



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 01:42 pm GMT

PDB ID : 5LZI  
Title : Porcine heat-labile enterotoxin R13H in complex with inhibitor MM146  
Authors : Heggelund, J.E.; Mackenzie, A.; Kregel, U.  
Deposited on : 2016-09-29  
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

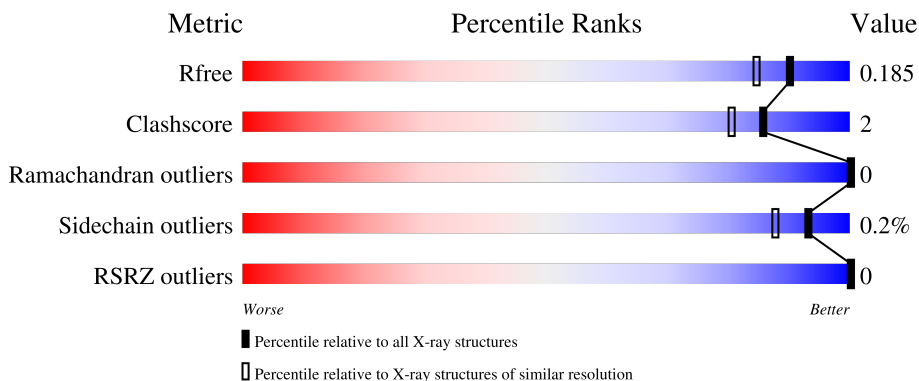
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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  $\geq 3$ , 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	103	91% (green), 8% (yellow), 1% (orange), 0% (red), 0% (grey)
1	B	103	91% (green), 9% (yellow), 0% (orange), 0% (red), 0% (grey)
1	C	103	88% (green), 12% (yellow), 0% (orange), 0% (red), 0% (grey)
1	D	103	96% (green), 4% (yellow), 0% (orange), 0% (red), 0% (grey)
1	E	103	95% (green), 5% (yellow), 0% (orange), 0% (red), 0% (grey)

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5453 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.

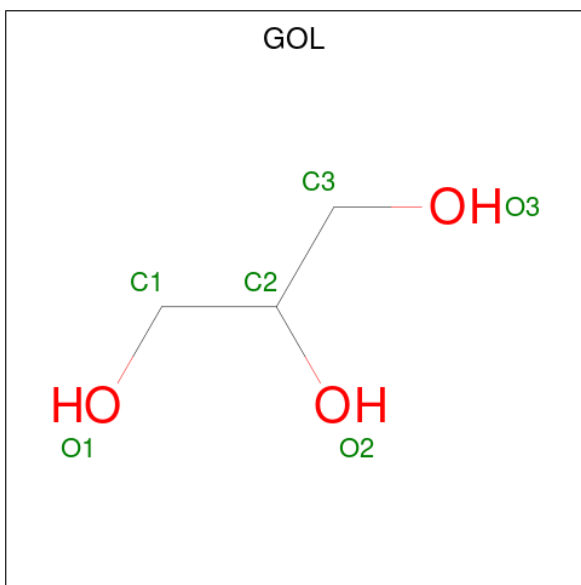
- Molecule 1 is a protein called Heat-labile enterotoxin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	103	867	542	145	174	6	0	5	0
1	B	103	870	549	144	170	7	0	6	0
1	C	103	857	540	141	169	7	0	5	0
1	D	103	845	530	141	167	7	0	3	0
1	E	103	840	526	140	167	7	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

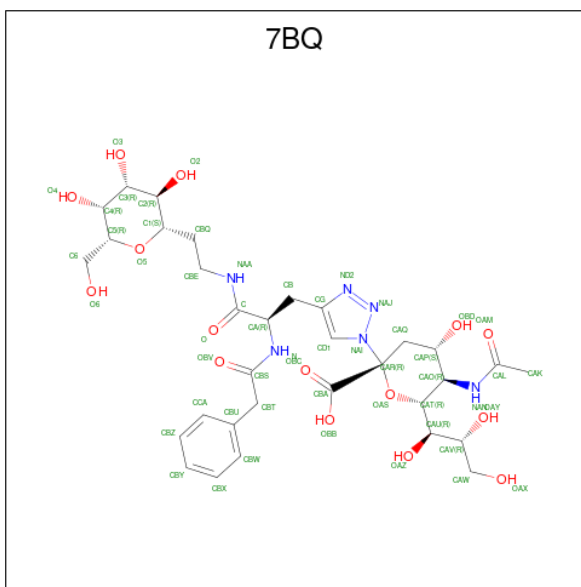
Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	ARG	engineered mutation	UNP P32890
B	13	HIS	ARG	engineered mutation	UNP P32890
C	13	HIS	ARG	engineered mutation	UNP P32890
D	13	HIS	ARG	engineered mutation	UNP P32890
E	13	HIS	ARG	engineered mutation	UNP P32890

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



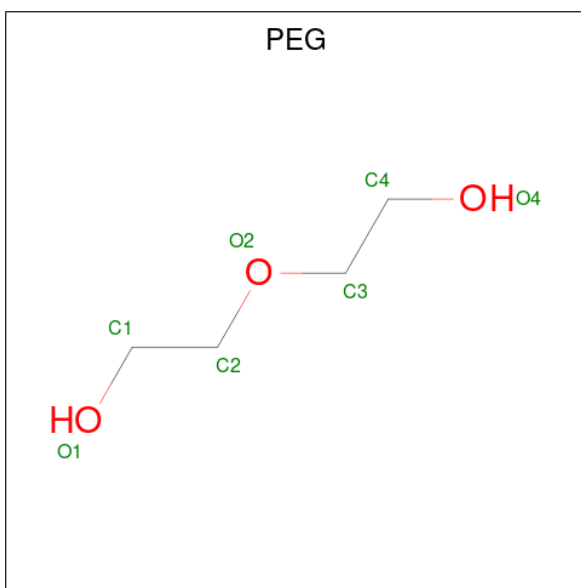
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is (2 {R},4 {S},5 {R},6 {R})-5-acetamido-2-[4-[(2 {R})-3-[2-[(2 {S},3 {R},4 {R},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]ethylamino]-3-oxidanylidene-2-(2-phenylethanoylamino)propyl]-1,2,3-triazol-1-yl]-4-oxidanyl-6-[(1 {R},2 {R})-1,2,3-tris(oxidanyl)propyl]oxane-2-carboxylic acid (three-letter code: 7BQ) (formula: C<sub>32</sub>H<sub>46</sub>N<sub>6</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
3	A	1	106	64	12	30	0	1

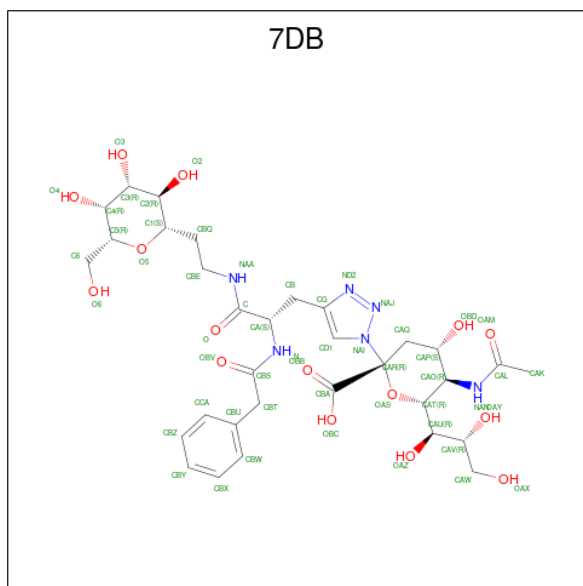
- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0

