



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 12:15 PM EDT

PDB ID : 7MFS  
Title : N-Acetylmannosamine-6-phosphate 2-epimerase from *Staphylococcus aureus*  
(strain MRSA USA300) with substrate and product bound  
Authors : Currie, M.J.; Dobson, R.C.J.  
Deposited on : 2021-04-11  
Resolution : 1.51 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.

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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 : 2.27  
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) : 2.27

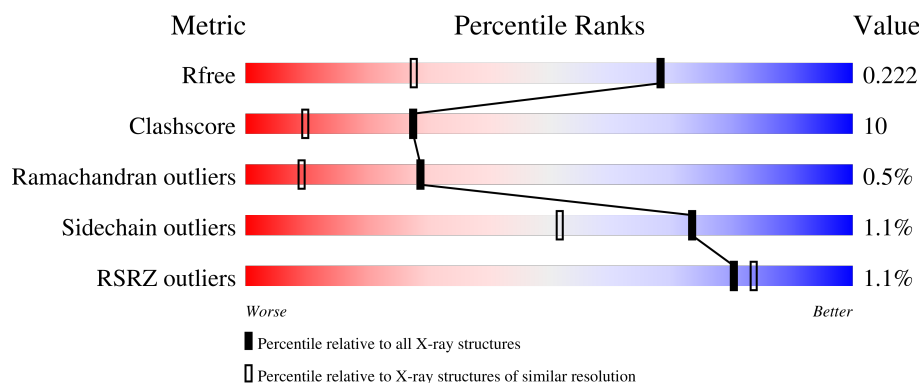
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	AAA	222	<div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	BBB	222	<div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div>

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
4	RFW	BBB	305[B]	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4408 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.

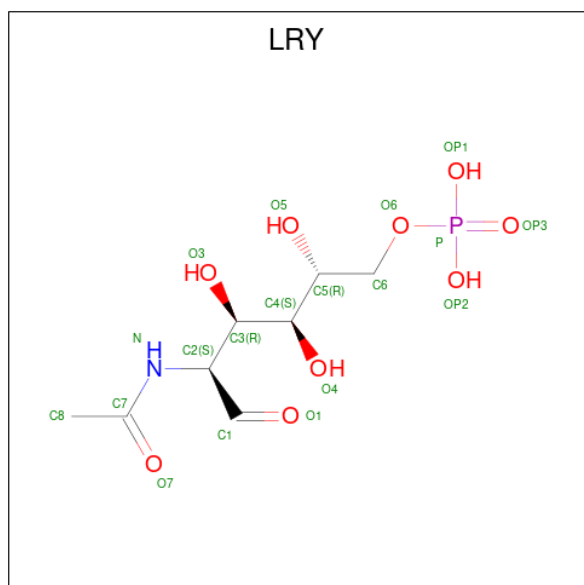
- Molecule 1 is a protein called N-acetylmannosamine-6-phosphate 2-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	BBB	222	Total	C	N	O	S	0	19	0
			1848	1175	302	360	11			
1	AAA	222	Total	C	N	O	S	0	24	0
			1884	1201	311	361	11			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

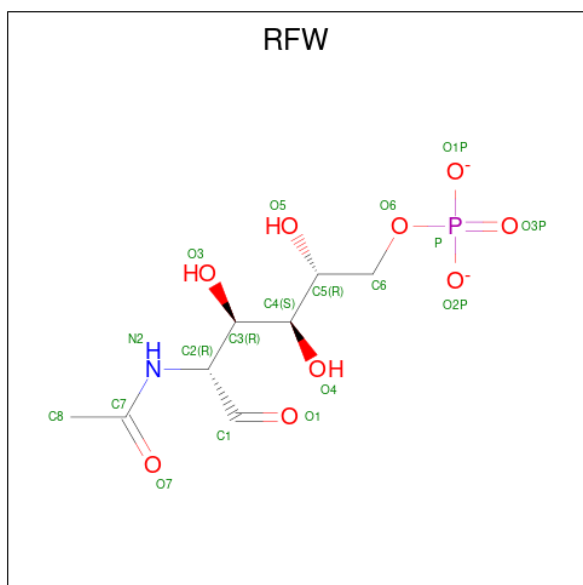
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	BBB	3	Total	Cl	0	0
			3	3		
2	AAA	1	Total	Cl	0	0
			1	1		

- Molecule 3 is N-acetylmannosamine-6-phosphate (three-letter code: LRY) (formula: C<sub>8</sub>H<sub>16</sub>NO<sub>9</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	BBB	1	Total	C	N	O	P	0	1
			19	8	1	9	1		
3	AAA	1	Total	C	N	O	P	0	1
			19	8	1	9	1		

- Molecule 4 is N-acetyl-D-glucosamine-6-phosphate (three-letter code: RFW) (formula:  $C_8H_{14}NO_9P$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	BBB	1	Total	C	N	O	P	0	1
			19	8	1	9	1		
4	AAA	1	Total	C	N	O	P	0	1
			19	8	1	9	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	BBB	298	Total	O	0	0
			298	298		
5	AAA	298	Total	O	0	0
			298	298		

