



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 17, 2021 – 07:41 AM EDT

PDB ID : 1JYV
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

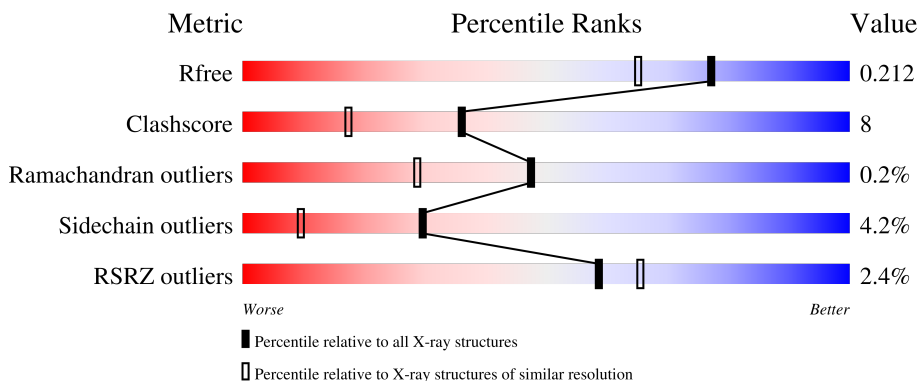
1 Overall quality at a glance

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}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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

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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

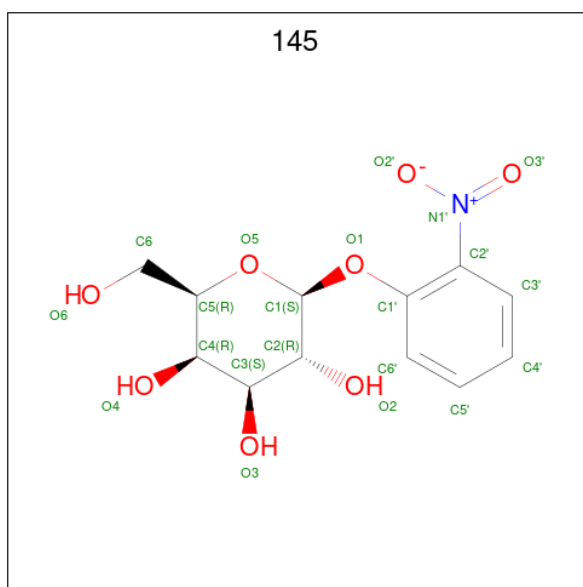
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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		

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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

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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

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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

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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

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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

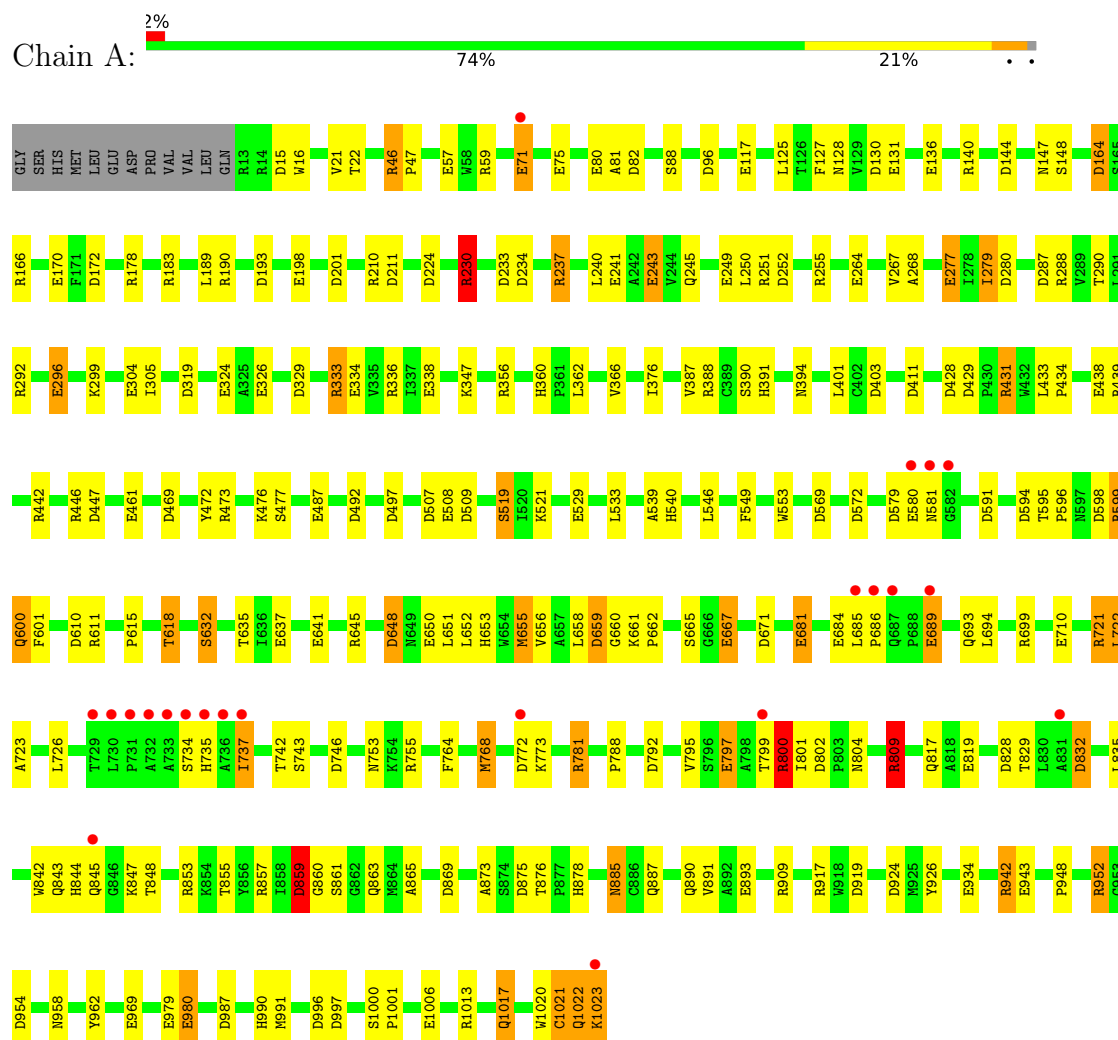
- Molecule 6 is water.

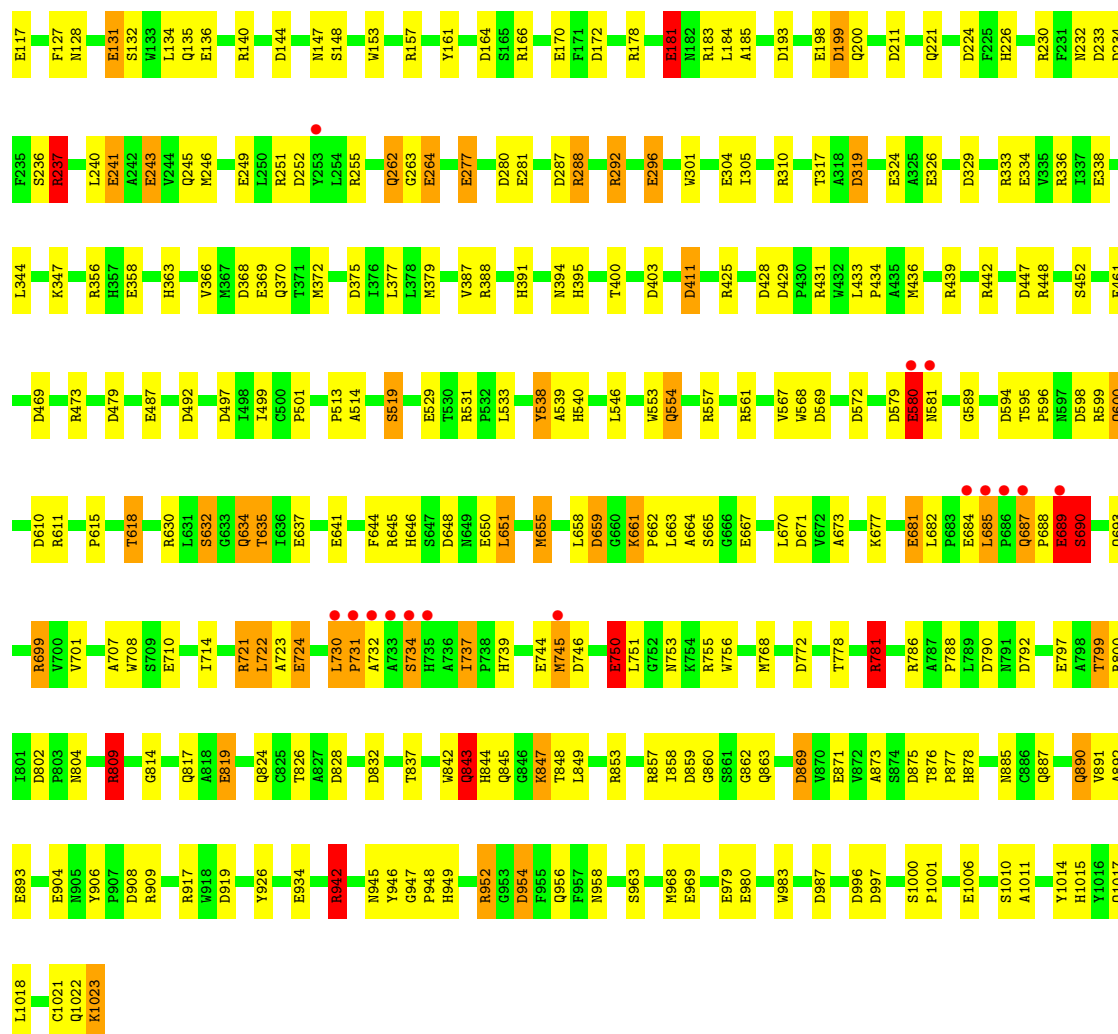
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1060	Total O 1060 1060	0	0
6	B	1013	Total O 1013 1013	0	0
6	C	987	Total O 987 987	0	0
6	D	1021	Total O 1021 1021	0	0