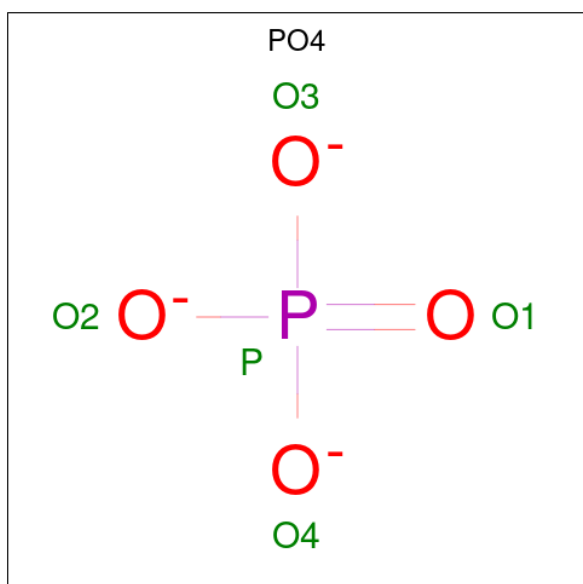
- Molecule 5 is (2 {R},4 {S},5 {R},6 {R})-5-acetamido-2-[4-[(2 {S})-3-[2-[(2 {S},3 {R},4 {R}),5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]ethylamino]-3-oxidanylidene-2-(2-phenylethanoylamino)propyl]-1,2,3-triazol-1-yl]-4-oxidanyl-6-[(1 {R},2 {R})-1,2,3-tris(

oxidanyl)propyl]oxane-2-carboxylic acid (three-letter code: 7DB) (formula: C<sub>32</sub>H<sub>46</sub>N<sub>6</sub>O<sub>15</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
5	B	1	Total	C	N	O	0	0
			53	32	6	15		
5	C	1	Total	C	N	O	0	0
			53	32	6	15		
5	D	1	Total	C	N	O	0	0
			53	32	6	15		
5	E	1	Total	C	N	O	0	0
			53	32	6	15		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is water.

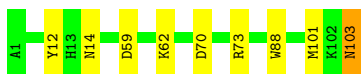
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	157	Total	O	0	0
			157	157		
7	B	144	Total	O	0	0
			144	144		
7	C	167	Total	O	0	0
			167	167		
7	D	174	Total	O	0	2
			176	176		
7	E	168	Total	O	0	2
			170	170		

### 3 Residue-property plots [i](#)


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

- Molecule 1: Heat-labile enterotoxin B chain

Chain A:  91% 8%




- Molecule 1: Heat-labile enterotoxin B chain

Chain B:  91% 9%



- Molecule 1: Heat-labile enterotoxin B chain

Chain C:  88% 12%



- Molecule 1: Heat-labile enterotoxin B chain

Chain D:  96%



- Molecule 1: Heat-labile enterotoxin B chain

Chain E:  95% 5%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.17Å 75.87Å 125.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.20 – 1.60 29.16 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.20-1.60) 92.7 (29.16-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.24 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0155, REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.147 , 0.176 0.161 , 0.185	Depositor DCC
$R_{free}$ test set	3766 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtrriage
Anisotropy	0.351	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5453	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 7DB, PO4, GOL, 7BQ, PEG

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	1.05	0/879	1.06	4/1182 (0.3%)
1	B	1.09	3/885 (0.3%)	1.06	3/1191 (0.3%)
1	C	1.01	1/875 (0.1%)	1.07	2/1180 (0.2%)
1	D	1.11	2/860 (0.2%)	1.04	2/1157 (0.2%)
1	E	1.06	2/852 (0.2%)	1.04	2/1147 (0.2%)
All	All	1.06	8/4351 (0.2%)	1.05	13/5857 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	79	GLU	CD-OE2	-7.62	1.17	1.25
1	E	44	SER	CB-OG	6.05	1.50	1.42
1	E	79	GLU	CD-OE1	-5.81	1.19	1.25
1	B	46	GLU	CD-OE1	5.76	1.31	1.25
1	C	11	GLU	CD-OE1	-5.70	1.19	1.25
1	B	79	GLU	CD-OE1	-5.65	1.19	1.25
1	D	11	GLU	CD-OE1	-5.36	1.19	1.25
1	B	79	GLU	CD-OE2	-5.07	1.20	1.25

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	MET	CG-SD-CE	-9.28	85.35	100.20
1	A	59	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	C	35	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	70	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	73	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	E	101[A]	MET	CG-SD-CE	5.97	109.75	100.20
1	E	101[B]	MET	CG-SD-CE	5.97	109.75	100.20
1	C	34	LYS	CD-CE-NZ	5.71	124.84	111.70

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	79	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	A	70	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	59	ASP	CB-CG-OD1	5.14	122.93	118.30
1	B	59	ASP	CB-CG-OD2	-5.03	113.77	118.30

There are no chirality outliers.

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	867	0	872	4	0
1	B	870	0	891	3	0
1	C	857	0	877	12	0
1	D	845	0	859	1	0
1	E	840	0	848	2	0
2	A	6	0	8	0	0
2	B	12	0	16	0	0
2	C	6	0	7	0	0
2	D	6	0	8	0	0
3	A	106	0	0	0	0
4	A	7	0	10	0	0
5	B	53	0	0	0	0
5	C	53	0	0	0	0
5	D	53	0	0	0	0
5	E	53	0	0	0	0
6	C	5	0	0	0	0
7	A	157	0	0	1	1
7	B	144	0	0	1	0
7	C	167	0	0	1	0
7	D	176	0	0	0	1
7	E	170	0	0	1	0
All	All	5453	0	4396	20	1

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 2.

All (20) 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:C:85[B]:LEU:CD2	1:C:99[B]:ILE:HG22	1.60	1.31
1:C:85[B]:LEU:HD23	1:C:99[B]:ILE:HG22	1.07	1.06
1:C:85[B]:LEU:CD2	1:C:99[B]:ILE:CG2	2.50	0.86
1:C:7:GLU:OE1	7:C:301:HOH:O	2.01	0.77
1:C:85[B]:LEU:HD23	1:C:99[B]:ILE:CG2	2.03	0.76
1:C:85[B]:LEU:HD21	1:C:99[B]:ILE:HG22	1.74	0.58
1:A:103:ASN:O	1:A:103:ASN:ND2	2.34	0.56
1:C:71:THR:HG21	1:C:99[B]:ILE:HD11	1.95	0.49
1:C:85[B]:LEU:HD21	1:C:99[B]:ILE:CG2	2.39	0.47
1:C:82:ILE:HA	1:C:101[A]:MET:HG2	1.96	0.47
1:B:82:ILE:CD1	1:B:99[A]:ILE:HD11	2.45	0.46
1:D:12:TYR:CZ	1:E:32:ALA:HB1	2.51	0.45
1:A:12:TYR:CZ	1:B:32:ALA:HB1	2.52	0.45
1:E:46[A]:GLU:OE1	7:E:301:HOH:O	2.20	0.45
1:A:14:ASN:O	1:A:88:TRP:HA	2.17	0.44
7:B:362:HOH:O	1:C:23:LYS:HE2	2.17	0.44
1:B:20:ILE:HG13	1:B:85[B]:LEU:CD1	2.49	0.43
1:A:62[B]:LYS:HD2	7:A:397:HOH:O	2.19	0.41
1:C:22:ASP:OD2	1:C:43:LYS:HE2	2.20	0.41
1:C:99[A]:ILE:HD13	1:C:99[A]:ILE:HG21	1.78	0.40

All (1) 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)
7:A:428:HOH:O	7:D:441:HOH:O[1_655]	2.12	0.08