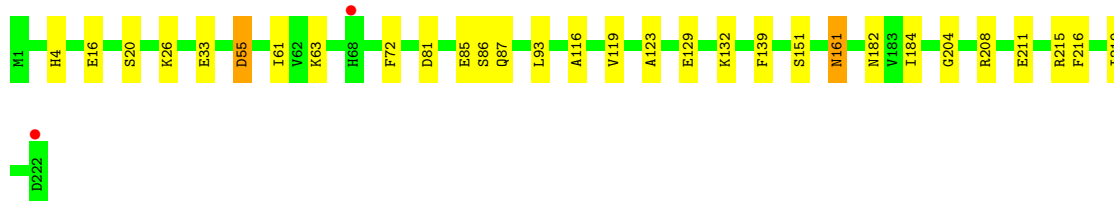
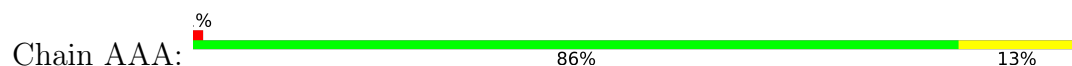
### 3 Residue-property plots [i](#)

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: N-acetylmannosamine-6-phosphate 2-epimerase



- Molecule 1: N-acetylmannosamine-6-phosphate 2-epimerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	43.93Å 76.47Å 174.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.25 – 1.51 46.25 – 1.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (46.25-1.51) 98.7 (46.25-1.51)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.85 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.180 , 0.210 0.191 , 0.222	Depositor DCC
$R_{free}$ test set	4620 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	11.4	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4408	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: CL, LRY, RFW

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	AAA	0.80	0/1952	0.89	1/2640 (0.0%)
1	BBB	0.82	0/1909	0.93	4/2587 (0.2%)
All	All	0.81	0/3861	0.91	5/5227 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	215	ARG	NE-CZ-NH1	-8.26	116.17	120.30
1	AAA	55	ASP	CB-CA-C	6.76	123.91	110.40
1	BBB	40	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	BBB	215	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	BBB	55	ASP	CB-CA-C	5.09	120.57	110.40

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	AAA	1884	0	1943	34	0
1	BBB	1848	0	1885	39	0
2	AAA	1	0	0	0	0
2	BBB	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	AAA	19	0	14	5	0
3	BBB	19	0	14	6	0
4	AAA	19	0	14	3	0
4	BBB	19	0	14	10	0
5	AAA	298	0	0	13	3
5	BBB	298	0	0	12	2
All	All	4408	0	3884	77	4

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 10.

