



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 30, 2021 – 10:10 PM JST

PDB ID : 7CYY  
Title : Crystal structure of Arabinose isomerase from hybrid AI8 with Adonitol  
Authors : Hoang, N.K.Q.; Dhanasingh, I.; Cao, T.P.; Sung, J.Y.; Shin, S.M.; Lee, D.W.;  
Lee, S.H.  
Deposited on : 2020-09-05  
Resolution : 2.60 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](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.

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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 : 2.23.1  
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) : 2.23.1

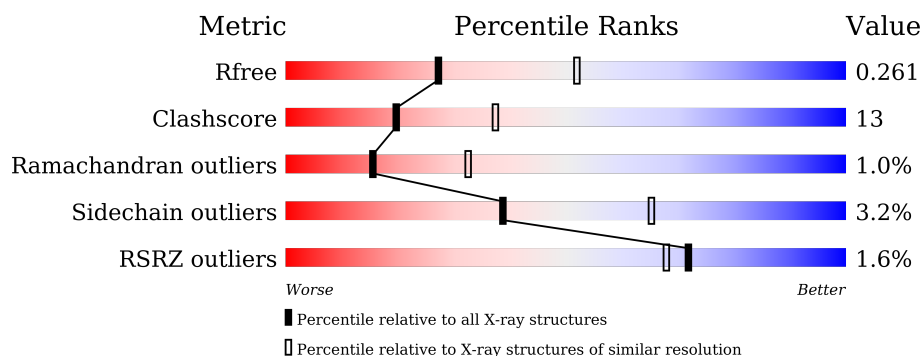
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">%</span> <span style="position: absolute; left: 74%; top: -10px;">74%</span> <span style="position: absolute; left: 95%; top: -10px;">25%</span> <span style="position: absolute; left: 100%; top: -10px;">.</span> </div> </div>
1	B	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">%</span> <span style="position: absolute; left: 70%; top: -10px;">70%</span> <span style="position: absolute; left: 95%; top: -10px;">28%</span> <span style="position: absolute; left: 100%; top: -10px;">..</span> </div> </div>
1	C	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">%</span> <span style="position: absolute; left: 69%; top: -10px;">69%</span> <span style="position: absolute; left: 95%; top: -10px;">30%</span> <span style="position: absolute; left: 100%; top: -10px;">.</span> </div> </div>
1	D	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">4%</span> <span style="position: absolute; left: 72%; top: -10px;">72%</span> <span style="position: absolute; left: 95%; top: -10px;">25%</span> <span style="position: absolute; left: 100%; top: -10px;">..</span> </div> </div>
1	E	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">%</span> <span style="position: absolute; left: 67%; top: -10px;">67%</span> <span style="position: absolute; left: 95%; top: -10px;">30%</span> <span style="position: absolute; left: 100%; top: -10px;">..</span> </div> </div>
1	F	497	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; left: 0; top: -10px;">2%</span> <span style="position: absolute; left: 69%; top: -10px;">69%</span> <span style="position: absolute; left: 95%; top: -10px;">29%</span> <span style="position: absolute; left: 100%; top: -10px;">..</span> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23776 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.

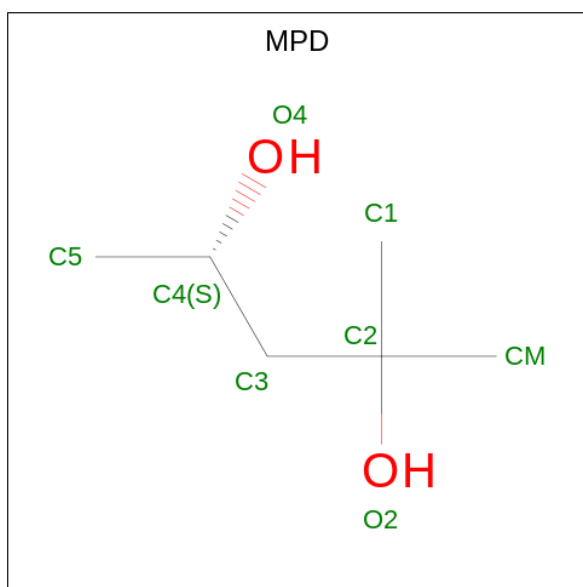
- Molecule 1 is a protein called L-arabinose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3925	2491	693	715	26			
1	B	494	Total	C	N	O	S	0	0	0
			3911	2484	691	710	26			
1	C	497	Total	C	N	O	S	0	0	0
			3932	2496	694	716	26			
1	D	490	Total	C	N	O	S	0	0	0
			3878	2460	687	706	25			
1	E	492	Total	C	N	O	S	0	0	0
			3895	2474	689	708	24			
1	F	493	Total	C	N	O	S	0	0	0
			3903	2478	690	711	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q5KYP7
B	1	MET	-	initiating methionine	UNP Q5KYP7
C	1	MET	-	initiating methionine	UNP Q5KYP7
D	1	MET	-	initiating methionine	UNP Q5KYP7
E	1	MET	-	initiating methionine	UNP Q5KYP7
F	1	MET	-	initiating methionine	UNP Q5KYP7

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

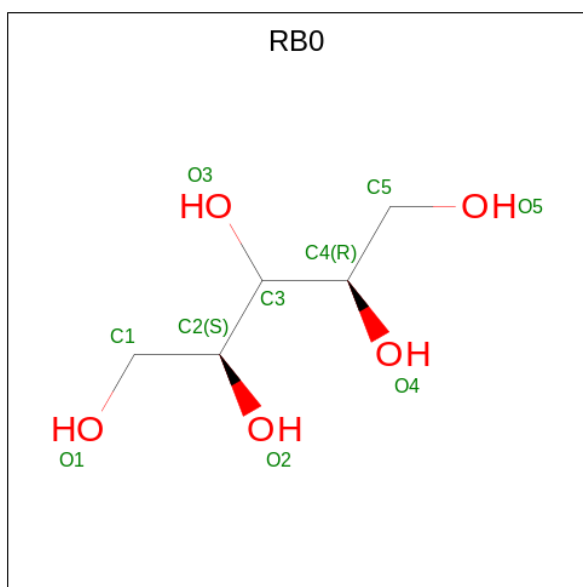


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mn	0	0
			2	2		
3	B	2	Total	Mn	0	0
			2	2		
3	C	1	Total	Mn	0	0
			1	1		
3	D	2	Total	Mn	0	0
			2	2		
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		

- Molecule 4 is D-ribitol (three-letter code: RB0) (formula: C<sub>5</sub>H<sub>12</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	0
			10	5	5		
4	D	1	Total	C	O	0	0
			10	5	5		
4	E	1	Total	C	O	0	0
			10	5	5		
4	F	1	Total	C	O	0	0
			10	5	5		
4	F	1	Total	C	O	0	0
			10	5	5		