## 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	106/103 (103%)	104 (98%)	2 (2%)	0	100	100
1	B	107/103 (104%)	106 (99%)	1 (1%)	0	100	100
1	C	106/103 (103%)	105 (99%)	1 (1%)	0	100	100
1	D	104/103 (101%)	102 (98%)	2 (2%)	0	100	100
1	E	103/103 (100%)	101 (98%)	2 (2%)	0	100	100
All	All	526/515 (102%)	518 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	100/95 (105%)	99 (99%)	1 (1%)	76	61
1	B	101/95 (106%)	101 (100%)	0	100	100
1	C	100/95 (105%)	100 (100%)	0	100	100
1	D	98/95 (103%)	98 (100%)	0	100	100
1	E	97/95 (102%)	97 (100%)	0	100	100
All	All	496/475 (104%)	495 (100%)	1 (0%)	93	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	D	201	-	5,5,5	0.50	0	5,5,5	1.48	1 (20%)
3	7BQ	A	202[B]	-	54,56,56	1.63	9 (16%)	64,80,80	1.65	10 (15%)
2	GOL	C	201	-	5,5,5	0.87	0	5,5,5	1.51	2 (40%)
4	PEG	A	203	-	6,6,6	0.69	0	5,5,5	0.84	0
5	7DB	E	201	-	54,56,56	1.55	10 (18%)	64,80,80	1.55	13 (20%)
5	7DB	C	202	-	54,56,56	1.84	10 (18%)	64,80,80	1.58	8 (12%)
5	7DB	D	202	-	54,56,56	1.65	9 (16%)	64,80,80	1.40	9 (14%)
2	GOL	B	202	-	5,5,5	0.66	0	5,5,5	1.50	1 (20%)
6	PO4	C	203	-	4,4,4	1.69	2 (50%)	6,6,6	1.43	1 (16%)
2	GOL	A	201	-	5,5,5	0.82	0	5,5,5	0.86	0
3	7BQ	A	202[A]	-	54,56,56	1.73	8 (14%)	64,80,80	1.63	17 (26%)
5	7DB	B	203	-	54,56,56	2.28	12 (22%)	64,80,80	1.49	9 (14%)
2	GOL	B	201	-	5,5,5	0.80	0	5,5,5	1.14	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	201	-	-	2/4/4/4	-
3	7BQ	A	202[B]	-	-	1/39/88/88	0/4/4/4
2	GOL	C	201	-	-	0/4/4/4	-
4	PEG	A	203	-	-	3/4/4/4	-
5	7DB	E	201	-	-	4/39/88/88	0/4/4/4
5	7DB	C	202	-	-	6/39/88/88	0/4/4/4
5	7DB	D	202	-	-	3/39/88/88	0/4/4/4
2	GOL	B	202	-	-	3/4/4/4	-
2	GOL	A	201	-	-	2/4/4/4	-
3	7BQ	A	202[A]	-	-	8/39/88/88	0/4/4/4
5	7DB	B	203	-	-	0/39/88/88	0/4/4/4
2	GOL	B	201	-	-	0/4/4/4	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	203	7DB	CAP-CAO	-9.34	1.45	1.53
3	A	202[A]	7BQ	CAP-CAO	-6.47	1.47	1.53
3	A	202[B]	7BQ	CBT-CBU	-6.38	1.41	1.51
5	C	202	7DB	CAP-CAO	-6.34	1.47	1.53
3	A	202[A]	7BQ	CBT-CBU	-6.18	1.41	1.51
5	B	203	7DB	CD1-NAI	-6.09	1.29	1.35
5	B	203	7DB	CAR-NAI	-6.04	1.44	1.50
5	C	202	7DB	CAR-CBA	-5.92	1.46	1.55
5	B	203	7DB	CBT-CBU	-5.41	1.42	1.51
5	D	202	7DB	CBT-CBU	-5.09	1.43	1.51
5	D	202	7DB	CAR-NAI	-4.21	1.46	1.50
5	E	201	7DB	CBT-CBU	-4.20	1.44	1.51
5	D	202	7DB	CD1-NAI	-4.13	1.31	1.35
5	C	202	7DB	CAV-CAU	4.11	1.61	1.53
3	A	202[B]	7BQ	CAO-NAN	4.09	1.52	1.45
3	A	202[B]	7BQ	CAR-CBA	-3.98	1.49	1.55
5	E	201	7DB	CAP-CAO	3.73	1.56	1.53
5	C	202	7DB	CD1-CG	-3.45	1.31	1.36
5	D	202	7DB	ND2-NAJ	-3.36	1.28	1.34
5	E	201	7DB	C-NAA	-3.35	1.26	1.33
5	D	202	7DB	CAP-CAO	-3.23	1.50	1.53
3	A	202[A]	7BQ	CB-CA	-3.17	1.46	1.54
5	B	203	7DB	OBD-CAP	3.16	1.50	1.43
3	A	202[B]	7BQ	CBE-NAA	3.16	1.53	1.46
3	A	202[B]	7BQ	CD1-NAI	-3.15	1.32	1.35

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	203	7DB	CAK-CAL	3.10	1.57	1.50
5	C	202	7DB	C3-C4	3.09	1.60	1.52
3	A	202[B]	7BQ	O3-C3	2.87	1.49	1.43
3	A	202[A]	7BQ	CAR-NAI	2.81	1.53	1.50
5	C	202	7DB	O2-C2	2.78	1.49	1.43
5	C	202	7DB	CBT-CBU	-2.72	1.47	1.51
3	A	202[A]	7BQ	ND2-NAJ	2.62	1.39	1.34
3	A	202[B]	7BQ	CAR-NAI	-2.55	1.47	1.50
5	C	202	7DB	CAK-CAL	2.53	1.55	1.50
5	E	201	7DB	OBD-CAP	2.52	1.48	1.43
5	B	203	7DB	OAY-CAV	2.48	1.48	1.43
5	B	203	7DB	OBC-CBA	-2.37	1.21	1.30
5	D	202	7DB	CBW-CBU	2.35	1.43	1.38
5	E	201	7DB	CB-CA	-2.33	1.48	1.54
5	D	202	7DB	C-NAA	-2.32	1.28	1.33
5	B	203	7DB	C2-C1	-2.31	1.48	1.53
5	B	203	7DB	O2-C2	2.31	1.48	1.43
3	A	202[B]	7BQ	CD1-CG	-2.30	1.32	1.36
5	C	202	7DB	O3-C3	2.30	1.48	1.43
3	A	202[A]	7BQ	CG-ND2	-2.30	1.31	1.34
5	C	202	7DB	CBS-N	2.27	1.38	1.34
5	E	201	7DB	CAO-NAN	2.26	1.49	1.45
3	A	202[A]	7BQ	CA-N	2.26	1.50	1.45
5	E	201	7DB	O2-C2	2.22	1.48	1.43
5	E	201	7DB	CA-C	2.22	1.58	1.52
6	C	203	PO4	P-O1	2.22	1.56	1.50
5	D	202	7DB	NAJ-NAI	2.15	1.38	1.34
5	B	203	7DB	CAO-NAN	2.15	1.49	1.45
5	D	202	7DB	CA-C	2.13	1.58	1.52
5	B	203	7DB	C-NAA	2.11	1.38	1.33
3	A	202[A]	7BQ	CAR-CBA	2.06	1.58	1.55
3	A	202[B]	7BQ	CA-N	2.05	1.50	1.45
6	C	203	PO4	P-O4	-2.04	1.48	1.54
5	E	201	7DB	CAK-CAL	2.03	1.54	1.50
5	E	201	7DB	C4-C5	-2.02	1.48	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202[B]	7BQ	OBC-CBA-CAR	-7.61	112.36	123.64
5	C	202	7DB	OBB-CBA-CAR	-5.58	115.37	123.64
3	A	202[B]	7BQ	OAS-CAT-CAO	-4.65	105.24	109.78

Continued on next page...