3 Residue-property plots

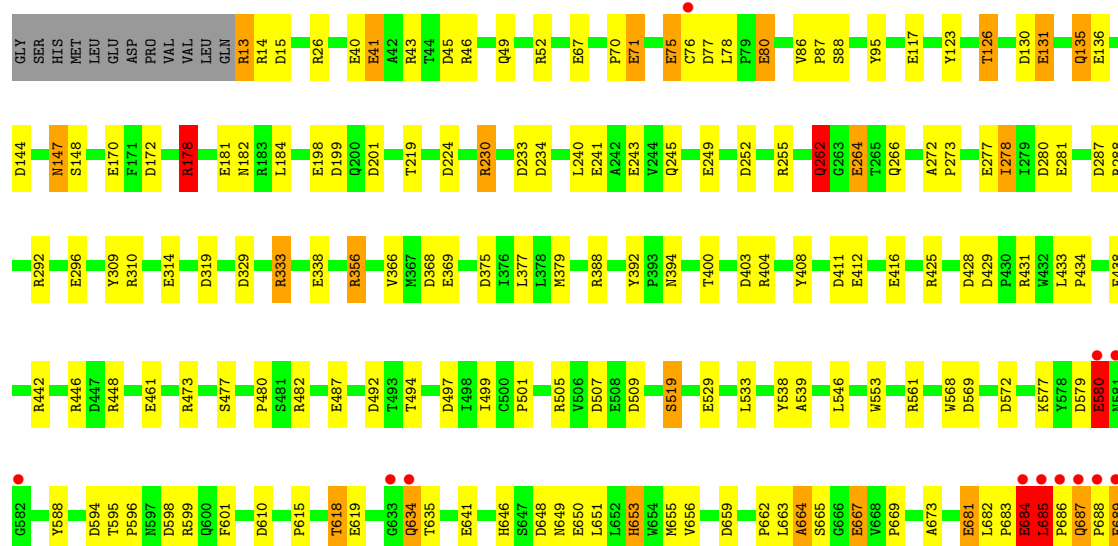
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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





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 29.85 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.75) 90.9 (29.85-1.75)	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 , 0.212	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)	0.34 , 89.4	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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS, 145, 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	1.10	44/8383 (0.5%)	1.62	155/11437 (1.4%)
1	B	1.11	48/8383 (0.6%)	1.64	177/11437 (1.5%)
1	C	1.10	46/8383 (0.5%)	1.64	173/11437 (1.5%)
1	D	1.11	43/8383 (0.5%)	1.59	163/11437 (1.4%)
All	All	1.10	181/33532 (0.5%)	1.62	668/45748 (1.5%)

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 181 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	684	GLU	CD-OE2	10.26	1.36	1.25
1	D	893	GLU	CD-OE2	9.38	1.35	1.25
1	D	71	GLU	CD-OE2	8.89	1.35	1.25
1	C	80	GLU	CD-OE2	8.45	1.34	1.25
1	C	1006	GLU	CD-OE2	8.41	1.34	1.25

The worst 5 of 668 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	19.59	130.09	120.30
1	B	942	ARG	NE-CZ-NH1	17.39	128.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	687	GLN	C-N-CD	-15.95	85.52	120.60
1	C	699	ARG	NE-CZ-NH1	15.62	128.11	120.30
1	B	942	ARG	NE-CZ-NH2	-14.81	112.89	120.30

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

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	108	0
1	B	8128	0	7712	141	0
1	C	8128	0	7712	125	0
1	D	8128	0	7712	132	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	7	0
5	B	100	0	150	5	0
5	C	108	0	162	5	0
5	D	112	0	168	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1060	0	0	16	3
6	B	1013	0	0	14	1
6	C	987	0	0	14	2
6	D	1021	0	0	15	0
All	All	37222	0	31598	518	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 8.

The worst 5 of 518 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%)	47 29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1011/1023 (99%)	968 (96%)	39 (4%)	4 (0%)	34 17
1	C	1011/1023 (99%)	966 (96%)	44 (4%)	1 (0%)	51 33
1	D	1011/1023 (99%)	972 (96%)	37 (4%)	2 (0%)	47 29
All	All	4044/4092 (99%)	3880 (96%)	155 (4%)	9 (0%)	47 29

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%)	836 (97%)	29 (3%)	37 14
1	B	865/875 (99%)	821 (95%)	44 (5%)	24 6
1	C	865/875 (99%)	829 (96%)	36 (4%)	30 9
1	D	865/875 (99%)	828 (96%)	37 (4%)	29 9
All	All	3460/3500 (99%)	3314 (96%)	146 (4%)	30 9

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	392	TYR
1	D	1018	LEU
1	D	581	ASN
1	D	734	SER
1	B	661	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	266	GLN
1	C	977	HIS
1	C	624	GLN
1	C	687	GLN
1	D	163	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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	C	8421	-	3,3,3	0.62	0	3,3,3	0.67	0
5	DMS	A	8415	-	3,3,3	1.10	0	3,3,3	0.70	0
5	DMS	C	8419	-	3,3,3	1.04	0	3,3,3	0.47	0
5	DMS	A	8419	-	3,3,3	0.78	0	3,3,3	0.33	0
5	DMS	B	8417	-	3,3,3	0.94	0	3,3,3	0.21	0
4	145	C	2002	-	21,22,22	0.82	1 (4%)	28,31,31	1.11	2 (7%)
5	DMS	C	8501	-	3,3,3	1.43	1 (33%)	3,3,3	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8414	-	3,3,3	1.11	0	3,3,3	0.45	0
5	DMS	C	8601	-	3,3,3	0.75	0	3,3,3	1.05	0
4	145	B	2001	3	21,22,22	1.09	2 (9%)	28,31,31	0.90	0
5	DMS	A	8408	-	3,3,3	0.65	0	3,3,3	1.67	1 (33%)
4	145	D	2001	3	21,22,22	1.13	2 (9%)	28,31,31	1.28	4 (14%)
5	DMS	D	8409	-	3,3,3	2.22	1 (33%)	3,3,3	0.61	0
5	DMS	A	8421	-	3,3,3	0.19	0	3,3,3	0.36	0
5	DMS	A	8602	-	3,3,3	0.84	0	3,3,3	0.55	0
5	DMS	D	8413	-	3,3,3	1.95	1 (33%)	3,3,3	0.67	0
5	DMS	A	8420	-	3,3,3	1.08	0	3,3,3	0.37	0
4	145	A	2002	-	21,22,22	0.83	0	28,31,31	1.23	2 (7%)
5	DMS	A	8501	-	3,3,3	1.16	0	3,3,3	0.33	0
5	DMS	D	8416	-	3,3,3	1.34	1 (33%)	3,3,3	0.50	0
5	DMS	C	8404	-	3,3,3	1.19	0	3,3,3	1.15	0
5	DMS	B	8409	-	3,3,3	2.21	1 (33%)	3,3,3	0.58	0
5	DMS	A	8410	-	3,3,3	1.10	0	3,3,3	0.35	0
5	DMS	B	8502	-	3,3,3	2.33	2 (66%)	3,3,3	0.45	0
5	DMS	D	8421	-	3,3,3	0.55	0	3,3,3	0.37	0
5	DMS	A	8414	-	3,3,3	1.23	0	3,3,3	0.14	0
5	DMS	B	8415	-	3,3,3	2.02	1 (33%)	3,3,3	1.40	1 (33%)
5	DMS	D	8420	-	3,3,3	1.31	1 (33%)	3,3,3	0.38	0
5	DMS	C	8414	-	3,3,3	1.06	0	3,3,3	0.82	0
5	DMS	C	8402	-	3,3,3	1.03	0	3,3,3	0.81	0
5	DMS	B	8408	-	3,3,3	1.45	1 (33%)	3,3,3	0.34	0
5	DMS	C	8503	-	3,3,3	1.06	0	3,3,3	0.21	0
5	DMS	A	8411	-	3,3,3	0.75	0	3,3,3	0.40	0
5	DMS	A	8403	-	3,3,3	1.45	1 (33%)	3,3,3	0.37	0
5	DMS	D	8407	-	3,3,3	2.84	2 (66%)	3,3,3	0.32	0
5	DMS	B	8405	-	3,3,3	1.42	0	3,3,3	0.55	0
5	DMS	A	8401	-	3,3,3	0.65	0	3,3,3	0.85	0
5	DMS	C	8415	-	3,3,3	2.69	2 (66%)	3,3,3	1.74	1 (33%)
5	DMS	B	8412	-	3,3,3	1.90	1 (33%)	3,3,3	0.19	0
5	DMS	B	8402	-	3,3,3	0.58	0	3,3,3	0.09	0
5	DMS	B	8421	-	3,3,3	0.70	0	3,3,3	1.00	0
5	DMS	C	8403	-	3,3,3	1.25	0	3,3,3	0.45	0
5	DMS	A	8412	-	3,3,3	0.62	0	3,3,3	0.36	0
5	DMS	D	8406	-	3,3,3	1.15	0	3,3,3	0.70	0
4	145	B	2002	-	21,22,22	0.84	0	28,31,31	1.34	3 (10%)
5	DMS	A	8409	-	3,3,3	2.04	1 (33%)	3,3,3	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8407	-	3,3,3	2.14	1 (33%)	3,3,3	0.25	0
5	DMS	A	8425	3	3,3,3	1.97	1 (33%)	3,3,3	0.65	0
5	DMS	A	8503	-	3,3,3	0.33	0	3,3,3	0.20	0
5	DMS	C	8602	-	3,3,3	1.08	0	3,3,3	0.28	0
5	DMS	C	8425	3	3,3,3	1.79	1 (33%)	3,3,3	0.39	0
5	DMS	C	8423	-	3,3,3	0.64	0	3,3,3	0.35	0
5	DMS	D	8703	-	3,3,3	2.32	2 (66%)	3,3,3	0.24	0
5	DMS	A	8417	-	3,3,3	2.09	1 (33%)	3,3,3	1.05	0
5	DMS	D	8404	-	3,3,3	1.09	0	3,3,3	0.47	0
5	DMS	B	8411	-	3,3,3	1.23	1 (33%)	3,3,3	0.42	0
5	DMS	C	8412	-	3,3,3	0.85	0	3,3,3	0.33	0
5	DMS	B	8504	-	3,3,3	1.06	0	3,3,3	0.84	0
5	DMS	D	8411	-	3,3,3	1.04	0	3,3,3	0.27	0
5	DMS	C	8504	-	3,3,3	0.82	0	3,3,3	0.29	0
5	DMS	B	8416	-	3,3,3	0.53	0	3,3,3	0.52	0
5	DMS	B	8404	-	3,3,3	1.28	0	3,3,3	1.38	1 (33%)
5	DMS	C	8420	-	3,3,3	1.89	1 (33%)	3,3,3	0.22	0
5	DMS	D	8423	-	3,3,3	1.31	0	3,3,3	0.30	0
5	DMS	A	8407	-	3,3,3	2.55	2 (66%)	3,3,3	0.23	0
5	DMS	C	8705	-	3,3,3	1.11	0	3,3,3	0.21	0
5	DMS	A	8416	-	3,3,3	0.55	0	3,3,3	0.40	0
5	DMS	B	8413	-	3,3,3	1.66	1 (33%)	3,3,3	0.14	0
5	DMS	D	8412	-	3,3,3	0.93	0	3,3,3	0.50	0
5	DMS	D	8401	-	3,3,3	0.96	0	3,3,3	0.83	0
5	DMS	D	8417	-	3,3,3	1.37	0	3,3,3	1.13	0
5	DMS	D	8701	-	3,3,3	1.86	0	3,3,3	0.47	0
5	DMS	B	8401	-	3,3,3	0.58	0	3,3,3	0.29	0
5	DMS	A	8406	-	3,3,3	0.35	0	3,3,3	1.07	0
5	DMS	B	8423	-	3,3,3	0.97	0	3,3,3	0.10	0
5	DMS	C	8417	-	3,3,3	1.04	0	3,3,3	0.84	0
5	DMS	D	8414	-	3,3,3	0.66	0	3,3,3	0.34	0
4	145	D	2002	-	21,22,22	0.52	0	28,31,31	1.27	3 (10%)
5	DMS	D	8705	-	3,3,3	1.67	0	3,3,3	0.81	0
5	DMS	A	8502	-	3,3,3	1.29	0	3,3,3	1.31	1 (33%)
5	DMS	C	8401	-	3,3,3	0.86	0	3,3,3	0.51	0
4	145	C	2001	3	21,22,22	0.77	0	28,31,31	1.19	5 (17%)
5	DMS	A	8405	-	3,3,3	0.85	0	3,3,3	0.30	0
5	DMS	D	8402	-	3,3,3	1.60	1 (33%)	3,3,3	0.39	0
5	DMS	B	8508	-	3,3,3	2.16	1 (33%)	3,3,3	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8410	-	3,3,3	0.72	0	3,3,3	0.31	0
5	DMS	C	8407	-	3,3,3	2.23	2 (66%)	3,3,3	0.55	0
5	DMS	B	8425	3	3,3,3	1.85	1 (33%)	3,3,3	0.59	0
5	DMS	B	8419	-	3,3,3	0.62	0	3,3,3	0.42	0
5	DMS	D	8415	-	3,3,3	2.49	1 (33%)	3,3,3	0.47	0
5	DMS	D	8508	-	3,3,3	1.78	1 (33%)	3,3,3	0.47	0
5	DMS	C	8416	-	3,3,3	0.75	0	3,3,3	0.11	0
4	145	A	2001	3	21,22,22	0.95	1 (4%)	28,31,31	1.45	4 (14%)
5	DMS	D	8419	-	3,3,3	0.40	0	3,3,3	0.18	0
5	DMS	C	8413	-	3,3,3	1.33	0	3,3,3	0.18	0
5	DMS	D	8503	-	3,3,3	0.73	0	3,3,3	0.33	0
5	DMS	C	8405	-	3,3,3	1.49	1 (33%)	3,3,3	0.57	0
5	DMS	D	8403	-	3,3,3	0.58	0	3,3,3	0.71	0
5	DMS	C	8411	-	3,3,3	1.05	0	3,3,3	0.42	0
5	DMS	D	8405	-	3,3,3	0.73	0	3,3,3	0.81	0
5	DMS	C	8409	-	3,3,3	2.08	1 (33%)	3,3,3	0.83	0
5	DMS	C	8410	-	3,3,3	1.26	0	3,3,3	0.21	0
5	DMS	B	8601	-	3,3,3	2.10	1 (33%)	3,3,3	1.03	0
5	DMS	A	8504	-	3,3,3	0.65	0	3,3,3	0.30	0
5	DMS	A	8423	-	3,3,3	1.26	0	3,3,3	0.86	0
5	DMS	D	8501	-	3,3,3	0.34	0	3,3,3	0.73	0
5	DMS	D	8408	-	3,3,3	0.81	0	3,3,3	0.22	0
5	DMS	C	8408	-	3,3,3	1.36	0	3,3,3	0.55	0
5	DMS	B	8420	-	3,3,3	1.52	1 (33%)	3,3,3	0.45	0
5	DMS	A	8404	-	3,3,3	1.07	0	3,3,3	0.70	0
5	DMS	A	8402	-	3,3,3	1.50	0	3,3,3	0.29	0
5	DMS	A	8413	-	3,3,3	2.07	2 (66%)	3,3,3	0.34	0
5	DMS	D	8410	-	3,3,3	1.50	0	3,3,3	0.46	0
5	DMS	B	8403	-	3,3,3	1.20	0	3,3,3	0.45	0
5	DMS	D	8425	3	3,3,3	0.37	0	3,3,3	0.66	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	B	2001	3	-	1/8/30/30	0/2/2/2
4	145	A	2002	-	-	0/8/30/30	0/2/2/2
4	145	C	2001	3	-	1/8/30/30	0/2/2/2