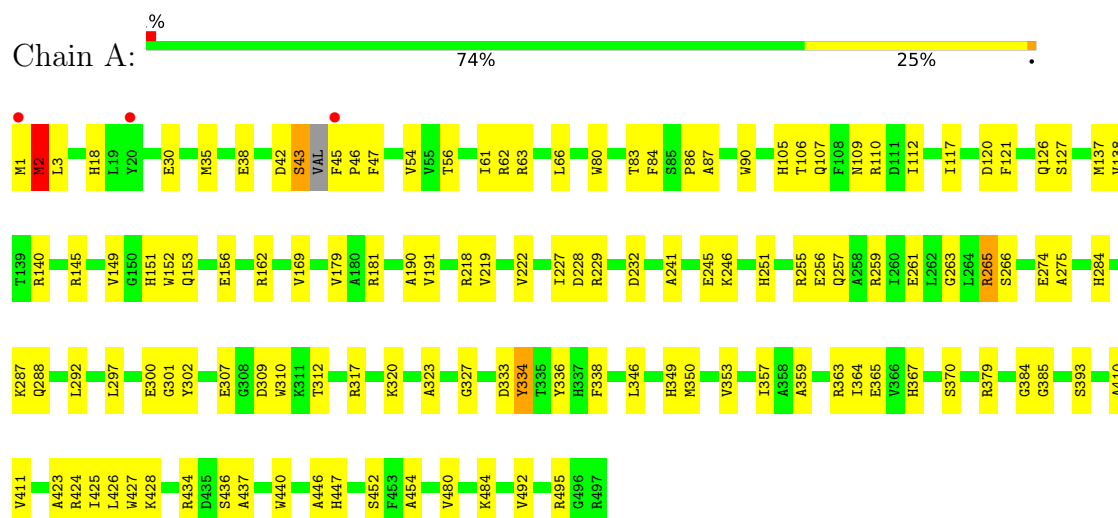
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	52	Total	O	0	0
			52	52		
5	C	42	Total	O	0	0
			42	42		
5	D	21	Total	O	0	0
			21	21		
5	E	23	Total	O	0	0
			23	23		
5	F	44	Total	O	0	0
			44	44		

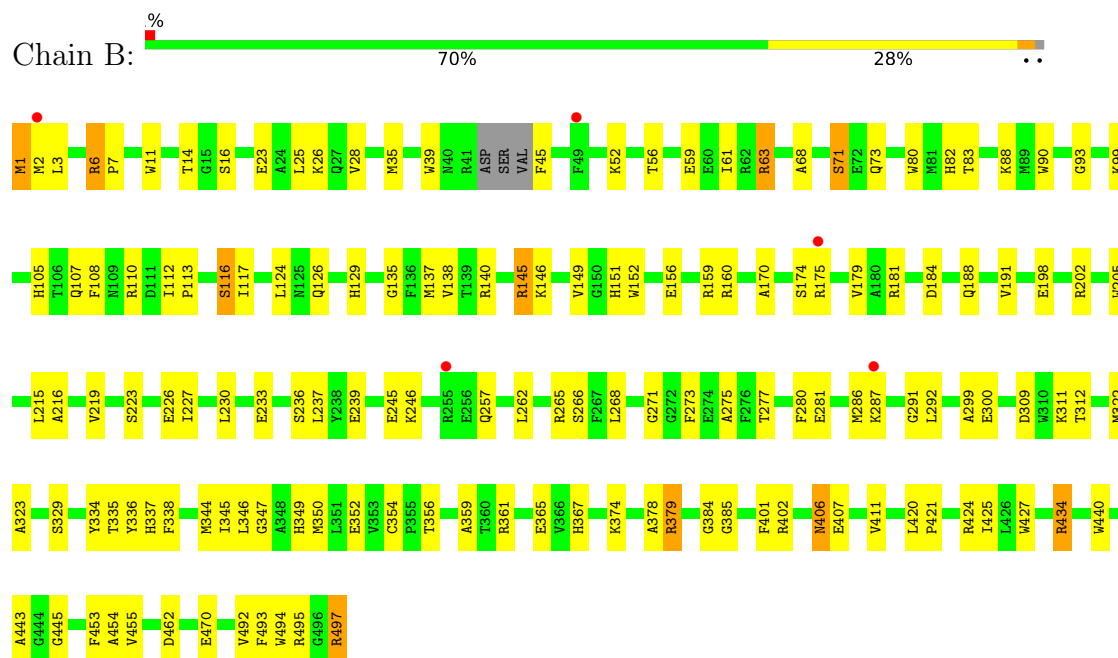
### 3 Residue-property plots [i](#)

