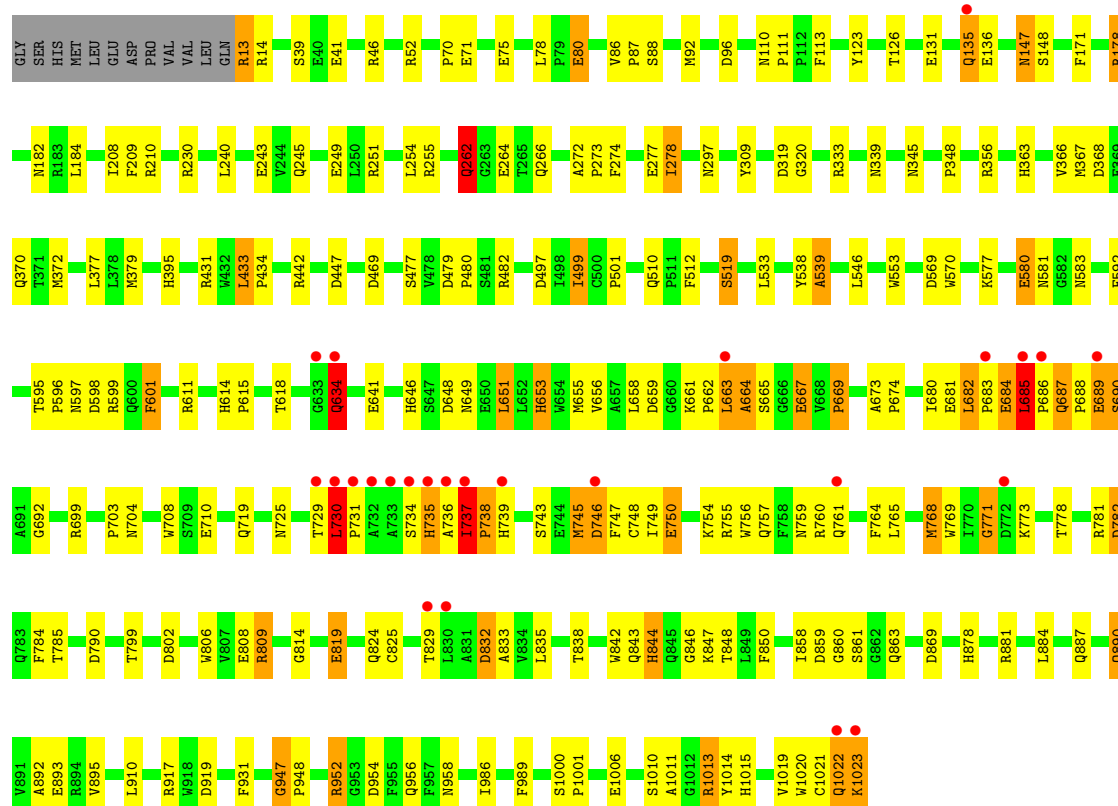
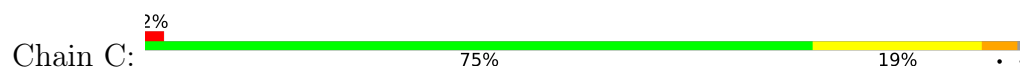


• Molecule 1: Beta-Galactosidase

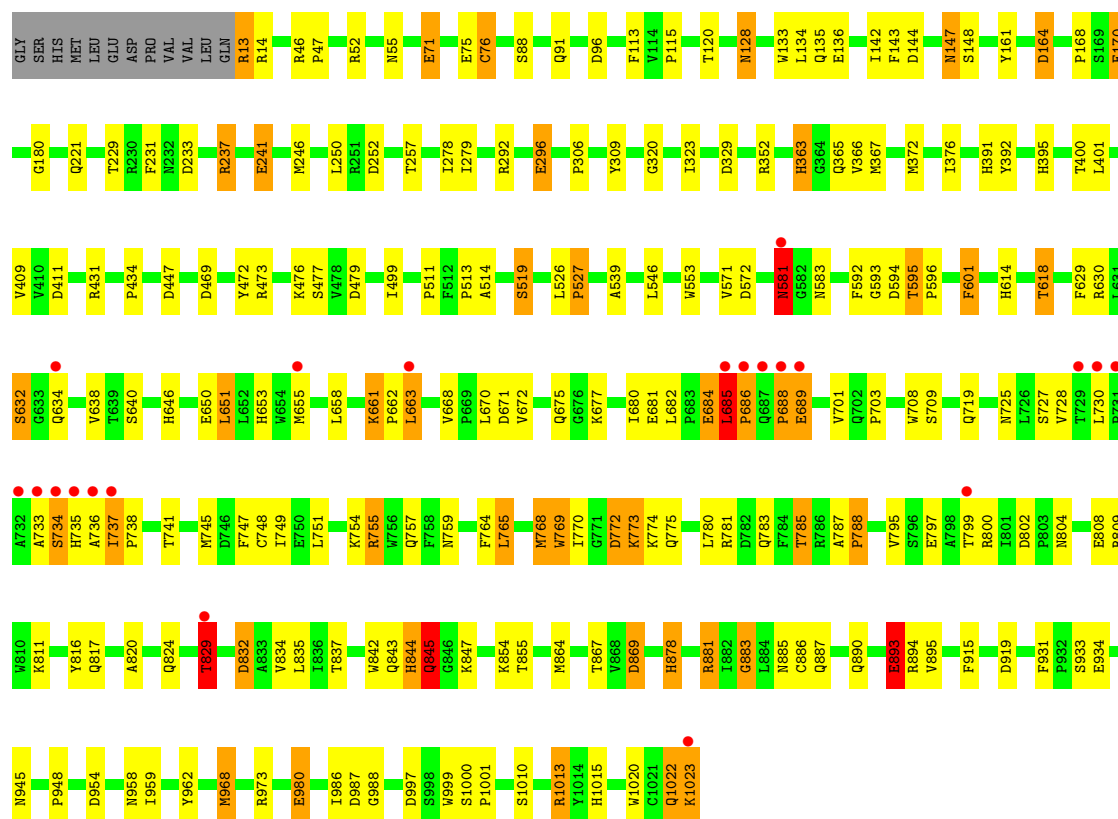
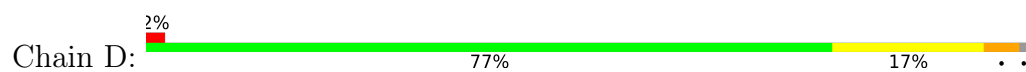




• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.49Å 167.46Å 200.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.75 29.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.75) 90.9 (29.90-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.180 , 0.240 0.162 , 0.213	Depositor DCC
R_{free} test set	7151 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37222	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3036e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 145, DMS, MG, NA

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	1.30	5/8383 (0.1%)	1.76	108/11437 (0.9%)
1	B	1.30	3/8383 (0.0%)	1.77	117/11437 (1.0%)
1	C	1.28	8/8383 (0.1%)	1.80	131/11437 (1.1%)
1	D	1.29	12/8383 (0.1%)	1.77	127/11437 (1.1%)
All	All	1.29	28/33532 (0.1%)	1.77	483/45748 (1.1%)

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	C	2	0
1	D	1	0
All	All	3	0

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-8.36	1.25	1.34
1	C	111	PRO	CA-C	-7.24	1.47	1.51
1	D	883	GLY	C-O	6.73	1.30	1.23
1	D	734	SER	N-CA	-6.47	1.38	1.46
1	B	86	VAL	CA-C	6.21	1.57	1.52

The worst 5 of 483 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	HIS	CA-CB-CG	-13.29	100.51	113.80
1	C	685	LEU	N-CA-CB	12.40	125.92	110.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	844	HIS	CA-CB-CG	-9.91	103.89	113.80
1	B	687	GLN	C-N-CD	-9.63	85.52	125.00
1	C	725	ASN	CA-CB-CG	-9.62	102.98	112.60

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	13	ARG	CA
1	C	685	LEU	CA
1	D	733	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8128	0	7712	124	0
1	B	8128	0	7712	163	0
1	C	8128	0	7712	133	0
1	D	8128	0	7712	147	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	42	0	27	2	0
4	B	42	0	27	1	0
4	C	42	0	27	2	0
4	D	42	0	27	4	0
5	A	108	0	162	15	0
5	B	100	0	150	18	0
5	C	108	0	162	14	0
5	D	112	0	168	24	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1060	0	0	20	3
6	B	1013	0	0	18	1
6	C	987	0	0	21	2
6	D	1021	0	0	18	0
All	All	37222	0	31598	595	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 595 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)
5:B:8407:DMS:C2	5:B:8407:DMS:S	2.01	1.48
5:B:8502:DMS:C1	5:B:8502:DMS:S	2.01	1.46
5:D:8407:DMS:C2	5:D:8407:DMS:S	2.04	1.46
5:C:8415:DMS:S	5:C:8415:DMS:C2	2.04	1.45
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.37	1.21

All (3) 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)
6:A:9649:HOH:O	6:C:9528:HOH:O[3_544]	2.07	0.13
6:A:9494:HOH:O	6:B:9578:HOH:O[2_454]	2.10	0.10
6:A:9651:HOH:O	6:C:9654:HOH:O[2_554]	2.18	0.02

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	1011/1023 (99%)	974 (96%)	35 (4%)	2 (0%)	43 27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1011/1023 (99%)	968 (96%)	39 (4%)	4 (0%)	30	15
1	C	1011/1023 (99%)	966 (96%)	44 (4%)	1 (0%)	48	32
1	D	1011/1023 (99%)	972 (96%)	37 (4%)	2 (0%)	43	27
All	All	4044/4092 (99%)	3880 (96%)	155 (4%)	9 (0%)	43	27

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	732	ALA
1	B	731	PRO
1	B	690	SER
1	A	164	ASP

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	865/875 (99%)	831 (96%)	34 (4%)	28	9
1	B	865/875 (99%)	819 (95%)	46 (5%)	20	5
1	C	865/875 (99%)	830 (96%)	35 (4%)	28	9
1	D	865/875 (99%)	830 (96%)	35 (4%)	28	9
All	All	3460/3500 (99%)	3310 (96%)	150 (4%)	26	8

