



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 08:36 AM EST

PDB ID : 4JPG  
Title : 2-((1H-benzo[d]imidazol-1-yl)methyl)-4H-pyrido[1,2-a]pyrimidin-4-ones as Novel PKM2 Activators  
Authors : Greasley, S.E.; Hickey, M.; Phonephaly, H.; Cronin, C.  
Deposited on : 2013-03-19  
Resolution : 2.33 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

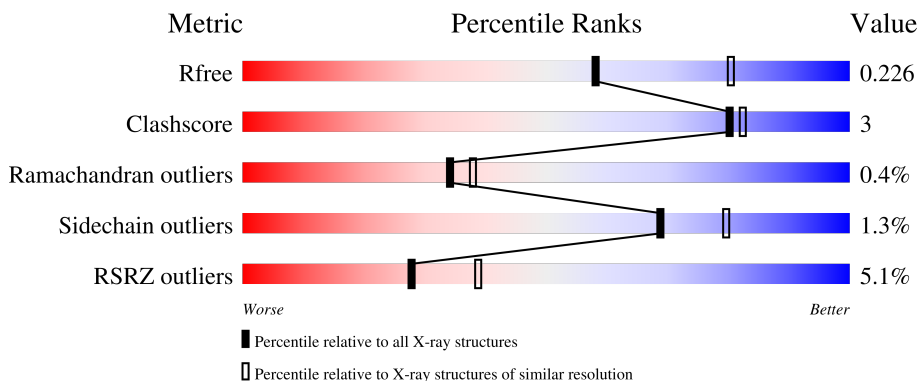
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	556	 4% 86% 7% 7%
1	B	556	 6% 82% 9% 8%
1	C	556	 2% 85% 8% 7%
1	D	556	 7% 86% 5% 8%

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 16344 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 Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	519	3905	2459	682	739	25	0	1	0
1	B	510	3816	2403	672	716	25	11	3	0
1	C	518	3921	2470	683	743	25	0	3	0
1	D	512	3844	2412	684	723	25	0	2	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	GLY	-	expression tag	UNP P14618
A	-23	SER	-	expression tag	UNP P14618
A	-22	MET	-	expression tag	UNP P14618
A	-21	LYS	-	expression tag	UNP P14618
A	-20	HIS	-	expression tag	UNP P14618
A	-19	HIS	-	expression tag	UNP P14618
A	-18	HIS	-	expression tag	UNP P14618
A	-17	HIS	-	expression tag	UNP P14618
A	-16	HIS	-	expression tag	UNP P14618
A	-15	HIS	-	expression tag	UNP P14618
A	-14	ASP	-	expression tag	UNP P14618
A	-13	TYR	-	expression tag	UNP P14618
A	-12	GLY	-	expression tag	UNP P14618
A	-11	ILE	-	expression tag	UNP P14618
A	-10	LEU	-	expression tag	UNP P14618
A	-9	THR	-	expression tag	UNP P14618
A	-8	THR	-	expression tag	UNP P14618
A	-7	GLU	-	expression tag	UNP P14618
A	-6	ASN	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	TYR	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	expression tag	UNP P14618
A	-2	GLN	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-24	GLY	-	expression tag	UNP P14618
B	-23	SER	-	expression tag	UNP P14618
B	-22	MET	-	expression tag	UNP P14618
B	-21	LYS	-	expression tag	UNP P14618
B	-20	HIS	-	expression tag	UNP P14618
B	-19	HIS	-	expression tag	UNP P14618
B	-18	HIS	-	expression tag	UNP P14618
B	-17	HIS	-	expression tag	UNP P14618
B	-16	HIS	-	expression tag	UNP P14618
B	-15	HIS	-	expression tag	UNP P14618
B	-14	ASP	-	expression tag	UNP P14618
B	-13	TYR	-	expression tag	UNP P14618
B	-12	GLY	-	expression tag	UNP P14618
B	-11	ILE	-	expression tag	UNP P14618
B	-10	LEU	-	expression tag	UNP P14618
B	-9	THR	-	expression tag	UNP P14618
B	-8	THR	-	expression tag	UNP P14618
B	-7	GLU	-	expression tag	UNP P14618
B	-6	ASN	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	TYR	-	expression tag	UNP P14618
B	-3	PHE	-	expression tag	UNP P14618
B	-2	GLN	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-24	GLY	-	expression tag	UNP P14618
C	-23	SER	-	expression tag	UNP P14618
C	-22	MET	-	expression tag	UNP P14618
C	-21	LYS	-	expression tag	UNP P14618
C	-20	HIS	-	expression tag	UNP P14618
C	-19	HIS	-	expression tag	UNP P14618
C	-18	HIS	-	expression tag	UNP P14618
C	-17	HIS	-	expression tag	UNP P14618
C	-16	HIS	-	expression tag	UNP P14618
C	-15	HIS	-	expression tag	UNP P14618
C	-14	ASP	-	expression tag	UNP P14618
C	-13	TYR	-	expression tag	UNP P14618
C	-12	GLY	-	expression tag	UNP P14618