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	7DB	CAP-CAO-NAN	-4.50	101.47	110.38
5	B	203	7DB	OBB-CBA-CAR	-4.35	117.20	123.64
5	E	201	7DB	OBB-CBA-CAR	-4.18	117.44	123.64
5	D	202	7DB	OAS-CAT-CAU	-4.01	101.11	107.29
3	A	202[A]	7BQ	OBC-CBA-CAR	-3.89	117.87	123.64
5	B	203	7DB	O5-C5-C4	3.81	116.61	109.69
5	B	203	7DB	C1-O5-C5	-3.77	106.57	113.16
5	D	202	7DB	OBB-CBA-CAR	-3.61	118.29	123.64
5	C	202	7DB	OAS-CAT-CAO	-3.49	106.37	109.78
5	E	201	7DB	CBQ-C1-C2	-3.45	108.48	114.02
5	B	203	7DB	CBU-CBT-CBS	-3.35	102.64	112.57
5	B	203	7DB	O2-C2-C3	-3.25	102.84	110.35
5	B	203	7DB	CAQ-CAP-CAO	3.22	114.93	109.98
3	A	202[A]	7BQ	C1-O5-C5	-3.21	107.55	113.16
3	A	202[A]	7BQ	CBE-NAA-C	-3.20	116.88	122.59
3	A	202[B]	7BQ	OAX-CAW-CAV	3.14	117.92	111.07
3	A	202[A]	7BQ	CD1-NAI-NAJ	-3.12	105.93	112.31
3	A	202[A]	7BQ	CA-C-NAA	3.07	122.73	116.54
5	E	201	7DB	O2-C2-C3	-3.03	103.35	110.35
3	A	202[A]	7BQ	CAV-CAU-CAT	-3.02	107.31	113.03
5	E	201	7DB	CBU-CBT-CBS	-3.01	103.64	112.57
5	D	202	7DB	CD1-CG-ND2	-3.00	106.88	111.34
3	A	202[A]	7BQ	CA-N-CBS	2.91	129.14	121.65
5	E	201	7DB	O-C-CA	2.88	126.51	120.45
5	B	203	7DB	CBE-NAA-C	-2.81	117.57	122.59
2	D	201	GOL	O1-C1-C2	-2.75	97.03	110.20
5	D	202	7DB	CAK-CAL-NAN	-2.74	111.46	116.10
5	E	201	7DB	CB-CA-C	2.73	117.34	110.25
5	B	203	7DB	CD1-CG-ND2	-2.71	107.31	111.34
3	A	202[A]	7BQ	OAX-CAW-CAV	-2.65	105.29	111.07
6	C	203	PO4	O4-P-O3	2.64	116.43	107.97
5	E	201	7DB	OAS-CAT-CAO	-2.63	107.22	109.78
3	A	202[B]	7BQ	CD1-CG-ND2	-2.62	107.44	111.34
5	E	201	7DB	C1-O5-C5	-2.60	108.62	113.16
3	A	202[A]	7BQ	CBU-CBT-CBS	-2.59	104.89	112.57
5	D	202	7DB	CAW-CAV-CAU	-2.59	106.80	112.41
5	E	201	7DB	CA-C-NAA	-2.59	111.33	116.54
5	E	201	7DB	C2-C3-C4	-2.58	106.33	110.82
3	A	202[B]	7BQ	CBQ-C1-C2	-2.52	109.98	114.02
3	A	202[B]	7BQ	OAM-CAL-NAN	2.49	126.54	121.95
5	C	202	7DB	O4-C4-C5	2.47	115.44	109.30
2	C	201	GOL	C3-C2-C1	-2.43	102.27	111.70

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	7DB	O-C-CA	2.40	125.50	120.45
2	B	202	GOL	O3-C3-C2	-2.37	98.83	110.20
3	A	202[A]	7BQ	O-C-CA	-2.36	115.50	120.45
5	D	202	7DB	CD1-NAI-NAJ	-2.34	107.52	112.31
3	A	202[A]	7BQ	CBT-CBS-N	-2.33	112.12	115.88
5	E	201	7DB	OAS-CAT-CAU	-2.33	103.69	107.29
5	D	202	7DB	OBD-CAP-CAQ	-2.32	104.51	109.91
3	A	202[A]	7BQ	CAP-CAO-NAN	-2.29	105.84	110.38
5	D	202	7DB	CAQ-CAR-NAI	2.27	111.85	109.35
5	C	202	7DB	CD1-NAI-NAJ	-2.24	107.72	112.31
2	C	201	GOL	O2-C2-C3	2.24	118.97	109.12
3	A	202[B]	7BQ	CAT-CAO-NAN	2.21	114.58	110.91
3	A	202[A]	7BQ	OAS-CAT-CAU	-2.20	103.90	107.29
5	D	202	7DB	O5-C5-C4	2.19	113.68	109.69
2	B	201	GOL	O2-C2-C1	2.19	118.75	109.12
3	A	202[A]	7BQ	CB-CA-N	2.15	115.32	110.79
5	E	201	7DB	CB-CG-ND2	-2.14	118.91	123.57
5	E	201	7DB	CAQ-CAR-NAI	2.10	111.66	109.35
3	A	202[A]	7BQ	CBT-CBU-CCA	-2.09	117.90	120.89
3	A	202[B]	7BQ	CBU-CBT-CBS	-2.09	106.39	112.57
3	A	202[B]	7BQ	CBE-NAA-C	-2.08	118.88	122.59
5	B	203	7DB	OBV-CBS-N	-2.07	119.46	122.95
5	C	202	7DB	OBD-CAP-CAQ	-2.05	105.13	109.91
3	A	202[A]	7BQ	O5-C1-C2	-2.02	106.02	109.69
3	A	202[A]	7BQ	CD1-CG-ND2	-2.02	108.34	111.34
3	A	202[B]	7BQ	CAQ-CAR-NAI	-2.01	107.14	109.35
5	C	202	7DB	O3-C3-C4	-2.01	105.71	110.35

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GOL	C1-C2-C3-O3
2	A	201	GOL	O2-C2-C3-O3
2	B	202	GOL	C1-C2-C3-O3
2	D	201	GOL	O1-C1-C2-C3
3	A	202[A]	7BQ	CB-CA-N-CBS
2	D	201	GOL	O1-C1-C2-O2
4	A	203	PEG	O1-C1-C2-O2
4	A	203	PEG	O2-C3-C4-O4
3	A	202[A]	7BQ	CAU-CAV-CAW-OAX
2	B	202	GOL	O1-C1-C2-C3

Continued on next page...