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	13	ARG
1	D	845	GLN
1	D	519	SER
1	D	685	LEU
1	B	600	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	363	HIS
1	D	583	ASN
1	D	824	GLN
1	B	624	GLN
1	B	600	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 148 ligands modelled in this entry, 33 are monoatomic - leaving 115 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	DMS	A	8414	-	3,3,3	1.27	0	3,3,3	0.13	0
5	DMS	B	8403	-	3,3,3	1.23	0	3,3,3	0.46	0
5	DMS	A	8405	-	3,3,3	0.86	0	3,3,3	0.30	0
5	DMS	A	8406	-	3,3,3	0.36	0	3,3,3	1.08	0
5	DMS	B	8414	-	3,3,3	1.16	0	3,3,3	0.45	0
4	145	A	2002	-	22,22,22	0.94	1 (4%)	28,31,31	1.26	3 (10%)
5	DMS	B	8404	-	3,3,3	1.31	0	3,3,3	1.39	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8508	-	3,3,3	2.22	1 (33%)	3,3,3	0.37	0
5	DMS	D	8425	3	3,3,3	0.37	0	3,3,3	0.66	0
5	DMS	D	8417	-	3,3,3	1.40	0	3,3,3	1.14	0
5	DMS	B	8417	-	3,3,3	0.98	0	3,3,3	0.21	0
5	DMS	C	8416	-	3,3,3	0.77	0	3,3,3	0.10	0
5	DMS	A	8412	-	3,3,3	0.63	0	3,3,3	0.36	0
5	DMS	C	8705	-	3,3,3	1.14	0	3,3,3	0.21	0
5	DMS	B	8425	3	3,3,3	1.89	1 (33%)	3,3,3	0.60	0
5	DMS	C	8420	-	3,3,3	1.93	1 (33%)	3,3,3	0.22	0
5	DMS	C	8408	-	3,3,3	1.39	0	3,3,3	0.56	0
4	145	C	2002	-	22,22,22	0.92	1 (4%)	28,31,31	1.13	2 (7%)
5	DMS	A	8423	-	3,3,3	1.28	0	3,3,3	0.87	0
5	DMS	A	8503	-	3,3,3	0.33	0	3,3,3	0.20	0
5	DMS	C	8402	-	3,3,3	1.06	0	3,3,3	0.82	0
5	DMS	C	8602	-	3,3,3	1.11	0	3,3,3	0.28	0
5	DMS	B	8420	-	3,3,3	1.56	1 (33%)	3,3,3	0.45	0
5	DMS	D	8401	-	3,3,3	0.97	0	3,3,3	0.84	0
5	DMS	D	8412	-	3,3,3	0.95	0	3,3,3	0.50	0
5	DMS	B	8409	-	3,3,3	2.27	1 (33%)	3,3,3	0.58	0
5	DMS	C	8403	-	3,3,3	1.27	0	3,3,3	0.47	0
5	DMS	D	8410	-	3,3,3	1.53	1 (33%)	3,3,3	0.46	0
5	DMS	C	8407	-	3,3,3	2.29	2 (66%)	3,3,3	0.55	0
5	DMS	C	8504	-	3,3,3	0.86	0	3,3,3	0.29	0
5	DMS	C	8414	-	3,3,3	1.10	0	3,3,3	0.83	0
5	DMS	A	8403	-	3,3,3	1.49	1 (33%)	3,3,3	0.38	0
5	DMS	D	8416	-	3,3,3	1.39	1 (33%)	3,3,3	0.50	0
5	DMS	D	8423	-	3,3,3	1.34	0	3,3,3	0.30	0
5	DMS	B	8402	-	3,3,3	0.59	0	3,3,3	0.08	0
5	DMS	D	8701	-	3,3,3	1.90	1 (33%)	3,3,3	0.47	0
5	DMS	C	8601	-	3,3,3	0.76	0	3,3,3	1.06	0
5	DMS	C	8413	-	3,3,3	1.35	0	3,3,3	0.18	0
5	DMS	D	8705	-	3,3,3	1.73	0	3,3,3	0.82	0
5	DMS	B	8405	-	3,3,3	1.45	0	3,3,3	0.56	0
5	DMS	B	8411	-	3,3,3	1.26	1 (33%)	3,3,3	0.42	0
4	145	D	2002	-	22,22,22	0.72	1 (4%)	28,31,31	1.28	3 (10%)
5	DMS	C	8419	-	3,3,3	1.07	0	3,3,3	0.47	0
5	DMS	C	8421	-	3,3,3	0.63	0	3,3,3	0.67	0
5	DMS	D	8404	-	3,3,3	1.12	0	3,3,3	0.47	0
5	DMS	B	8416	-	3,3,3	0.55	0	3,3,3	0.53	0
5	DMS	B	8408	-	3,3,3	1.48	1 (33%)	3,3,3	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	145	B	2002	-	22,22,22	0.96	1 (4%)	28,31,31	1.38	4 (14%)
5	DMS	C	8425	3	3,3,3	1.83	1 (33%)	3,3,3	0.39	0
5	DMS	C	8415	-	3,3,3	2.77	2 (66%)	3,3,3	1.75	1 (33%)
5	DMS	A	8602	-	3,3,3	0.86	0	3,3,3	0.55	0
5	DMS	A	8402	-	3,3,3	1.54	0	3,3,3	0.29	0
5	DMS	C	8410	-	3,3,3	1.29	0	3,3,3	0.21	0
5	DMS	B	8407	-	3,3,3	2.20	1 (33%)	3,3,3	0.25	0
5	DMS	A	8407	-	3,3,3	2.61	2 (66%)	3,3,3	0.23	0
5	DMS	A	8409	-	3,3,3	2.09	1 (33%)	3,3,3	0.59	0
5	DMS	D	8501	-	3,3,3	0.33	0	3,3,3	0.74	0
5	DMS	D	8408	-	3,3,3	0.84	0	3,3,3	0.23	0
5	DMS	A	8410	-	3,3,3	1.13	0	3,3,3	0.35	0
5	DMS	A	8416	-	3,3,3	0.56	0	3,3,3	0.40	0
5	DMS	B	8415	-	3,3,3	2.07	1 (33%)	3,3,3	1.41	1 (33%)
4	145	B	2001	3	22,22,22	1.19	3 (13%)	28,31,31	0.91	0
5	DMS	A	8425	3	3,3,3	2.02	1 (33%)	3,3,3	0.65	0
5	DMS	A	8501	-	3,3,3	1.19	0	3,3,3	0.33	0
5	DMS	D	8403	-	3,3,3	0.59	0	3,3,3	0.72	0
5	DMS	D	8415	-	3,3,3	2.55	2 (66%)	3,3,3	0.47	0
5	DMS	D	8703	-	3,3,3	2.39	2 (66%)	3,3,3	0.24	0
5	DMS	A	8502	-	3,3,3	1.32	1 (33%)	3,3,3	1.31	1 (33%)
5	DMS	D	8407	-	3,3,3	2.92	2 (66%)	3,3,3	0.32	0
5	DMS	D	8409	-	3,3,3	2.27	1 (33%)	3,3,3	0.62	0
5	DMS	C	8405	-	3,3,3	1.52	1 (33%)	3,3,3	0.57	0
5	DMS	A	8419	-	3,3,3	0.82	0	3,3,3	0.33	0
5	DMS	C	8411	-	3,3,3	1.07	0	3,3,3	0.42	0
5	DMS	B	8410	-	3,3,3	0.73	0	3,3,3	0.32	0
5	DMS	B	8504	-	3,3,3	1.09	0	3,3,3	0.85	0
5	DMS	A	8408	-	3,3,3	0.68	0	3,3,3	1.68	1 (33%)
4	145	D	2001	3	22,22,22	1.22	3 (13%)	28,31,31	1.34	5 (17%)
5	DMS	C	8409	-	3,3,3	2.13	1 (33%)	3,3,3	0.83	0
5	DMS	C	8417	-	3,3,3	1.08	0	3,3,3	0.84	0
5	DMS	B	8502	-	3,3,3	2.39	2 (66%)	3,3,3	0.45	0
5	DMS	C	8503	-	3,3,3	1.08	0	3,3,3	0.22	0
5	DMS	A	8415	-	3,3,3	1.12	0	3,3,3	0.71	0
5	DMS	A	8411	-	3,3,3	0.77	0	3,3,3	0.40	0
5	DMS	B	8601	-	3,3,3	2.16	1 (33%)	3,3,3	1.03	0
5	DMS	A	8417	-	3,3,3	2.18	1 (33%)	3,3,3	1.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8420	-	3,3,3	1.37	1 (33%)	3,3,3	0.38	0
5	DMS	D	8508	-	3,3,3	1.83	1 (33%)	3,3,3	0.48	0
5	DMS	B	8421	-	3,3,3	0.71	0	3,3,3	1.00	0
5	DMS	D	8414	-	3,3,3	0.70	0	3,3,3	0.34	0
5	DMS	C	8404	-	3,3,3	1.22	1 (33%)	3,3,3	1.16	0
5	DMS	D	8411	-	3,3,3	1.06	0	3,3,3	0.27	0
5	DMS	B	8419	-	3,3,3	0.64	0	3,3,3	0.41	0
5	DMS	D	8402	-	3,3,3	1.63	1 (33%)	3,3,3	0.39	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.33	0
5	DMS	A	8401	-	3,3,3	0.66	0	3,3,3	0.85	0
5	DMS	B	8413	-	3,3,3	1.70	1 (33%)	3,3,3	0.14	0
5	DMS	C	8401	-	3,3,3	0.88	0	3,3,3	0.51	0
5	DMS	B	8423	-	3,3,3	0.99	0	3,3,3	0.11	0
5	DMS	C	8423	-	3,3,3	0.67	0	3,3,3	0.35	0
5	DMS	D	8405	-	3,3,3	0.74	0	3,3,3	0.82	0
4	145	A	2001	3	22,22,22	1.06	3 (13%)	28,31,31	1.46	4 (14%)
4	145	C	2001	3	22,22,22	0.90	1 (4%)	28,31,31	1.19	5 (17%)
5	DMS	A	8421	-	3,3,3	0.19	0	3,3,3	0.36	0
5	DMS	B	8412	-	3,3,3	1.96	1 (33%)	3,3,3	0.19	0
5	DMS	C	8501	-	3,3,3	1.47	1 (33%)	3,3,3	1.02	0
5	DMS	A	8420	-	3,3,3	1.11	0	3,3,3	0.37	0
5	DMS	A	8404	-	3,3,3	1.10	0	3,3,3	0.70	0
5	DMS	D	8421	-	3,3,3	0.56	0	3,3,3	0.37	0
5	DMS	B	8401	-	3,3,3	0.59	0	3,3,3	0.29	0
5	DMS	D	8413	-	3,3,3	1.99	1 (33%)	3,3,3	0.67	0
5	DMS	A	8504	-	3,3,3	0.68	0	3,3,3	0.30	0
5	DMS	D	8503	-	3,3,3	0.75	0	3,3,3	0.33	0
5	DMS	A	8413	-	3,3,3	2.12	2 (66%)	3,3,3	0.34	0
5	DMS	D	8406	-	3,3,3	1.18	0	3,3,3	0.71	0
5	DMS	D	8419	-	3,3,3	0.42	0	3,3,3	0.17	0