All (77) 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:BBB:211[B]:GLU:OE1	5:BBB:403:HOH:O	1.55	1.24
1:AAA:85[B]:GLU:OE2	5:AAA:403:HOH:O	1.56	1.21
1:AAA:63:LYS:HZ3	3:AAA:302[A]:LRY:H2	1.11	1.15
1:AAA:85[A]:GLU:OE1	5:AAA:404:HOH:O	1.68	1.11
4:BBB:305[B]:RFW:O7	4:BBB:305[B]:RFW:H1	1.46	1.07
1:AAA:63:LYS:NZ	3:AAA:302[A]:LRY:H2	1.73	1.02
1:BBB:63:LYS:NZ	3:BBB:304[A]:LRY:H2	1.83	0.93
4:BBB:305[B]:RFW:O7	4:BBB:305[B]:RFW:C1	2.20	0.89
1:AAA:208[B]:ARG:NH1	1:AAA:211:GLU:HG3	1.90	0.85
1:BBB:208[B]:ARG:NH2	5:BBB:403:HOH:O	2.09	0.83
1:BBB:63:LYS:HZ3	3:BBB:304[A]:LRY:H2	1.44	0.83
1:AAA:161:ASN:HB2	5:AAA:641:HOH:O	1.84	0.77
1:BBB:55:ASP:C	5:BBB:433:HOH:O	2.26	0.73
4:AAA:303[B]:RFW:O5	4:AAA:303[B]:RFW:H2	1.89	0.72
1:BBB:63:LYS:HZ1	3:BBB:304[A]:LRY:C2	2.03	0.71
1:BBB:63:LYS:HZ1	3:BBB:304[A]:LRY:C1	2.05	0.70
1:AAA:55:ASP:C	5:AAA:451:HOH:O	2.30	0.70
1:BBB:63:LYS:NZ	3:BBB:304[A]:LRY:C2	2.54	0.70
1:BBB:63:LYS:NZ	4:BBB:305[B]:RFW:O1	2.27	0.66
1:AAA:211:GLU:HG3	5:AAA:554:HOH:O	1.96	0.65
1:BBB:89:GLU:OE2	5:BBB:405:HOH:O	2.15	0.65
4:BBB:305[B]:RFW:O5	4:BBB:305[B]:RFW:H2	2.00	0.62
1:AAA:116:ALA:O	1:AAA:119[A]:VAL:HG22	2.00	0.61
1:AAA:208[B]:ARG:NH1	1:AAA:211:GLU:CG	2.62	0.61
1:BBB:63:LYS:HZ1	3:BBB:304[A]:LRY:H2	1.59	0.61
1:AAA:208[B]:ARG:HH11	1:AAA:211:GLU:CG	2.13	0.61
1:BBB:172[A]:SER:OG	5:BBB:404:HOH:O	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:208[B]:ARG:HH11	1:AAA:211:GLU:HG3	1.63	0.60
1:BBB:211[B]:GLU:HG3	5:BBB:611:HOH:O	2.01	0.60
1:BBB:63:LYS:CE	4:BBB:305[B]:RFW:O1	2.51	0.59
1:AAA:63:LYS:NZ	3:AAA:302[A]:LRY:C2	2.59	0.59
1:BBB:86:SER:O	1:BBB:87[B]:GLN:HB2	2.03	0.58
1:AAA:208[B]:ARG:NH2	5:AAA:413:HOH:O	2.32	0.58
1:BBB:89:GLU:CD	5:BBB:408:HOH:O	2.43	0.57
1:AAA:132[B]:LYS:NZ	5:AAA:416:HOH:O	2.36	0.57
1:BBB:87[A]:GLN:NE2	5:BBB:407:HOH:O	2.26	0.57
1:AAA:182:ASN:HA	1:AAA:184:ILE:HD11	1.86	0.56
1:AAA:4[B]:HIS:HE1	5:AAA:480:HOH:O	1.88	0.56
1:BBB:221:GLU:HG3	5:BBB:523:HOH:O	2.05	0.56
1:AAA:129:GLU:HG3	5:AAA:592:HOH:O	2.04	0.56
1:AAA:151[B]:SER:OG	5:AAA:405:HOH:O	2.13	0.56
1:BBB:216:PHE:O	1:BBB:219[A]:ILE:HG22	2.07	0.55
1:AAA:215[A]:ARG:HD2	5:AAA:673:HOH:O	2.05	0.54
1:AAA:61:ILE:CD1	1:AAA:63:LYS:HE3	2.38	0.53
1:BBB:45[B]:GLU:CD	5:BBB:430:HOH:O	2.49	0.51
1:AAA:61:ILE:HD12	1:AAA:63:LYS:HE3	1.91	0.51
1:AAA:63:LYS:NZ	4:AAA:303[B]:RFW:O3	2.43	0.51
1:BBB:87[B]:GLN:NE2	1:BBB:87[B]:GLN:HA	2.26	0.51
1:AAA:16:GLU:OE1	1:AAA:208[B]:ARG:HD3	2.12	0.50
1:BBB:215:ARG:HD2	5:BBB:670:HOH:O	2.13	0.49
1:BBB:86:SER:O	1:BBB:87[B]:GLN:CB	2.60	0.48
1:AAA:208[B]:ARG:NH2	5:AAA:425:HOH:O	2.47	0.48
1:BBB:63:LYS:NZ	4:BBB:305[B]:RFW:C1	2.77	0.48
1:AAA:81:ASP:O	1:AAA:85[B]:GLU:HG3	2.14	0.48
1:AAA:63:LYS:HZ1	3:AAA:302[A]:LRY:H2	1.75	0.47
1:BBB:204:GLY:HA2	1:BBB:208[B]:ARG:HG3	1.97	0.47
4:AAA:303[B]:RFW:O7	4:AAA:303[B]:RFW:C1	2.63	0.46
1:AAA:216:PHE:O	1:AAA:219:ILE:HG22	2.16	0.46
1:AAA:204:GLY:HA2	1:AAA:208[B]:ARG:HB2	1.98	0.46
1:BBB:210:LYS:HE3	1:AAA:33:GLU:HB3	1.98	0.46
1:AAA:86:SER:C	1:AAA:87[B]:GLN:HG2	2.36	0.45
3:AAA:302[A]:LRY:O5	3:AAA:302[A]:LRY:C1	2.64	0.45
1:BBB:17:PRO:HD2	5:AAA:649:HOH:O	2.16	0.44
1:BBB:204:GLY:HA2	1:BBB:208[B]:ARG:CG	2.48	0.44
1:BBB:157:LEU:HD23	5:BBB:574:HOH:O	2.17	0.44
1:BBB:7[A]:ILE:HD12	1:BBB:38:GLY:HA3	1.99	0.44
1:BBB:149:TYR:CG	4:BBB:305[B]:RFW:H8B	2.54	0.43
1:BBB:149:TYR:CD1	4:BBB:305[B]:RFW:C8	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:3:PRO:HG2	1:BBB:37:VAL:HB	2.01	0.42
1:BBB:116:ALA:O	1:BBB:119[B]:VAL:HG22	2.20	0.41
1:BBB:18[A]:LEU:HD23	1:AAA:26[A]:LYS:HB3	2.03	0.41
1:BBB:87[B]:GLN:NE2	1:BBB:87[B]:GLN:CA	2.84	0.41
1:AAA:63:LYS:HA	1:AAA:72:PHE:O	2.20	0.41
1:AAA:123:ALA:HB2	1:AAA:139:PHE:CD2	2.55	0.41
1:BBB:63:LYS:NZ	4:BBB:305[B]:RFW:H3	2.36	0.41
1:BBB:63:LYS:HZ1	4:BBB:305[B]:RFW:H3	1.85	0.40
1:BBB:37:VAL:HG13	2:BBB:303:CL:CL	2.59	0.40

All (4) 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)
5:AAA:633:HOH:O	5:AAA:633:HOH:O[2_549]	1.49	0.71
5:BBB:558:HOH:O	5:AAA:636:HOH:O[1_455]	1.90	0.30
5:BBB:558:HOH:O	5:BBB:589:HOH:O[1_455]	2.11	0.09
5:AAA:511:HOH:O	5:AAA:570:HOH:O[2_549]	2.18	0.02

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	AAA	244/222 (110%)	235 (96%)	8 (3%)	1 (0%)	34	13
1	BBB	240/222 (108%)	234 (98%)	5 (2%)	1 (0%)	34	13
All	All	484/444 (109%)	469 (97%)	13 (3%)	2 (0%)	29	13

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	20	SER

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Mol	Chain	Res	Type
1	BBB	20	SER

### 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	AAA	215/190 (113%)	213 (99%)	2 (1%)	78	60
1	BBB	210/190 (110%)	208 (99%)	2 (1%)	76	56
All	All	425/380 (112%)	421 (99%)	4 (1%)	73	60

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	93	LEU
1	BBB	106	ASP
1	AAA	93	LEU
1	AAA	161	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