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: L-arabinose isomerase

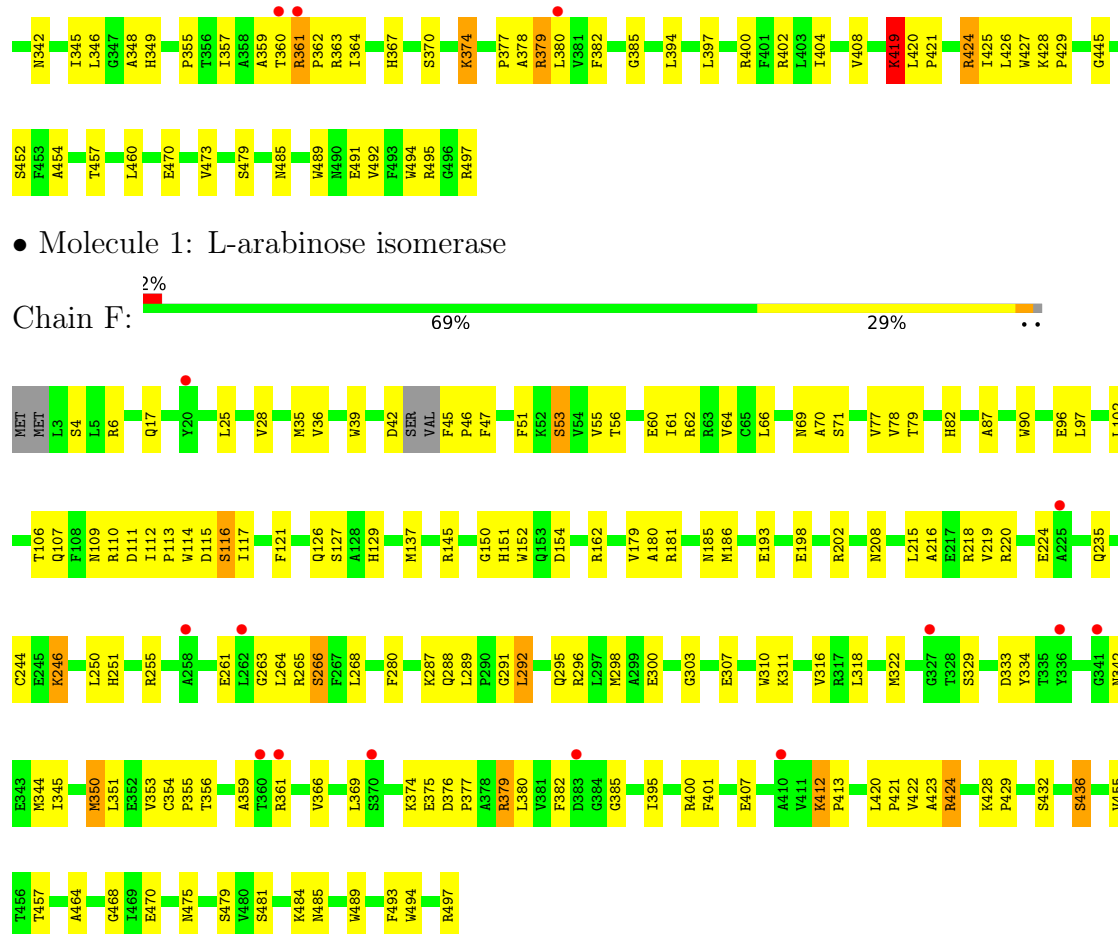


#### • Molecule 1: L-arabinose isomerase



#### • Molecule 1: L-arabinose isomerase





- Molecule 1: L-arabinose isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	205.58Å 82.12Å 192.73Å 90.00° 117.93° 90.00°	Depositor
Resolution (Å)	48.18 – 2.60 48.73 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.18-2.60) 98.3 (48.73-2.58)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.186 , 0.261 0.186 , 0.261	Depositor DCC
$R_{free}$ test set	4500 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.1	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	23776	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, RB0, MN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.48	0/4023	0.63	0/5440
1	B	0.45	0/4009	0.59	0/5421
1	C	0.46	0/4031	0.61	1/5453 (0.0%)
1	D	0.47	0/3974	0.65	2/5372 (0.0%)
1	E	0.46	1/3993 (0.0%)	0.60	1/5401 (0.0%)
1	F	0.45	0/4001	0.58	0/5412
All	All	0.46	1/24031 (0.0%)	0.61	4/32499 (0.0%)

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	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	419	LYS	CE-NZ	-5.37	1.35	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	187	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	E	360	THR	C-N-CA	-7.55	102.82	121.70
1	C	142	GLY	C-N-CA	-6.86	104.56	121.70
1	D	142	GLY	C-N-CA	-5.71	107.43	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	53	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3925	0	3815	89	1
1	B	3911	0	3806	113	1
1	C	3932	0	3825	111	0
1	D	3878	0	3766	110	0
1	E	3895	0	3785	112	0
1	F	3903	0	3789	99	1
2	A	8	0	14	3	0
2	C	8	0	14	5	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	B	10	0	11	1	0
4	D	20	0	20	1	0
4	E	10	0	12	1	0
4	F	20	0	23	0	0
5	A	65	0	0	1	0
5	B	52	0	0	1	0
5	C	42	0	0	3	0
5	D	21	0	0	3	0
5	E	23	0	0	2	0
5	F	44	0	0	1	0
All	All	23776	0	22880	590	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 590 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:D:187:ARG:NH1	5:D:601:HOH:O	1.64	1.25
1:C:492:VAL:HG12	1:C:495:ARG:NH2	1.72	1.05
1:B:493:PHE:O	1:B:497:ARG:NH1	1.95	0.99
1:C:319:MET:CE	1:C:450:CYS:HB3	1.92	0.99
1:D:91:ILE:HD11	1:D:137:MET:HE3	1.44	0.96

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:ARG:NH1	1:F:70:ALA:O[1_565]	2.05	0.15
1:A:38:GLU:OE2	1:A:229:ARG:NH1[2_555]	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	492/497 (99%)	472 (96%)	15 (3%)	5 (1%)	15	32
1	B	490/497 (99%)	473 (96%)	15 (3%)	2 (0%)	34	57
1	C	495/497 (100%)	468 (94%)	21 (4%)	6 (1%)	13	27
1	D	484/497 (97%)	448 (93%)	30 (6%)	6 (1%)	13	27
1	E	488/497 (98%)	467 (96%)	17 (4%)	4 (1%)	19	39
1	F	489/497 (98%)	459 (94%)	25 (5%)	5 (1%)	15	32
All	All	2938/2982 (98%)	2787 (95%)	123 (4%)	28 (1%)	15	32

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ASP
1	C	116	SER
1	D	244	CYS

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Mol	Chain	Res	Type
1	E	117	ILE
1	A	2	MET

### 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	407/408 (100%)	395 (97%)	12 (3%)	42	68
1	B	405/408 (99%)	391 (96%)	14 (4%)	36	62
1	C	408/408 (100%)	397 (97%)	11 (3%)	44	71
1	D	402/408 (98%)	390 (97%)	12 (3%)	41	67
1	E	403/408 (99%)	390 (97%)	13 (3%)	39	65
1	F	404/408 (99%)	388 (96%)	16 (4%)	31	57
All	All	2429/2448 (99%)	2351 (97%)	78 (3%)	39	65

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	374	LYS
1	F	361	ARG
1	E	419	LYS
1	F	154	ASP
1	F	424	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	415	HIS
1	E	188	GLN
1	F	73	GLN
1	E	477	HIS
1	C	188	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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 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	$\# Z  > 2$
2	MPD	A	501	-	7,7,7	0.33	0	9,10,10	0.32	0
4	RB0	D	501	3	9,9,9	0.89	0	11,11,11	1.43	1 (9%)
4	RB0	F	502	3	9,9,9	0.69	0	11,11,11	1.19	2 (18%)
4	RB0	E	501	3	9,9,9	0.78	0	11,11,11	1.27	1 (9%)
4	RB0	D	502	3	9,9,9	0.82	0	11,11,11	1.25	1 (9%)
4	RB0	F	501	3	9,9,9	0.71	0	11,11,11	2.07	5 (45%)
2	MPD	C	501	-	7,7,7	0.34	0	9,10,10	0.32	0
4	RB0	B	501	3	9,9,9	0.80	0	11,11,11	0.88	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
2	MPD	A	501	-	-	2/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	RB0	D	501	3	-	9/12/12/12	-
4	RB0	F	502	3	-	8/12/12/12	-
4	RB0	E	501	3	-	6/12/12/12	-
4	RB0	D	502	3	-	6/12/12/12	-
4	RB0	F	501	3	-	4/12/12/12	-
2	MPD	C	501	-	-	0/5/5/5	-
4	RB0	B	501	3	-	12/12/12/12	-

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	501	RB0	C4-C3-C2	-4.12	104.80	113.36
4	D	502	RB0	C5-C4-C3	-2.84	106.26	112.41
4	F	501	RB0	O3-C3-C2	2.68	115.28	108.81
4	E	501	RB0	O4-C4-C3	2.55	115.30	109.10
4	D	501	RB0	O1-C1-C2	-2.46	105.72	111.07

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	RB0	C1-C2-C3-O3
4	B	501	RB0	C1-C2-C3-C4
4	B	501	RB0	O2-C2-C3-O3
4	B	501	RB0	O2-C2-C3-C4
4	B	501	RB0	C3-C4-C5-O5