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
4	145	A	2001	3	-	1/8/30/30	0/2/2/2
4	145	C	2001	3	-	1/8/30/30	0/2/2/2
4	145	B	2002	-	-	1/8/30/30	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	145	D	2002	-	-	0/8/30/30	0/2/2/2
4	145	D	2001	3	-	1/8/30/30	0/2/2/2
4	145	C	2002	-	-	0/8/30/30	0/2/2/2
4	145	A	2002	-	-	0/8/30/30	0/2/2/2
4	145	B	2001	3	-	1/8/30/30	0/2/2/2

The worst 5 of 60 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8415	DMS	C2-S	4.02	2.04	1.76
5	D	8407	DMS	C2-S	3.96	2.04	1.76
5	D	8409	DMS	O-S	3.71	1.74	1.50
5	A	8417	DMS	C1-S	-3.71	1.49	1.76
5	D	8415	DMS	O-S	3.68	1.74	1.50

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2002	145	C3'-C2'-N1'	4.36	121.13	116.47
4	A	2001	145	O1-C1'-C2'	4.14	122.30	117.31
4	B	2002	145	C3'-C2'-N1'	3.82	120.56	116.47
4	A	2001	145	C3'-C2'-N1'	-3.00	113.27	116.47
5	C	8415	DMS	C2-S-C1	2.97	113.64	98.42

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	145	O5-C5-C6-O6
4	D	2001	145	O5-C5-C6-O6
4	B	2001	145	O5-C5-C6-O6
4	A	2001	145	O5-C5-C6-O6
4	B	2002	145	C4-C5-C6-O6

There are no ring outliers.

51 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	145	1	0
5	B	8508	DMS	2	0
5	D	8425	DMS	3	0

Continued on next page...

Continued from previous page...

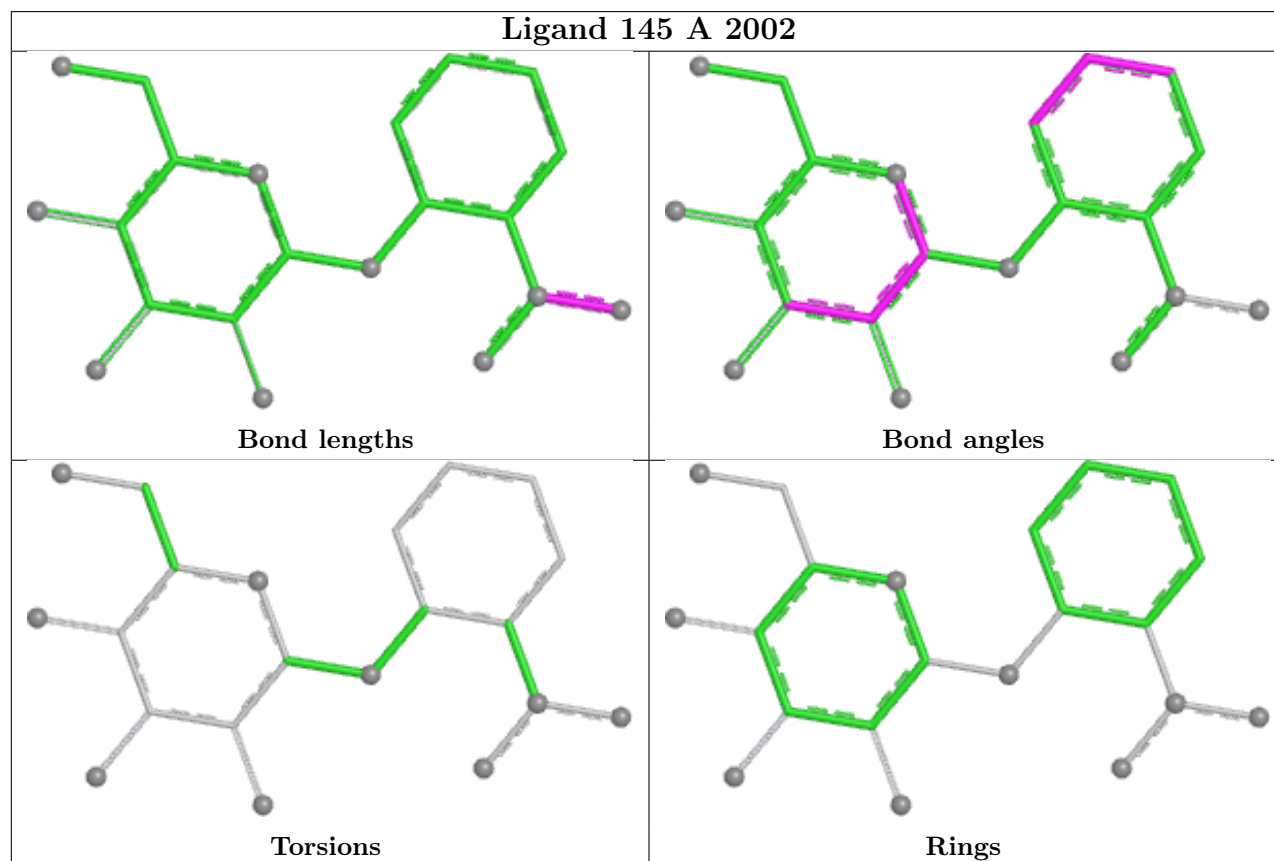
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8417	DMS	1	0
5	B	8417	DMS	2	0
5	A	8412	DMS	4	0
5	C	8705	DMS	1	0
5	C	8420	DMS	1	0
4	C	2002	145	2	0
5	A	8423	DMS	2	0
5	A	8503	DMS	1	0
5	C	8602	DMS	2	0
5	B	8420	DMS	1	0
5	D	8412	DMS	3	0
5	B	8409	DMS	1	0
5	D	8410	DMS	2	0
5	A	8403	DMS	1	0
5	D	8416	DMS	3	0
5	D	8423	DMS	1	0
4	D	2002	145	3	0
5	C	8419	DMS	2	0
5	B	8416	DMS	3	0
4	B	2002	145	1	0
5	C	8425	DMS	2	0
5	C	8415	DMS	1	0
5	A	8602	DMS	1	0
5	C	8410	DMS	2	0
5	B	8407	DMS	2	0
5	A	8407	DMS	1	0
5	D	8408	DMS	1	0
5	A	8410	DMS	1	0
5	A	8416	DMS	1	0
5	B	8415	DMS	2	0
5	D	8703	DMS	4	0
5	D	8407	DMS	2	0
5	B	8410	DMS	1	0
5	B	8504	DMS	2	0
4	D	2001	145	1	0
5	C	8417	DMS	1	0
5	B	8502	DMS	1	0
5	C	8503	DMS	1	0
5	A	8415	DMS	1	0
5	A	8417	DMS	1	0
5	D	8420	DMS	1	0
5	D	8508	DMS	1	0

Continued on next page...

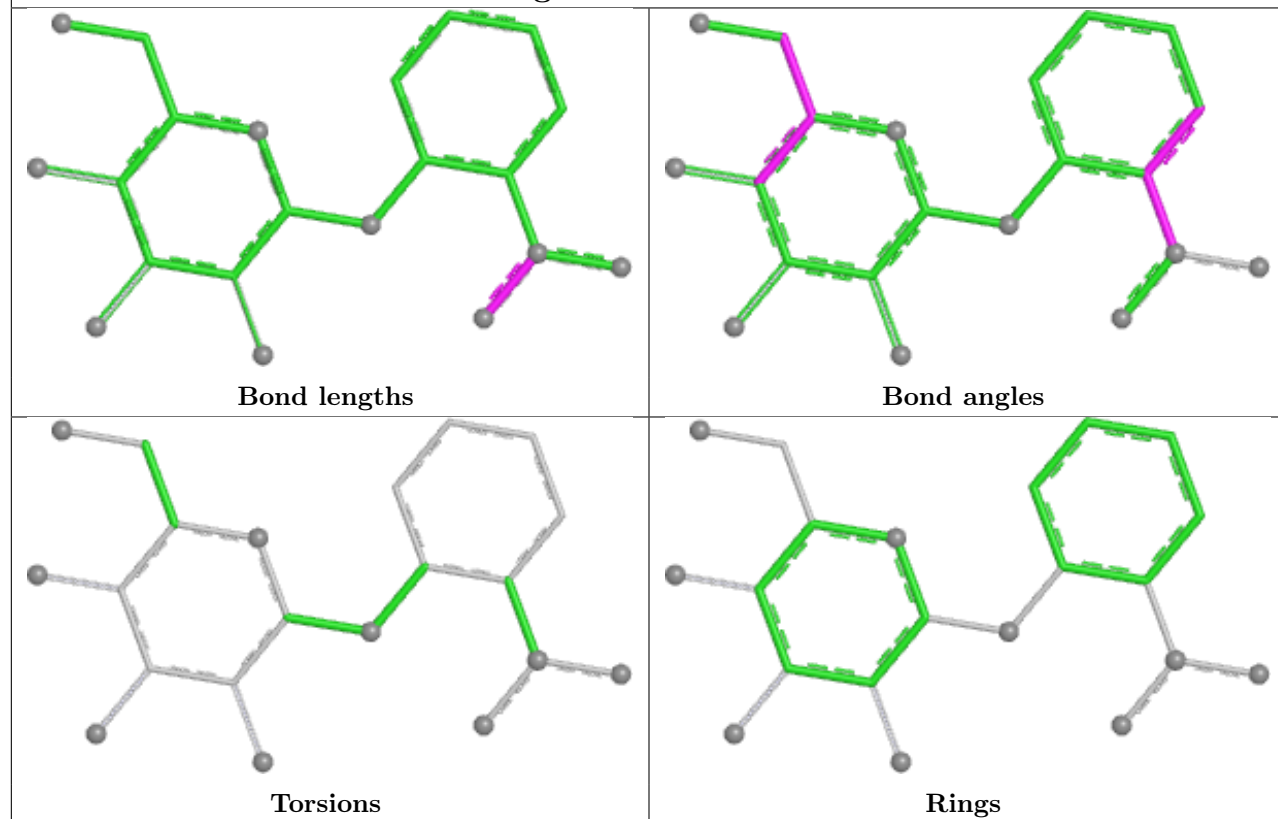
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8423	DMS	1	0
5	C	8423	DMS	1	0
4	A	2001	145	1	0
5	A	8404	DMS	1	0
5	D	8503	DMS	1	0
5	D	8419	DMS	1	0