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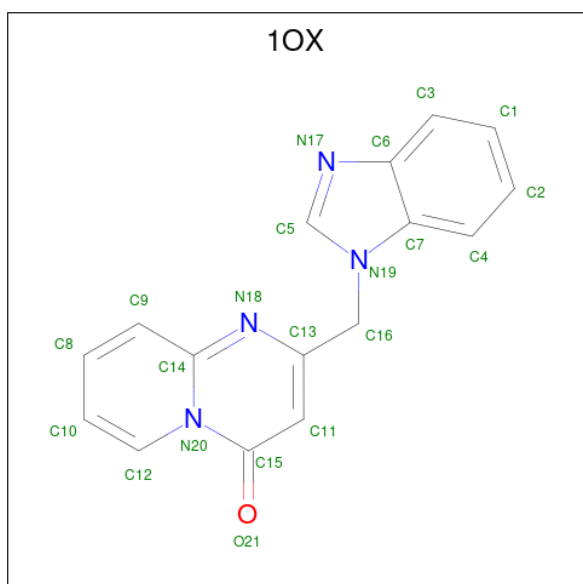
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	ILE	-	expression tag	UNP P14618
C	-10	LEU	-	expression tag	UNP P14618
C	-9	THR	-	expression tag	UNP P14618
C	-8	THR	-	expression tag	UNP P14618
C	-7	GLU	-	expression tag	UNP P14618
C	-6	ASN	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	TYR	-	expression tag	UNP P14618
C	-3	PHE	-	expression tag	UNP P14618
C	-2	GLN	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-24	GLY	-	expression tag	UNP P14618
D	-23	SER	-	expression tag	UNP P14618
D	-22	MET	-	expression tag	UNP P14618
D	-21	LYS	-	expression tag	UNP P14618
D	-20	HIS	-	expression tag	UNP P14618
D	-19	HIS	-	expression tag	UNP P14618
D	-18	HIS	-	expression tag	UNP P14618
D	-17	HIS	-	expression tag	UNP P14618
D	-16	HIS	-	expression tag	UNP P14618
D	-15	HIS	-	expression tag	UNP P14618
D	-14	ASP	-	expression tag	UNP P14618
D	-13	TYR	-	expression tag	UNP P14618
D	-12	GLY	-	expression tag	UNP P14618
D	-11	ILE	-	expression tag	UNP P14618
D	-10	LEU	-	expression tag	UNP P14618
D	-9	THR	-	expression tag	UNP P14618
D	-8	THR	-	expression tag	UNP P14618
D	-7	GLU	-	expression tag	UNP P14618
D	-6	ASN	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	TYR	-	expression tag	UNP P14618
D	-3	PHE	-	expression tag	UNP P14618
D	-2	GLN	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618