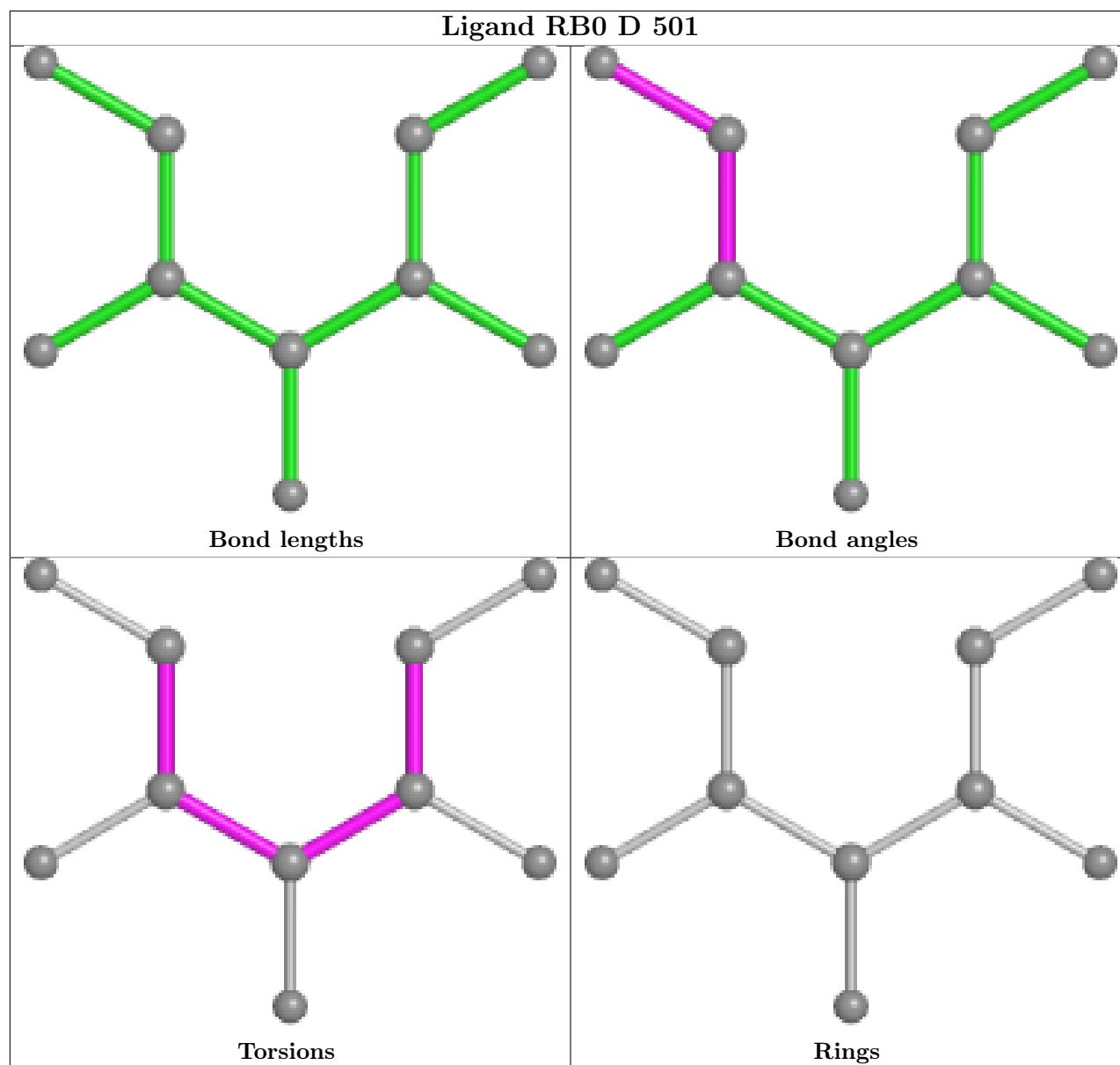
There are no ring outliers.

5 monomers are involved in 11 short contacts:

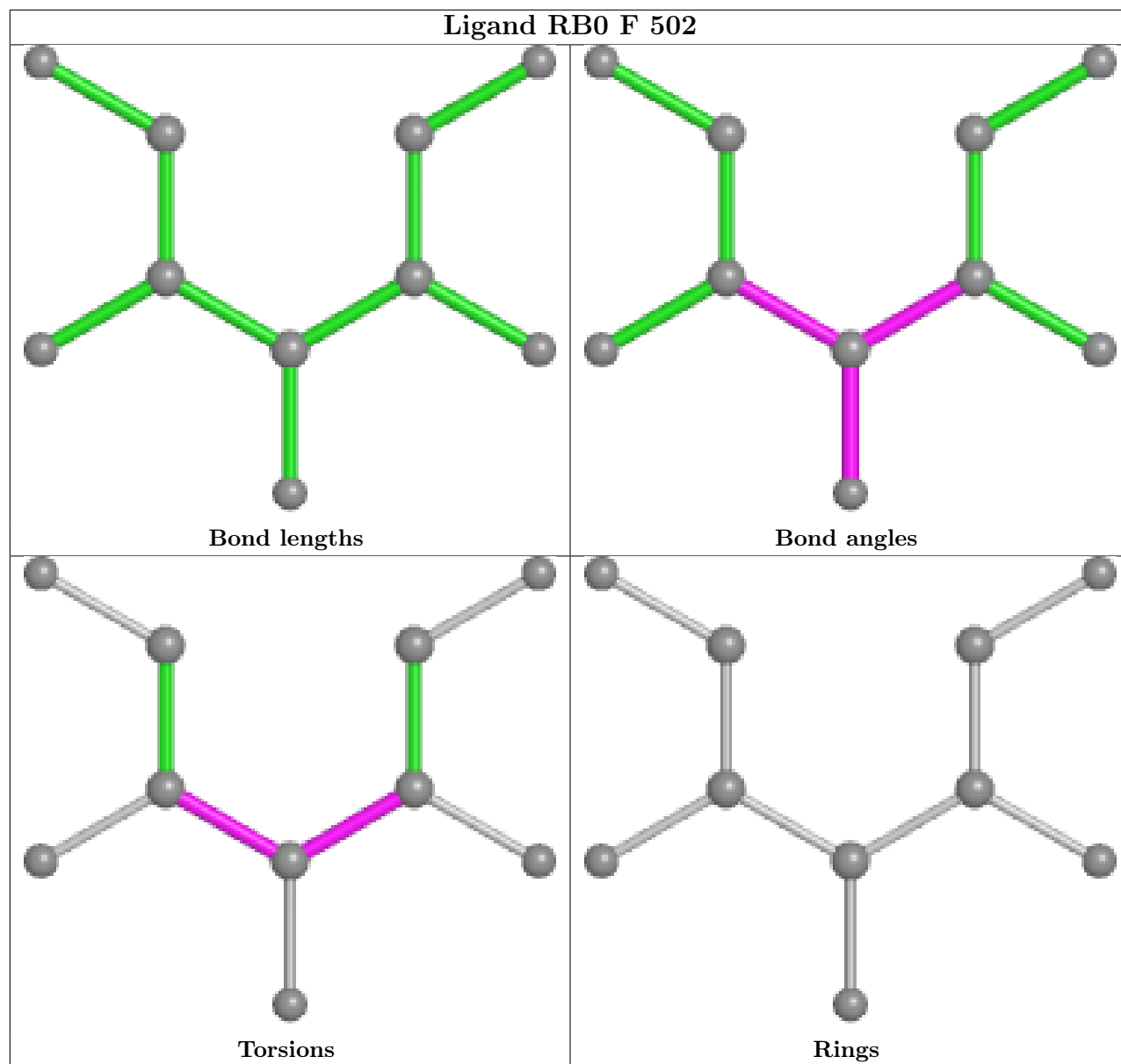
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	MPD	3	0
4	D	501	RB0	1	0
4	E	501	RB0	1	0
2	C	501	MPD	5	0
4	B	501	RB0	1	0