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	LRY	BBB	304[A]	4	17,18,18	0.87	0	21,25,25	1.09	1 (4%)
4	RFW	BBB	305[B]	3	17,18,18	0.50	0	21,25,25	0.99	1 (4%)
3	LRY	AAA	302[A]	4	17,18,18	0.71	0	21,25,25	0.79	0
4	RFW	AAA	303[B]	3	17,18,18	0.37	0	21,25,25	0.61	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
3	LRY	BBB	304[A]	4	-	6/22/24/24	-
4	RFW	BBB	305[B]	3	-	2/22/24/24	-
3	LRY	AAA	302[A]	4	-	5/22/24/24	-
4	RFW	AAA	303[B]	3	-	10/22/24/24	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BBB	304[A]	LRY	OP2-P-O6	3.28	115.45	106.73
4	BBB	305[B]	RFW	C2-N2-C7	-3.15	119.68	123.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	BBB	305[B]	RFW	C1-C2-N2-C7
4	AAA	303[B]	RFW	C6-O6-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	AAA	303[B]	RFW	C6-O6-P-O2P
4	AAA	303[B]	RFW	C1-C2-N2-C7
3	BBB	304[A]	LRY	C8-C7-N-C2
3	BBB	304[A]	LRY	O3-C3-C4-C5
3	AAA	302[A]	LRY	O3-C3-C4-C5
3	BBB	304[A]	LRY	C1-C2-C3-O3
3	AAA	302[A]	LRY	C1-C2-C3-O3
3	BBB	304[A]	LRY	C2-C3-C4-C5
3	BBB	304[A]	LRY	O7-C7-N-C2
4	AAA	303[B]	RFW	C6-O6-P-O3P
4	AAA	303[B]	RFW	C1-C2-C3-O3
3	AAA	302[A]	LRY	C2-C3-C4-C5
4	AAA	303[B]	RFW	C1-C2-C3-C4
4	AAA	303[B]	RFW	C8-C7-N2-C2
4	AAA	303[B]	RFW	O5-C5-C6-O6
4	AAA	303[B]	RFW	N2-C2-C3-C4
3	BBB	304[A]	LRY	C1-C2-C3-C4
3	AAA	302[A]	LRY	C1-C2-C3-C4
4	BBB	305[B]	RFW	C2-C3-C4-C5
4	AAA	303[B]	RFW	O7-C7-N2-C2
3	AAA	302[A]	LRY	O3-C3-C4-O4

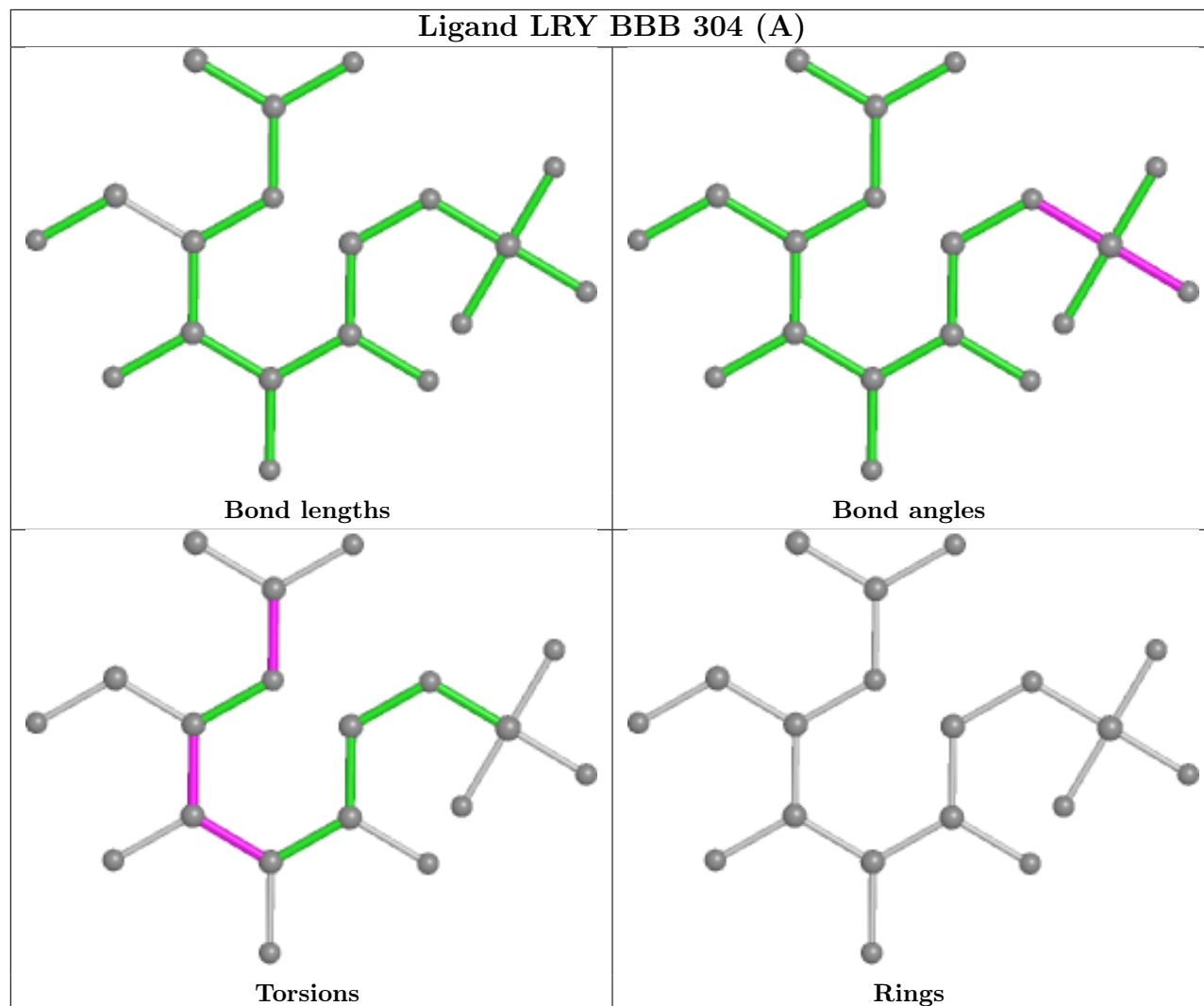
There are no ring outliers.