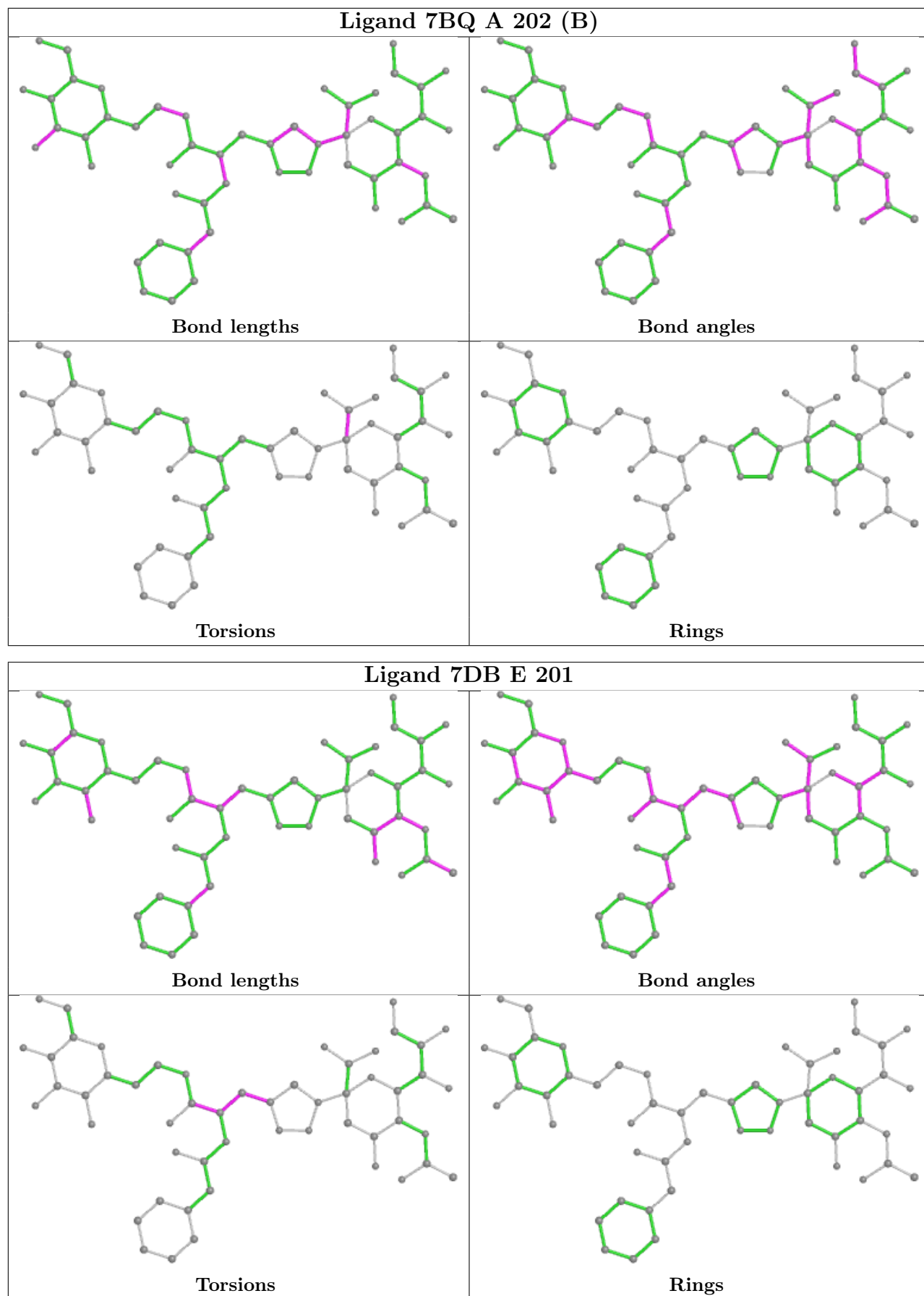
*Continued from previous page...*

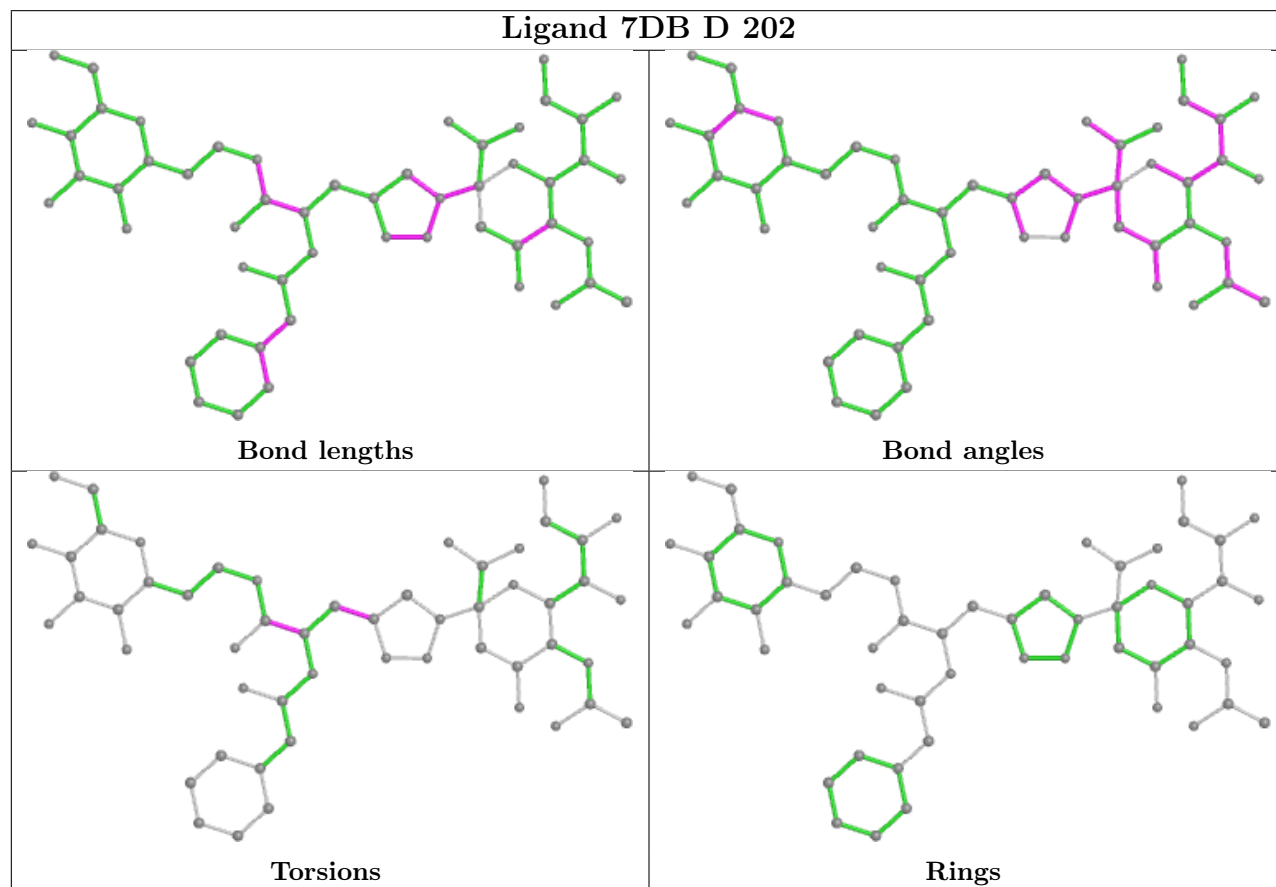
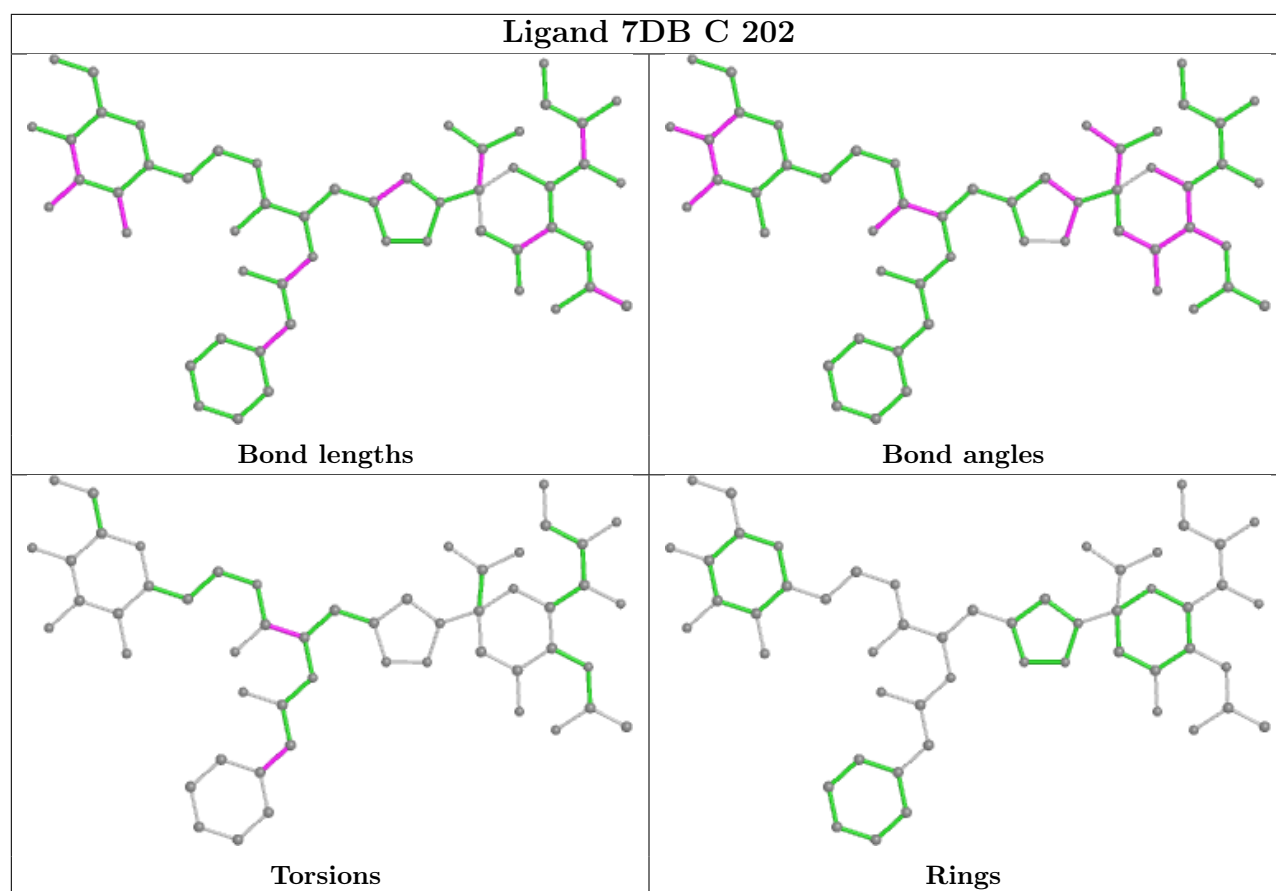
Mol	Chain	Res	Type	Atoms
3	A	202[A]	7BQ	OAY-CAV-CAW-OAX
3	A	202[A]	7BQ	NAA-C-CA-N
5	C	202	7DB	O-C-CA-N
5	D	202	7DB	O-C-CA-N
5	E	201	7DB	CA-CB-CG-CD1
5	C	202	7DB	NAA-C-CA-N
3	A	202[A]	7BQ	O-C-CA-N
3	A	202[A]	7BQ	CAQ-CAR-CBA-OBC
3	A	202[B]	7BQ	CAQ-CAR-CBA-OBC
2	B	202	GOL	O1-C1-C2-O2
5	C	202	7DB	CBS-CBT-CBU-CBW
5	E	201	7DB	C-CA-CB-CG
5	E	201	7DB	O-C-CA-N
5	C	202	7DB	CBS-CBT-CBU-CCA
3	A	202[A]	7BQ	NAA-C-CA-CB
5	D	202	7DB	CA-CB-CG-CD1
5	D	202	7DB	NAA-C-CA-N
3	A	202[A]	7BQ	O-C-CA-CB
4	A	203	PEG	C4-C3-O2-C2
5	E	201	7DB	NAA-C-CA-N
5	C	202	7DB	O-C-CA-CB
5	C	202	7DB	NAA-C-CA-CB