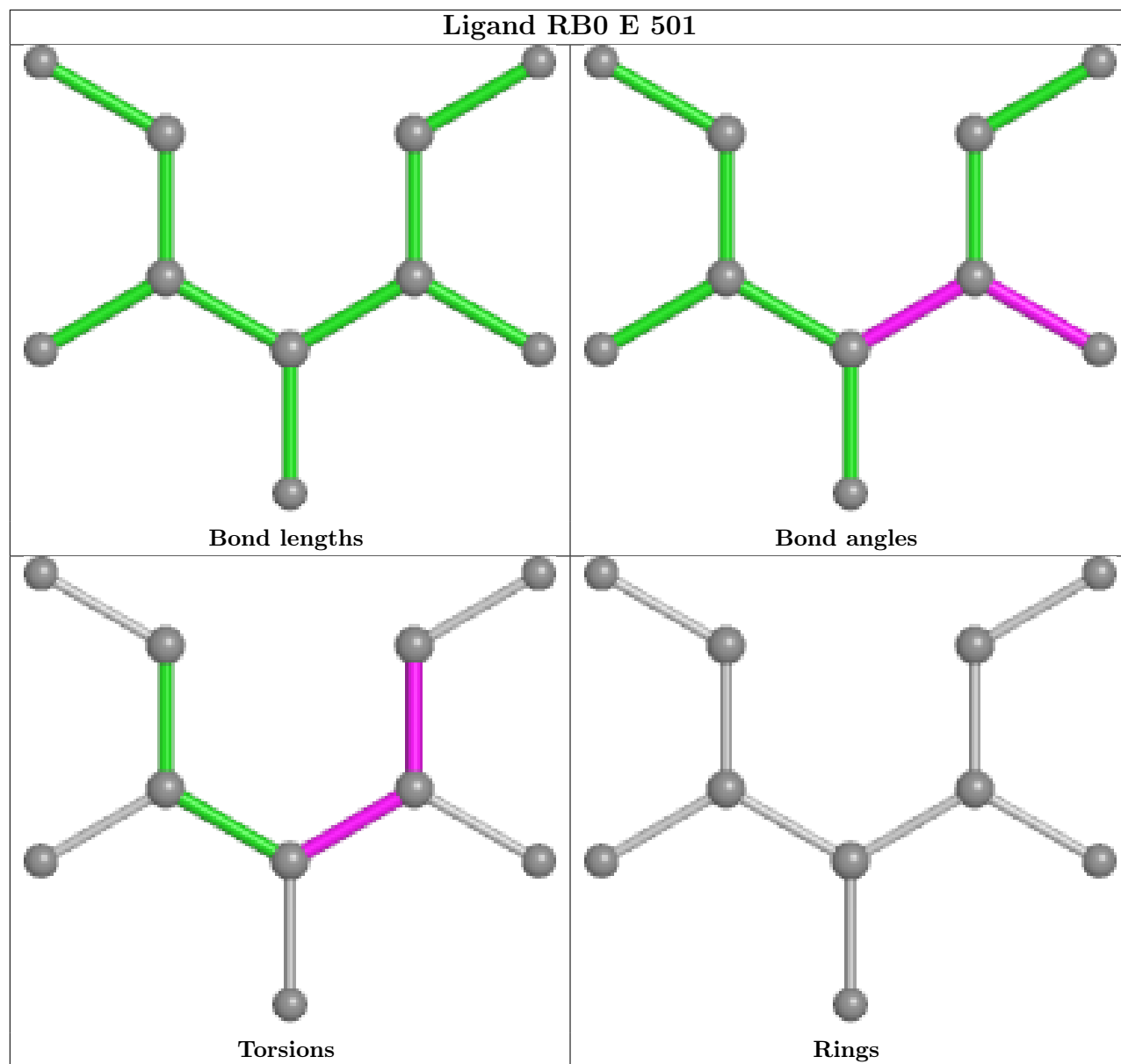
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

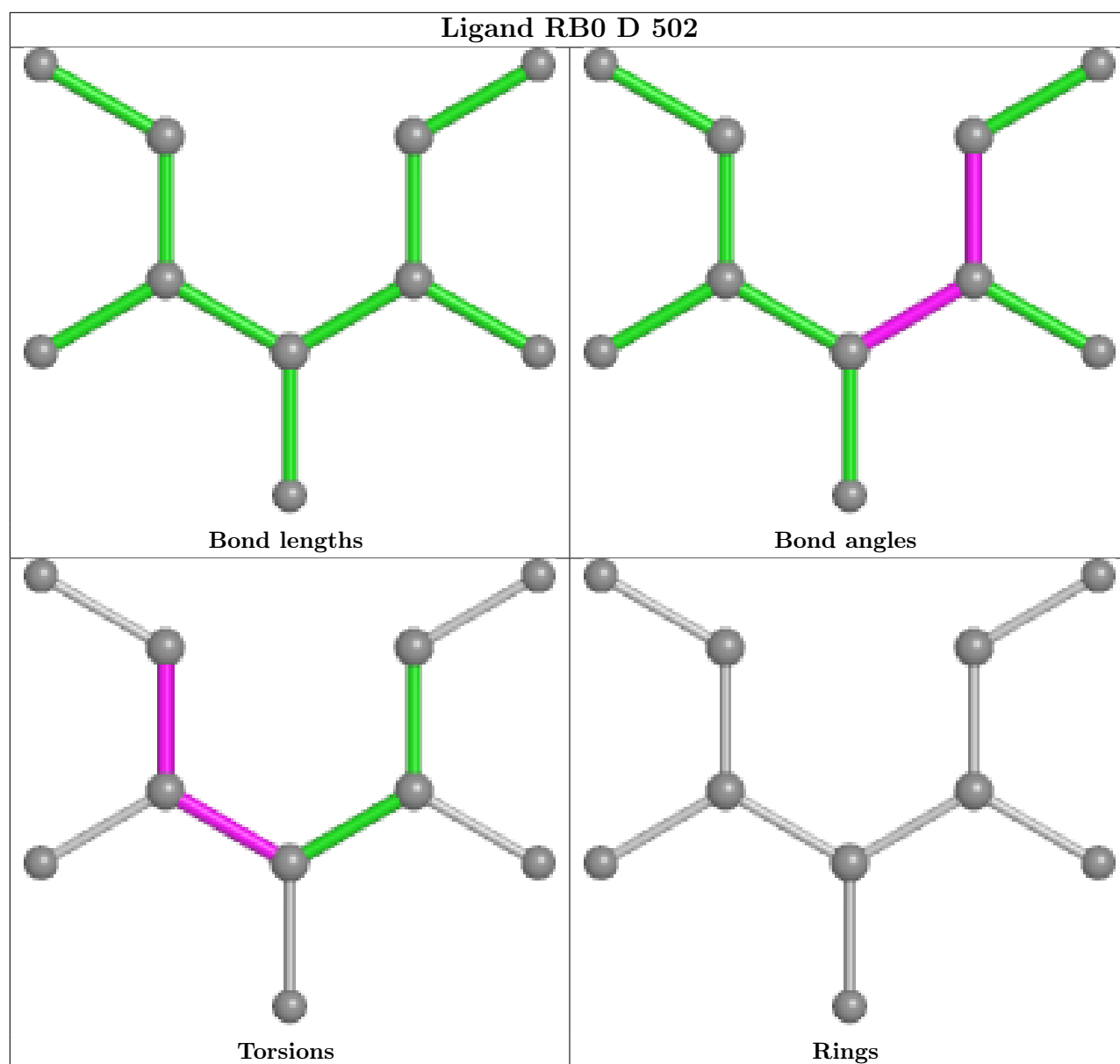
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

