



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2025 – 02:11 PM EST

PDB ID : 9DQ7  
Title : Borrelia burgdorferi LDH with NADH, oxamate and FBS  
Authors : Lynch, M.J.  
Deposited on : 2024-09-23  
Resolution : 2.11 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

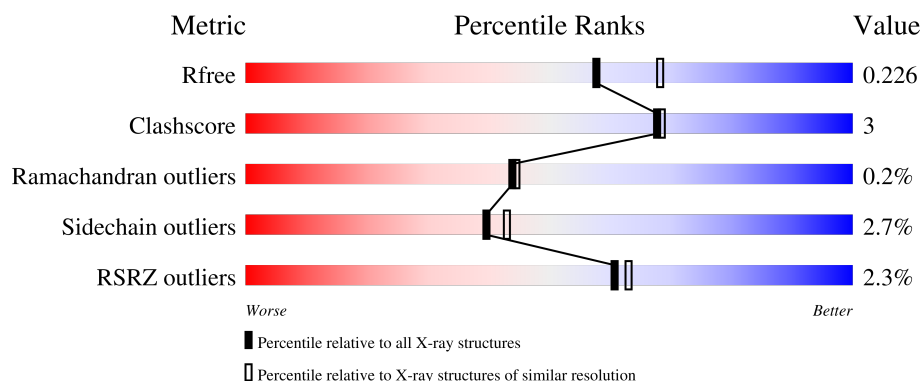
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 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))
$R_{free}$	164625	7689 (2.14-2.10)
Clashscore	180529	8431 (2.14-2.10)
Ramachandran outliers	177936	8366 (2.14-2.10)
Sidechain outliers	177891	8367 (2.14-2.10)
RSRZ outliers	164620	7689 (2.14-2.10)

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	314	<div> <div>0%</div> <div>93%</div> <div>7%</div> </div>
1	B	314	<div> <div>2%</div> <div>92%</div> <div>7%</div> </div>
1	C	314	<div> <div>4%</div> <div>93%</div> <div>6%</div> </div>
1	P	314	<div> <div>2%</div> <div>92%</div> <div>7%</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
3	OXM	B	401	-	X	-	-
3	OXM	C	402	-	X	-	-

2 Entry composition ⓘ

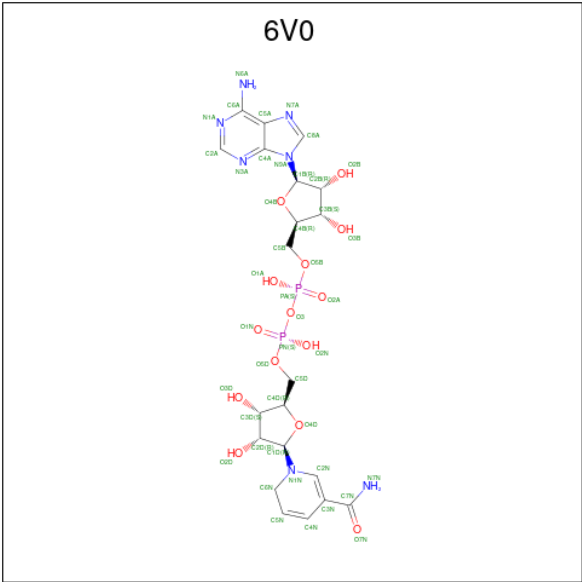
There are 6 unique types of molecules in this entry. The entry contains 20417 atoms, of which 10102 are hydrogens and 0 are deuteriums.

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-lactate dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	P	314	Total	C	H	N	O	S	0	0	0
			4924	1564	2492	397	461	10			
1	A	314	Total	C	H	N	O	S	0	0	0
			4923	1564	2491	397	461	10			
1	B	314	Total	C	H	N	O	S	0	0	0
			4923	1564	2491	397	461	10			
1	C	314	Total	C	H	N	O	S	0	0	0
			4924	1564	2492	397	461	10			

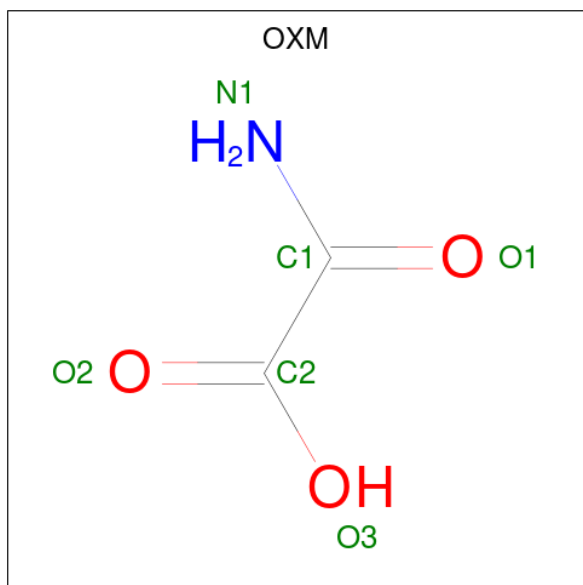
- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(5-aminocarbonyl-2 {H}-pyridin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (three-letter code: 6V0) (formula: C<sub>21</sub>H<sub>29</sub>N<sub>7</sub>O<sub>14</sub>P<sub>2</sub>).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			71	21	27	7	14		
2	B	1	Total	C	H	N	O	0	0
			71	21	27	7	14		
2	C	1	Total	C	H	N	O	0	0
			71	21	27	7	14		

- Molecule 3 is OXAMIC ACID (three-letter code: OXM) (formula:  $C_2H_3NO_3$ ).

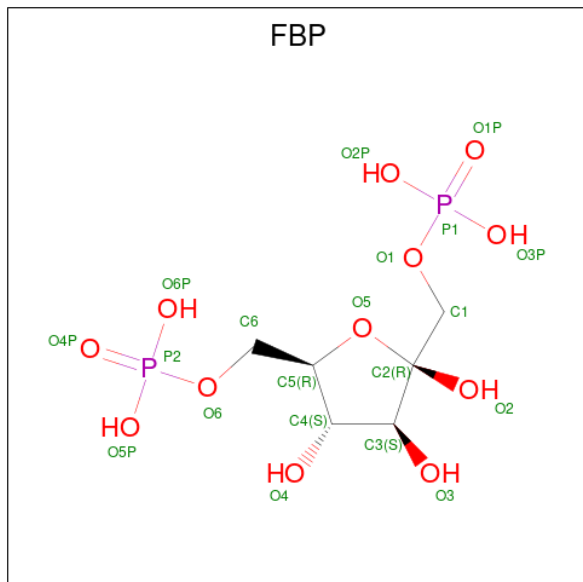


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	P	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	A	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	B	1	Total	C	H	N	O	0	0
			8	2	2	1	3		
3	C	1	Total	C	H	N	O	0	0
			8	2	2	1	3		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula:  $C_6H_{14}O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	O	P	0	0
			30	6	10	12	2		
5	B	1	Total	C	H	O	P	0	0
			30	6	10	12	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	90	Total	O	0	0
			90	90		
6	A	86	Total	O	0	0
			86	86		
6	B	80	Total	O	0	0
			80	80		
6	C	89	Total	O	0	0
			89	89		

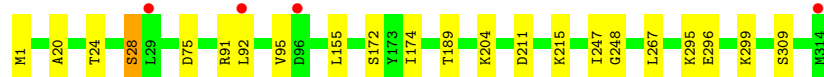
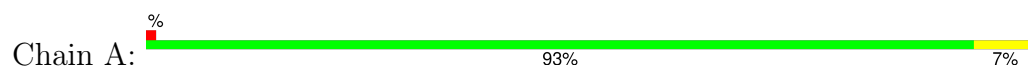
### 3 Residue-property plots [i](#)

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-lactate dehydrogenase



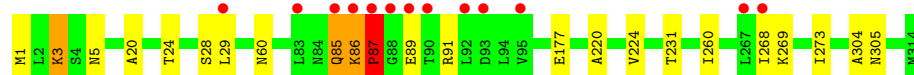
- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase



- Molecule 1: L-lactate dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.96Å 91.25Å 166.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.11 48.98 – 2.11	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.98-2.11) 98.7 (48.98-2.11)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.175 , 0.222 0.183 , 0.226	Depositor DCC
$R_{free}$ test set	69721 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 39.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: FBP, OXM, CA, 6V0

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	0.31	0/2473	0.51	0/3341
1	B	0.35	0/2473	0.52	0/3341
1	C	0.33	0/2473	0.52	0/3341
1	P	0.35	0/2473	0.52	0/3341
All	All	0.33	0/9892	0.52	0/13364

There are no bond length outliers.