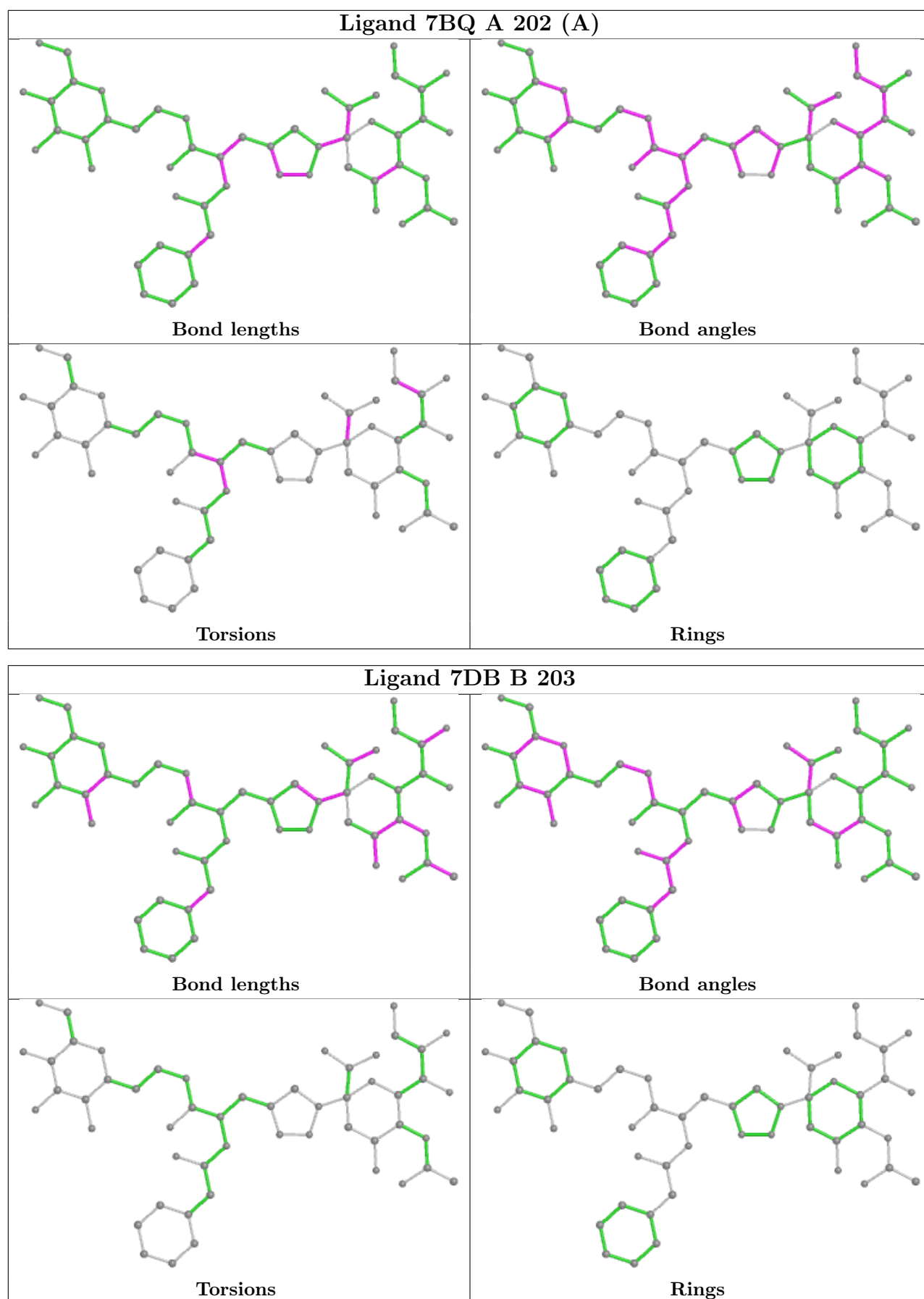
There are no ring outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	103/103 (100%)	-0.56	0 100 100	7, 13, 23, 48	0
1	B	103/103 (100%)	-0.39	0 100 100	8, 18, 29, 40	0
1	C	103/103 (100%)	-0.48	0 100 100	9, 15, 26, 35	0
1	D	103/103 (100%)	-0.37	0 100 100	9, 17, 27, 46	0
1	E	103/103 (100%)	-0.55	0 100 100	7, 14, 25, 42	0
All	All	515/515 (100%)	-0.47	0 100 100	7, 15, 28, 48	0

There are no RSRZ outliers to report.