- Molecule 2 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
			Total	C	O	P		
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is 2-(1H-benzimidazol-1-ylmethyl)-4H-pyrido[1,2-a]pyrimidin-4-one (three-letter code: 1OX) (formula: C<sub>16</sub>H<sub>12</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	1
			42	32	8	2		
3	D	1	Total	C	N	O	0	1
			42	32	8	2		

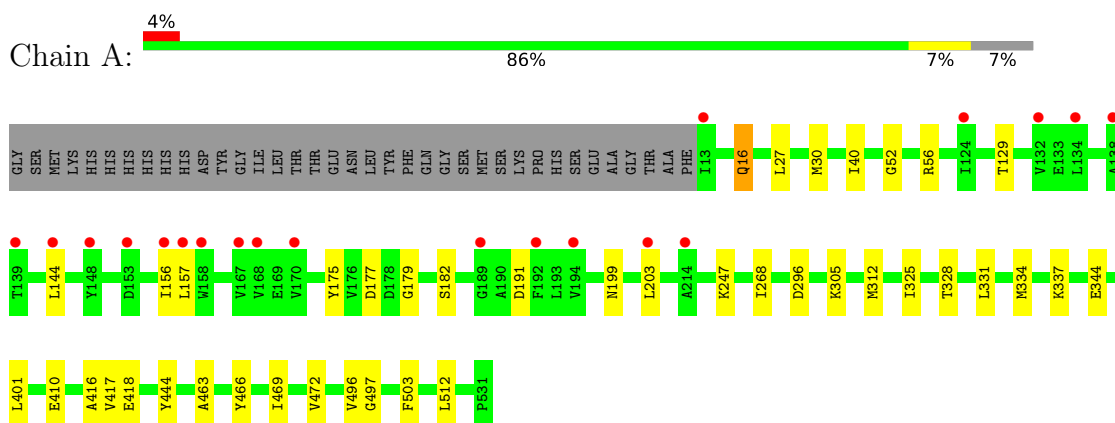
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	194	Total	O	0	0
			194	194		
4	B	184	Total	O	0	0
			184	184		
4	C	165	Total	O	0	0
			165	165		
4	D	151	Total	O	0	0
			151	151		

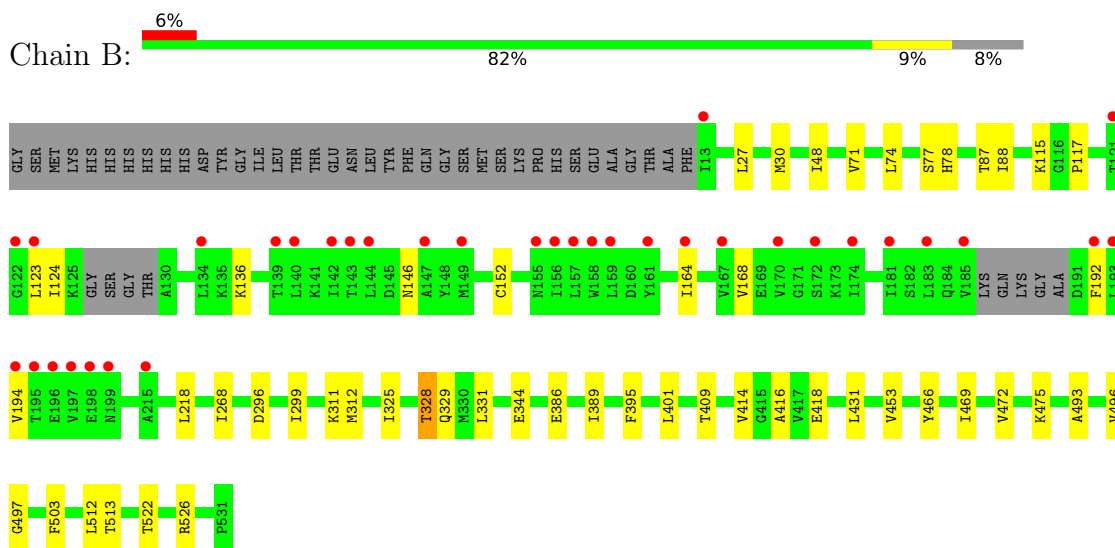
### 3 Residue-property plots [i](#)

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.