There are no bond angle outliers.

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	2432	2491	2490	19	0
1	B	2432	2491	2490	20	0
1	C	2432	2492	2490	17	0
1	P	2432	2492	2490	14	0
2	A	44	27	0	2	0
2	B	44	27	0	2	0
2	C	44	27	0	2	0
2	P	44	27	0	2	0
3	A	6	2	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	2	2	1	0
3	C	6	2	2	0	0
3	P	6	2	2	0	0
4	C	1	0	0	0	0
4	P	1	0	0	0	0
5	A	20	10	9	0	0
5	B	20	10	9	1	0
6	A	86	0	0	2	0
6	B	80	0	0	1	0
6	C	89	0	0	0	0
6	P	90	0	0	5	0
All	All	10315	10102	9986	69	0

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 3.

All (69) 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)
2:A:401:6V0:C1D	2:A:401:6V0:O4D	1.64	1.23
2:P:401:6V0:O4D	2:P:401:6V0:C1D	1.64	1.20
2:B:403:6V0:C1B	2:B:403:6V0:O4B	1.66	1.20
2:A:401:6V0:O4B	2:A:401:6V0:C1B	1.66	1.18
2:B:403:6V0:O4D	2:B:403:6V0:C1D	1.64	1.18
5:B:402:FBP:C5	5:B:402:FBP:O5	1.63	1.18
2:C:401:6V0:C1B	2:C:401:6V0:O4B	1.66	1.14
2:P:401:6V0:O4B	2:P:401:6V0:C1B	1.67	1.14
2:C:401:6V0:O4D	2:C:401:6V0:C1D	1.64	1.12
1:A:91:ARG:O	1:A:95:VAL:HG23	1.74	0.88
1:B:95:VAL:O	1:B:99:SER:OG	2.02	0.77
1:B:48:MET:HE2	1:C:224:VAL:HG22	1.72	0.69
1:A:247:ILE:HG22	1:B:29:LEU:CD1	2.25	0.66
1:B:29:LEU:HD22	1:B:31:HIS:CE1	2.31	0.66
1:C:268:ILE:HD11	1:C:305:ASN:OD1	1.96	0.65
1:A:248:GLY:HA2	1:B:29:LEU:HD21	1.77	0.65
1:P:295:LYS:HG2	6:P:528:HOH:O	1.97	0.64
1:A:28:SER:OG	1:A:28:SER:O	2.17	0.63
1:P:248:GLY:HA2	1:C:29:LEU:HD11	1.83	0.61
1:B:299:LYS:HE2	6:B:579:HOH:O	2.00	0.60
1:C:268:ILE:HG21	1:C:304:ALA:HB1	1.85	0.57
1:A:295:LYS:HE2	1:A:299:LYS:NZ	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:532:HOH:O	1:B:193:MET:CE	2.54	0.56
1:P:29:LEU:HD22	1:C:29:LEU:HB3	1.87	0.56
1:A:91:ARG:NE	1:A:91:ARG:HA	2.21	0.55
1:C:220:ALA:O	1:C:224:VAL:HG23	2.07	0.54
1:P:95:VAL:HG22	1:P:124:PRO:HG3	1.90	0.54
6:P:568:HOH:O	1:C:1:MET:HA	2.08	0.53
1:A:20:ALA:O	1:A:24:THR:HG23	2.08	0.53
1:A:247:ILE:HG22	1:B:29:LEU:HD11	1.88	0.53
1:A:92:LEU:C	1:A:92:LEU:HD13	2.29	0.53
1:A:91:ARG:HA	1:A:91:ARG:HE	1.74	0.52
1:C:28:SER:O	1:C:28:SER:OG	2.27	0.52
6:P:532:HOH:O	1:B:193:MET:HE2	2.08	0.51
1:P:247:ILE:HG22	1:C:29:LEU:HD21	1.92	0.51
1:P:267:LEU:HD12	1:P:267:LEU:H	1.76	0.51
1:A:295:LYS:HE2	1:A:299:LYS:HZ2	1.76	0.50
1:A:155:LEU:HD22	1:A:174:ILE:HG12	1.96	0.47
1:C:3:LYS:HE3	1:C:5:ASN:OD1	2.15	0.47
1:P:36:ILE:HD11	1:P:67:THR:O	2.16	0.46
1:B:48:MET:CE	1:C:224:VAL:HG22	2.41	0.46
1:A:299:LYS:NZ	6:A:501:HOH:O	2.47	0.46
1:B:106:ILE:CD1	1:B:132:THR:HG23	2.46	0.45
1:B:20:ALA:O	1:B:24:THR:HG23	2.17	0.45
1:C:85:GLN:HG2	1:C:89:GLU:HA	1.98	0.45
1:A:295:LYS:HG3	1:A:296:GLU:N	2.31	0.44
1:P:313:LYS:HD2	1:P:313:LYS:O	2.17	0.44
6:P:532:HOH:O	1:B:193:MET:HE1	2.17	0.44
1:C:86:LYS:N	1:C:87:PRO:CD	2.81	0.44
1:B:85:GLN:O	1:B:86:LYS:HG2	2.17	0.44
1:C:20:ALA:O	1:C:24:THR:HG23	2.18	0.44
1:A:172:SER:HB2	1:A:189:THR:HG23	2.00	0.43
1:P:247:ILE:HG22	1:C:29:LEU:CD2	2.48	0.43
1:P:250:GLN:HB3	1:P:252:VAL:HG13	2.00	0.43
1:P:140:ILE:HD12	1:P:141:HIS:N	2.33	0.43
1:A:92:LEU:HD13	1:A:92:LEU:O	2.18	0.43
1:B:91:ARG:NH2	3:B:401:OXM:O2	2.51	0.43
1:B:106:ILE:HD12	1:B:132:THR:HG23	2.01	0.42
1:B:268:ILE:HD13	1:B:304:ALA:HB3	2.01	0.42
1:A:267:LEU:HD12	1:A:267:LEU:O	2.20	0.42
1:C:260:ILE:HG13	1:C:273:ILE:HG22	2.02	0.42
1:P:292:ILE:HD11	1:P:297:LEU:HA	2.01	0.42
1:P:92:LEU:O	1:P:95:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:106:ILE:CD1	1:P:132:THR:HG23	2.49	0.42
1:C:269:LYS:HB3	1:C:269:LYS:HE2	1.94	0.41
6:A:578:HOH:O	1:B:1:MET:HE2	2.19	0.41
1:B:268:ILE:HG23	1:B:308:LYS:HD3	2.03	0.41
1:A:75:ASP:HA	1:B:1:MET:SD	2.61	0.40
1:A:211:ASP:O	1:A:215:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

## 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	312/314 (99%)	299 (96%)	13 (4%)	0	100	100
1	B	312/314 (99%)	298 (96%)	13 (4%)	1 (0%)	37	36
1	C	312/314 (99%)	297 (95%)	14 (4%)	1 (0%)	37	36
1	P	312/314 (99%)	303 (97%)	9 (3%)	0	100	100
All	All	1248/1256 (99%)	1197 (96%)	49 (4%)	2 (0%)	44	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	LEU
1	C	87	PRO