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	A	201	6/6	0.78	0.24	39,44,52,53	0
4	PEG	A	203	7/7	0.79	0.19	35,37,46,56	0
2	GOL	B	201	6/6	0.88	0.19	19,29,39,42	0

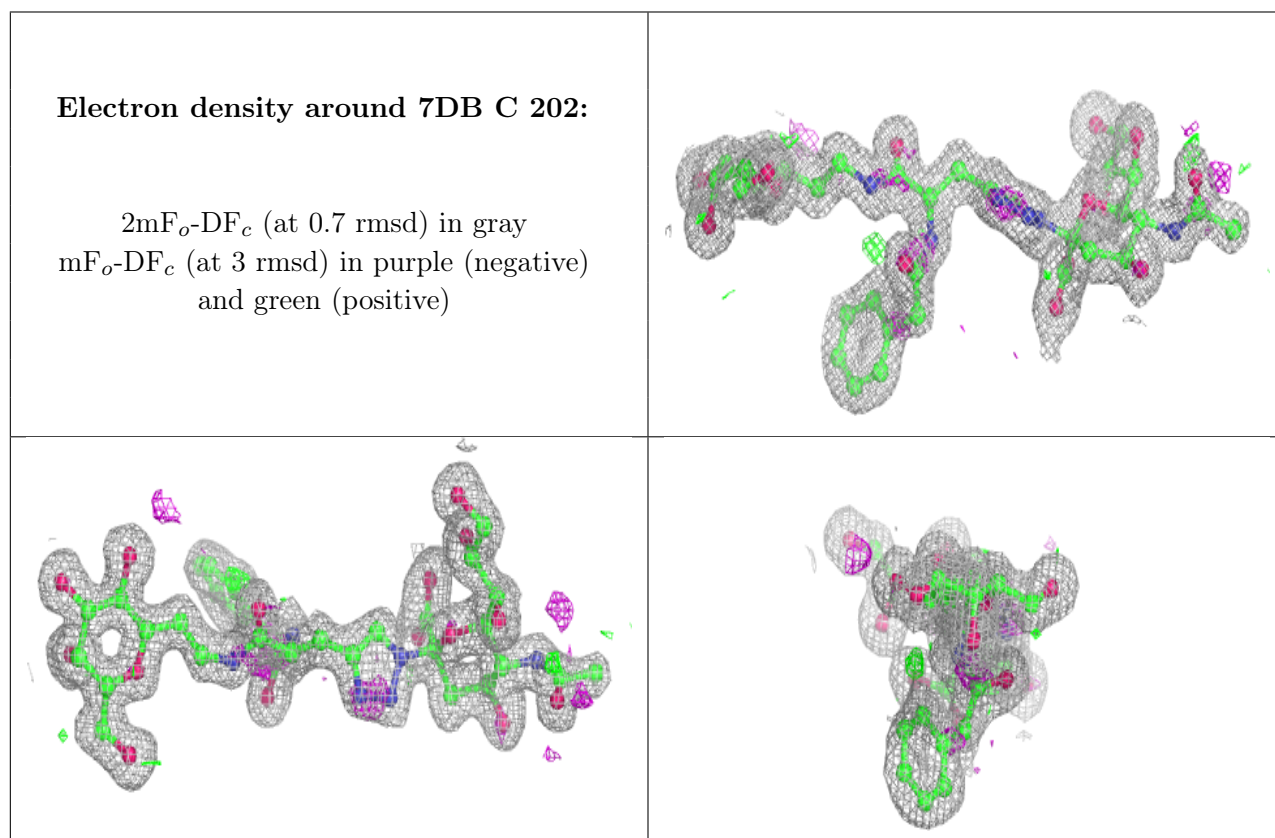
*Continued on next page...*



Continued from previous page...

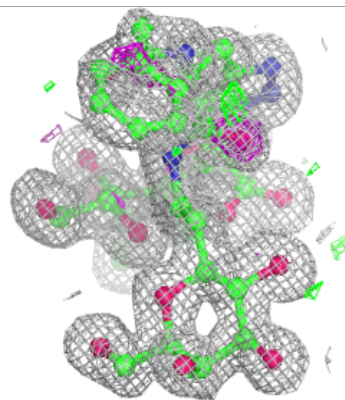
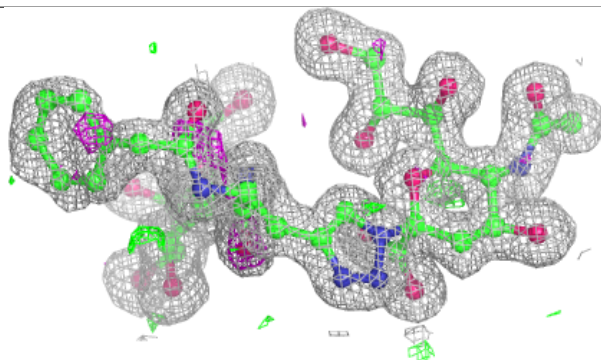
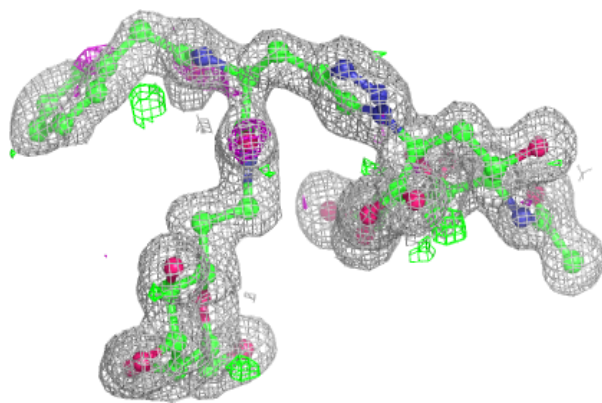
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	B	202	6/6	0.91	0.18	18,30,31,32	0
2	GOL	D	201	6/6	0.92	0.29	24,38,47,50	0
6	PO4	C	203	5/5	0.92	0.23	42,44,52,55	0
5	7DB	C	202	53/53	0.94	0.12	9,16,24,26	0
2	GOL	C	201	6/6	0.95	0.07	14,18,20,23	0
5	7DB	D	202	53/53	0.96	0.09	9,12,31,33	0
5	7DB	E	201	53/53	0.96	0.12	8,11,37,41	0
5	7DB	B	203	53/53	0.96	0.12	11,15,60,64	0
3	7BQ	A	202[A]	53/53	0.97	0.09	9,11,22,25	53
3	7BQ	A	202[B]	53/53	0.97	0.09	7,9,17,18	53

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.



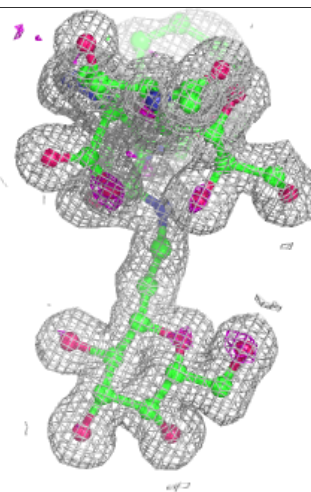
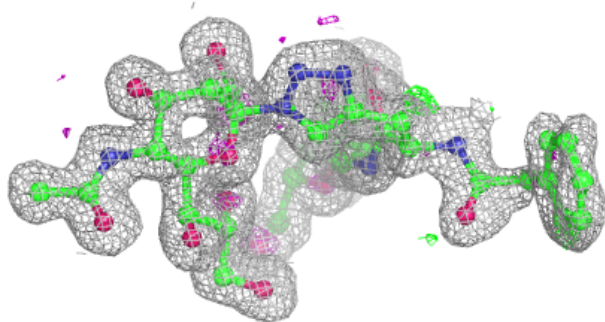
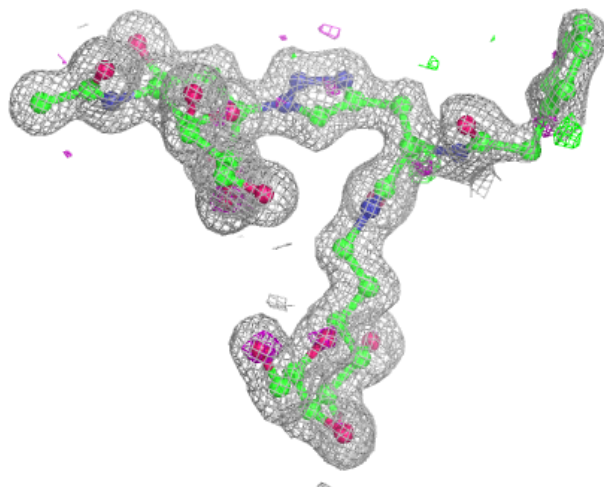
**Electron density around 7DB D 202:**