4 monomers are involved in 24 short contacts:

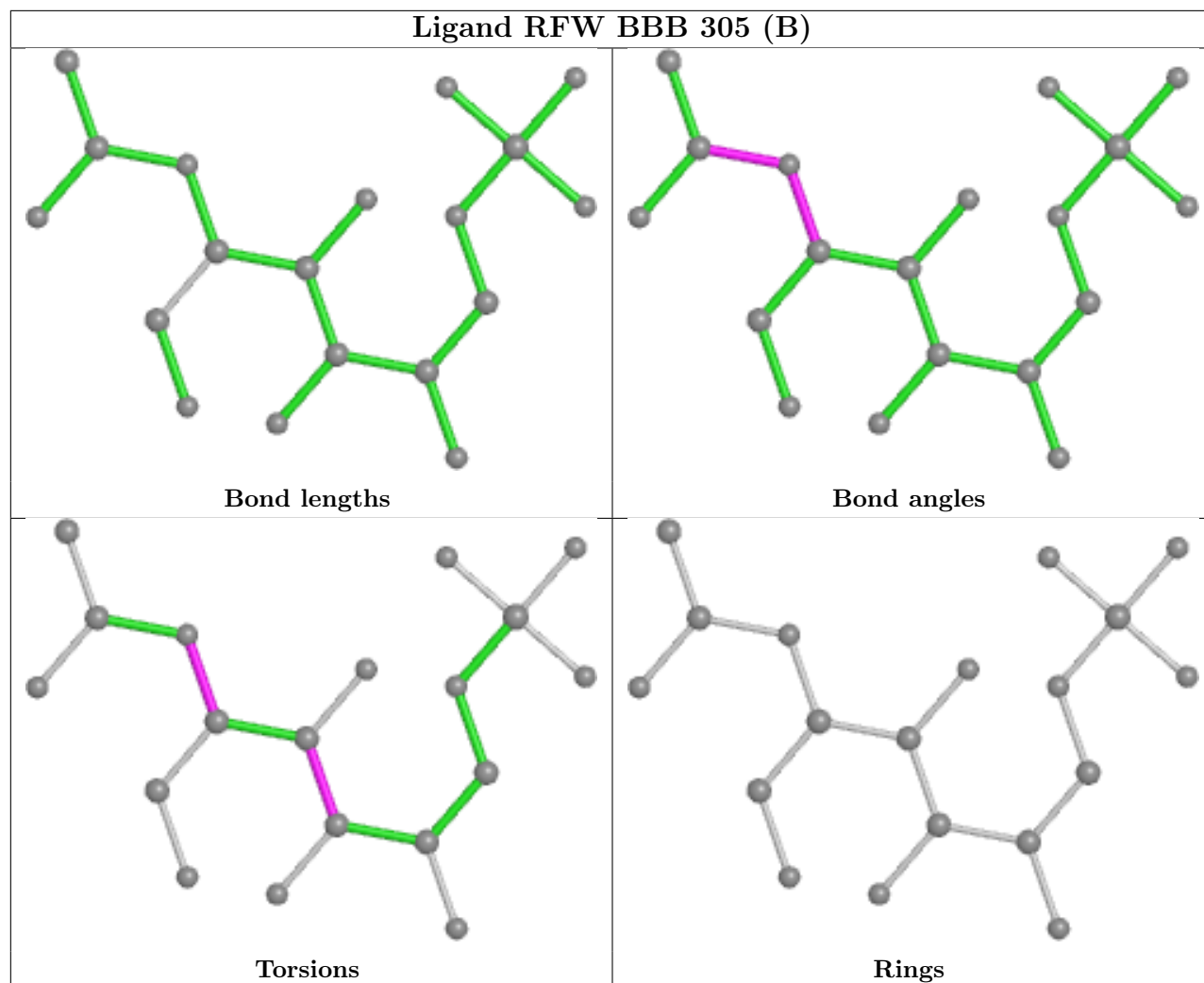
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	BBB	304[A]	LRY	6	0
4	BBB	305[B]	RFW	10	0
3	AAA	302[A]	LRY	5	0
4	AAA	303[B]	RFW	3	0

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.