### 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	270/270 (100%)	266 (98%)	4 (2%)	60	67
1	B	270/270 (100%)	260 (96%)	10 (4%)	29	30
1	C	270/270 (100%)	262 (97%)	8 (3%)	36	38
1	P	270/270 (100%)	263 (97%)	7 (3%)	41	45
All	All	1080/1080 (100%)	1051 (97%)	29 (3%)	40	43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	1	MET
1	P	28	SER
1	P	29	LEU
1	P	100	LYS
1	P	115	ASP
1	P	231	THR
1	P	313	LYS
1	A	1	MET
1	A	28	SER
1	A	204	LYS
1	A	309	SER
1	B	1	MET
1	B	60	ASN
1	B	69	LYS
1	B	96	ASP
1	B	99	SER
1	B	111	SER
1	B	142	LYS
1	B	302	SER
1	B	308	LYS
1	B	314	MET
1	C	3	LYS
1	C	60	ASN
1	C	85	GLN
1	C	86	LYS
1	C	87	PRO
1	C	91	ARG
1	C	177	GLU
1	C	231	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	241	ASN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	OXM	C	402	-	5,5,5	2.53	2 (40%)	2,6,6	1.43	0
2	6V0	P	401	-	43,48,48	4.68	20 (46%)	49,73,73	1.57	7 (14%)
3	OXM	A	402	-	5,5,5	2.56	3 (60%)	2,6,6	1.25	0
5	FBP	A	403	-	18,20,20	4.03	5 (27%)	21,32,32	1.08	1 (4%)
2	6V0	C	401	-	43,48,48	4.62	18 (41%)	49,73,73	1.36	5 (10%)
3	OXM	P	402	-	5,5,5	2.56	3 (60%)	2,6,6	1.01	0
2	6V0	B	403	-	43,48,48	4.66	19 (44%)	49,73,73	1.38	5 (10%)
5	FBP	B	402	-	18,20,20	3.90	5 (27%)	21,32,32	0.69	0
2	6V0	A	401	-	43,48,48	4.58	19 (44%)	49,73,73	1.33	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	OXM	B	401	-	5,5,5	2.54	2 (40%)	2,6,6	1.28	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	OXM	C	402	-	-	4/4/4/4	-
2	6V0	P	401	-	-	7/26/72/72	0/5/5/5
3	OXM	A	402	-	-	0/4/4/4	-
5	FBP	A	403	-	-	0/13/32/32	0/1/1/1
2	6V0	C	401	-	-	3/26/72/72	0/5/5/5
3	OXM	P	402	-	-	1/4/4/4	-
2	6V0	B	403	-	-	4/26/72/72	0/5/5/5
5	FBP	B	402	-	-	0/13/32/32	0/1/1/1
2	6V0	A	401	-	-	4/26/72/72	0/5/5/5
3	OXM	B	401	-	-	4/4/4/4	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	401	6V0	O4B-C1B	20.08	1.67	1.40
2	B	403	6V0	O4B-C1B	19.66	1.66	1.40
2	C	401	6V0	O4B-C1B	19.35	1.66	1.40
2	A	401	6V0	O4B-C1B	19.16	1.66	1.40
5	A	403	FBP	O5-C2	-10.54	1.26	1.43
2	C	401	6V0	O4D-C1D	9.91	1.64	1.42
2	A	401	6V0	O4D-C1D	9.75	1.64	1.42
2	B	403	6V0	O4D-C1D	9.70	1.64	1.42
2	P	401	6V0	O4D-C1D	9.65	1.64	1.42
5	B	402	FBP	O5-C5	9.07	1.63	1.43
5	A	403	FBP	C4-C5	-9.03	1.30	1.53
5	B	402	FBP	O5-C2	-9.01	1.29	1.43
5	B	402	FBP	C4-C5	-8.69	1.31	1.53
2	B	403	6V0	PN-O3	8.48	1.68	1.59
2	P	401	6V0	PN-O3	8.44	1.68	1.59
2	C	401	6V0	PN-O3	8.11	1.68	1.59
2	A	401	6V0	PN-O3	8.08	1.68	1.59
2	P	401	6V0	C4N-C5N	7.94	1.53	1.33
2	B	403	6V0	C4N-C5N	7.93	1.53	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	6V0	C4N-C5N	7.87	1.53	1.33
5	A	403	FBP	O5-C5	7.82	1.61	1.43
2	C	401	6V0	C4N-C5N	7.81	1.53	1.33
2	C	401	6V0	C2D-C1D	-7.35	1.30	1.53
2	P	401	6V0	C2D-C1D	-7.19	1.30	1.53
2	B	403	6V0	C2D-C1D	-7.19	1.30	1.53
2	A	401	6V0	C2D-C1D	-7.18	1.30	1.53
2	A	401	6V0	O4B-C4B	-6.76	1.30	1.45
2	B	403	6V0	O4D-C4D	-6.76	1.30	1.45
2	C	401	6V0	O4B-C4B	-6.67	1.30	1.45
2	C	401	6V0	O4D-C4D	-6.62	1.30	1.45
2	P	401	6V0	O4D-C4D	-6.61	1.30	1.45
2	B	403	6V0	O4B-C4B	-6.52	1.30	1.45
2	A	401	6V0	O4D-C4D	-6.51	1.30	1.45
2	P	401	6V0	O4B-C4B	-6.26	1.31	1.45
2	C	401	6V0	C2N-C3N	5.85	1.54	1.37
2	B	403	6V0	C2N-C3N	5.77	1.54	1.37
2	A	401	6V0	C2N-C3N	5.76	1.54	1.37
2	P	401	6V0	C2N-C3N	5.67	1.53	1.37
2	B	403	6V0	C4N-C3N	5.21	1.54	1.43
2	C	401	6V0	C4N-C3N	5.19	1.53	1.43
2	P	401	6V0	C4N-C3N	5.18	1.53	1.43
2	A	401	6V0	C4N-C3N	5.15	1.53	1.43
3	A	402	OXM	C1-N1	4.35	1.46	1.33
3	B	401	OXM	C1-N1	4.30	1.45	1.33
3	P	402	OXM	C1-N1	4.21	1.45	1.33
3	C	402	OXM	C1-N1	4.19	1.45	1.33
2	C	401	6V0	PA-O3	4.15	1.64	1.59
2	B	403	6V0	PA-O3	4.05	1.63	1.59
2	A	401	6V0	PA-O3	3.95	1.63	1.59
2	P	401	6V0	PA-O3	3.88	1.63	1.59
5	A	403	FBP	O3-C3	-3.58	1.35	1.42
2	A	401	6V0	C7N-N7N	3.43	1.43	1.33
2	C	401	6V0	C7N-N7N	3.41	1.43	1.33
5	B	402	FBP	O3-C3	-3.34	1.36	1.42
2	B	403	6V0	C7N-N7N	3.34	1.43	1.33
2	P	401	6V0	C7N-N7N	3.22	1.42	1.33
5	B	402	FBP	O4-C4	3.19	1.50	1.43
2	A	401	6V0	C6A-N6A	3.18	1.45	1.34
2	P	401	6V0	C6A-N6A	3.11	1.45	1.34
2	C	401	6V0	C6A-N6A	3.10	1.45	1.34
2	B	403	6V0	C6A-N6A	3.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	401	6V0	O3D-C3D	-2.96	1.35	1.43
2	B	403	6V0	O3D-C3D	-2.93	1.35	1.43
5	A	403	FBP	O4-C4	2.91	1.50	1.43
2	A	401	6V0	O3D-C3D	-2.88	1.35	1.43
2	C	401	6V0	O3D-C3D	-2.85	1.35	1.43
2	B	403	6V0	O3B-C3B	-2.64	1.36	1.43
2	A	401	6V0	O7N-C7N	-2.62	1.18	1.24
2	A	401	6V0	O3B-C3B	-2.62	1.36	1.43
2	P	401	6V0	O7N-C7N	-2.59	1.18	1.24
2	C	401	6V0	O3B-C3B	-2.58	1.36	1.43
2	C	401	6V0	O7N-C7N	-2.56	1.18	1.24
2	B	403	6V0	O7N-C7N	-2.55	1.18	1.24
2	P	401	6V0	O3B-C3B	-2.55	1.36	1.43
2	C	401	6V0	C2N-N1N	2.44	1.43	1.35
2	A	401	6V0	C2N-N1N	2.38	1.42	1.35
2	B	403	6V0	C2N-N1N	2.38	1.42	1.35
3	C	402	OXM	O1-C1	-2.33	1.19	1.24
3	P	402	OXM	C1-C2	-2.32	1.52	1.55
2	B	403	6V0	PA-O5B	2.27	1.68	1.59
3	P	402	OXM	O1-C1	-2.27	1.19	1.24
3	A	402	OXM	O1-C1	-2.26	1.19	1.24
2	P	401	6V0	C2N-N1N	2.26	1.42	1.35
3	B	401	OXM	O1-C1	-2.23	1.19	1.24
2	P	401	6V0	C2B-C3B	2.23	1.59	1.53
2	P	401	6V0	O2B-C2B	2.17	1.48	1.43
2	B	403	6V0	C5D-C4D	2.15	1.58	1.51
2	P	401	6V0	PA-O5B	2.14	1.67	1.59
2	A	401	6V0	O2B-C2B	2.13	1.48	1.43
2	C	401	6V0	PA-O5B	2.13	1.67	1.59
2	A	401	6V0	PA-O5B	2.13	1.67	1.59
3	A	402	OXM	C1-C2	-2.09	1.53	1.55
2	A	401	6V0	O2D-C2D	2.08	1.48	1.43
2	P	401	6V0	C5D-C4D	2.08	1.57	1.51
2	B	403	6V0	O2D-C2D	2.07	1.48	1.43
2	C	401	6V0	O2B-C2B	2.00	1.47	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	401	6V0	C4B-O4B-C1B	-6.05	104.39	109.92
2	A	401	6V0	C4B-O4B-C1B	-4.78	105.55	109.92
2	P	401	6V0	N3A-C2A-N1A	-4.69	122.30	128.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	403	6V0	N3A-C2A-N1A	-4.67	122.33	128.67
2	B	403	6V0	C4B-O4B-C1B	-4.63	105.68	109.92
2	C	401	6V0	N3A-C2A-N1A	-4.54	122.50	128.67
2	A	401	6V0	N3A-C2A-N1A	-4.52	122.53	128.67
2	C	401	6V0	C4B-O4B-C1B	-4.47	105.83	109.92
2	A	401	6V0	C5N-C4N-C3N	-3.19	114.17	121.50
2	P	401	6V0	O4B-C1B-N9A	3.17	112.95	108.75
2	P	401	6V0	C5N-C4N-C3N	-3.07	114.46	121.50
2	C	401	6V0	C5N-C4N-C3N	-2.99	114.65	121.50
2	B	403	6V0	C5N-C4N-C3N	-2.96	114.71	121.50
2	C	401	6V0	C2N-C3N-C4N	2.79	121.44	117.97
2	P	401	6V0	C4A-C5A-N7A	-2.73	106.45	109.34
2	C	401	6V0	C4A-C5A-N7A	-2.67	106.52	109.34
2	P	401	6V0	C2N-C3N-C4N	2.66	121.29	117.97
2	B	403	6V0	C4A-C5A-N7A	-2.63	106.56	109.34
2	A	401	6V0	C4A-C5A-N7A	-2.41	106.79	109.34
2	P	401	6V0	C1B-N9A-C4A	-2.40	122.42	126.64
2	B	403	6V0	C2N-C3N-C4N	2.33	120.88	117.97
2	A	401	6V0	C2N-C3N-C4N	2.28	120.81	117.97
5	A	403	FBP	O2P-P1-O1	2.08	112.09	106.67