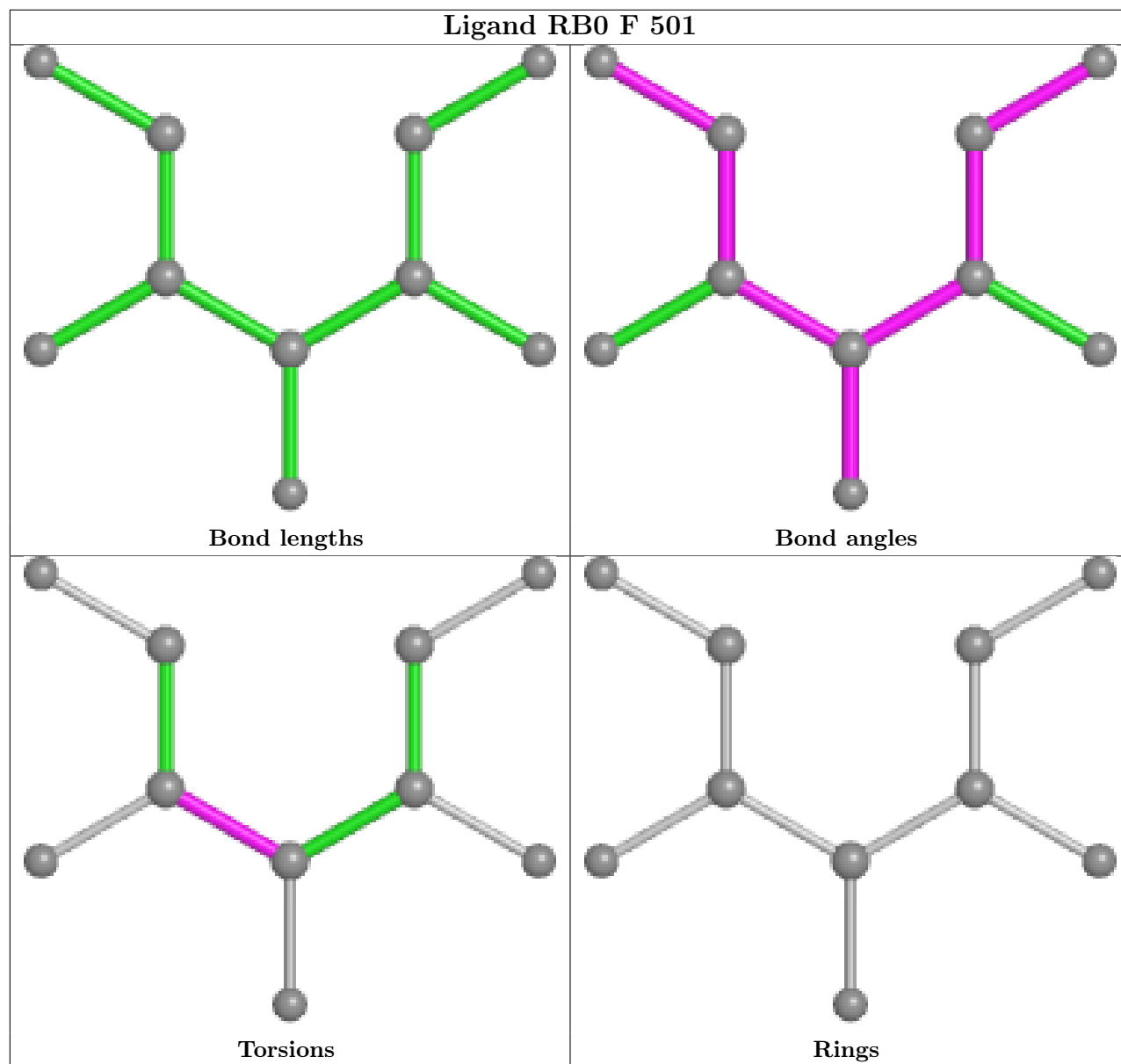


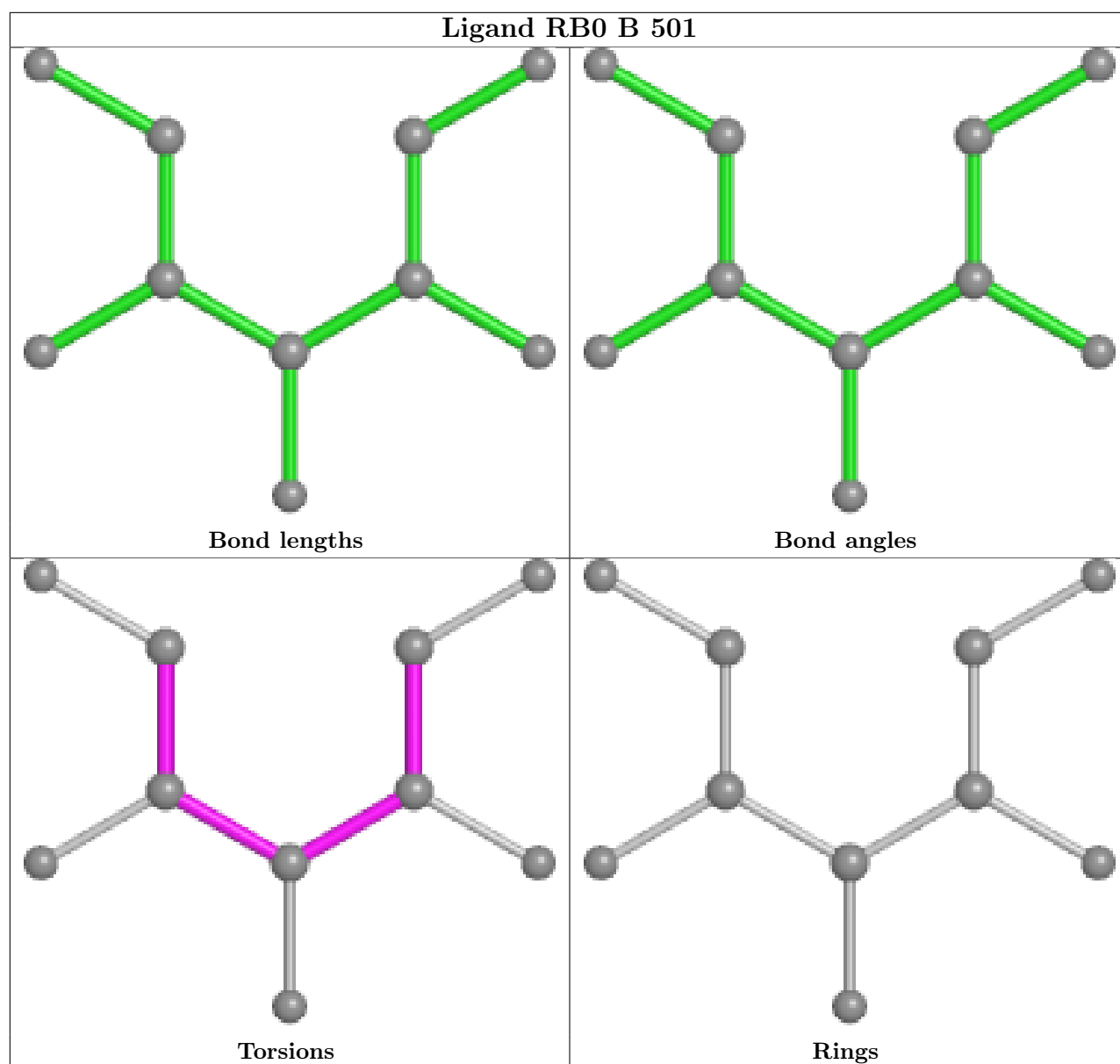












## 5.7 Other polymers [i](#)

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	496/497 (99%)	-0.42	3 (0%) 89 88	28, 42, 63, 88	0
1	B	494/497 (99%)	-0.28	5 (1%) 82 80	32, 49, 72, 97	0
1	C	497/497 (100%)	-0.39	4 (0%) 86 84	32, 48, 73, 91	0
1	D	490/497 (98%)	-0.17	18 (3%) 41 34	30, 49, 84, 120	0
1	E	492/497 (98%)	-0.19	4 (0%) 86 84	32, 49, 71, 93	0
1	F	493/497 (99%)	-0.16	12 (2%) 59 53	33, 52, 77, 104	0
All	All	2962/2982 (99%)	-0.27	46 (1%) 72 68	28, 48, 75, 120	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	248	GLY	7.5
1	B	2	MET	4.7
1	D	2	MET	4.5
1	D	249	PRO	4.3
1	D	380	LEU	3.9

### 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

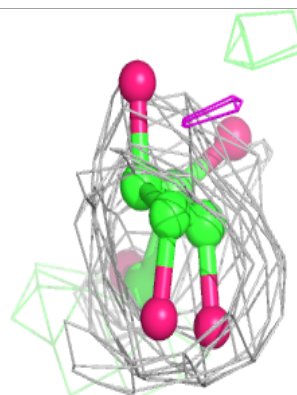
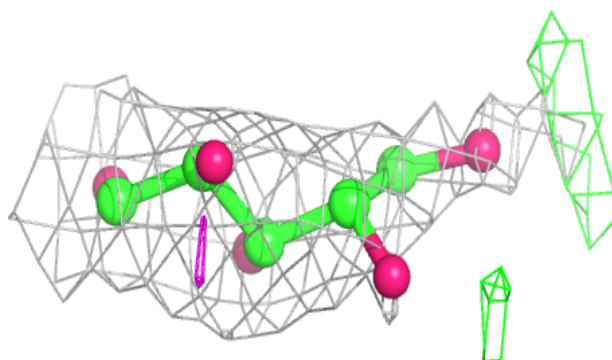
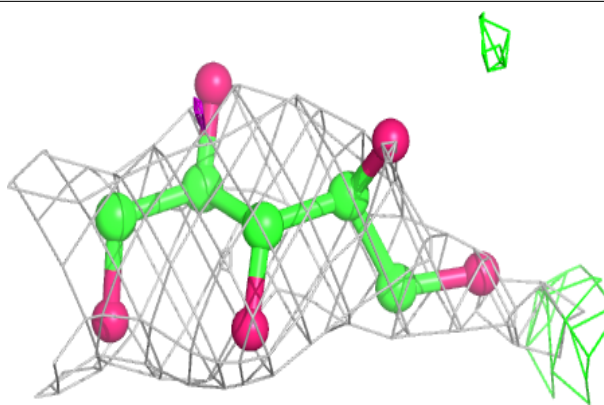