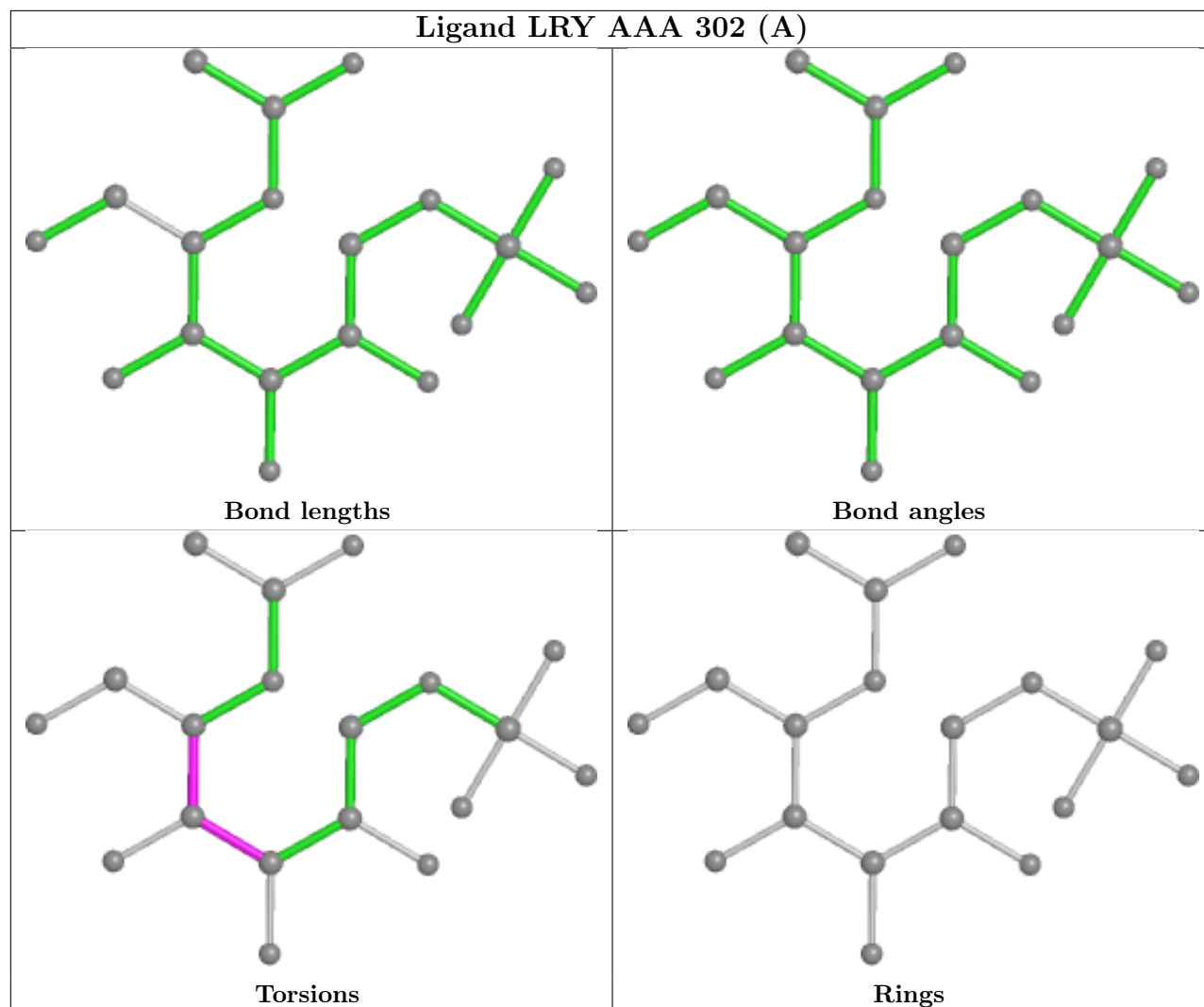


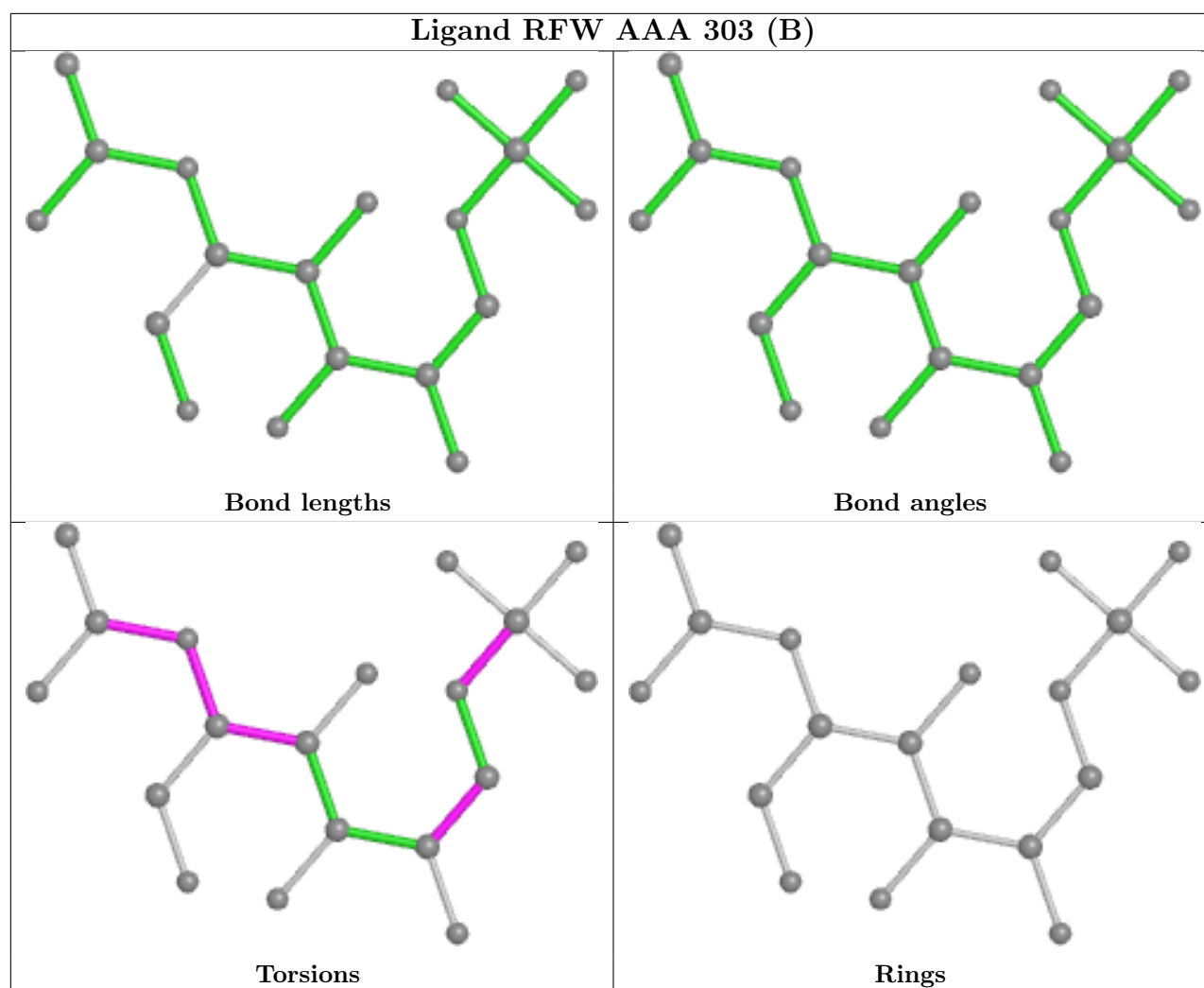
## Ligand RFW BBB 305 (B)