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	6V0	C4N-C3N-C7N-N7N
3	P	402	OXM	O1-C1-C2-O3
3	B	401	OXM	N1-C1-C2-O2
3	B	401	OXM	N1-C1-C2-O3
3	B	401	OXM	O1-C1-C2-O2
3	B	401	OXM	O1-C1-C2-O3
3	C	402	OXM	N1-C1-C2-O3
3	C	402	OXM	O1-C1-C2-O3
2	P	401	6V0	C3B-C4B-C5B-O5B
2	P	401	6V0	O4B-C4B-C5B-O5B
2	P	401	6V0	C4N-C3N-C7N-O7N
2	B	403	6V0	C4N-C3N-C7N-O7N
2	C	401	6V0	C2D-C1D-N1N-C2N
2	A	401	6V0	C4N-C3N-C7N-O7N
2	A	401	6V0	C2D-C1D-N1N-C2N
2	B	403	6V0	C2D-C1D-N1N-C2N
2	P	401	6V0	C2D-C1D-N1N-C2N

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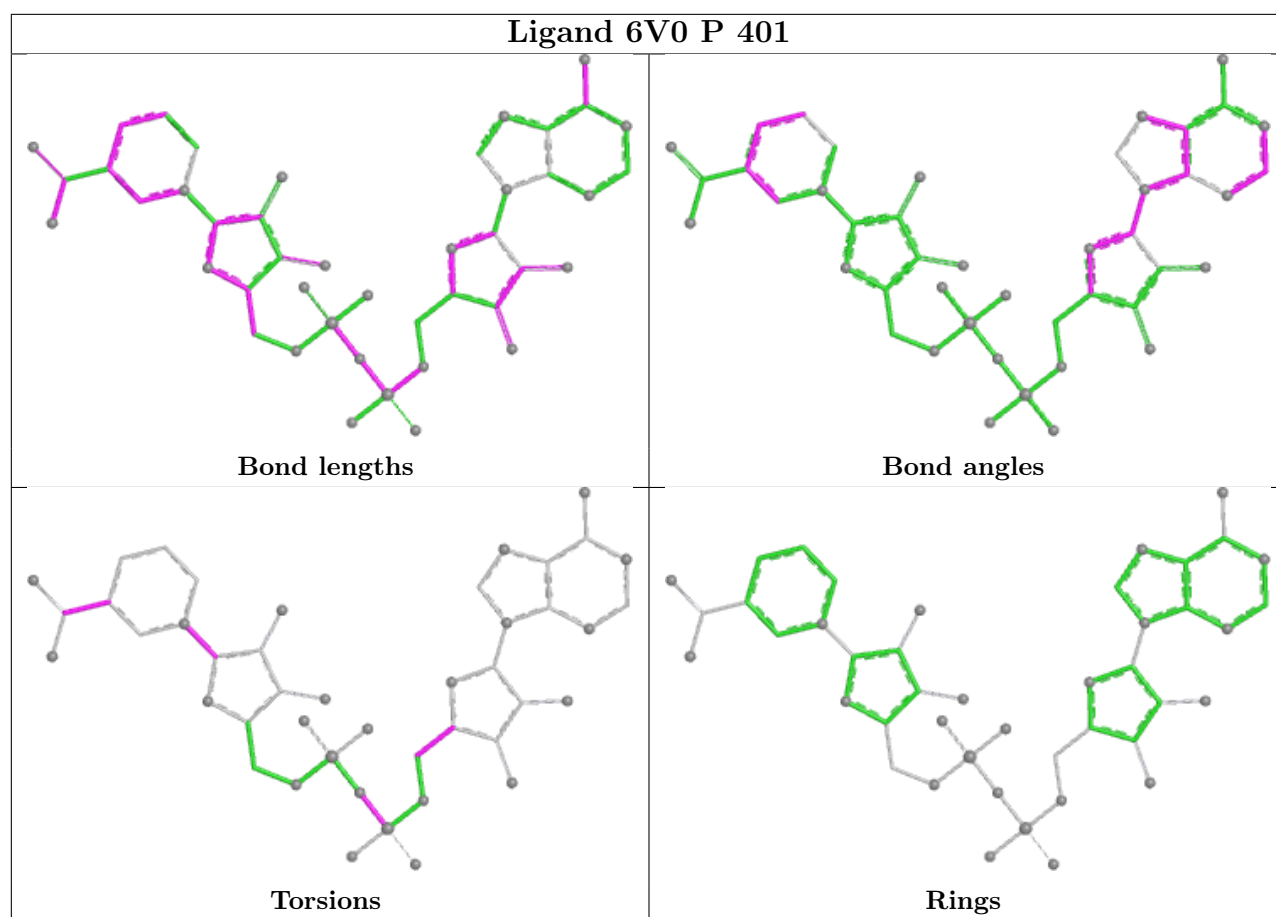
Mol	Chain	Res	Type	Atoms
2	C	401	6V0	O4D-C1D-N1N-C2N
2	P	401	6V0	PN-O3-PA-O2A
2	A	401	6V0	O4D-C1D-N1N-C2N
2	B	403	6V0	O4D-C1D-N1N-C2N
2	C	401	6V0	C2D-C1D-N1N-C6N
2	P	401	6V0	O4D-C1D-N1N-C2N
3	C	402	OXM	O1-C1-C2-O2
3	C	402	OXM	N1-C1-C2-O2
2	B	403	6V0	O4B-C4B-C5B-O5B
2	P	401	6V0	PN-O3-PA-O1A

There are no ring outliers.