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

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8415	DMS	C2-S	3.90	2.04	1.75
5	D	8407	DMS	C2-S	3.84	2.04	1.75
5	D	8409	DMS	O-S	3.63	1.74	1.50
5	D	8415	DMS	O-S	3.59	1.74	1.50
5	A	8417	DMS	C1-S	-3.57	1.49	1.75

The worst 5 of 28 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	2.95	113.64	98.44

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	B	2001	145	O5-C5-C6-O6
4	D	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.

24 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2002	145	2	0
4	D	2001	145	1	0
5	A	8602	DMS	1	0

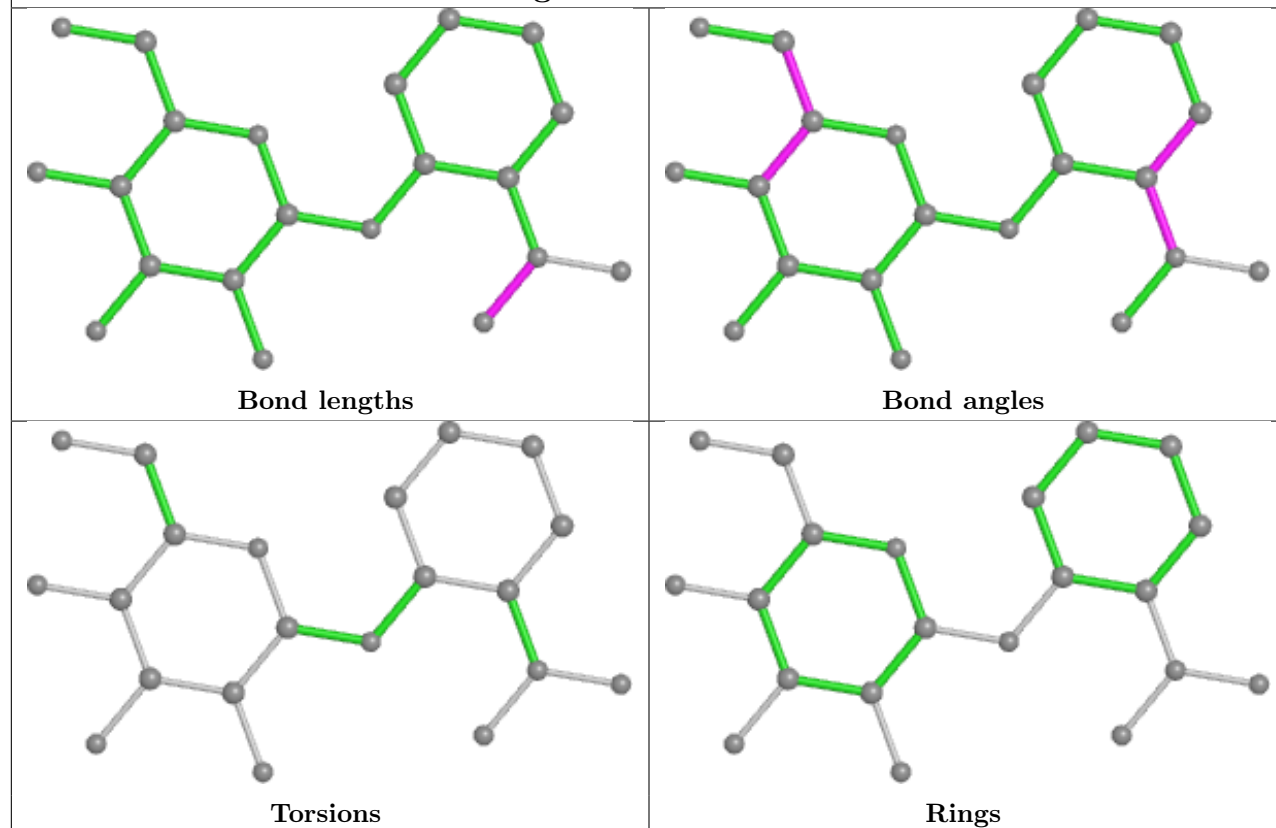
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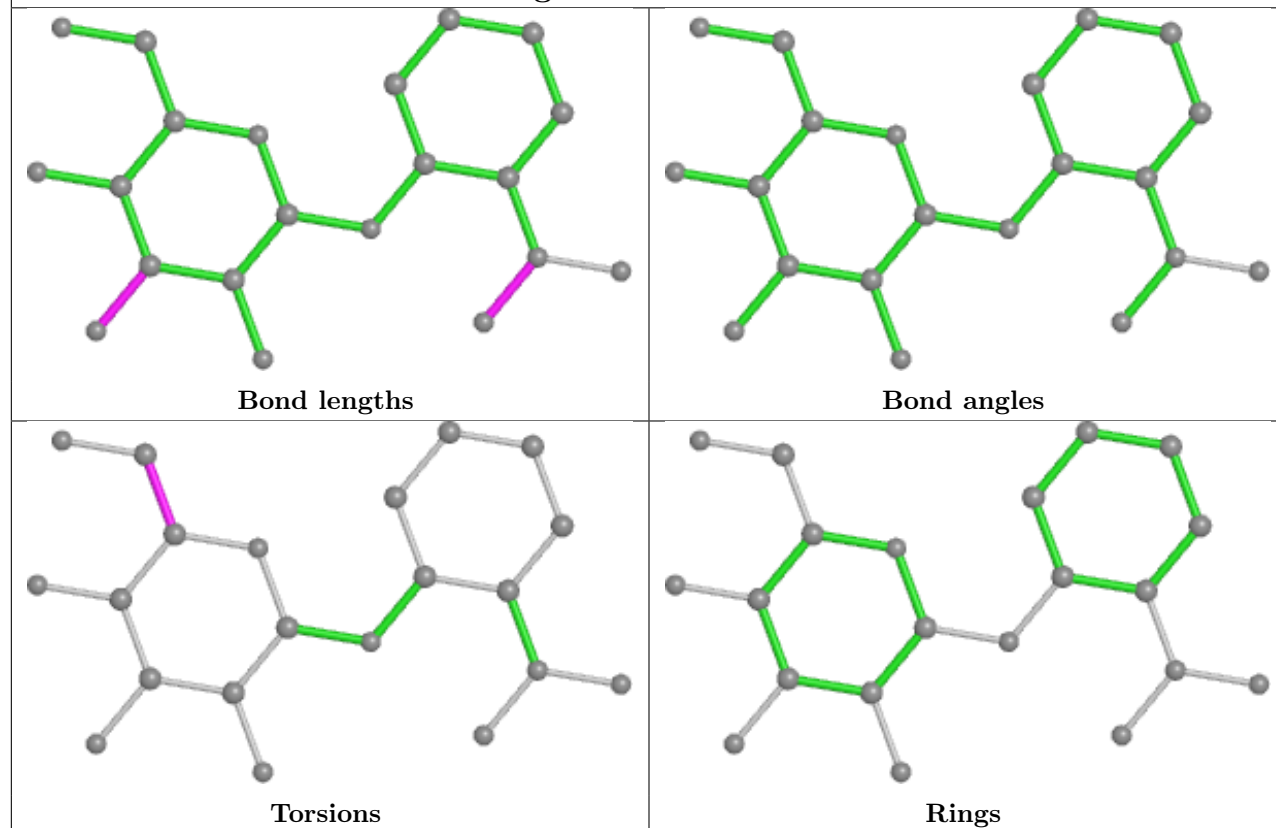
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	145	1	0
5	D	8416	DMS	1	0
5	B	8502	DMS	1	0
5	C	8503	DMS	1	0
5	D	8407	DMS	2	0
5	C	8415	DMS	1	0
5	A	8412	DMS	4	0
4	B	2002	145	1	0
5	B	8407	DMS	2	0
5	A	8503	DMS	1	0
5	C	8602	DMS	1	0
5	C	8425	DMS	1	0
5	D	8703	DMS	7	0
5	B	8416	DMS	1	0
5	C	8420	DMS	1	0
5	D	8412	DMS	3	0
4	D	2002	145	3	0
5	A	8502	DMS	1	0
4	A	2001	145	1	0
5	B	8420	DMS	1	0
5	D	8425	DMS	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.