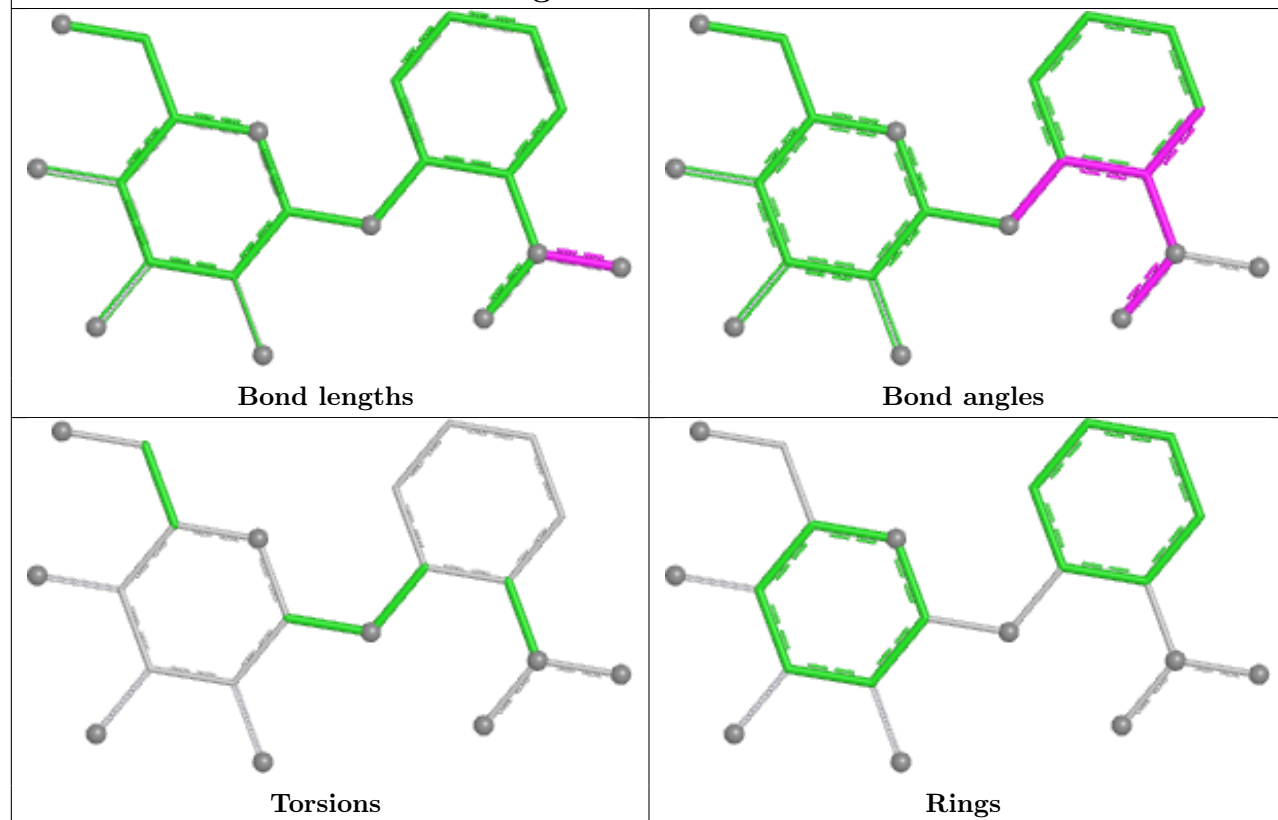
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

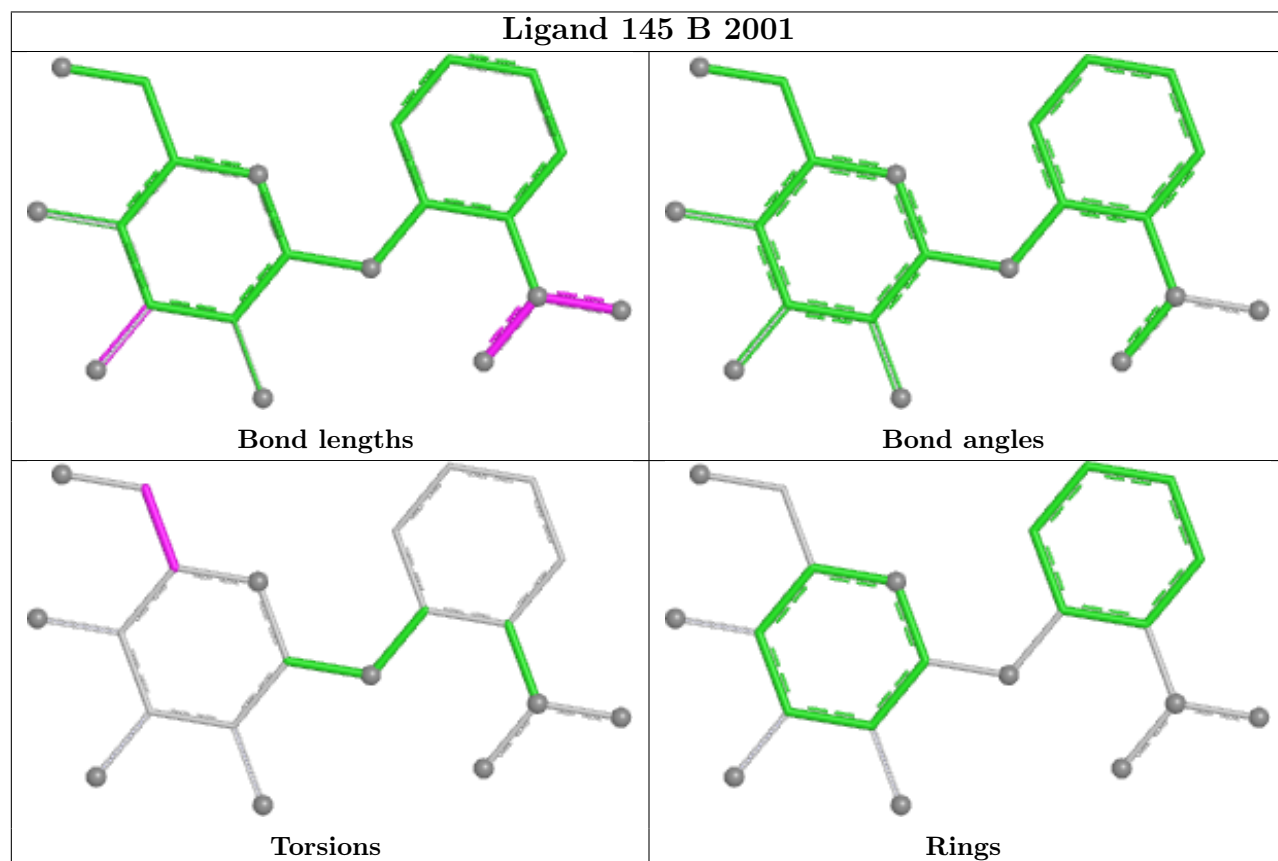
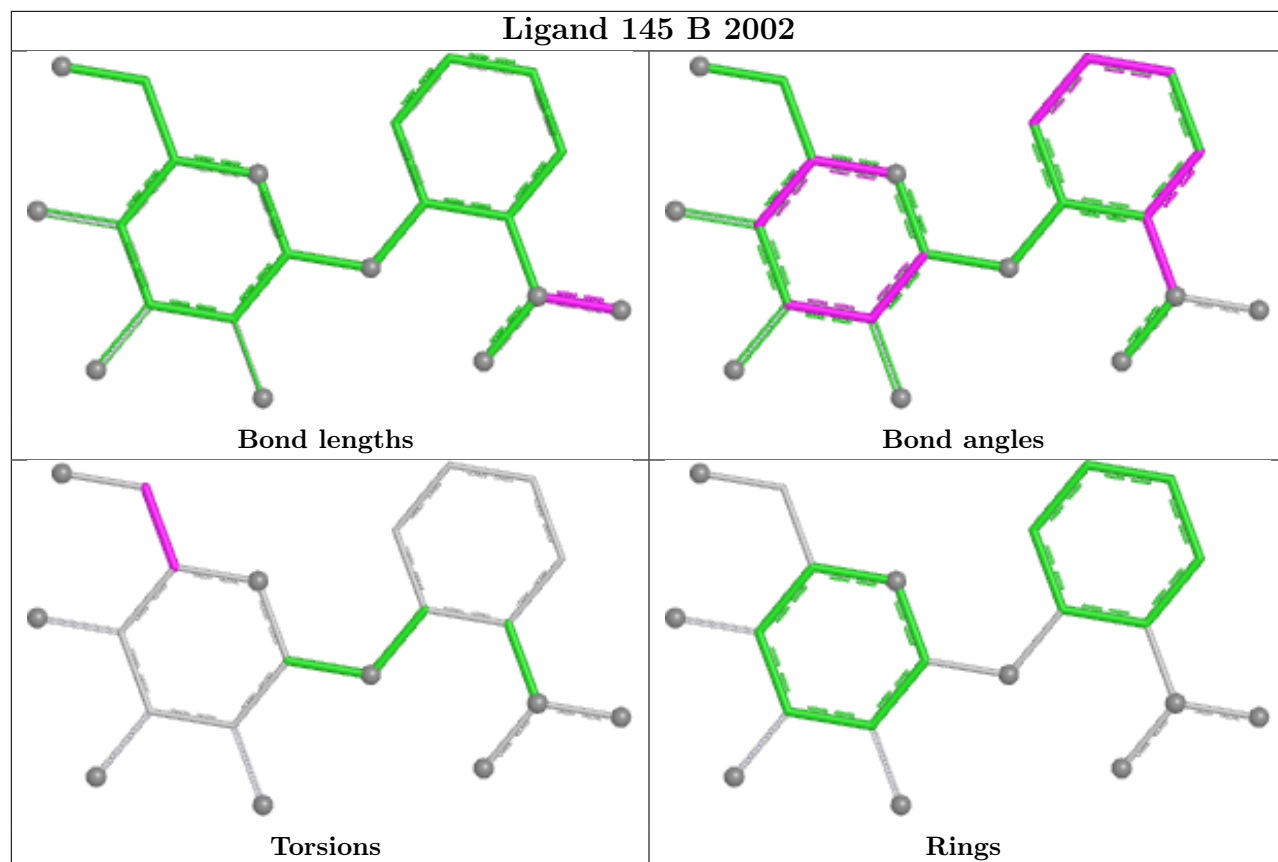