## Ligand LRY AAA 302 (A)





## 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	AAA	222/222 (100%)	-0.00	2 (0%) 84 87	5, 11, 20, 57	0
1	BBB	222/222 (100%)	-0.03	3 (1%) 75 79	5, 10, 20, 52	0
All	All	444/444 (100%)	-0.02	5 (1%) 80 84	5, 11, 20, 57	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	222	ASP	5.8
1	BBB	222	ASP	3.9
1	BBB	68	HIS	3.0
1	BBB	171	GLN	2.2
1	AAA	68	HIS	2.0

### 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](#)

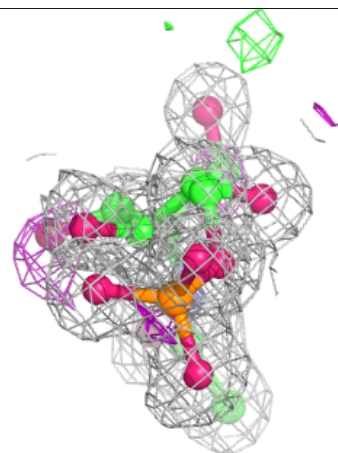
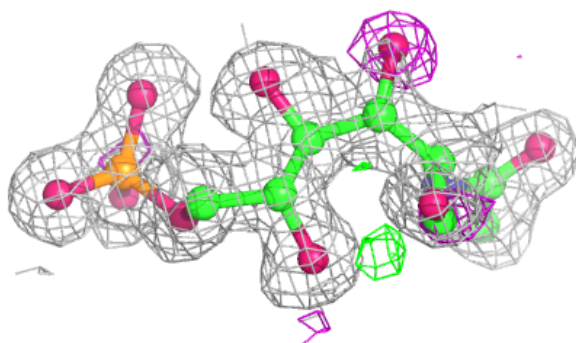
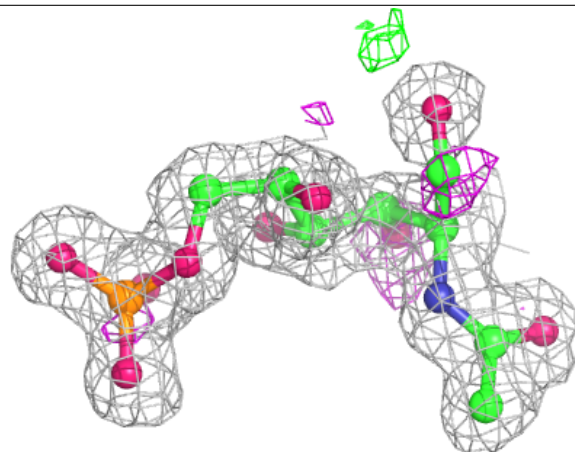
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	LRY	AAA	302[A]	19/19	0.93	0.12	5,9,15,15	19
3	LRY	BBB	304[A]	19/19	0.96	0.10	4,9,12,13	19
4	RFW	AAA	303[B]	19/19	0.96	0.13	46,51,61,64	19
4	RFW	BBB	305[B]	19/19	0.97	0.11	16,23,33,36	19
2	CL	BBB	301	1/1	0.99	0.05	17,17,17,17	0
2	CL	BBB	302	1/1	0.99	0.09	24,24,24,24	0
2	CL	BBB	303	1/1	0.99	0.07	24,24,24,24	0
2	CL	AAA	301	1/1	0.99	0.05	16,16,16,16	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.