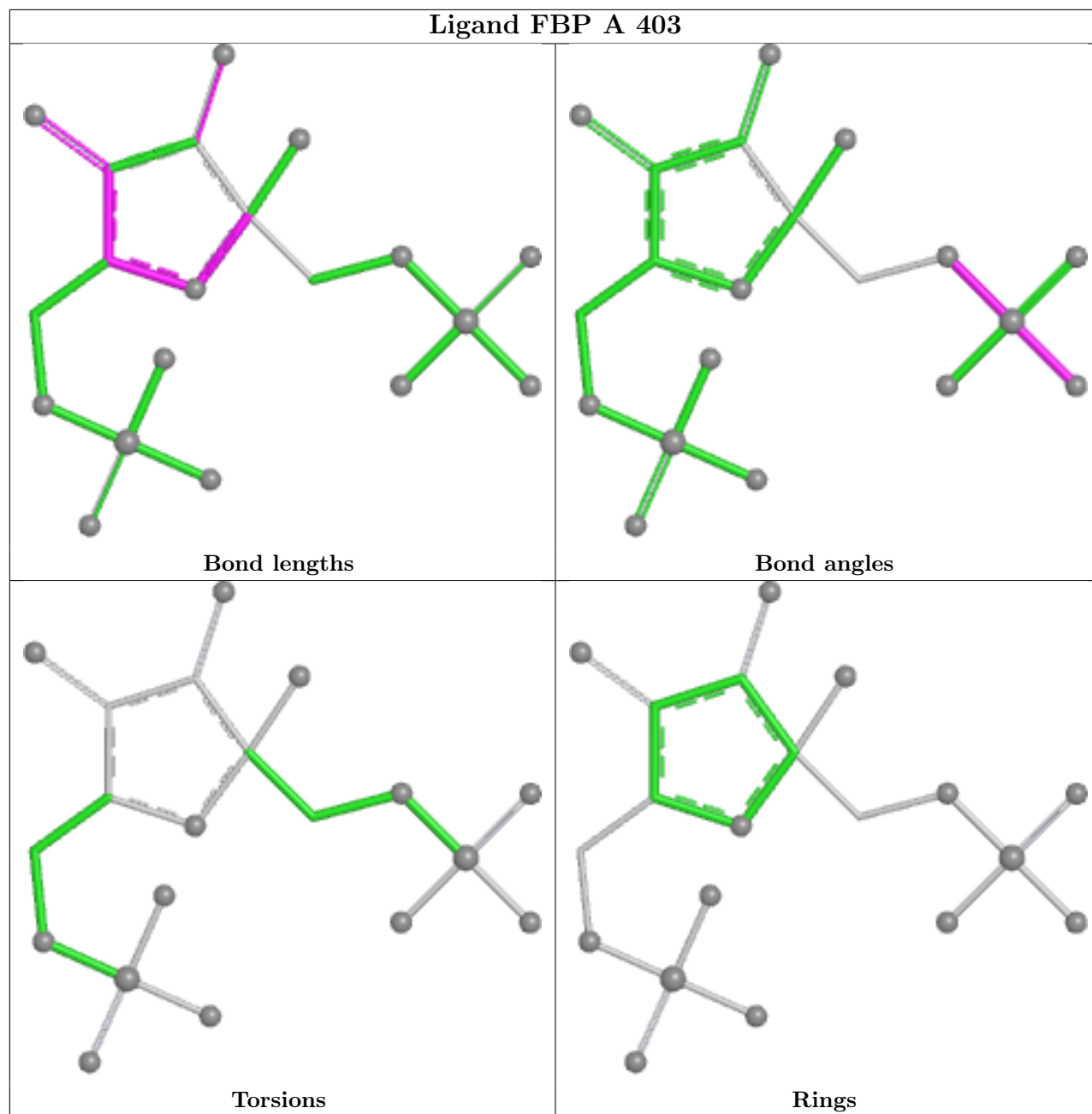
6 monomers are involved in 10 short contacts:

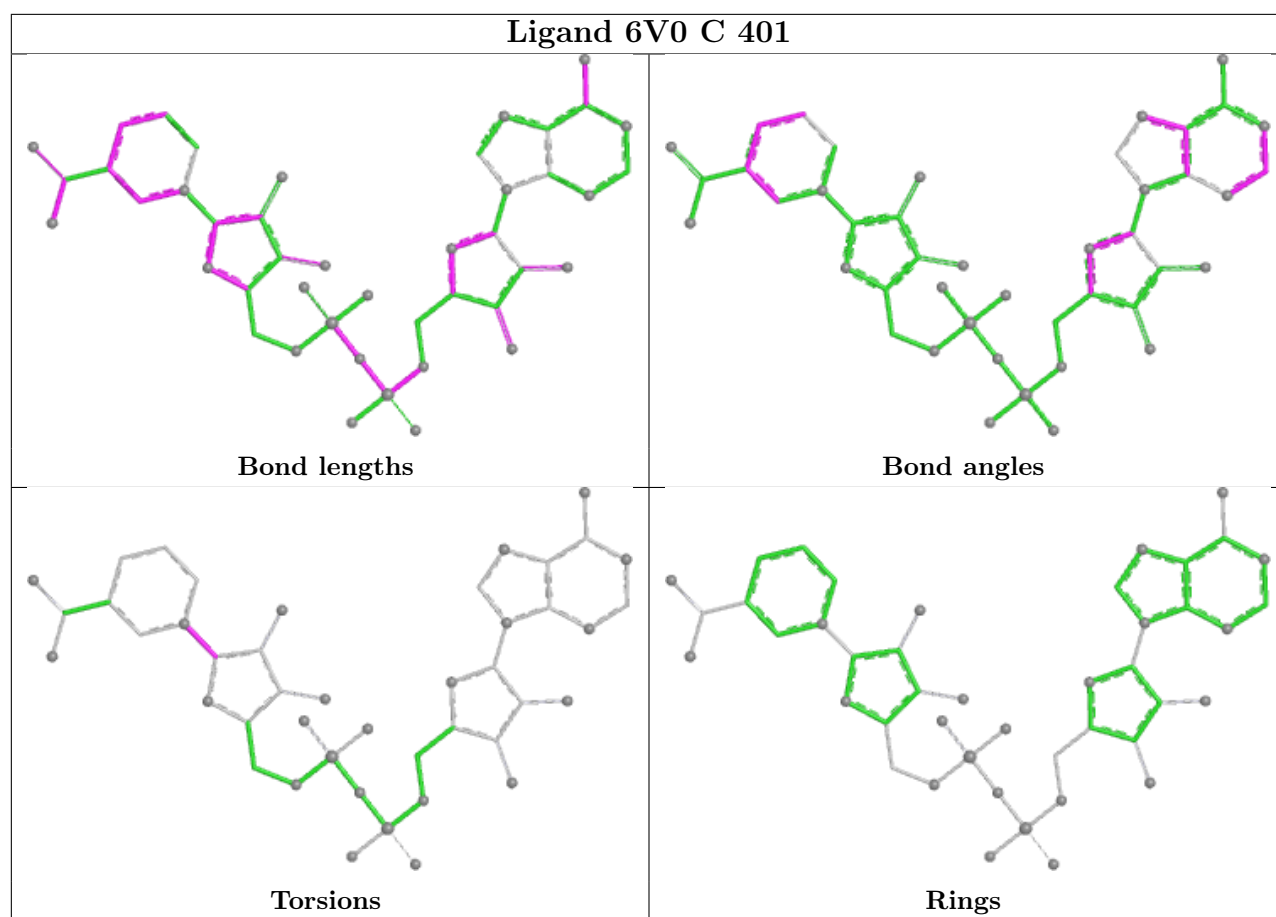
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	401	6V0	2	0
2	C	401	6V0	2	0
2	B	403	6V0	2	0
5	B	402	FBP	1	0
2	A	401	6V0	2	0
3	B	401	OXM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