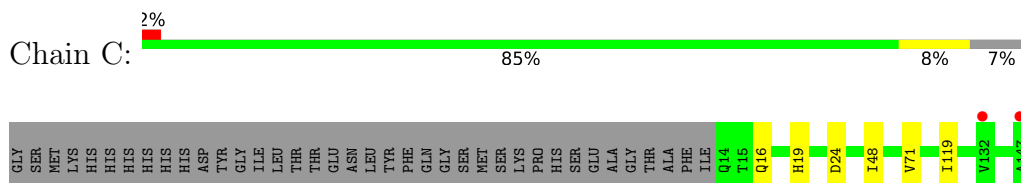
- Molecule 1: Pyruvate kinase isozymes M1/M2



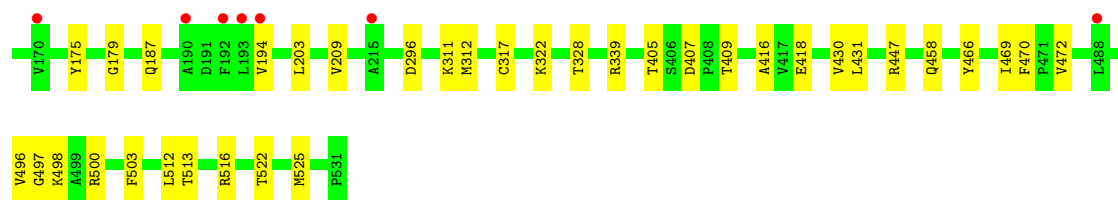
- Molecule 1: Pyruvate kinase isozymes M1/M2



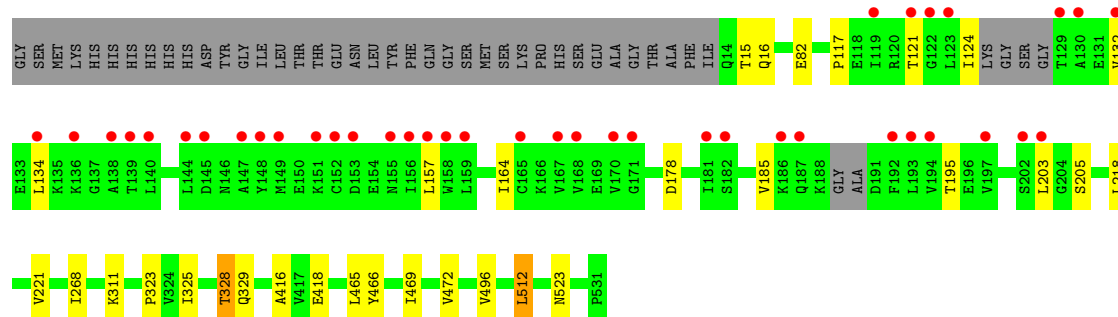
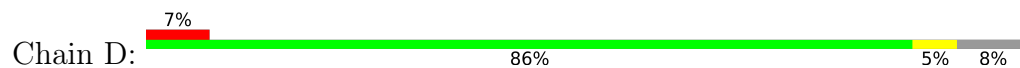
- Molecule 1: Pyruvate kinase isozymes M1/M2







● Molecule 1: Pyruvate kinase isozymes M1/M2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.97Å 153.61Å 93.48Å 90.00° 103.45° 90.00°	Depositor
Resolution (Å)	45.46 – 2.33 45.46 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.46-2.33) 99.7 (45.46-2.33)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.84 (at 2.34Å)	Xtrriage
Refinement program	BUSTER 2.11.4	Depositor
R, $R_{free}$	0.177 , 0.219 0.180 , 0.226	Depositor DCC
$R_{free}$ test set	4734 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtrriage
Anisotropy	0.144	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16344	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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, 1OX