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



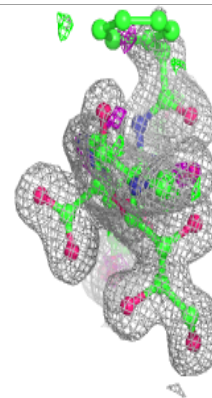
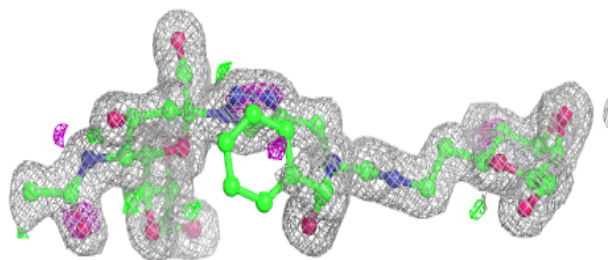
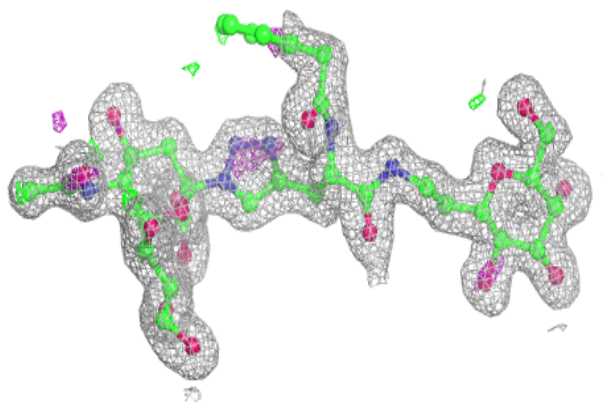
**Electron density around 7DB E 201:**

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



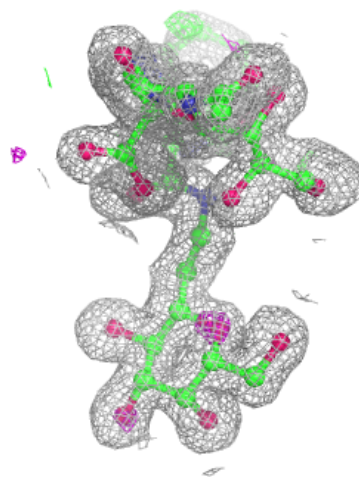
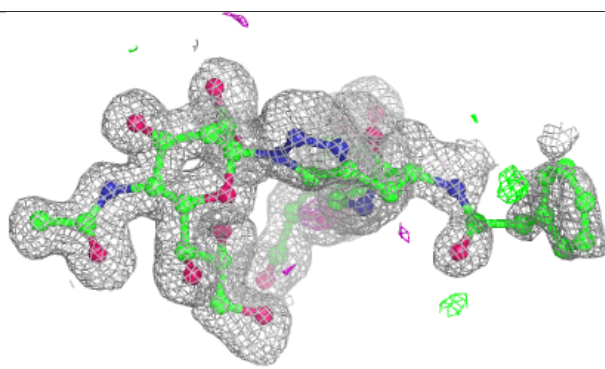
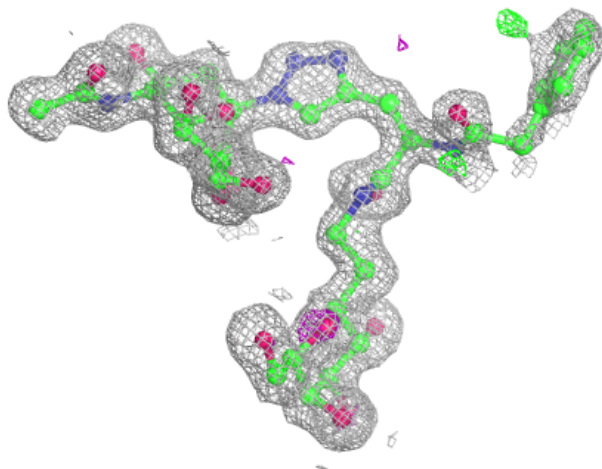
**Electron density around 7DB B 203:**

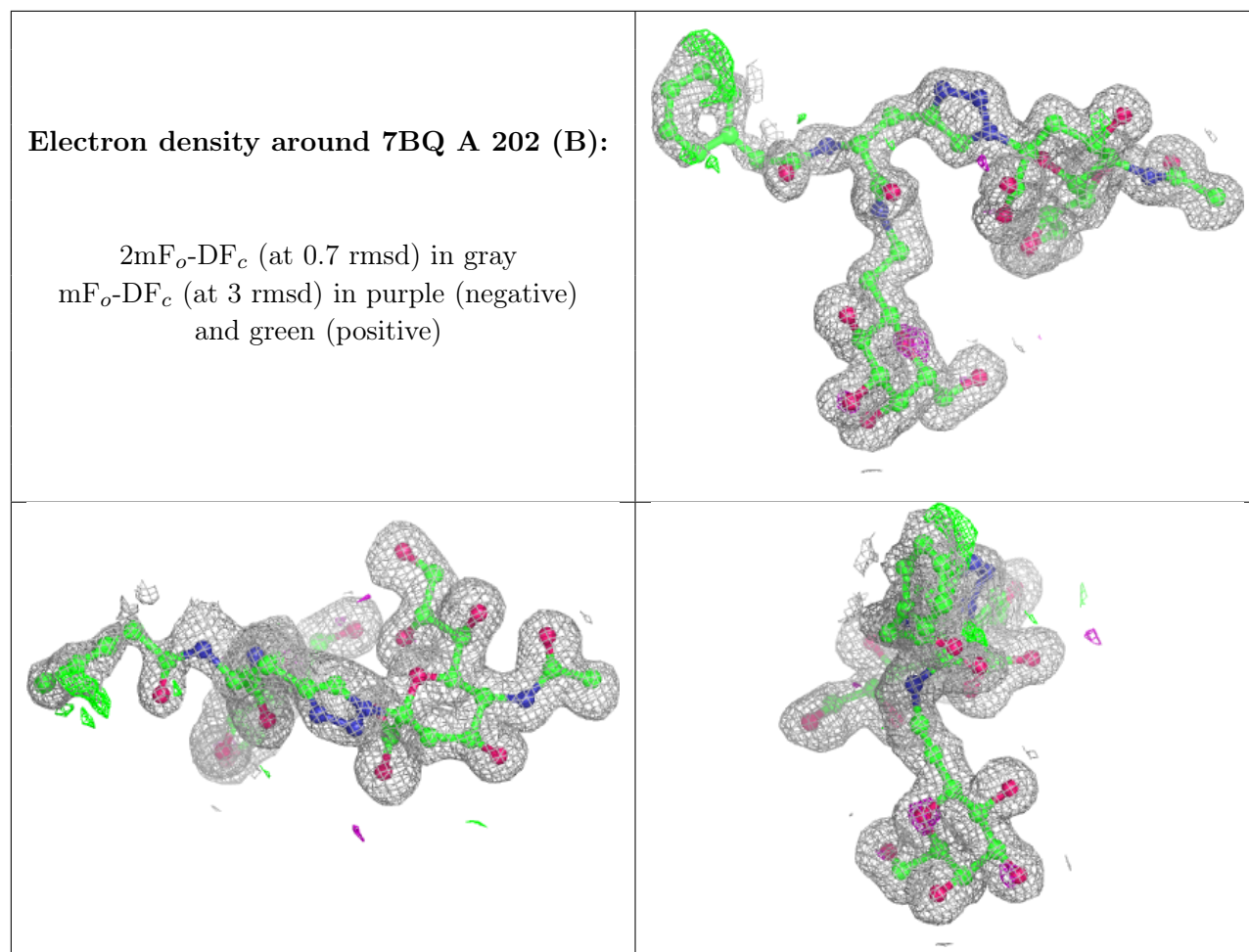
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 7BQ A 202 (A):**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.