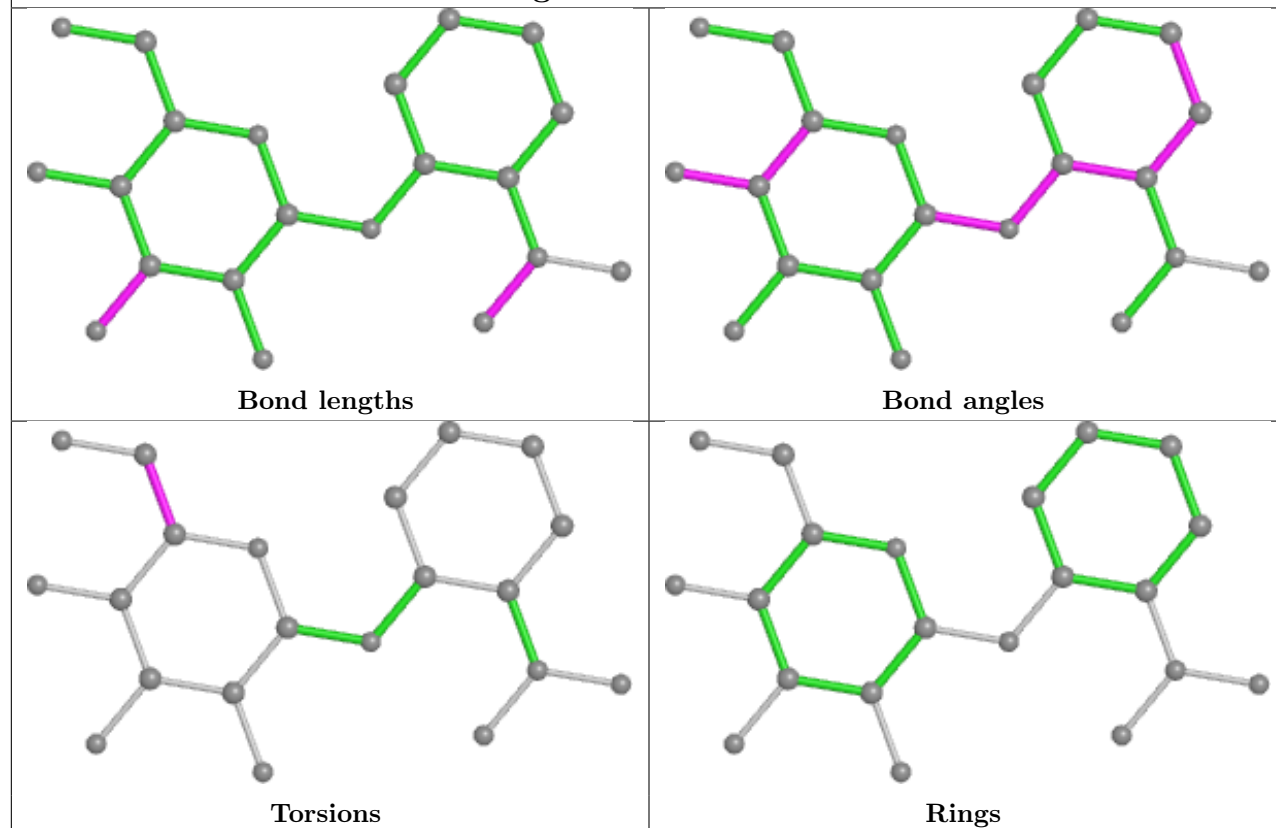
Ligand 145 C 2002



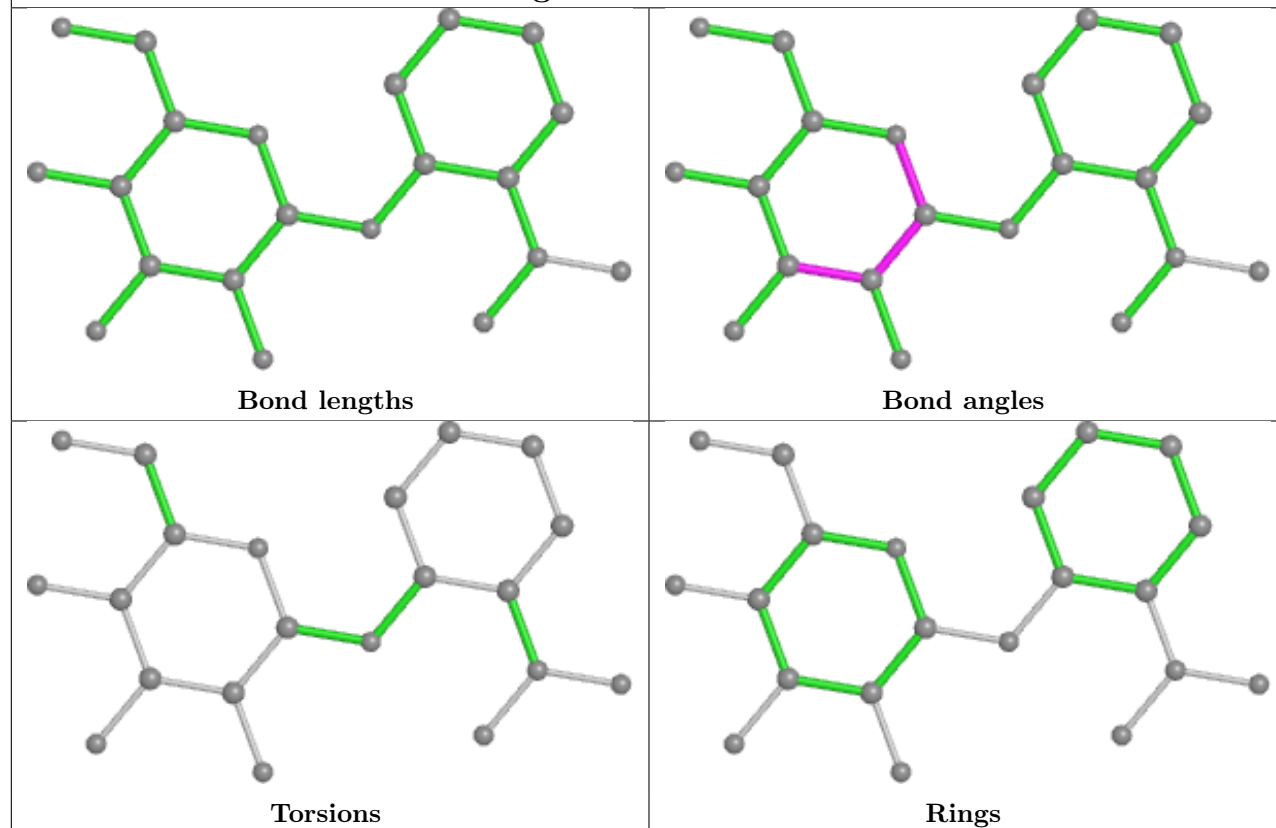
Ligand 145 B 2001



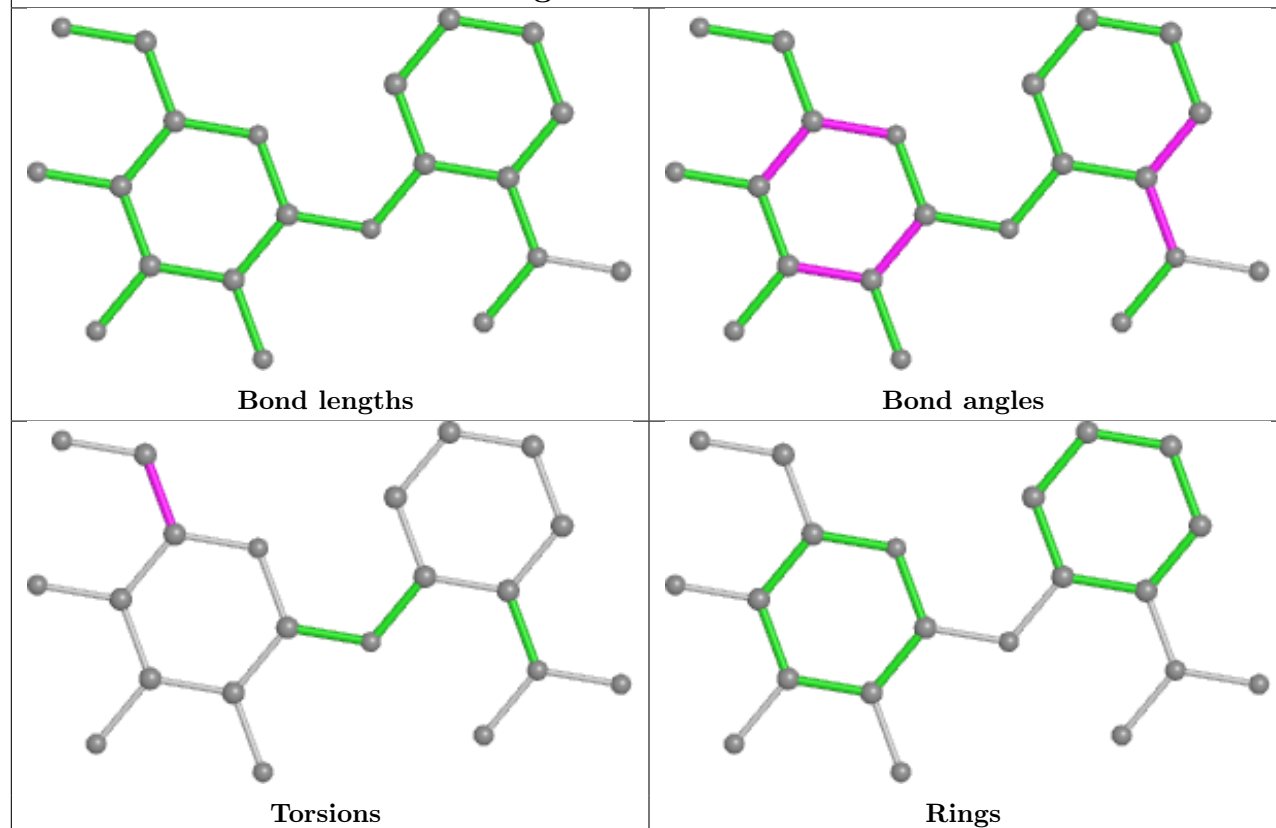
Ligand 145 D 2001



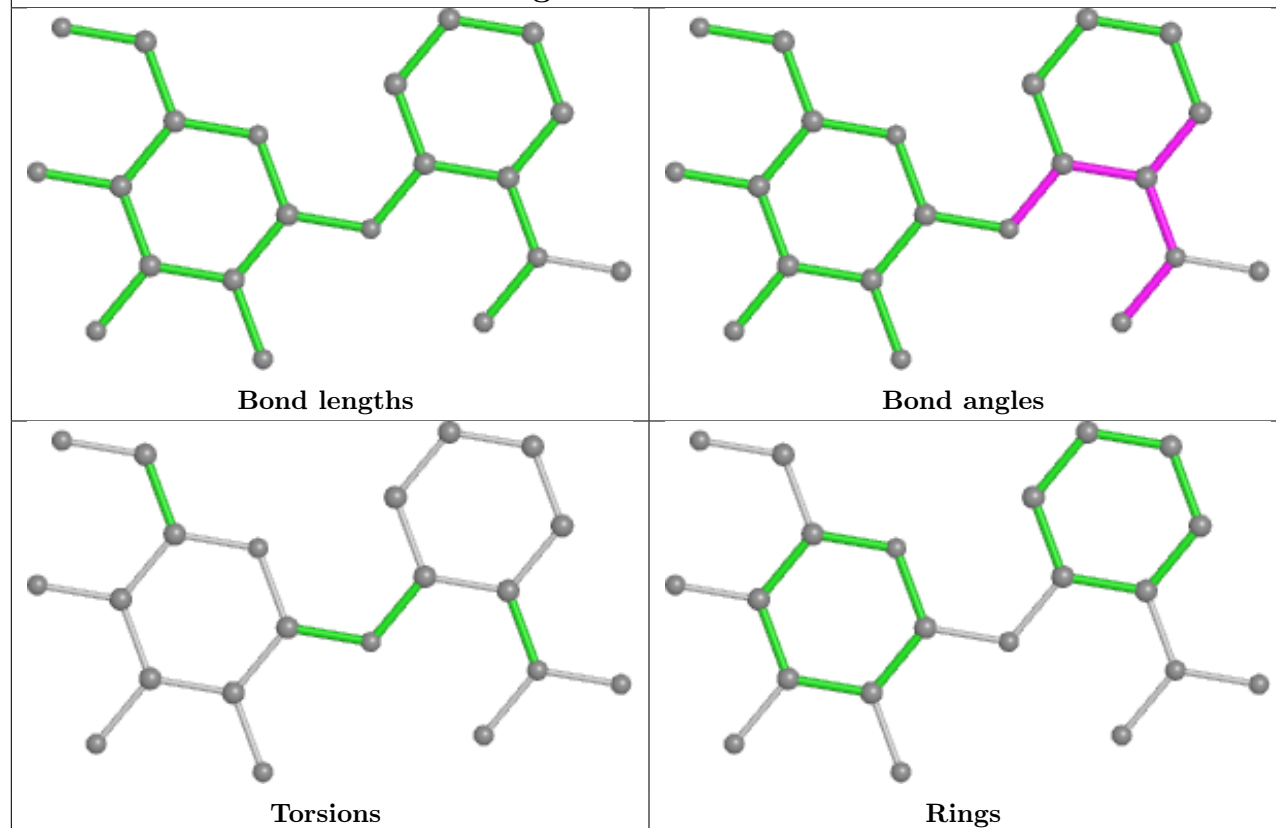
Ligand 145 A 2002



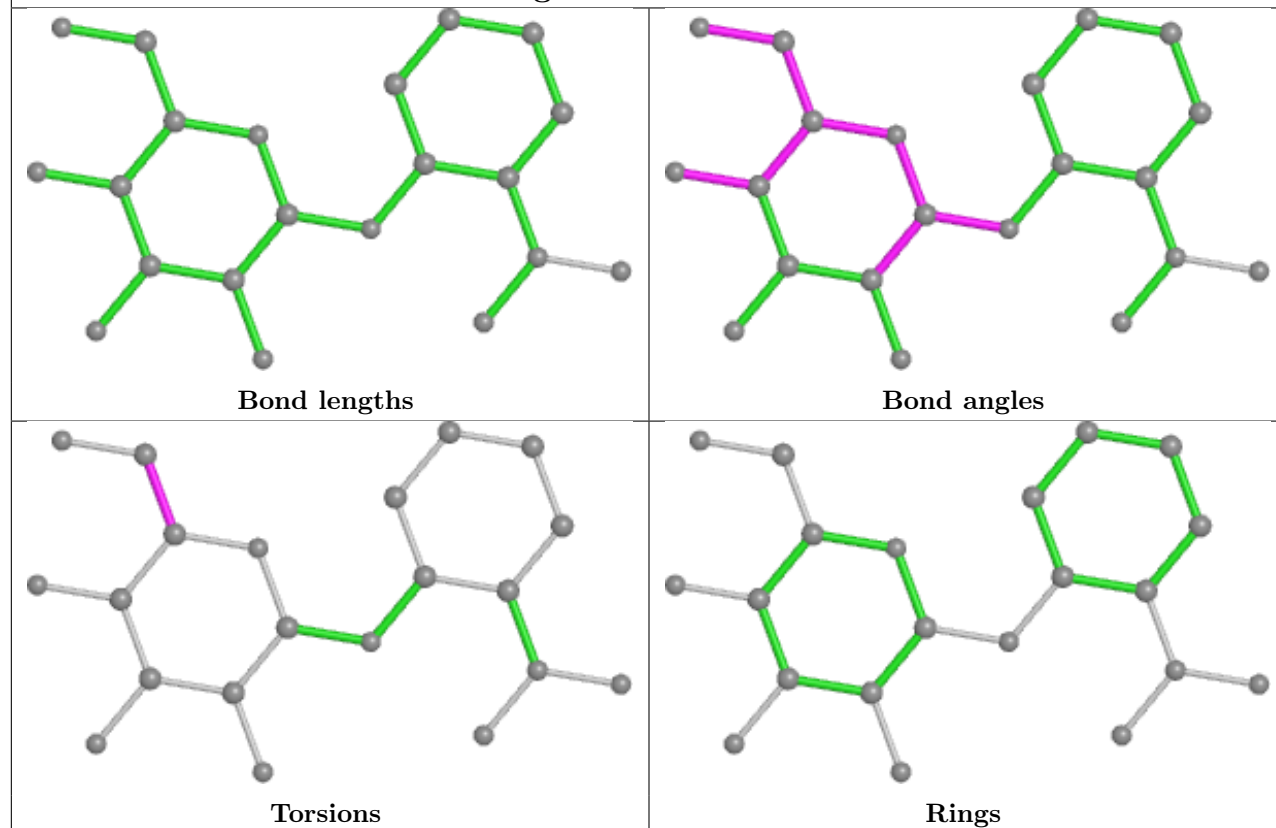
Ligand 145 B 2002



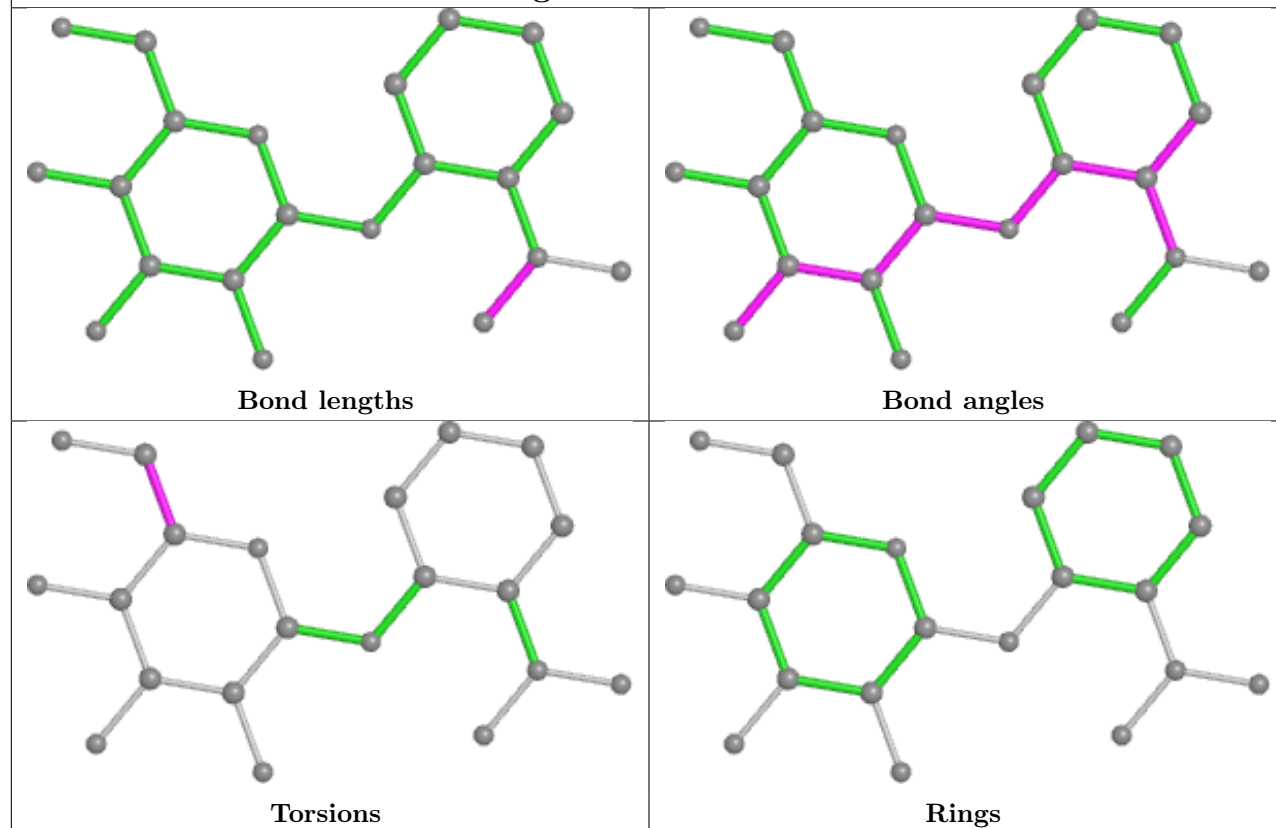
Ligand 145 D 2002



Ligand 145 C 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%)	-0.30	22 (2%) 62 69	11, 18, 46, 100	0
1	B	1011/1023 (98%)	-0.23	16 (1%) 72 79	11, 19, 48, 99	0
1	C	1011/1023 (98%)	-0.19	28 (2%) 53 58	11, 20, 51, 100	0
1	D	1011/1023 (98%)	-0.23	33 (3%) 46 53	11, 19, 50, 100	0
All	All	4044/4092 (98%)	-0.24	99 (2%) 59 65	11, 19, 49, 100	0

The worst 5 of 99 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	11.0
1	C	732	ALA	10.4
1	C	730	LEU	9.3
1	D	732	ALA	9.1
1	B	731	PRO	8.8

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 monosaccharides 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(\AA^2)	Q<0.9
5	DMS	C	8503	4/4	0.79	0.22	46,82,100,100	0
5	DMS	C	8705	4/4	0.80	0.19	35,45,50,100	0
3	NA	D	3104	1/1	0.83	0.11	36,36,36,36	0
2	MG	A	3003	1/1	0.84	0.19	61,61,61,61	0
2	MG	B	3003	1/1	0.85	0.26	48,48,48,48	0
5	DMS	B	8417	4/4	0.88	0.13	30,33,36,69	0
5	DMS	D	8417	4/4	0.88	0.18	26,41,80,100	0
4	145	C	2002	21/21	0.89	0.12	24,34,43,47	0
5	DMS	B	8415	4/4	0.89	0.12	30,34,37,73	0
4	145	A	2002	21/21	0.90	0.13	20,30,41,43	0
5	DMS	B	8416	4/4	0.90	0.19	46,55,71,100	0
5	DMS	B	8407	4/4	0.90	0.14	27,39,40,47	0
5	DMS	A	8421	4/4	0.91	0.16	51,60,61,74	0
5	DMS	C	8415	4/4	0.91	0.14	26,32,41,61	0
5	DMS	D	8407	4/4	0.91	0.12	26,50,53,55	0
5	DMS	C	8419	4/4	0.91	0.12	35,37,40,57	0
5	DMS	D	8703	4/4	0.91	0.15	32,38,49,53	0
4	145	B	2002	21/21	0.92	0.13	23,31,41,50	0
4	145	D	2002	21/21	0.92	0.14	23,35,50,55	0
5	DMS	D	8420	4/4	0.92	0.13	27,51,77,94	0
5	DMS	A	8407	4/4	0.92	0.13	25,38,39,47	0
5	DMS	C	8423	4/4	0.93	0.11	38,42,44,58	0
5	DMS	A	8503	4/4	0.93	0.17	31,100,100,100	0
5	DMS	A	8602	4/4	0.93	0.19	54,58,100,100	0
5	DMS	B	8419	4/4	0.93	0.17	33,56,58,66	0
5	DMS	B	8504	4/4	0.93	0.10	35,35,69,100	0
5	DMS	A	8423	4/4	0.93	0.19	36,59,67,100	0