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	0.52	0/3978	0.65	0/5389
1	B	0.51	0/3883	0.65	0/5264
1	C	0.50	0/3994	0.63	0/5410
1	D	0.48	0/3906	0.64	0/5292
All	All	0.50	0/15761	0.64	0/21355

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	3905	0	3900	21	0
1	B	3816	0	3770	32	0
1	C	3921	0	3920	21	0
1	D	3844	0	3778	17	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	B	42	0	24	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	42	0	24	3	0
4	A	194	0	0	1	0
4	B	184	0	0	3	0
4	C	165	0	0	3	0
4	D	151	0	0	1	0
All	All	16344	0	15456	85	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 (85) 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:B:418[B]:GLU:HG3	1:D:418:GLU:HG2	1.37	1.06
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.65	0.79
1:B:418[B]:GLU:HG3	1:D:418:GLU:CG	2.21	0.69
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.80	0.64
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.37	0.60
1:C:187:GLN:HB2	1:C:194:VAL:HB	1.84	0.60
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.84	0.59
1:D:82:GLU:HG2	4:D:845:HOH:O	2.01	0.58
1:A:401:LEU:HD12	1:B:27:LEU:HD23	1.86	0.58
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.40	0.56
1:A:182:SER:HB3	1:A:199:ASN:HB2	1.86	0.56
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.87	0.56
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.88	0.56
4:C:865:HOH:O	3:D:602[B]:1OX:H6	2.06	0.56
1:B:311:LYS:HD3	3:B:602[A]:1OX:H3	1.88	0.56
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.88	0.54
1:A:157:LEU:HD13	1:A:203:LEU:HD21	1.91	0.53
1:A:52:GLY:O	1:A:56:ARG:HG3	2.09	0.53
1:A:305:LYS:NZ	4:A:892:HOH:O	2.42	0.52
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.91	0.52
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.93	0.51
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.93	0.50
1:B:74:LEU:HD11	1:B:88:ILE:HG13	1.93	0.50
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.94	0.50
1:D:121:THR:HB	1:D:157:LEU:HD11	1.94	0.49
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.94	0.49
1:D:311:LYS:HD3	3:D:602[A]:1OX:H3	1.95	0.49
1:C:19:HIS:HD2	4:C:712:HOH:O	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:SER:HA	1:B:115:LYS:HG3	1.95	0.48
1:B:192:PHE:HE1	1:B:194:VAL:HG23	1.77	0.48
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.96	0.48
1:C:430:VAL:HG22	1:C:512:LEU:HD12	1.96	0.48
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.95	0.48
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.43	0.47
1:C:466:TYR:HB2	1:C:469:ILE:HD12	1.97	0.47
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.97	0.47
1:C:458:GLN:HG3	4:C:864:HOH:O	2.14	0.47