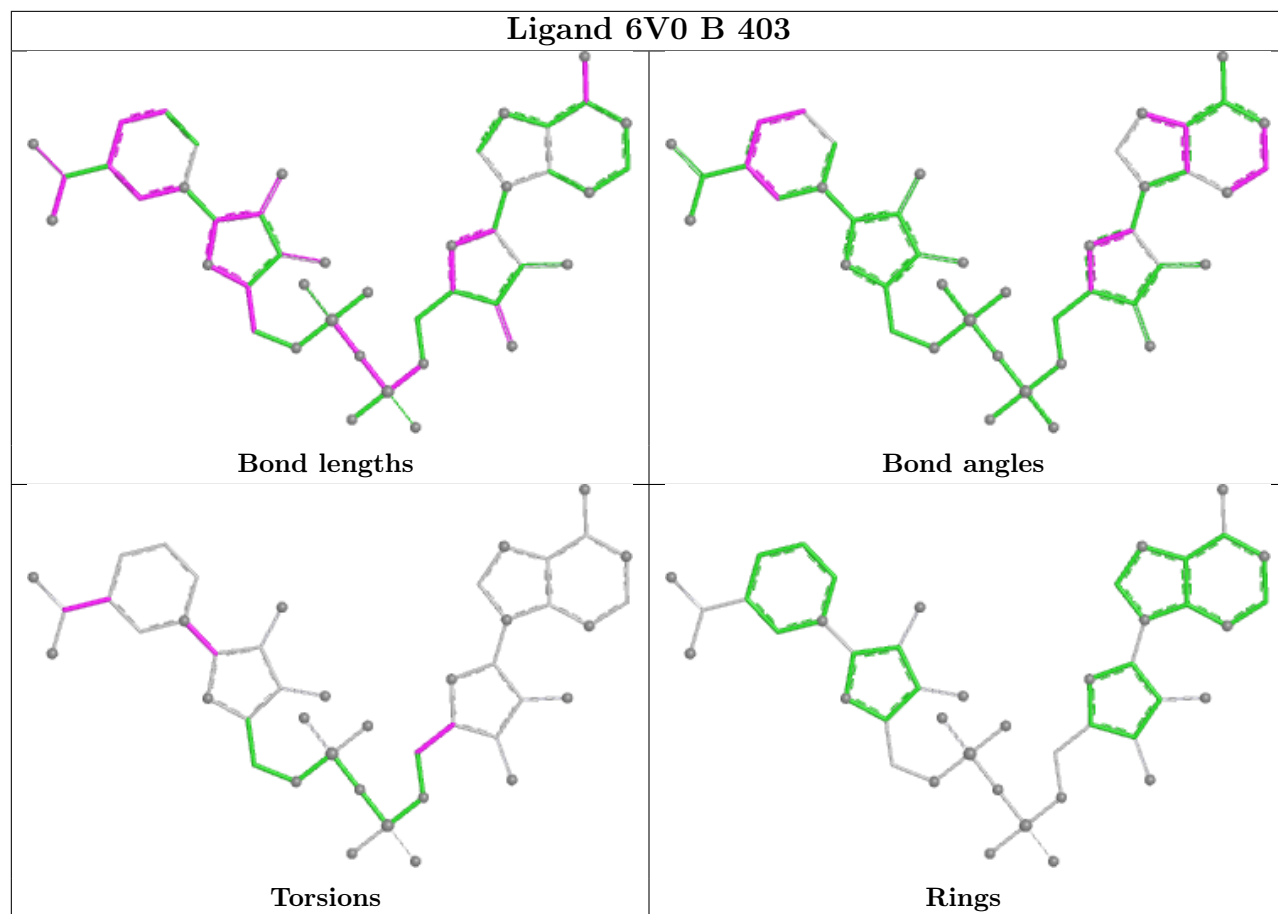


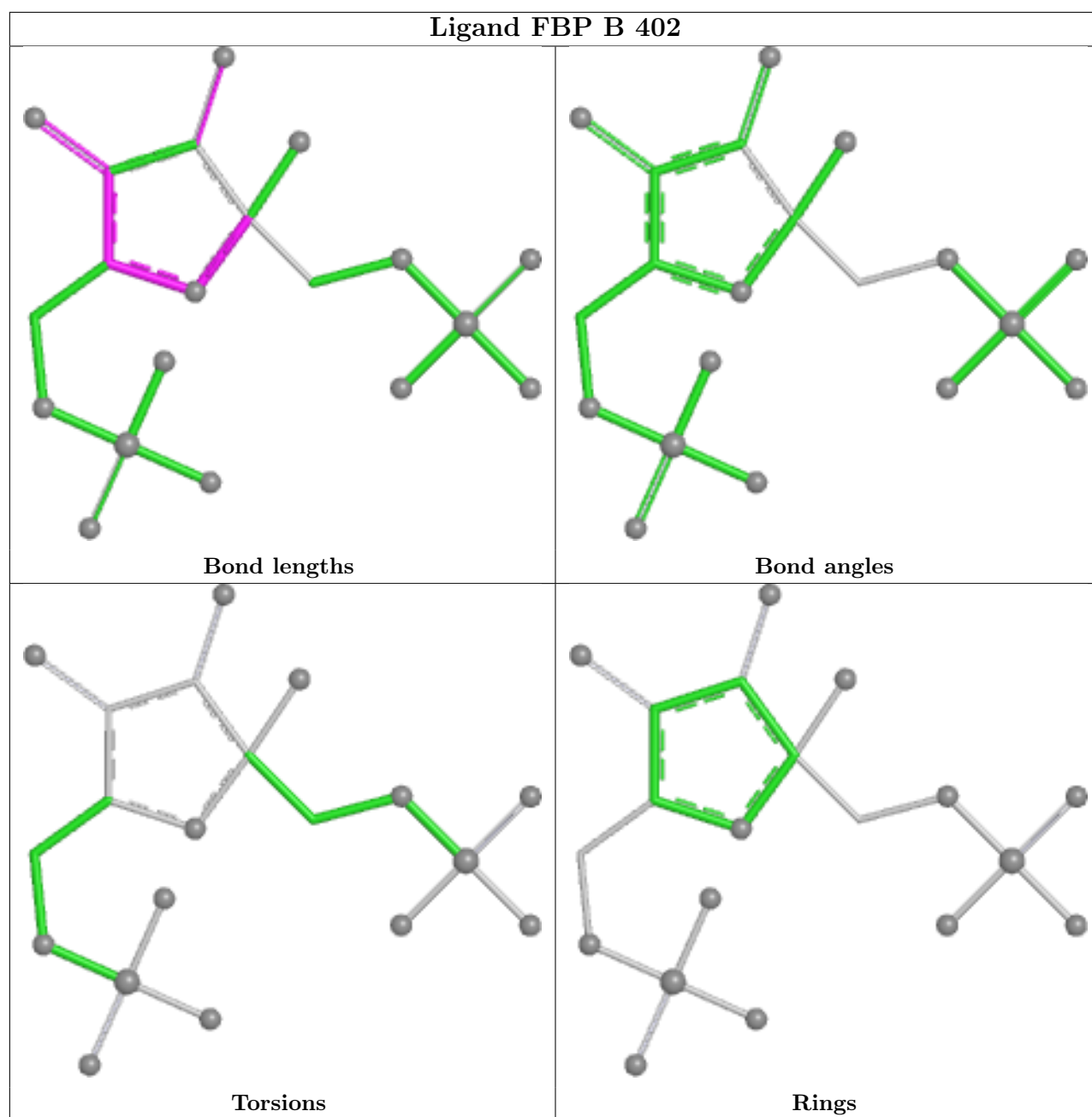
## Ligand FBP A 403



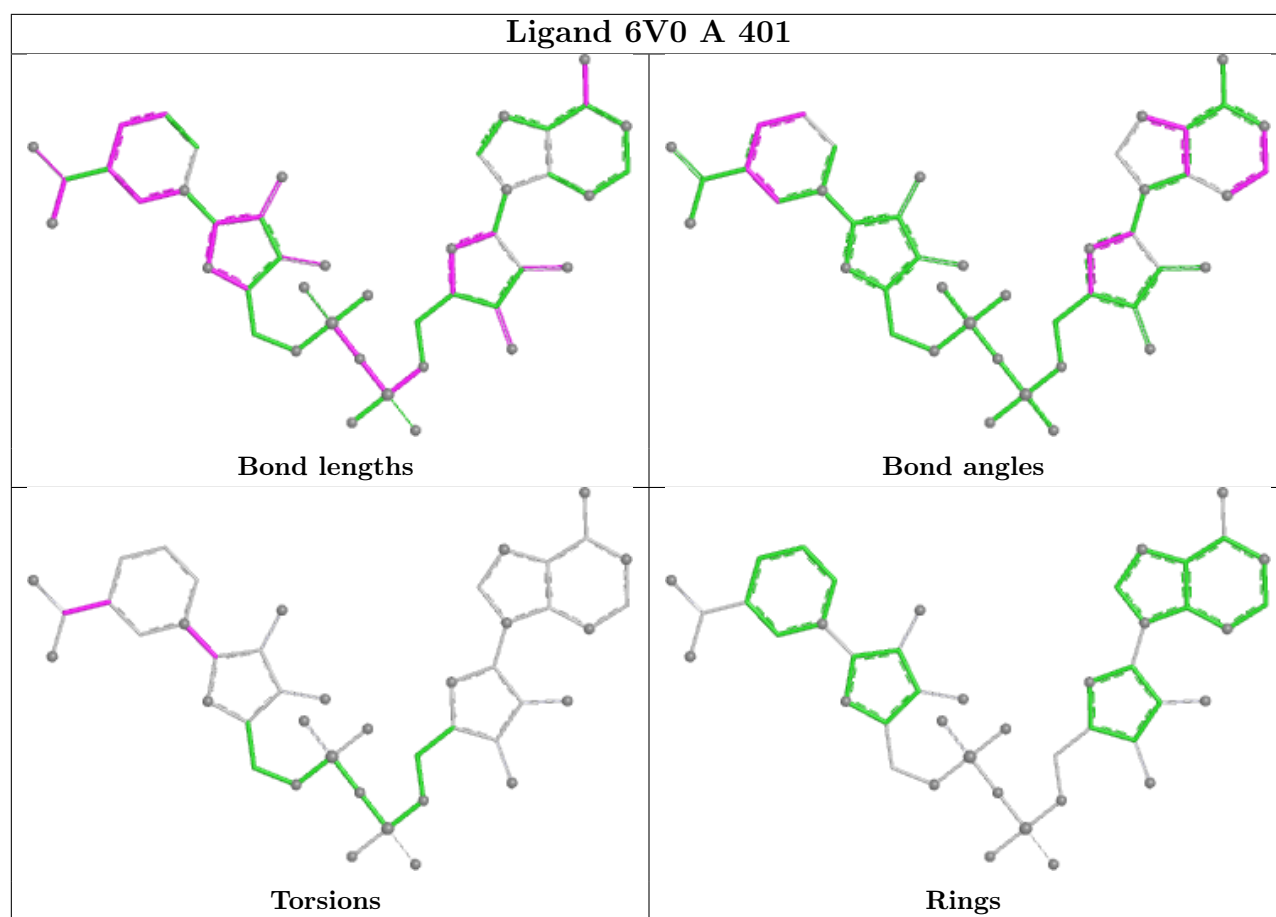


## Ligand 6V0 B 403









## 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	314/314 (100%)	-0.11	4 (1%) 74 76	21, 36, 60, 84	0
1	B	314/314 (100%)	-0.04	7 (2%) 62 64	23, 35, 65, 96	0
1	C	314/314 (100%)	0.01	13 (4%) 42 44	22, 36, 68, 134	0
1	P	314/314 (100%)	-0.10	5 (1%) 70 72	22, 35, 57, 73	0
All	All	1256/1256 (100%)	-0.06	29 (2%) 61 63	21, 35, 62, 134	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	PRO	5.1
1	C	268	ILE	4.4
1	A	92	LEU	4.4
1	P	29	LEU	4.0
1	B	1	MET	3.8
1	B	29	LEU	3.7
1	C	88	GLY	3.7
1	P	314	MET	3.6
1	C	90	THR	3.3
1	P	97	LYS	3.3
1	C	86	LYS	3.1
1	A	96	ASP	2.9
1	C	93	ASP	2.9
1	C	89	GLU	2.8
1	C	29	LEU	2.7
1	B	266	GLY	2.7
1	B	314	MET	2.6
1	C	85	GLN	2.5
1	B	87	PRO	2.5