5	DMS	D	8503	4/4	0.93	0.18	31,76,100,100	0
5	DMS	A	8501	4/4	0.93	0.12	20,28,34,38	0
5	DMS	D	8705	4/4	0.93	0.15	26,36,43,45	0
5	DMS	A	8414	4/4	0.94	0.14	27,38,66,100	0
5	DMS	A	8415	4/4	0.94	0.15	24,63,100,100	0
5	DMS	C	8425	4/4	0.94	0.14	42,44,49,71	0
5	DMS	A	8417	4/4	0.94	0.20	25,30,33,100	0
5	DMS	B	8420	4/4	0.94	0.11	39,42,46,52	0
5	DMS	B	8423	4/4	0.94	0.12	37,56,72,72	0
5	DMS	B	8425	4/4	0.94	0.13	29,35,36,43	0
5	DMS	A	8406	4/4	0.94	0.18	16,52,70,78	0
5	DMS	D	8425	4/4	0.94	0.19	22,24,28,56	4
5	DMS	D	8501	4/4	0.94	0.09	25,31,36,46	0
5	DMS	C	8409	4/4	0.94	0.13	29,40,45,47	0
2	MG	C	3006	1/1	0.94	0.14	41,41,41,41	0
5	DMS	C	8416	4/4	0.94	0.23	64,66,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	C	8602	4/4	0.95	0.12	43,49,52,100	0
5	DMS	C	8407	4/4	0.95	0.12	30,39,40,50	0
5	DMS	D	8404	4/4	0.95	0.11	21,31,44,100	0
4	145	A	2001	21/21	0.95	0.10	14,17,45,95	0
5	DMS	D	8416	4/4	0.95	0.25	34,35,54,77	0
5	DMS	A	8413	4/4	0.95	0.14	33,35,42,51	0
5	DMS	B	8413	4/4	0.95	0.15	47,48,50,100	0
5	DMS	C	8417	4/4	0.95	0.12	23,35,47,52	0
5	DMS	B	8414	4/4	0.95	0.14	22,49,74,100	0
5	DMS	A	8502	4/4	0.95	0.12	29,30,54,72	0
5	DMS	D	8508	4/4	0.95	0.10	34,39,44,51	0
2	MG	A	3005	1/1	0.95	0.06	31,31,31,31	0
5	DMS	B	8508	4/4	0.95	0.13	29,49,50,57	0
5	DMS	B	8502	4/4	0.96	0.09	30,31,44,100	0
5	DMS	C	8504	4/4	0.96	0.09	47,50,51,69	0
2	MG	D	3005	1/1	0.96	0.08	27,27,27,27	0
5	DMS	A	8425	4/4	0.96	0.09	28,32,41,42	0
4	145	C	2001	21/21	0.96	0.08	13,17,38,55	0
5	DMS	A	8416	4/4	0.96	0.23	24,53,80,100	0
5	DMS	D	8415	4/4	0.96	0.11	25,49,64,100	0
5	DMS	C	8413	4/4	0.96	0.14	32,33,45,45	0
4	145	B	2001	21/21	0.96	0.09	11,15,38,47	0
5	DMS	A	8504	4/4	0.96	0.10	21,36,41,87	0
5	DMS	D	8423	4/4	0.96	0.10	31,39,55,58	0
5	DMS	A	8420	4/4	0.96	0.10	37,44,52,62	0
5	DMS	B	8421	4/4	0.96	0.10	32,43,53,100	0
5	DMS	C	8420	4/4	0.96	0.10	40,41,57,100	0
4	145	D	2001	21/21	0.96	0.08	12,19,47,57	0
5	DMS	B	8410	4/4	0.96	0.12	29,42,60,100	0
5	DMS	C	8501	4/4	0.96	0.09	18,28,36,48	0
5	DMS	C	8601	4/4	0.97	0.10	37,38,41,43	0
3	NA	B	3104	1/1	0.97	0.09	32,32,32,32	0
5	DMS	C	8408	4/4	0.97	0.09	25,41,48,100	0