Ligand 145 C 2002

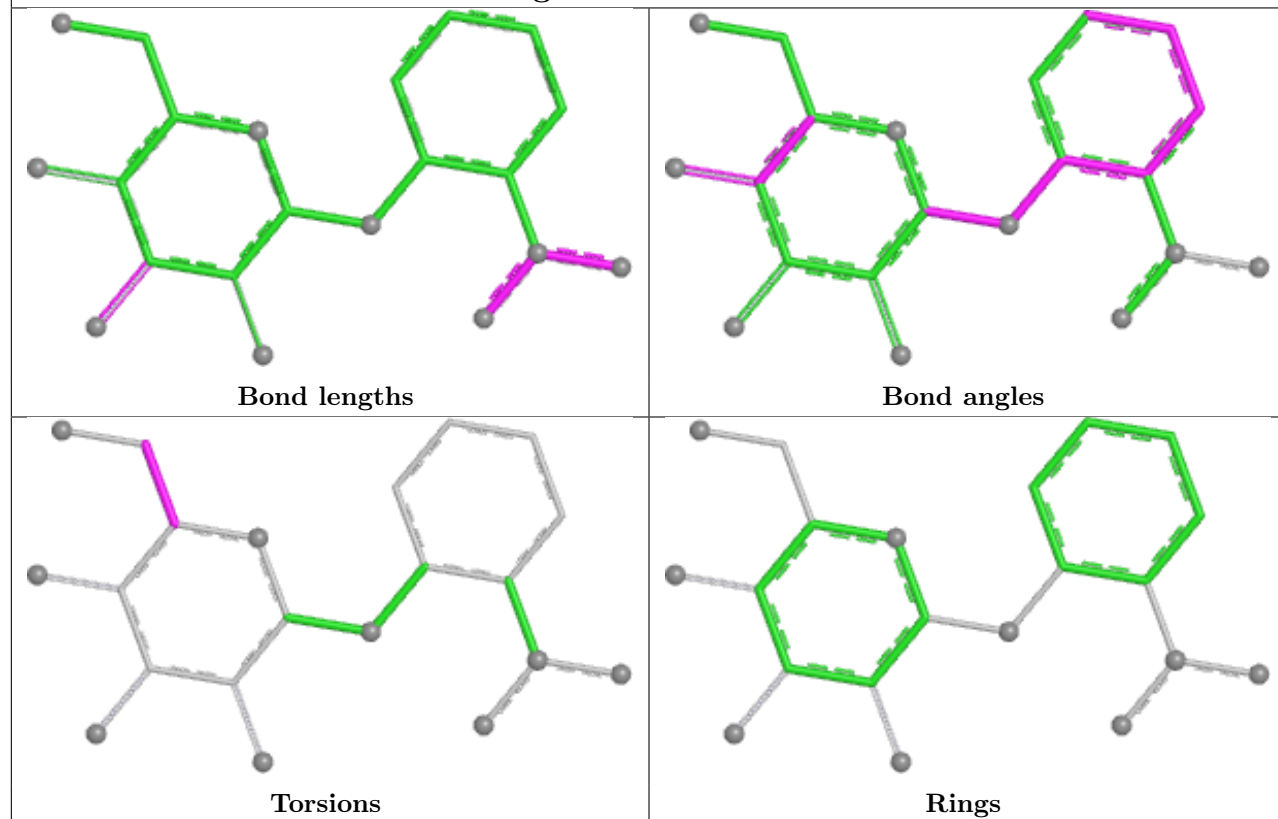


Ligand 145 D 2002

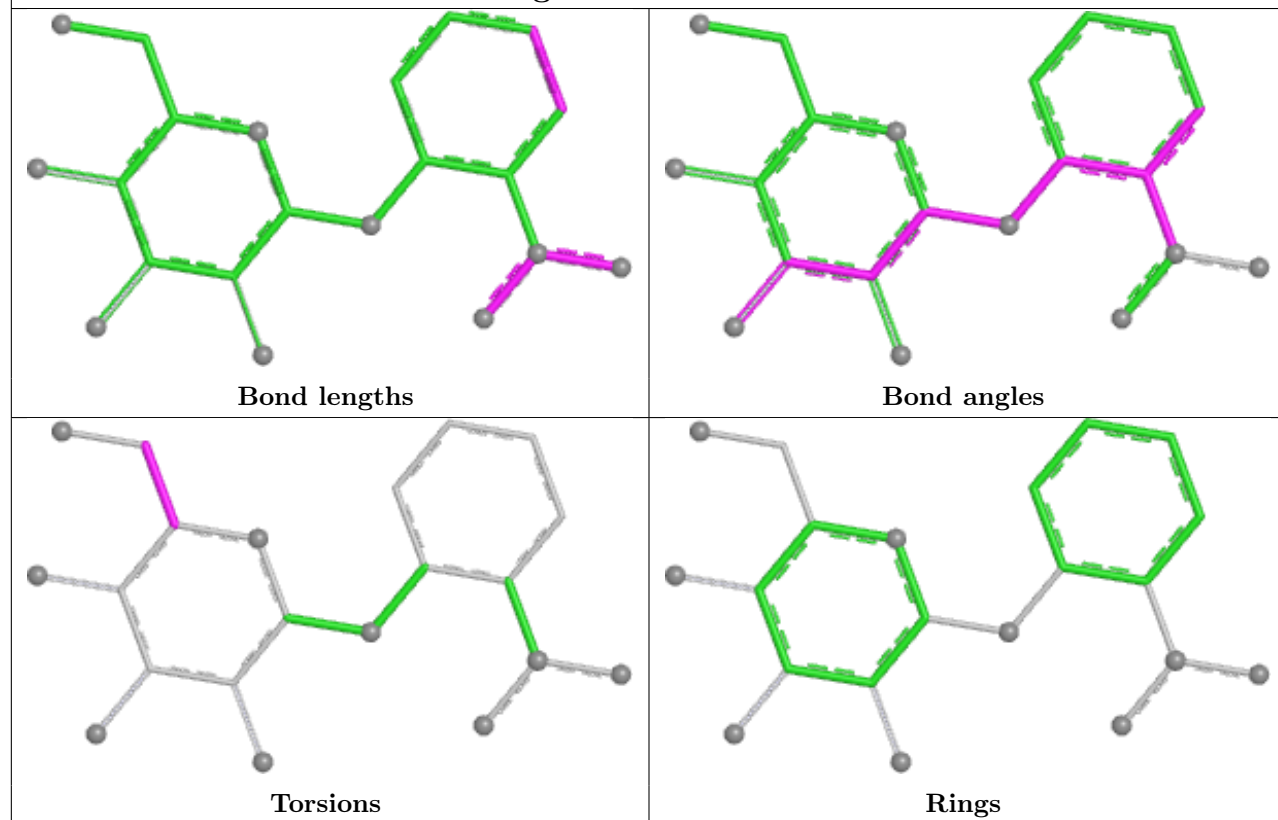


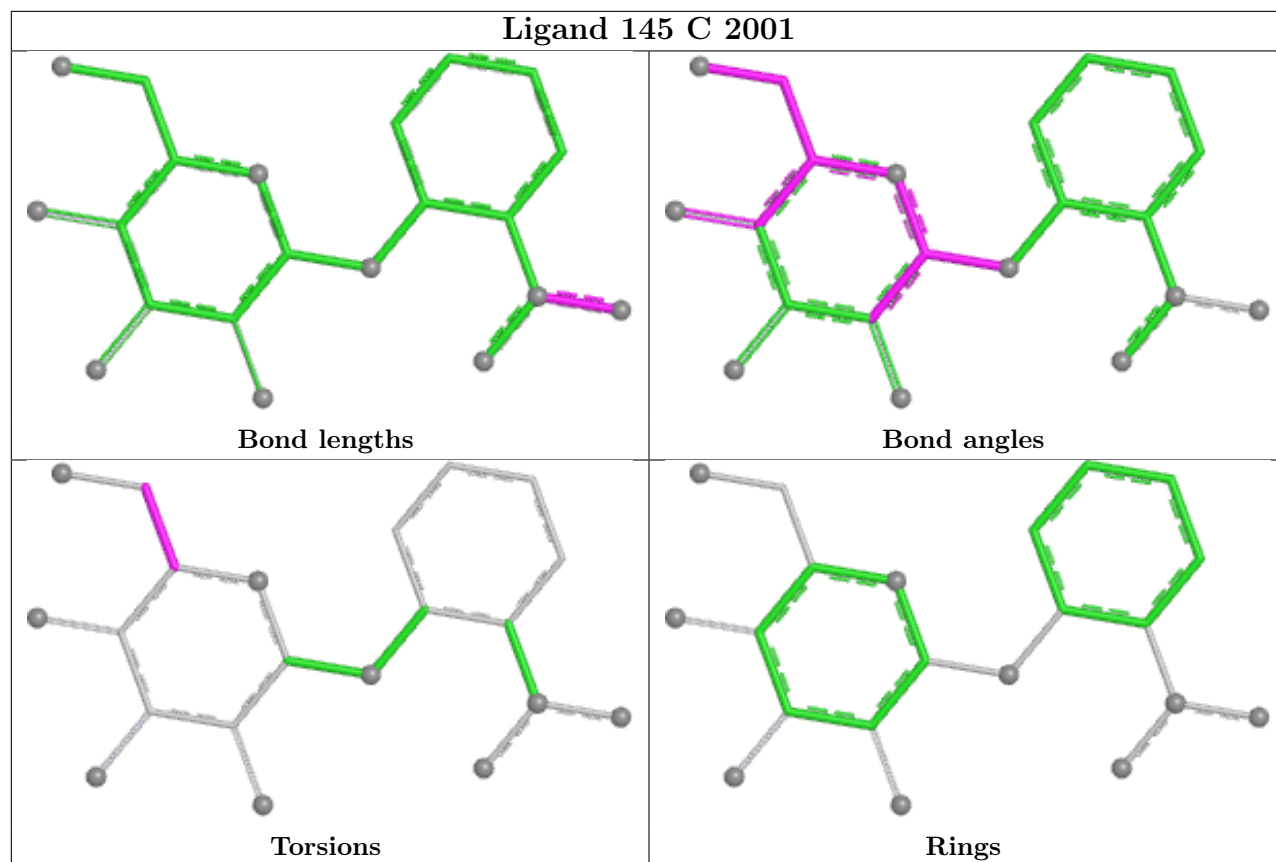


Ligand 145 D 2001



Ligand 145 A 2001





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	1011/1023 (98%)	-0.44	20 (1%) 65 71	11, 18, 46, 100	1 (0%)
1	B	1011/1023 (98%)	-0.35	24 (2%) 59 66	11, 19, 48, 99	1 (0%)
1	C	1011/1023 (98%)	-0.31	25 (2%) 58 64	11, 20, 51, 100	1 (0%)
1	D	1011/1023 (98%)	-0.37	21 (2%) 63 70	11, 19, 50, 100	1 (0%)
All	All	4044/4092 (98%)	-0.37	90 (2%) 62 69	11, 19, 49, 100	4 (0%)