1	A	29	LEU	2.4
1	B	83	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	P	28	SER	2.4
1	A	314	MET	2.3
1	C	95	VAL	2.2
1	C	92	LEU	2.2
1	P	285	LYS	2.1
1	B	85	GLN	2.1
1	C	83	LEU	2.1
1	C	267	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

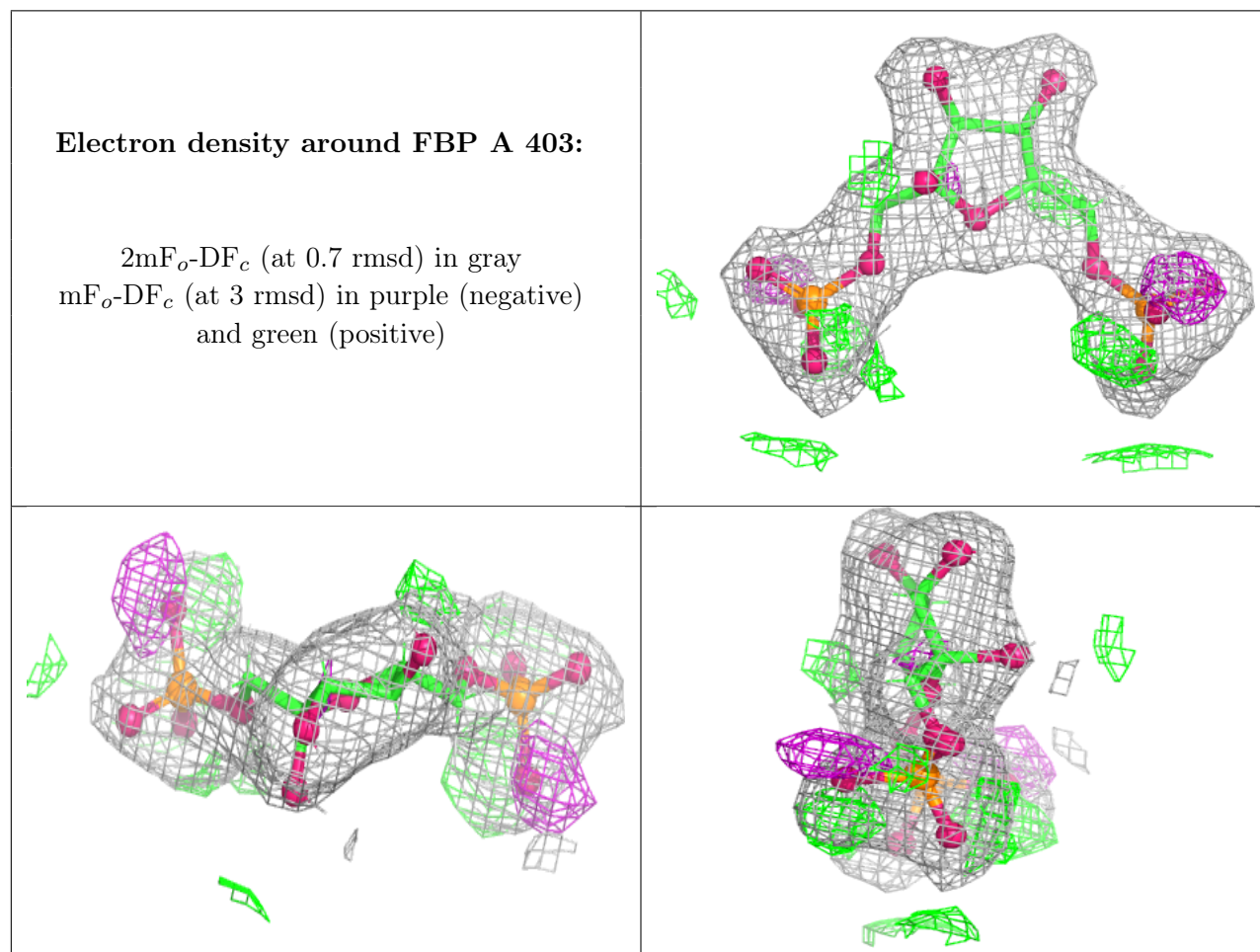
## 6.4 Ligands ⓘ

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
3	OXM	P	402	6/6	0.84	0.20	36,40,48,48	0
3	OXM	C	402	6/6	0.84	0.15	37,44,56,56	0
3	OXM	B	401	6/6	0.88	0.18	36,43,53,53	0
5	FBP	A	403	20/20	0.91	0.10	27,36,46,51	0
3	OXM	A	402	6/6	0.93	0.14	39,41,49,49	0
2	6V0	P	401	44/44	0.94	0.08	25,35,47,50	0
2	6V0	C	401	44/44	0.95	0.07	24,35,44,47	0
2	6V0	A	401	44/44	0.95	0.08	27,34,44,45	0
4	CA	P	403	1/1	0.95	0.05	37,37,37,37	0
4	CA	C	403	1/1	0.95	0.27	30,30,30,30	0
2	6V0	B	403	44/44	0.95	0.08	25,36,46,50	0
5	FBP	B	402	20/20	0.96	0.07	22,30,40,44	0