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<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	MPD	C	501	8/8	0.81	0.45	63,75,82,84	0
2	MPD	A	501	8/8	0.82	0.35	63,77,81,82	0
4	RB0	F	501	10/10	0.88	0.20	57,61,70,74	0
4	RB0	F	502	10/10	0.89	0.20	64,67,79,85	0
4	RB0	E	501	10/10	0.90	0.22	55,56,66,67	0
4	RB0	D	501	10/10	0.92	0.19	50,62,73,73	0
4	RB0	D	502	10/10	0.96	0.13	61,66,69,73	0
4	RB0	B	501	10/10	0.96	0.17	54,60,74,74	0
3	MN	E	502	1/1	0.97	0.09	50,50,50,50	0
3	MN	D	504	1/1	0.98	0.14	59,59,59,59	0
3	MN	B	502	1/1	0.99	0.10	52,52,52,52	0
3	MN	B	503	1/1	0.99	0.05	55,55,55,55	0
3	MN	D	503	1/1	0.99	0.06	60,60,60,60	0
3	MN	A	502	1/1	0.99	0.06	56,56,56,56	0
3	MN	A	503	1/1	0.99	0.13	45,45,45,45	0
3	MN	F	503	1/1	0.99	0.06	56,56,56,56	0
3	MN	C	502	1/1	1.00	0.09	54,54,54,54	0

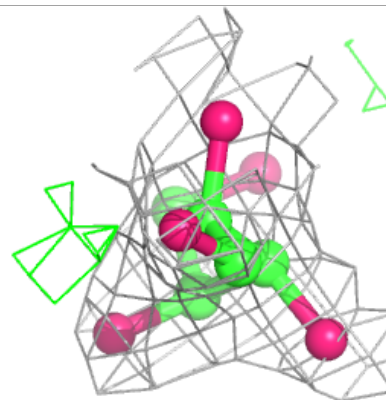
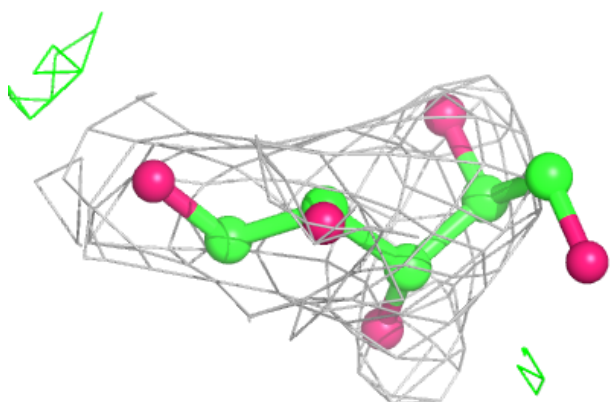
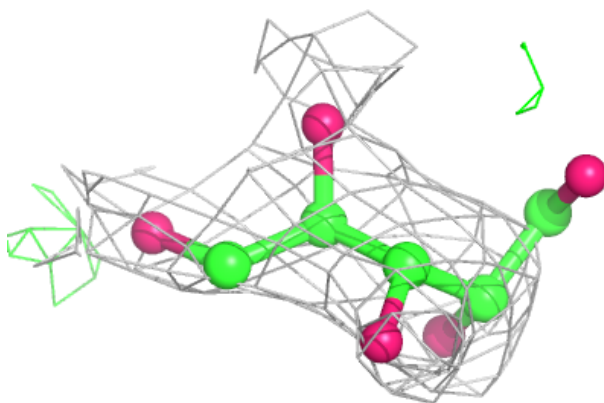
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around RB0 F 501:**