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.95	0.47
1:B:117:PRO:HB2	1:B:218:LEU:HD13	1.96	0.47
1:B:475:LYS:NZ	4:B:879:HOH:O	2.48	0.47
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.97	0.46
1:D:268:ILE:HG21	1:D:325:ILE:HD12	1.97	0.46
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.98	0.46
1:B:74:LEU:HD22	1:B:87:THR:HG21	1.98	0.46
1:B:124:ILE:HG12	1:B:152:CYS:HB2	1.98	0.46
1:B:431:LEU:HD22	1:B:513:THR:HG22	1.98	0.46
3:B:602[B]:1OX:H6	4:B:702:HOH:O	2.16	0.45
1:D:117:PRO:HB2	1:D:218:LEU:HD13	1.99	0.45
1:A:417:VAL:HG21	1:A:444:TYR:HB2	1.99	0.45
1:C:16:GLN:NE2	1:C:447[A]:ARG:HD3	2.31	0.45
3:B:602[A]:1OX:H6	4:B:701:HOH:O	2.16	0.45
1:D:124:ILE:H	1:D:205:SER:HB2	1.82	0.44
1:A:268:ILE:HG21	1:A:325:ILE:HD12	1.99	0.44
1:C:470:PHE:CZ	1:C:500:ARG:HD2	2.53	0.44
1:A:334:MET:HA	1:A:337:LYS:O	2.17	0.44
1:A:144:LEU:HD12	1:A:191:ASP:HA	2.00	0.44
1:A:312:MET:HA	1:B:30:MET:O	2.18	0.44
1:D:185:VAL:HA	1:D:195:THR:HG22	2.00	0.43
1:A:16:GLN:HG2	1:A:40:ILE:HG23	2.00	0.43
1:D:134:LEU:HD11	1:D:203:LEU:HD22	2.00	0.43
1:D:323:PRO:HB3	1:D:465:LEU:O	2.18	0.43
1:C:48:ILE:HG12	1:C:71:VAL:HB	2.00	0.43
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.53	0.43
1:B:268:ILE:HG21	1:B:325:ILE:HD12	2.00	0.43
1:A:30:MET:O	1:B:312:MET:HA	2.19	0.42
1:B:414:VAL:HG13	1:D:418:GLU:HG3	2.01	0.42
1:C:311:LYS:HD3	3:D:602[B]:1OX:H3	2.01	0.42
1:C:317:CYS:HB3	1:C:322:LYS:O	2.20	0.42
1:C:119:ILE:HG22	1:C:209:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:THR:HB	1:C:407:ASP:H	1.84	0.42
1:D:416:ALA:HB2	1:D:512:LEU:HD21	2.01	0.42
1:A:27:LEU:HD23	1:B:401:LEU:HD12	2.02	0.42
1:B:526:ARG:HA	1:D:523:ASN:O	2.19	0.42
1:A:416:ALA:HB2	1:A:512:LEU:HD21	2.02	0.42
1:B:48:ILE:HG12	1:B:71:VAL:HB	2.02	0.42
1:C:312:MET:C	1:C:312:MET:SD	2.98	0.41
1:B:192:PHE:CE1	1:B:194:VAL:HG23	2.54	0.41
1:B:395:PHE:CZ	1:B:418[B]:GLU:HG2	2.55	0.41
1:B:386:GLU:HA	1:B:389:ILE:HD12	2.03	0.41
1:B:409[A]:THR:HG23	1:B:522:THR:HB	2.01	0.41
1:A:418:GLU:HB2	1:C:418:GLU:HG2	2.03	0.41
1:B:331:LEU:HD23	1:B:344:GLU:HB3	2.01	0.41
1:C:409:THR:HG22	1:C:522:THR:O	2.21	0.41
1:C:431:LEU:HG	1:C:513:THR:HG22	2.04	0.40
1:B:296:ASP:HA	1:B:299:ILE:HD12	2.03	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	518/556 (93%)	508 (98%)	8 (2%)	2 (0%)	34 38
1	B	507/556 (91%)	496 (98%)	8 (2%)	3 (1%)	25 26
1	C	519/556 (93%)	507 (98%)	11 (2%)	1 (0%)	47 55
1	D	508/556 (91%)	493 (97%)	12 (2%)	3 (1%)	25 26
All	All	2052/2224 (92%)	2004 (98%)	39 (2%)	9 (0%)	34 38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	LYS
1	B	146	ASN
1	D	15	THR
1	D	16	GLN
1	A	328	THR
1	B	328	THR
1	C	328	THR
1	A	177	ASP
1	D	328	THR