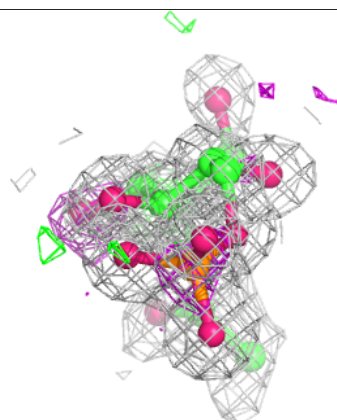
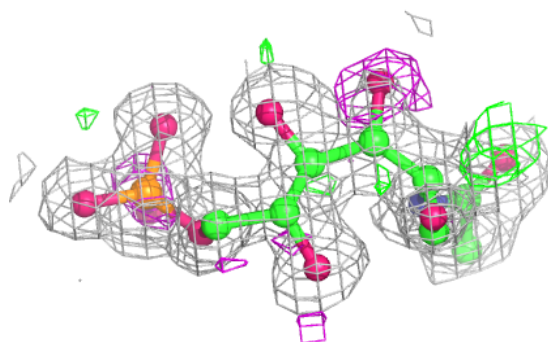
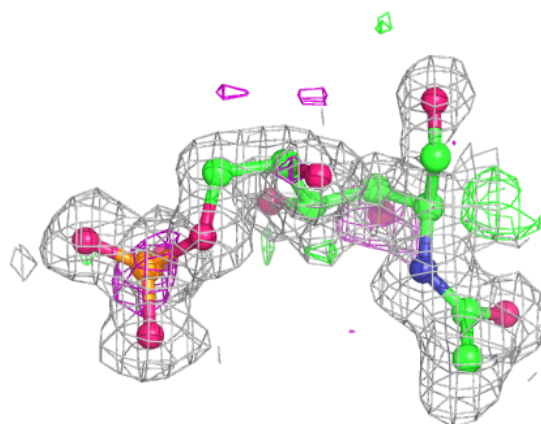
**Electron density around LRY AAA 302 (A):**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

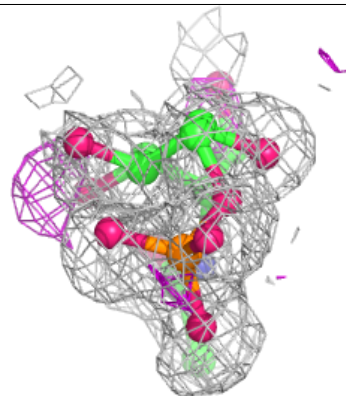
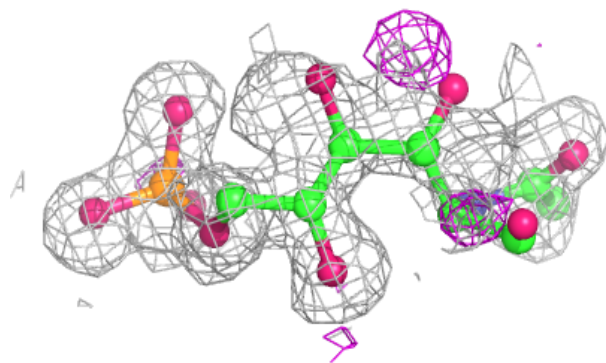
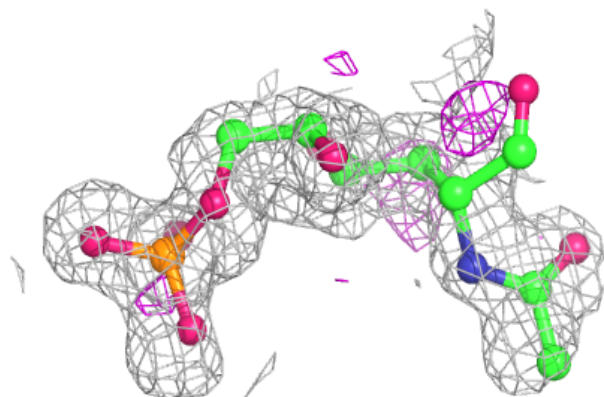


**Electron density around LRY BBB 304 (A):**

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

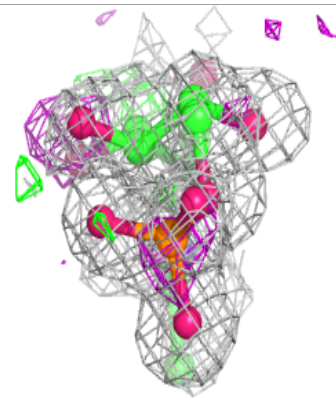
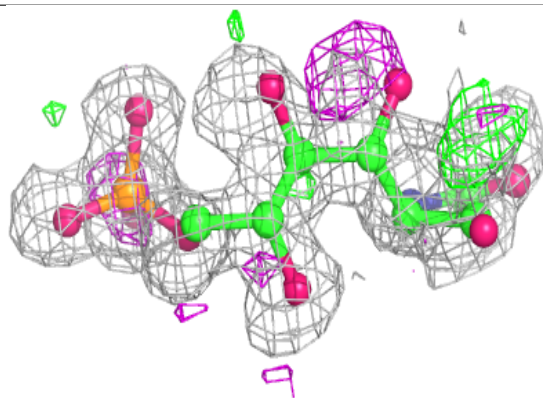
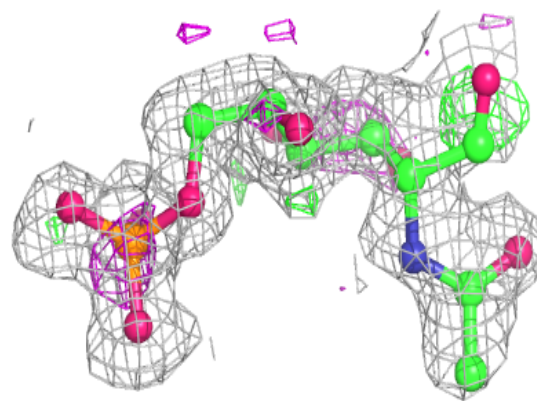
**Electron density around RFW AAA 303 (B):**

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



**Electron density around RFW BBB 305 (B):**

$2mF_o - DF_c$  (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.