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

**Electron density around RB0 F 502:**

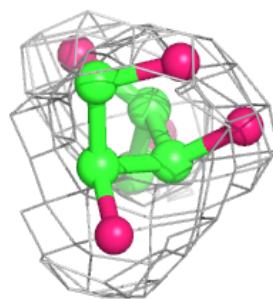
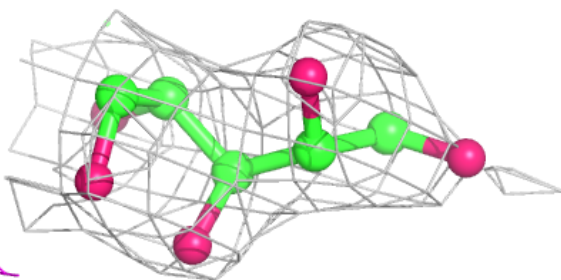
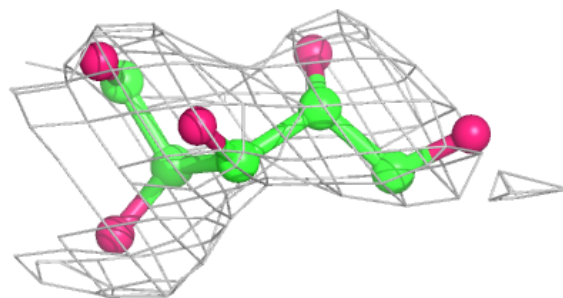
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



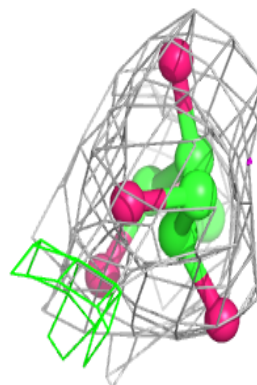
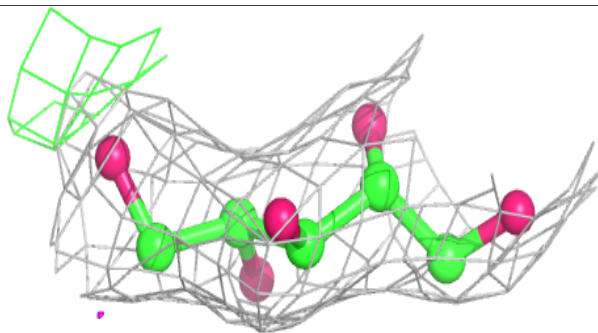
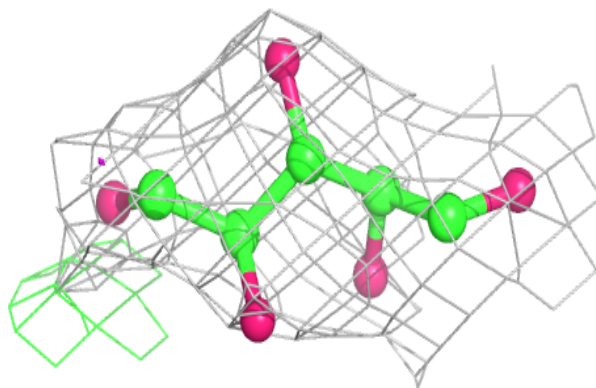


**Electron density around RB0 E 501:**

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

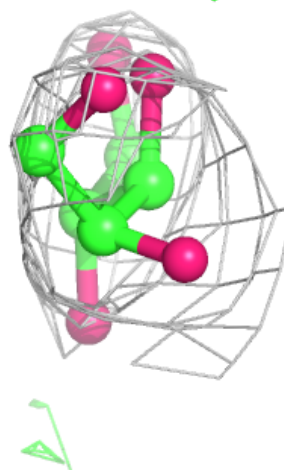
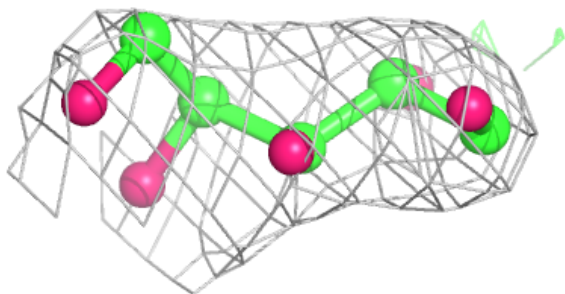
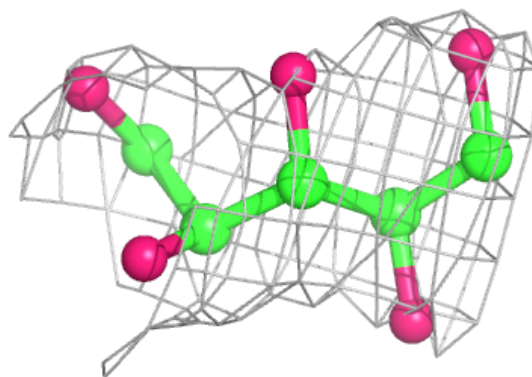
**Electron density around RB0 D 501:**

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



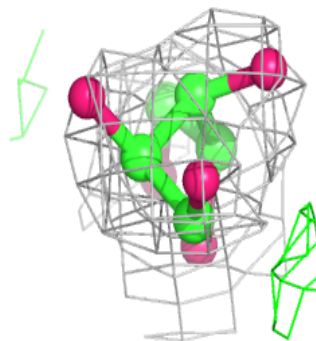
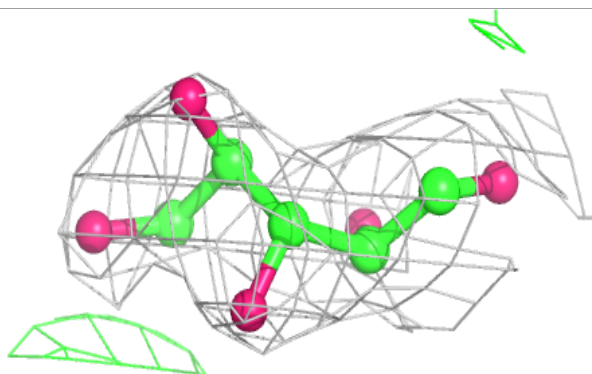
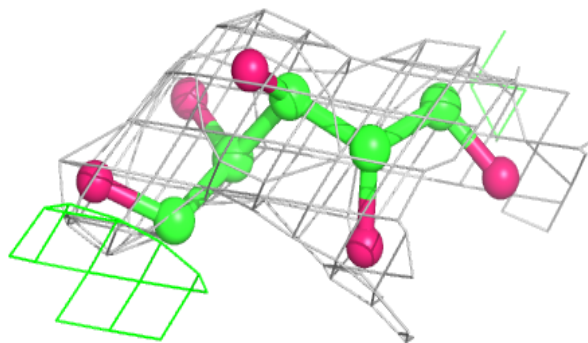
**Electron density around RB0 D 502:**

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



**Electron density around RB0 B 501:**

$2mF_o-DF_c$  (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.