3	NA	C	3103	1/1	0.97	0.05	26,26,26,26	0
5	DMS	D	8406	4/4	0.97	0.11	26,27,31,35	0
5	DMS	C	8410	4/4	0.97	0.13	24,34,37,39	0
5	DMS	D	8409	4/4	0.97	0.12	29,37,43,100	0
5	DMS	D	8413	4/4	0.97	0.12	31,33,40,55	0
3	NA	C	3104	1/1	0.97	0.14	30,30,30,30	0
5	DMS	A	8404	4/4	0.97	0.08	22,27,36,40	0
3	NA	D	3103	1/1	0.97	0.06	26,26,26,26	0
5	DMS	D	8419	4/4	0.97	0.10	34,36,55,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	A	8419	4/4	0.97	0.11	36,44,49,52	0
5	DMS	D	8421	4/4	0.97	0.13	32,54,78,100	0
5	DMS	B	8404	4/4	0.97	0.07	20,21,36,39	0
2	MG	C	3105	1/1	0.97	0.10	26,26,26,26	0
5	DMS	B	8408	4/4	0.97	0.10	31,36,40,100	0
5	DMS	B	8409	4/4	0.97	0.11	25,34,44,45	0
5	DMS	A	8409	4/4	0.97	0.12	30,41,46,100	0
5	DMS	A	8410	4/4	0.97	0.12	28,36,39,52	0
5	DMS	B	8601	4/4	0.97	0.10	33,35,37,42	0
5	DMS	D	8414	4/4	0.98	0.15	26,44,58,100	0
5	DMS	C	8411	4/4	0.98	0.11	24,28,30,35	0
5	DMS	B	8402	4/4	0.98	0.07	16,21,22,23	0
5	DMS	C	8414	4/4	0.98	0.10	26,35,50,100	0
3	NA	A	3104	1/1	0.98	0.09	25,25,25,25	0
5	DMS	C	8404	4/4	0.98	0.06	21,24,28,31	0
5	DMS	C	8405	4/4	0.98	0.08	27,31,31,32	0
5	DMS	D	8402	4/4	0.98	0.09	18,23,24,26	0
3	NA	B	3101	1/1	0.98	0.06	16,16,16,16	0
5	DMS	A	8408	4/4	0.98	0.07	22,35,39,47	0
5	DMS	C	8421	4/4	0.98	0.09	37,49,62,63	0
5	DMS	D	8408	4/4	0.98	0.08	17,31,35,38	0
2	MG	A	3105	1/1	0.98	0.12	31,31,31,31	0
2	MG	D	3105	1/1	0.98	0.09	31,31,31,31	0
2	MG	D	3001	1/1	0.99	0.04	15,15,15,15	0
2	MG	D	3002	1/1	0.99	0.05	17,17,17,17	0
2	MG	B	3002	1/1	0.99	0.05	17,17,17,17	0
2	MG	A	3002	1/1	0.99	0.04	17,17,17,17	0
3	NA	A	3101	1/1	0.99	0.06	17,17,17,17	0
3	NA	A	3102	1/1	0.99	0.05	15,15,15,15	0
3	NA	A	3103	1/1	0.99	0.07	25,25,25,25	0
2	MG	B	3105	1/1	0.99	0.08	27,27,27,27	0
2	MG	C	3001	1/1	0.99	0.05	15,15,15,15	0
3	NA	B	3102	1/1	0.99	0.04	16,16,16,16	0
5	DMS	D	8403	4/4	0.99	0.08	18,25,25,27	0
5	DMS	A	8401	4/4	0.99	0.08	12,14,16,18	0
5	DMS	D	8405	4/4	0.99	0.08	24,25,25,30	0
5	DMS	A	8402	4/4	0.99	0.07	16,17,22,28	0
5	DMS	A	8403	4/4	0.99	0.08	21,24,27,27	0
5	DMS	C	8402	4/4	0.99	0.06	18,22,23,28	0
5	DMS	C	8403	4/4	0.99	0.12	23,24,25,27	0
5	DMS	D	8410	4/4	0.99	0.10	25,34,43,53	0
5	DMS	D	8411	4/4	0.99	0.04	23,25,28,59	0