The worst 5 of 90 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	730	LEU	5.6
1	A	730	LEU	5.1
1	B	733	ALA	5.0
1	C	686	PRO	4.8
1	A	686	PRO	4.8

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
5	DMS	C	8503	4/4	0.72	0.24	46,82,100,100	0
2	MG	A	3003	1/1	0.74	0.18	61,61,61,61	0
5	DMS	D	8417	4/4	0.76	0.24	26,41,80,100	0
5	DMS	C	8705	4/4	0.82	0.19	35,45,50,100	0
5	DMS	D	8420	4/4	0.84	0.17	27,51,77,94	0
5	DMS	A	8423	4/4	0.85	0.22	36,59,67,100	0
5	DMS	B	8416	4/4	0.85	0.16	46,55,71,100	0
5	DMS	B	8415	4/4	0.86	0.15	30,34,37,73	0
5	DMS	A	8421	4/4	0.87	0.17	51,60,61,74	0
5	DMS	A	8602	4/4	0.87	0.22	54,58,100,100	0
5	DMS	A	8415	4/4	0.88	0.22	24,63,100,100	0
2	MG	B	3003	1/1	0.88	0.14	48,48,48,48	0
5	DMS	B	8421	4/4	0.88	0.17	32,43,53,100	0
5	DMS	B	8423	4/4	0.88	0.17	37,56,72,72	0
5	DMS	B	8417	4/4	0.89	0.12	30,33,36,69	0
5	DMS	C	8416	4/4	0.89	0.19	64,66,100,100	0
5	DMS	A	8416	4/4	0.89	0.18	24,53,80,100	0
5	DMS	D	8503	4/4	0.89	0.19	31,76,100,100	0
5	DMS	B	8504	4/4	0.90	0.16	35,35,69,100	0
5	DMS	D	8407	4/4	0.90	0.14	26,50,53,55	0
5	DMS	B	8407	4/4	0.90	0.16	27,39,40,47	0
5	DMS	C	8423	4/4	0.90	0.13	38,42,44,58	0
5	DMS	A	8503	4/4	0.90	0.21	31,100,100,100	0
5	DMS	D	8703	4/4	0.90	0.17	32,38,49,53	0
5	DMS	A	8502	4/4	0.91	0.15	29,30,54,72	0
5	DMS	D	8416	4/4	0.91	0.14	34,35,54,77	0
5	DMS	C	8419	4/4	0.91	0.12	35,37,40,57	0
5	DMS	A	8407	4/4	0.91	0.12	25,38,39,47	0
5	DMS	B	8414	4/4	0.91	0.15	22,49,74,100	0
5	DMS	C	8415	4/4	0.91	0.14	26,32,41,61	0
5	DMS	C	8504	4/4	0.92	0.13	47,50,51,69	0
5	DMS	C	8407	4/4	0.92	0.14	30,39,40,50	0
5	DMS	B	8413	4/4	0.92	0.16	47,48,50,100	0
5	DMS	D	8415	4/4	0.92	0.18	25,49,64,100	0
5	DMS	B	8419	4/4	0.92	0.13	33,56,58,66	0
5	DMS	C	8417	4/4	0.92	0.10	23,35,47,52	0
4	145	C	2002	21/21	0.92	0.09	24,34,43,47	0
5	DMS	D	8421	4/4	0.92	0.17	32,54,78,100	0
5	DMS	A	8417	4/4	0.92	0.12	25,30,33,100	0
5	DMS	B	8410	4/4	0.92	0.16	29,42,60,100	0
5	DMS	D	8705	4/4	0.92	0.14	26,36,43,45	0
4	145	A	2002	21/21	0.93	0.09	20,30,41,43	0
4	145	D	2002	21/21	0.93	0.09	23,35,50,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	145	B	2002	21/21	0.93	0.09	23,31,41,50	0
5	DMS	B	8508	4/4	0.93	0.10	29,49,50,57	0
5	DMS	C	8425	4/4	0.93	0.15	42,44,49,71	0
5	DMS	A	8414	4/4	0.93	0.15	27,38,66,100	0
5	DMS	D	8425	4/4	0.93	0.18	22,24,28,56	4
5	DMS	C	8409	4/4	0.93	0.12	29,40,45,47	0
5	DMS	D	8508	4/4	0.93	0.11	34,39,44,51	0
5	DMS	C	8602	4/4	0.93	0.16	43,49,52,100	0
5	DMS	B	8420	4/4	0.93	0.13	39,42,46,52	0
5	DMS	C	8421	4/4	0.94	0.12	37,49,62,63	0
3	NA	D	3104	1/1	0.94	0.11	36,36,36,36	0
5	DMS	A	8409	4/4	0.94	0.14	30,41,46,100	0
5	DMS	A	8413	4/4	0.94	0.12	33,35,42,51	0
5	DMS	A	8420	4/4	0.94	0.12	37,44,52,62	0
5	DMS	D	8423	4/4	0.94	0.10	31,39,55,58	0
5	DMS	A	8406	4/4	0.94	0.13	16,52,70,78	0
5	DMS	D	8501	4/4	0.94	0.09	25,31,36,46	0
5	DMS	B	8408	4/4	0.94	0.15	31,36,40,100	0
5	DMS	D	8404	4/4	0.94	0.13	21,31,44,100	0
5	DMS	C	8420	4/4	0.94	0.17	40,41,57,100	0
5	DMS	D	8414	4/4	0.94	0.16	26,44,58,100	0
5	DMS	C	8413	4/4	0.95	0.10	32,33,45,45	0
5	DMS	C	8414	4/4	0.95	0.12	26,35,50,100	0
5	DMS	B	8502	4/4	0.95	0.14	30,31,44,100	0
5	DMS	C	8601	4/4	0.95	0.10	37,38,41,43	0
2	MG	C	3006	1/1	0.95	0.10	41,41,41,41	0
3	NA	C	3104	1/1	0.95	0.10	30,30,30,30	0
5	DMS	B	8601	4/4	0.95	0.10	33,35,37,42	0
5	DMS	A	8501	4/4	0.95	0.09	20,28,34,38	0
5	DMS	D	8409	4/4	0.95	0.14	29,37,43,100	0
5	DMS	C	8408	4/4	0.95	0.13	25,41,48,100	0
5	DMS	B	8425	4/4	0.95	0.09	29,35,36,43	0
3	NA	B	3104	1/1	0.96	0.08	32,32,32,32	0
5	DMS	B	8404	4/4	0.96	0.07	20,21,36,39	0
5	DMS	D	8419	4/4	0.96	0.11	34,36,55,72	0
5	DMS	A	8425	4/4	0.96	0.08	28,32,41,42	0
5	DMS	A	8419	4/4	0.96	0.11	36,44,49,52	0
5	DMS	B	8409	4/4	0.96	0.10	25,34,44,45	0
5	DMS	A	8410	4/4	0.96	0.11	28,36,39,52	0
5	DMS	A	8404	4/4	0.96	0.09	22,27,36,40	0
5	DMS	C	8410	4/4	0.96	0.10	24,34,37,39	0
5	DMS	D	8413	4/4	0.96	0.11	31,33,40,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8504	4/4	0.96	0.13	21,36,41,87	0
5	DMS	C	8501	4/4	0.96	0.09	18,28,36,48	0
4	145	A	2001	21/21	0.97	0.08	14,17,45,95	0
5	DMS	A	8408	4/4	0.97	0.07	22,35,39,47	0
5	DMS	D	8410	4/4	0.97	0.10	25,34,43,53	0
3	NA	A	3103	1/1	0.97	0.07	25,25,25,25	0
4	145	B	2001	21/21	0.97	0.07	11,15,38,47	0
3	NA	A	3104	1/1	0.97	0.06	25,25,25,25	0
5	DMS	C	8402	4/4	0.97	0.06	18,22,23,28	0
5	DMS	C	8404	4/4	0.97	0.07	21,24,28,31	0
5	DMS	C	8405	4/4	0.97	0.08	27,31,31,32	0
4	145	C	2001	21/21	0.97	0.07	13,17,38,55	0
2	MG	A	3005	1/1	0.97	0.05	31,31,31,31	0
4	145	D	2001	21/21	0.97	0.07	12,19,47,57	0
2	MG	A	3105	1/1	0.97	0.07	31,31,31,31	0
5	DMS	C	8412	4/4	0.97	0.12	26,33,44,100	0
3	NA	D	3103	1/1	0.97	0.08	26,26,26,26	0
5	DMS	D	8402	4/4	0.97	0.07	18,23,24,26	0
2	MG	D	3005	1/1	0.97	0.08	27,27,27,27	0
5	DMS	D	8406	4/4	0.97	0.09	26,27,31,35	0
5	DMS	D	8412	4/4	0.98	0.10	26,28,31,100	0
5	DMS	B	8405	4/4	0.98	0.07	23,28,29,31	0
3	NA	B	3101	1/1	0.98	0.05	16,16,16,16	0
2	MG	C	3105	1/1	0.98	0.06	26,26,26,26	0
5	DMS	A	8402	4/4	0.98	0.06	16,17,22,28	0
5	DMS	C	8411	4/4	0.98	0.06	24,28,30,35	0
5	DMS	A	8403	4/4	0.98	0.06	21,24,27,27	0
5	DMS	B	8411	4/4	0.98	0.11	26,27,31,100	0
5	DMS	B	8412	4/4	0.98	0.08	27,33,35,37	0
5	DMS	A	8412	4/4	0.98	0.09	34,34,37,60	0
3	NA	C	3103	1/1	0.98	0.08	26,26,26,26	0
5	DMS	B	8402	4/4	0.98	0.06	16,21,22,23	0
5	DMS	C	8403	4/4	0.98	0.06	23,24,25,27	0
5	DMS	D	8408	4/4	0.98	0.06	17,31,35,38	0
5	DMS	B	8403	4/4	0.98	0.05	16,21,26,26	0
2	MG	D	3105	1/1	0.98	0.05	31,31,31,31	0
2	MG	B	3001	1/1	0.99	0.03	15,15,15,15	0
3	NA	B	3102	1/1	0.99	0.05	16,16,16,16	0
3	NA	B	3103	1/1	0.99	0.04	25,25,25,25	0
2	MG	D	3001	1/1	0.99	0.03	15,15,15,15	0
2	MG	D	3002	1/1	0.99	0.05	17,17,17,17	0
5	DMS	D	8411	4/4	0.99	0.07	23,25,28,59	0

Continued on next page...