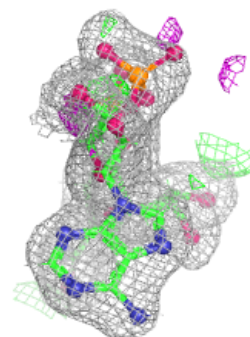
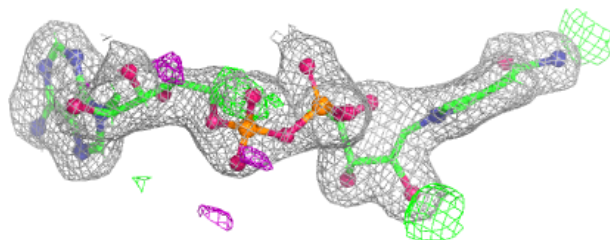
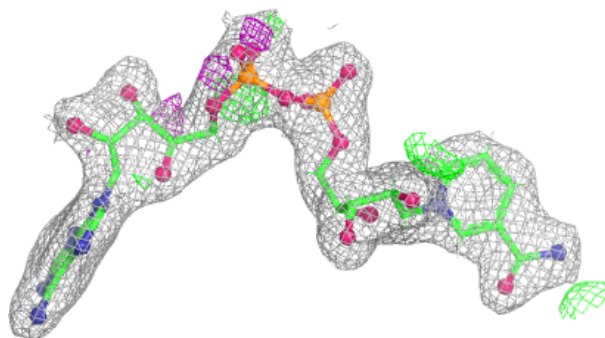
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

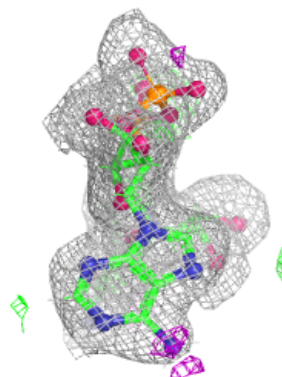
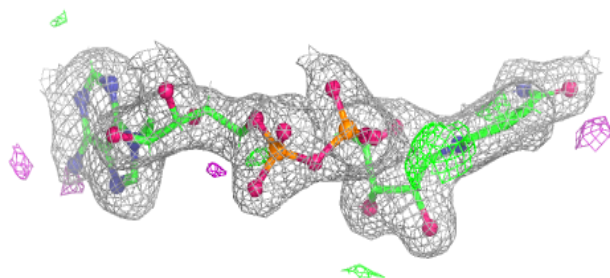
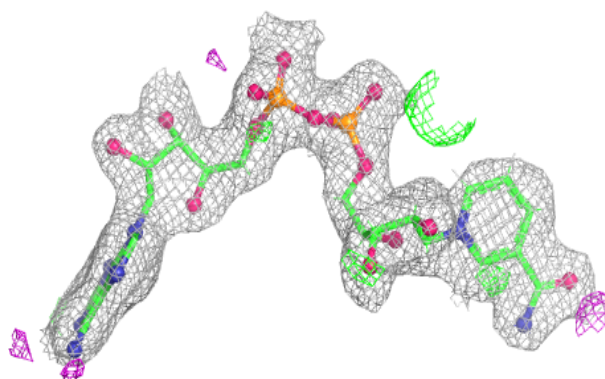


**Electron density around 6V0 P 401:**

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

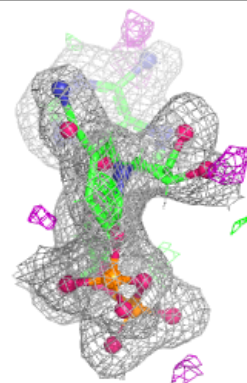
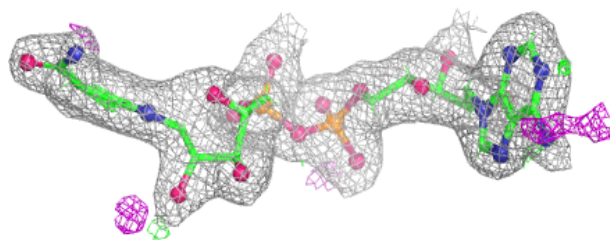
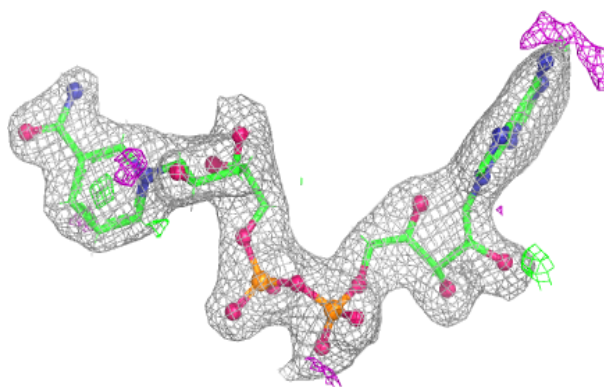
**Electron density around 6V0 C 401:**

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

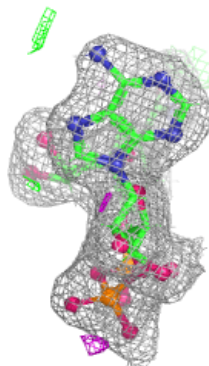
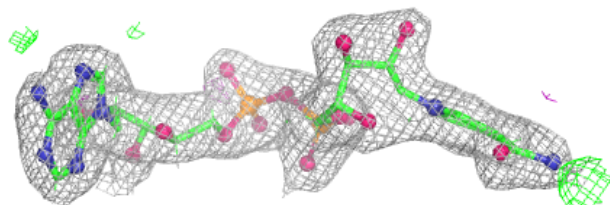
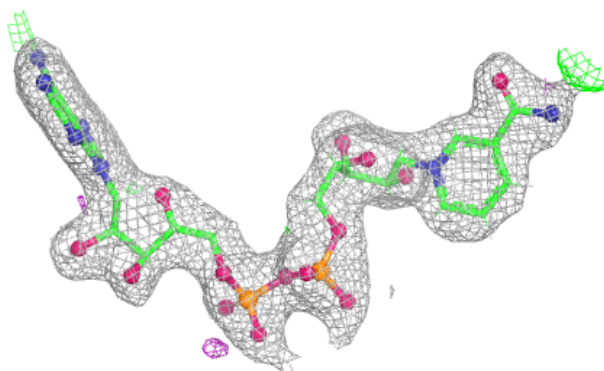


**Electron density around 6V0 A 401:**

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

**Electron density around 6V0 B 403:**

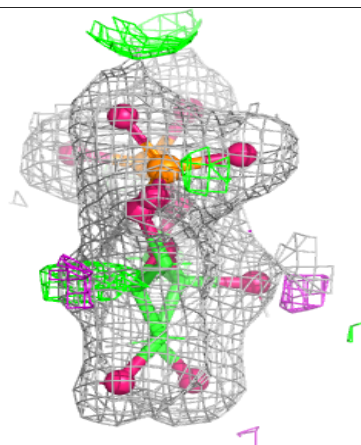
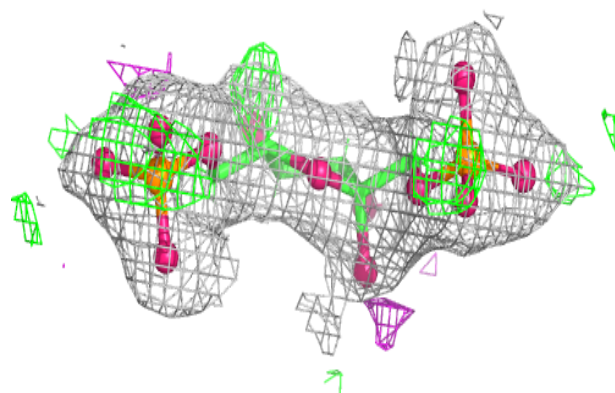
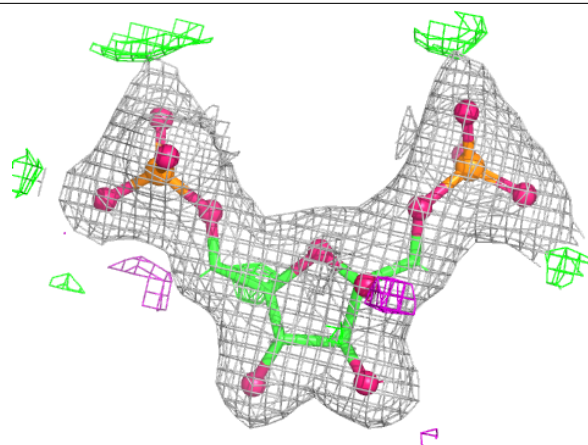
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around FBP B 402:**

$2mF_o - DF_c$  (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.