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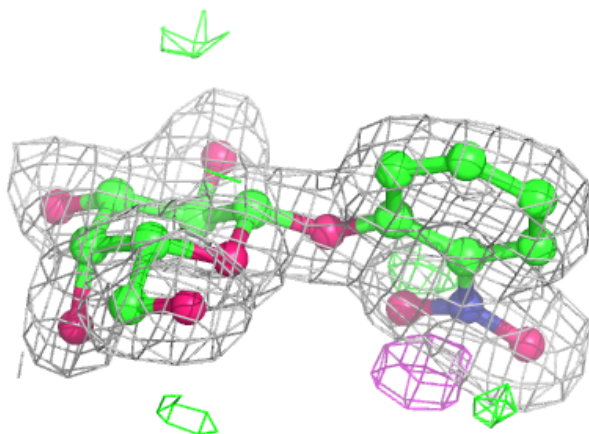
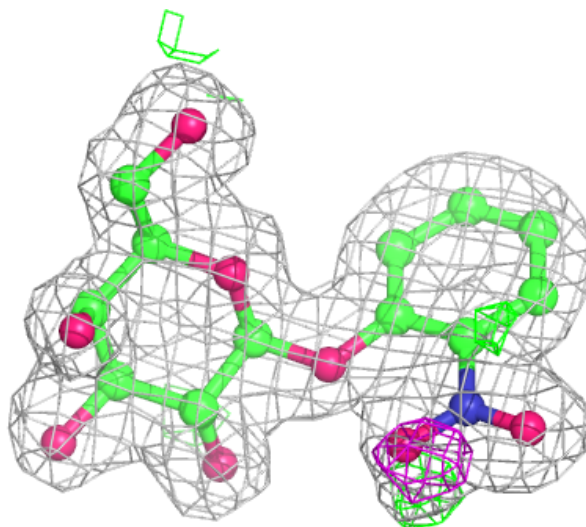
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	DMS	D	8412	4/4	0.99	0.08	26,28,31,100	0
3	NA	B	3103	1/1	0.99	0.04	25,25,25,25	0
5	DMS	A	8405	4/4	0.99	0.09	20,24,25,27	0
5	DMS	B	8401	4/4	0.99	0.08	15,17,17,20	0
2	MG	C	3002	1/1	0.99	0.05	15,15,15,15	0
5	DMS	B	8403	4/4	0.99	0.07	16,21,26,26	0
3	NA	C	3102	1/1	0.99	0.04	17,17,17,17	0
5	DMS	B	8405	4/4	0.99	0.09	23,28,29,31	0
5	DMS	C	8412	4/4	0.99	0.09	26,33,44,100	0
2	MG	A	3001	1/1	0.99	0.04	17,17,17,17	0
2	MG	B	3001	1/1	0.99	0.04	15,15,15,15	0
3	NA	D	3101	1/1	0.99	0.04	16,16,16,16	0
5	DMS	A	8411	4/4	0.99	0.07	23,24,28,31	0
5	DMS	B	8411	4/4	0.99	0.06	26,27,31,100	0
5	DMS	D	8701	4/4	0.99	0.08	15,16,20,38	0
5	DMS	B	8412	4/4	0.99	0.09	27,33,35,37	0
5	DMS	A	8412	4/4	0.99	0.12	34,34,37,60	0
5	DMS	D	8401	4/4	1.00	0.05	15,16,18,19	0
5	DMS	C	8401	4/4	1.00	0.07	15,17,21,23	0
3	NA	C	3101	1/1	1.00	0.03	15,15,15,15	0
3	NA	D	3102	1/1	1.00	0.05	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.

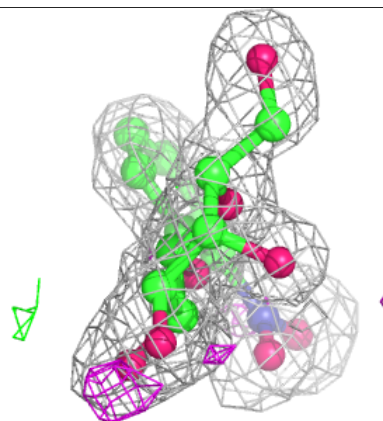
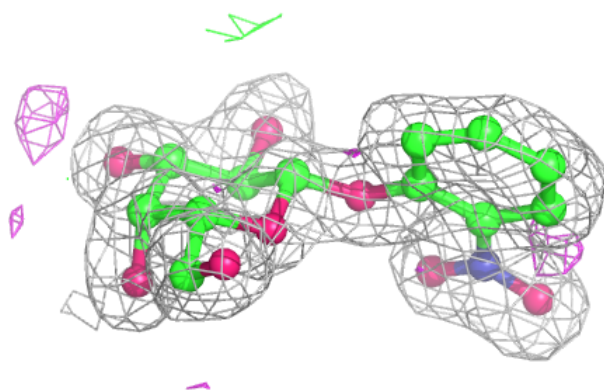
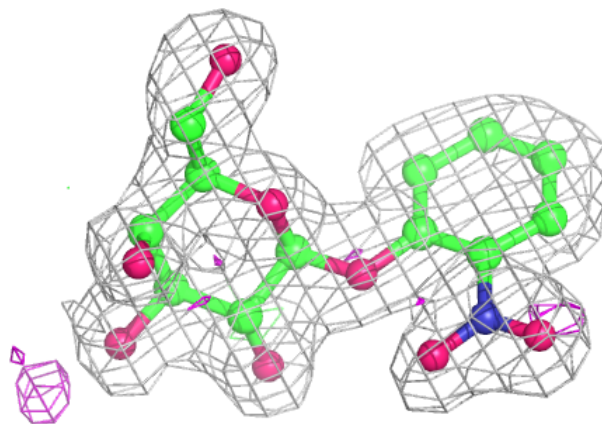
Electron density around 145 C 2002:

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



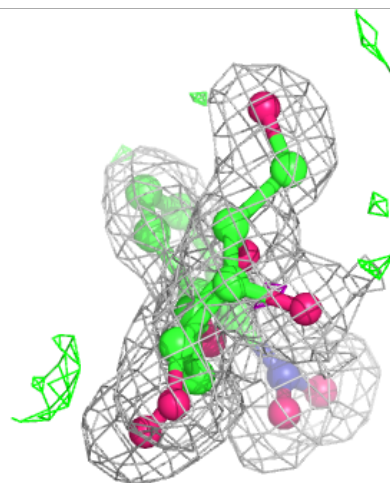
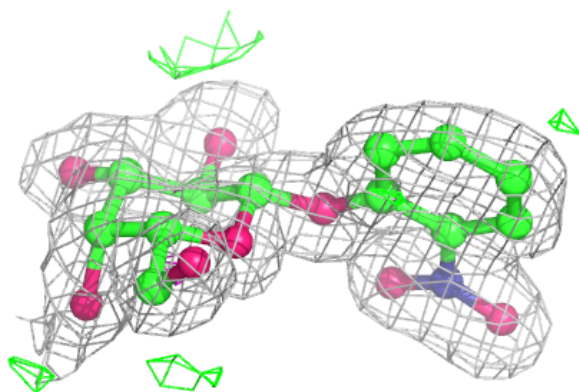
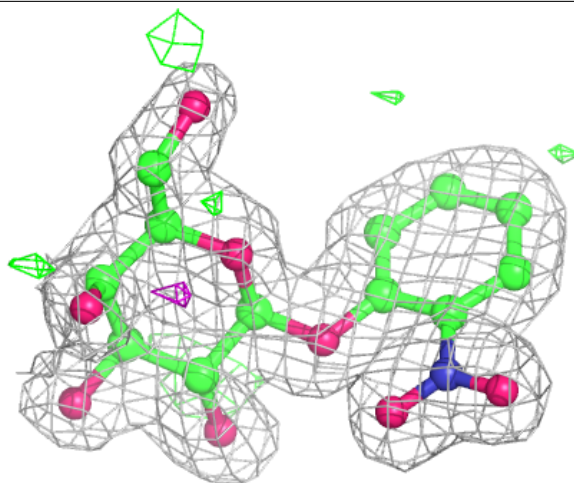
Electron density around 145 Å 2002:

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



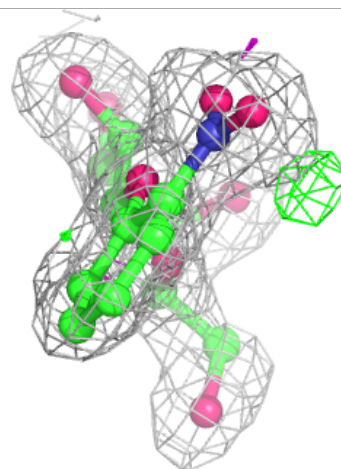
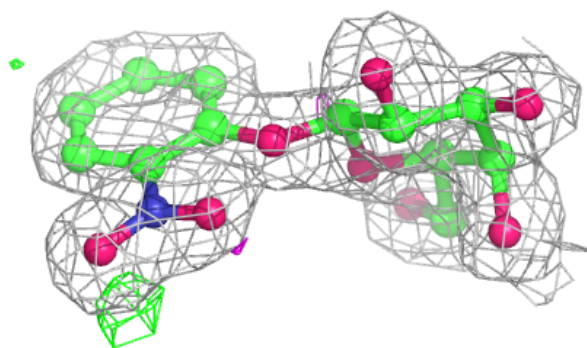
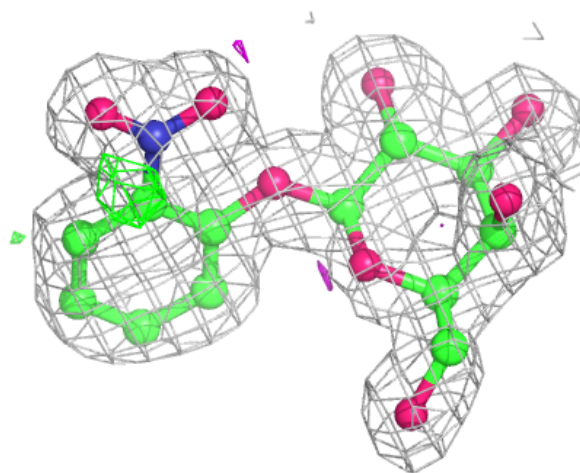
Electron density around 145 B 2002:

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



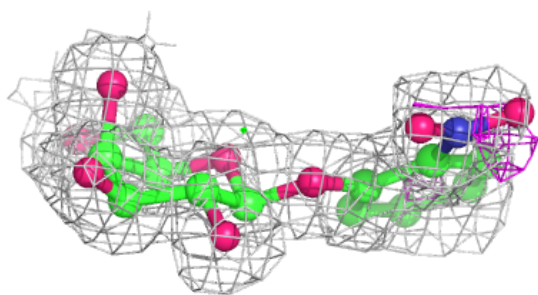
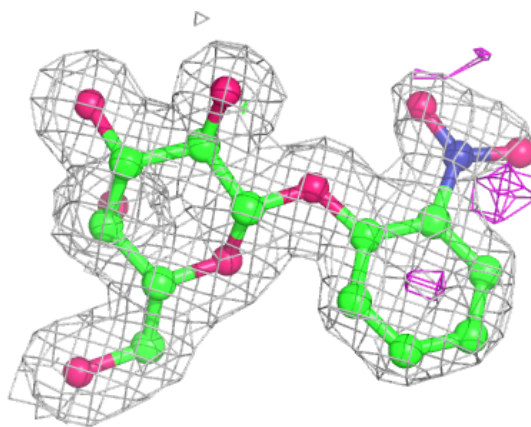
Electron density around 145 D 2002:

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



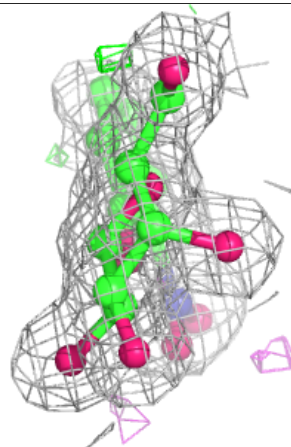
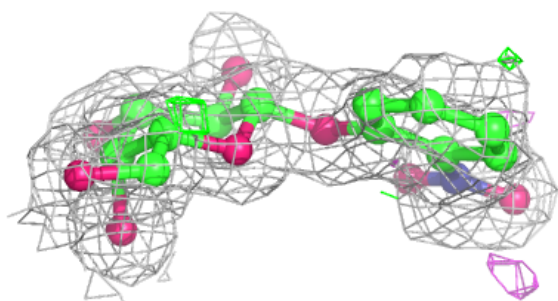
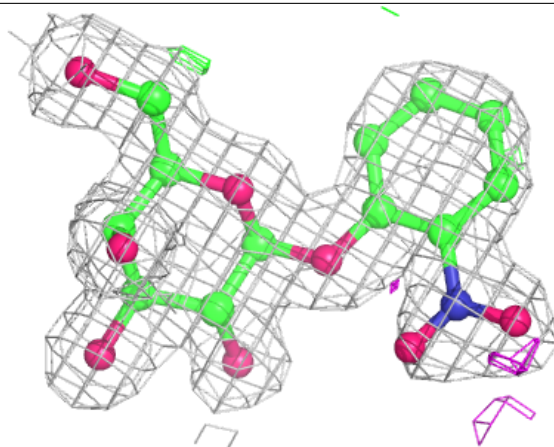
Electron density around 145 Å 2001:

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



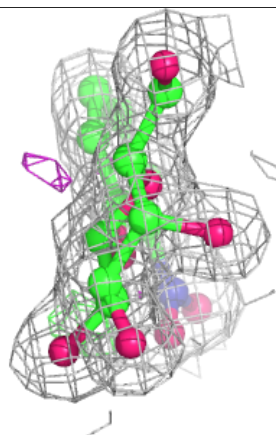
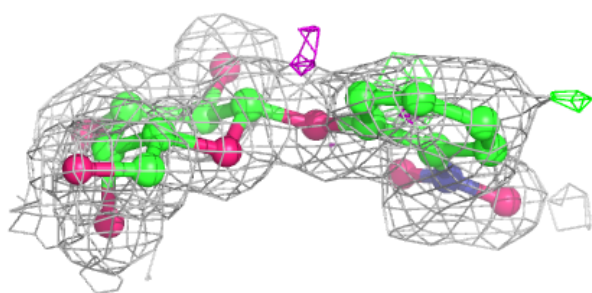
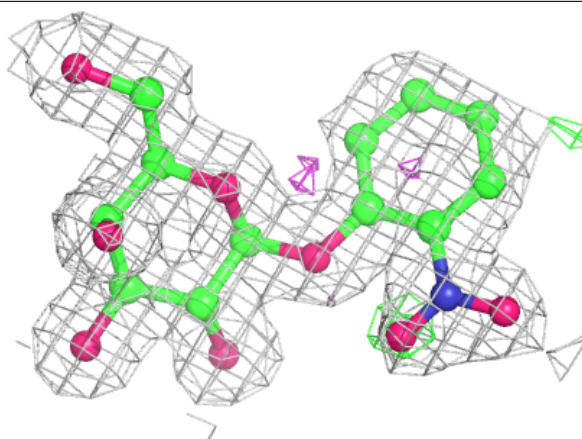
Electron density around 145 C 2001:

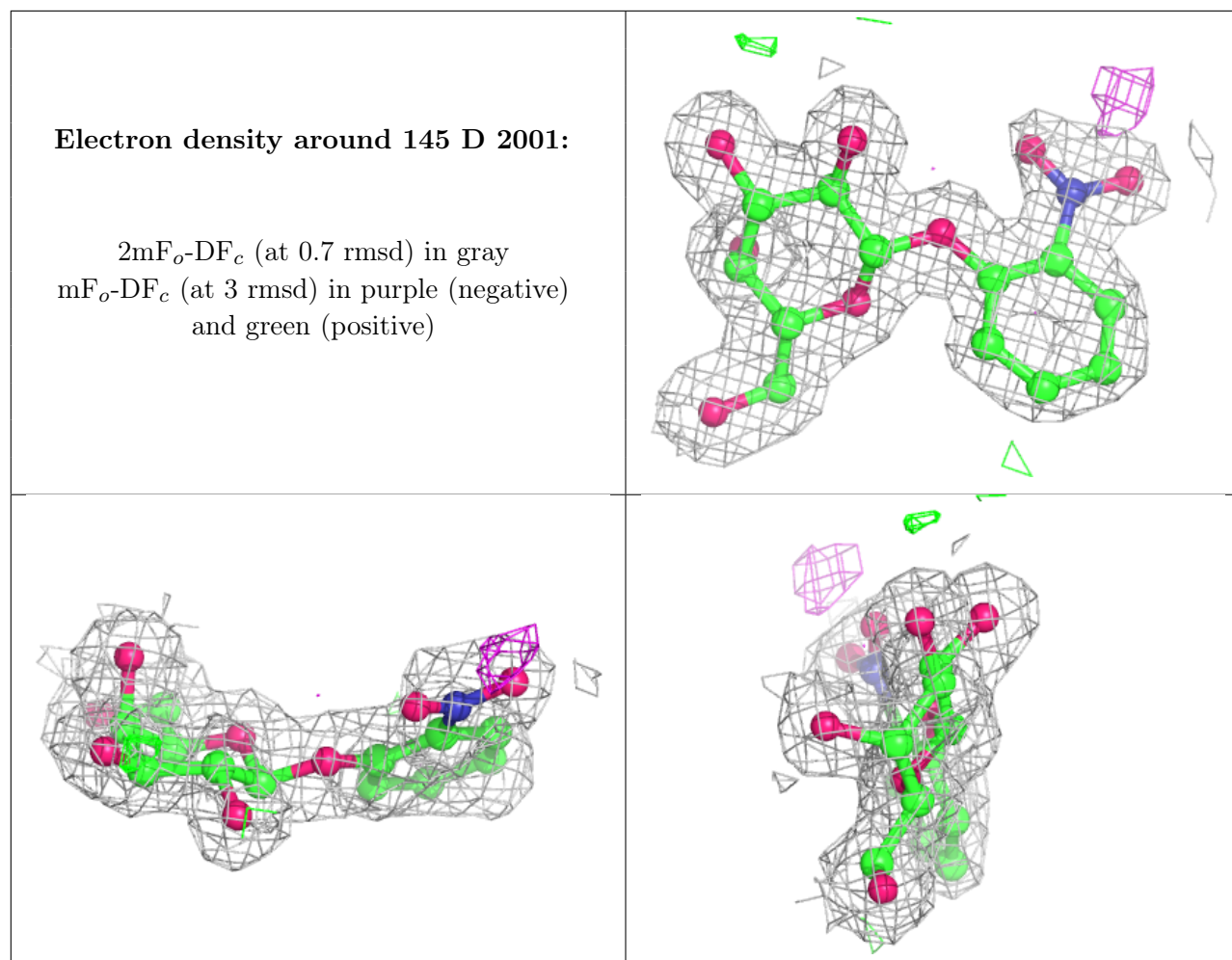
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 145 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.