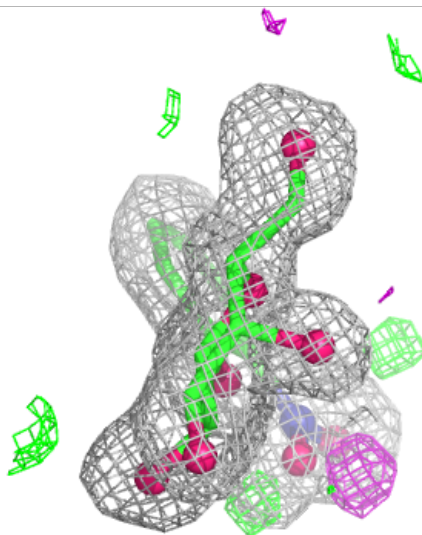
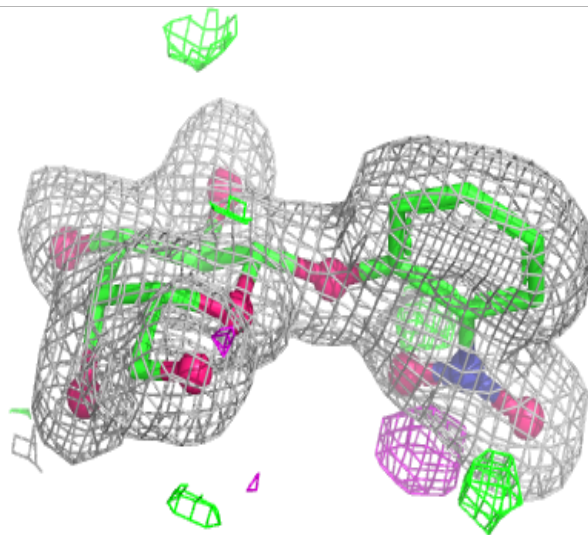
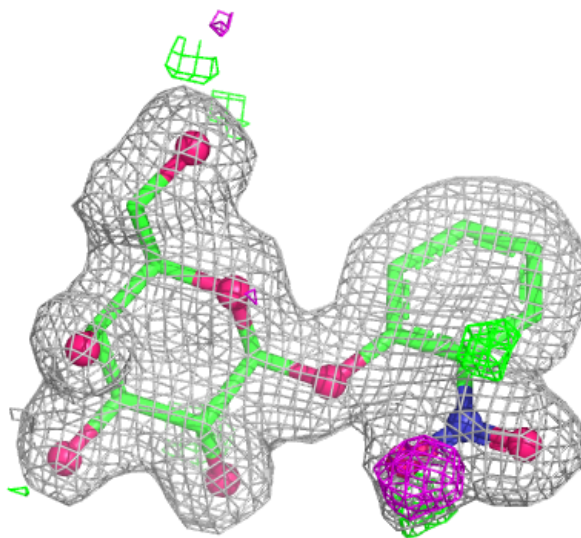
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8401	4/4	0.99	0.03	12,14,16,18	0
2	MG	B	3002	1/1	0.99	0.03	17,17,17,17	0
5	DMS	C	8401	4/4	0.99	0.03	15,17,21,23	0
3	NA	D	3101	1/1	0.99	0.05	16,16,16,16	0
3	NA	D	3102	1/1	0.99	0.02	15,15,15,15	0
5	DMS	A	8405	4/4	0.99	0.05	20,24,25,27	0
2	MG	A	3002	1/1	0.99	0.04	17,17,17,17	0
3	NA	A	3101	1/1	0.99	0.03	17,17,17,17	0
3	NA	A	3102	1/1	0.99	0.02	15,15,15,15	0
2	MG	B	3105	1/1	0.99	0.03	27,27,27,27	0
2	MG	A	3001	1/1	0.99	0.02	17,17,17,17	0
5	DMS	D	8401	4/4	0.99	0.04	15,16,18,19	0
5	DMS	A	8411	4/4	0.99	0.06	23,24,28,31	0
5	DMS	D	8403	4/4	0.99	0.05	18,25,25,27	0
5	DMS	D	8701	4/4	0.99	0.07	15,16,20,38	0
5	DMS	B	8401	4/4	0.99	0.04	15,17,17,20	0
5	DMS	D	8405	4/4	0.99	0.05	24,25,25,30	0
2	MG	C	3002	1/1	1.00	0.04	15,15,15,15	0
3	NA	C	3101	1/1	1.00	0.05	15,15,15,15	0
3	NA	C	3102	1/1	1.00	0.01	17,17,17,17	0
2	MG	C	3001	1/1	1.00	0.01	15,15,15,15	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.

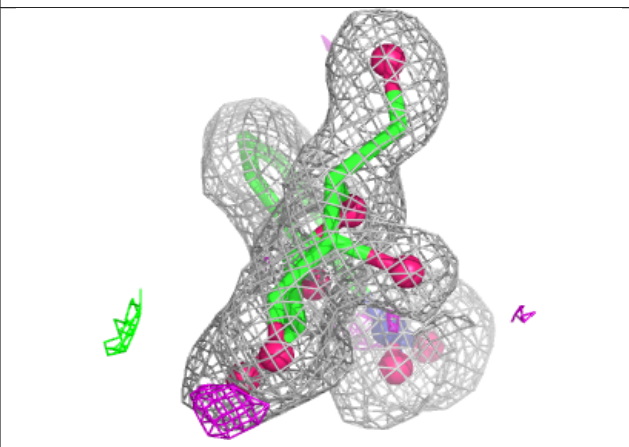
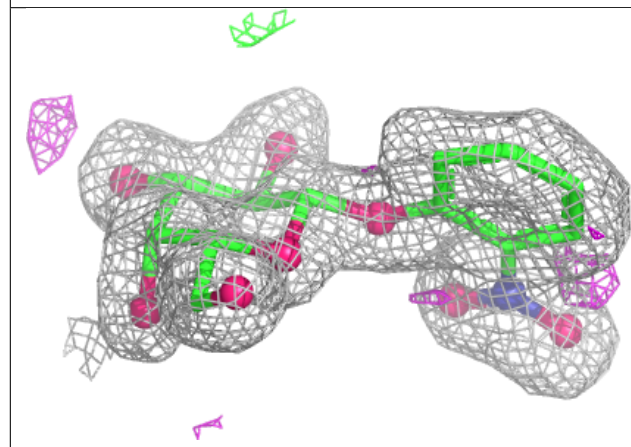
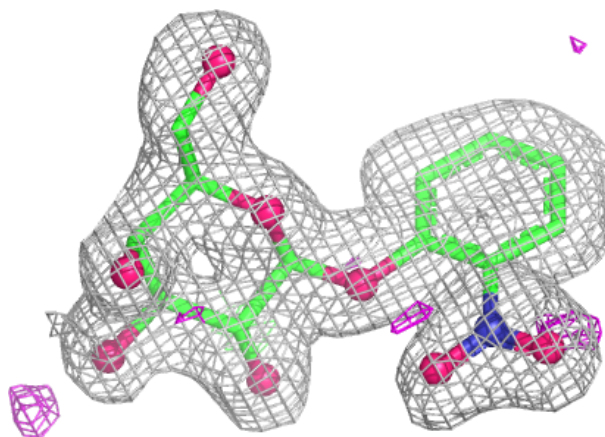
Electron density around 145 C 2002:

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



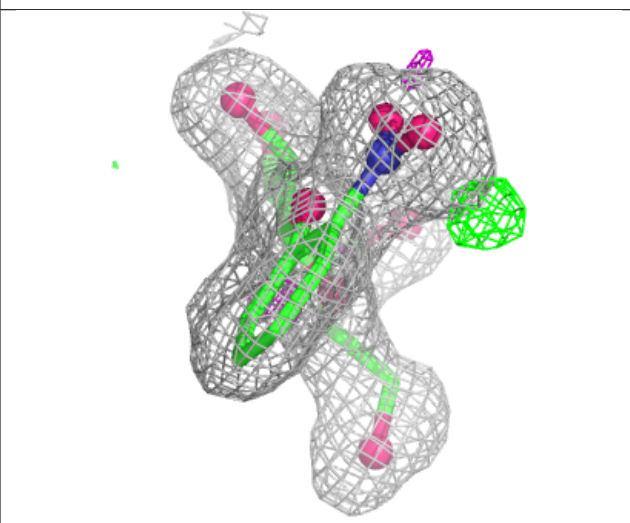
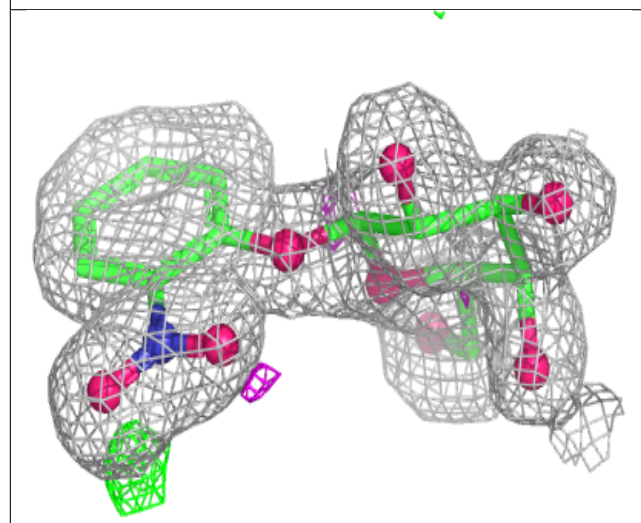
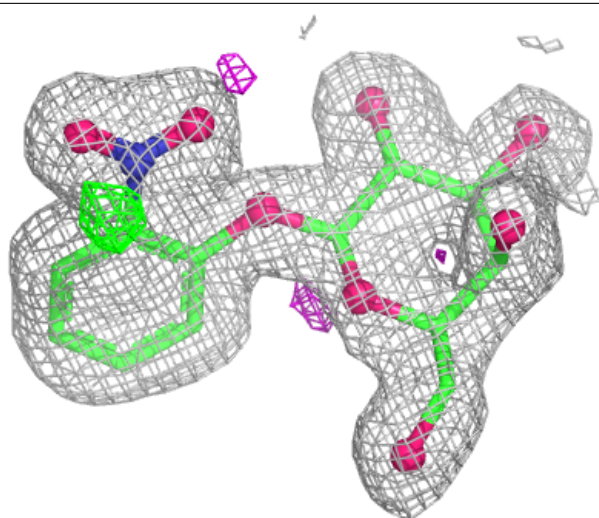
Electron density around 145 Å 2002:

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



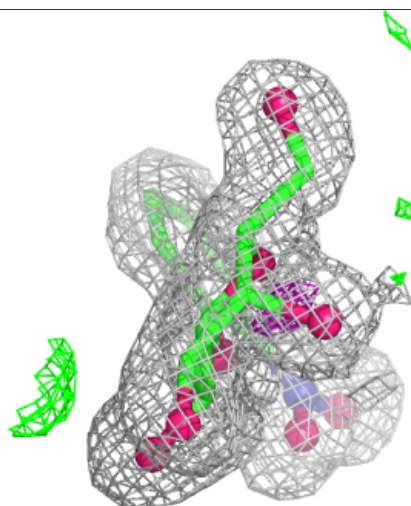
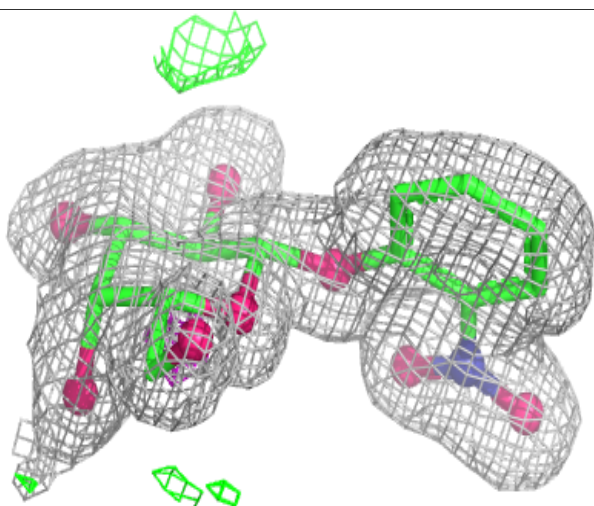
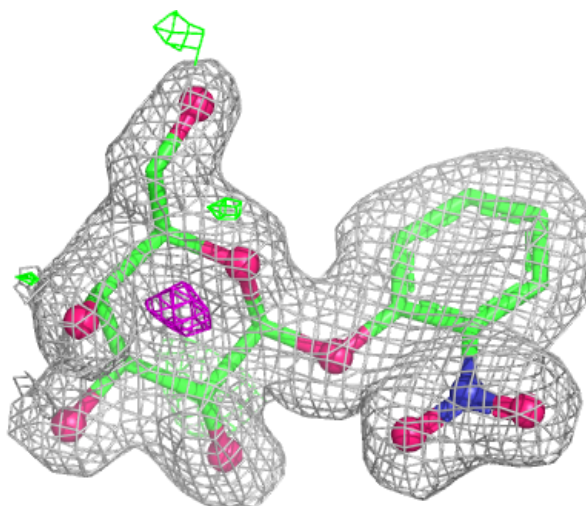
Electron density around 145 D 2002:

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



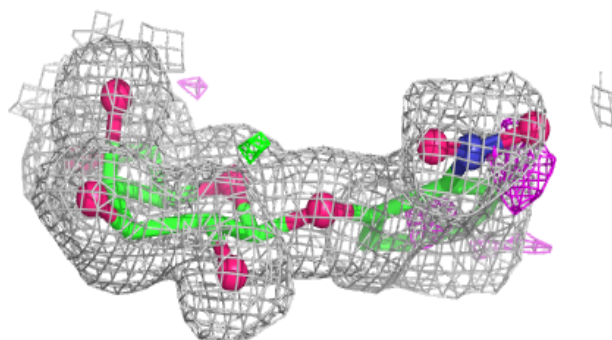
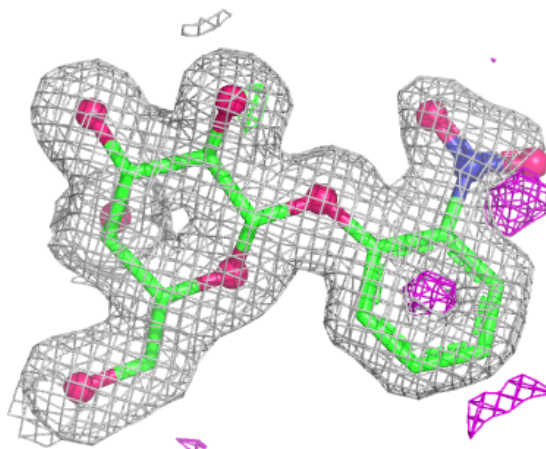
Electron density around 145 B 2002:

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



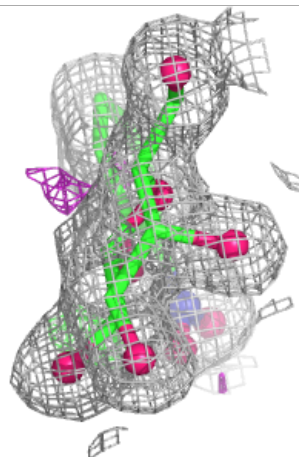
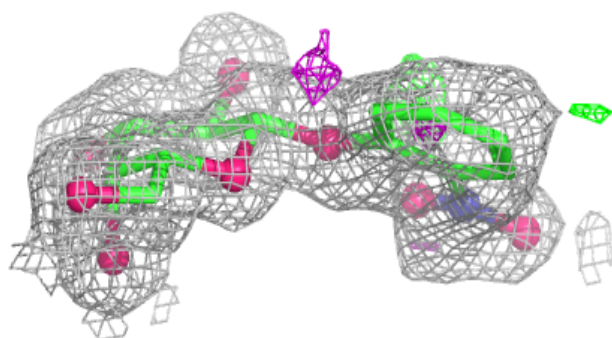
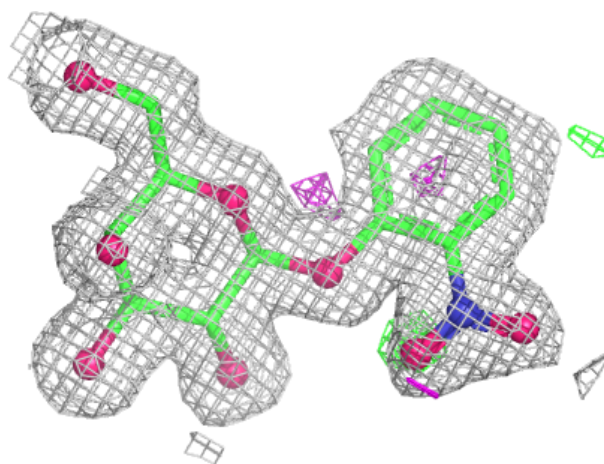
Electron density around 145 Å 2001:

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



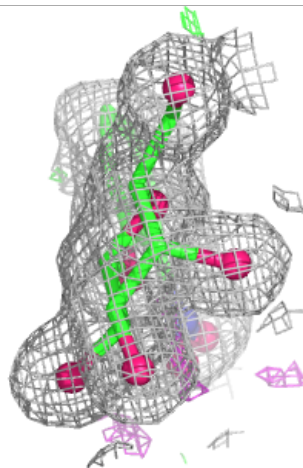
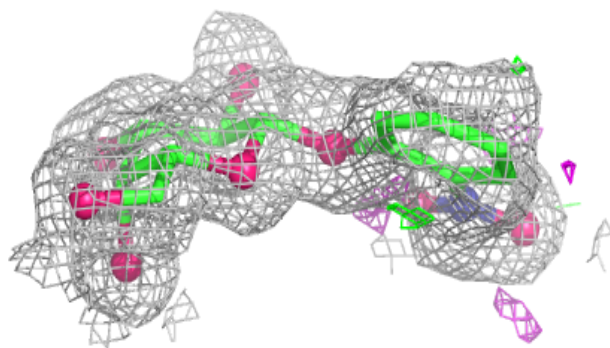
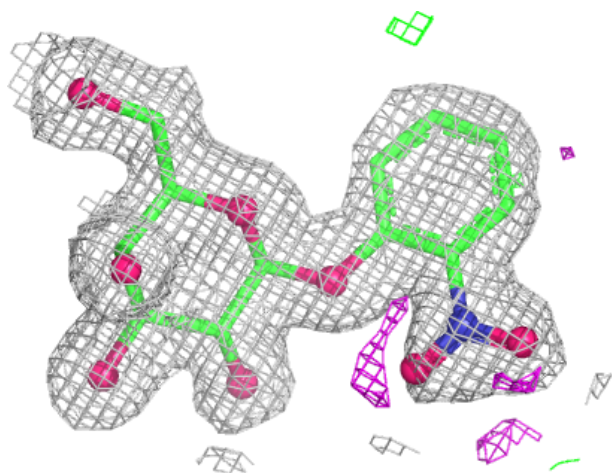
Electron density around 145 B 2001:

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



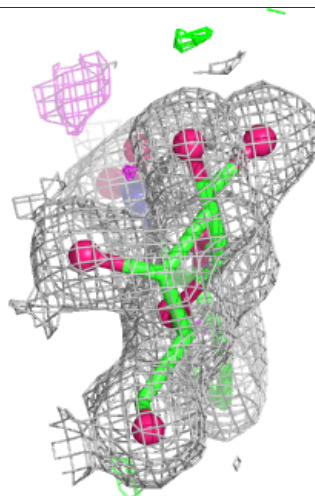
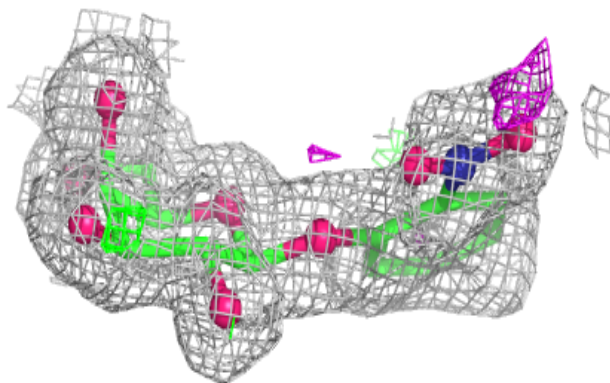
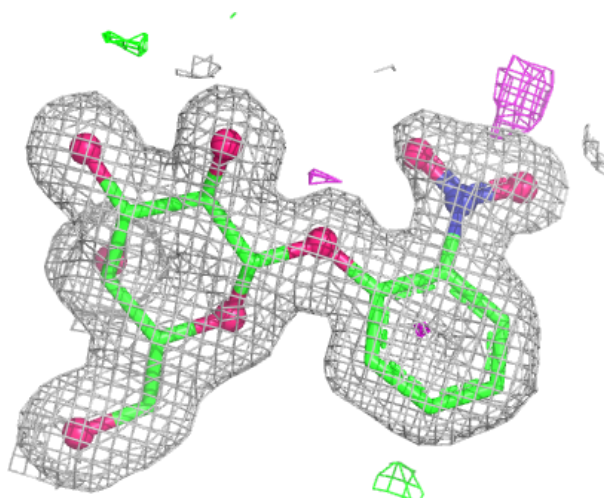
Electron density around 145 C 2001:

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



Electron density around 145 D 2001:

$2mF_o-DF_c$ (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.