### 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	409/458 (89%)	403 (98%)	6 (2%)	65	76
1	B	390/458 (85%)	386 (99%)	4 (1%)	76	85
1	C	410/458 (90%)	404 (98%)	6 (2%)	65	76
1	D	392/458 (86%)	387 (99%)	5 (1%)	69	79
All	All	1601/1832 (87%)	1580 (99%)	21 (1%)	69	79

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	129	THR
1	A	156	ILE
1	A	247	LYS
1	A	296	ASP
1	A	410	GLU
1	B	78	HIS
1	B	123	LEU
1	B	164	ILE
1	B	168	VAL
1	C	24	ASP
1	C	296	ASP
1	C	339	ARG

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Mol	Chain	Res	Type
1	C	498	LYS
1	C	516	ARG
1	C	525	MET
1	D	132	VAL
1	D	164	ILE
1	D	178	ASP
1	D	221	VAL
1	D	512	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	440	GLN
1	C	16	GLN
1	D	252	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	1OX	D	602[A]	-	22,24,24	1.75	4 (18%)	24,34,34	2.48	6 (25%)
2	FBP	D	601	-	18,20,20	0.71	0	23,32,32	1.16	1 (4%)
3	1OX	D	602[B]	-	22,24,24	1.80	4 (18%)	24,34,34	2.55	6 (25%)
2	FBP	A	601	-	18,20,20	0.68	0	23,32,32	1.00	1 (4%)
2	FBP	C	601	-	18,20,20	0.83	1 (5%)	23,32,32	0.93	0
3	1OX	B	602[A]	-	22,24,24	1.77	3 (13%)	24,34,34	2.59	8 (33%)
2	FBP	B	601	-	18,20,20	0.70	0	23,32,32	1.15	1 (4%)
3	1OX	B	602[B]	-	22,24,24	1.78	4 (18%)	24,34,34	2.65	8 (33%)

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	1OX	D	602[A]	-	-	0/3/4/4	0/4/4/4
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	1OX	D	602[B]	-	-	0/3/4/4	0/4/4/4
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	1OX	B	602[A]	-	-	0/3/4/4	0/4/4/4
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
3	1OX	B	602[B]	-	-	0/3/4/4	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	602[B]	1OX	C14-N18	5.82	1.41	1.32
3	B	602[B]	1OX	C14-N18	5.69	1.41	1.32
3	B	602[A]	1OX	C14-N18	5.42	1.40	1.32
3	D	602[A]	1OX	C14-N18	5.36	1.40	1.32
3	D	602[B]	1OX	C14-N20	-3.34	1.34	1.38
3	D	602[A]	1OX	C14-N20	-3.27	1.34	1.38
3	B	602[B]	1OX	C14-N20	-3.25	1.34	1.38
3	B	602[A]	1OX	C14-N20	-3.21	1.34	1.38
2	C	601	FBP	O2-C2	2.38	1.44	1.40
3	D	602[A]	1OX	C12-N20	-2.23	1.34	1.38
3	D	602[A]	1OX	C11-C15	2.17	1.48	1.43
3	D	602[B]	1OX	C12-N20	-2.15	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602[A]	1OX	C12-N20	-2.05	1.34	1.38
3	D	602[B]	1OX	C9-C14	-2.03	1.38	1.41
3	B	602[B]	1OX	C9-C14	-2.02	1.38	1.41
3	B	602[B]	1OX	C12-N20	-2.02	1.34	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602[B]	1OX	C15-C11-C13	-7.21	113.79	120.78
3	B	602[B]	1OX	C11-C15-N20	7.16	121.89	113.68
3	B	602[A]	1OX	C15-C11-C13	-7.01	113.99	120.78
3	D	602[B]	1OX	C15-C11-C13	-6.91	114.08	120.78
3	D	602[A]	1OX	C15-C11-C13	-6.84	114.16	120.78
3	D	602[B]	1OX	C11-C15-N20	6.80	121.47	113.68
3	B	602[A]	1OX	C11-C15-N20	6.41	121.02	113.68
3	D	602[A]	1OX	C11-C15-N20	6.03	120.59	113.68
3	B	602[A]	1OX	C9-C14-N20	4.66	121.06	116.85
3	D	602[A]	1OX	C9-C14-N20	4.38	120.80	116.85
3	B	602[B]	1OX	C9-C14-N20	3.83	120.31	116.85
3	D	602[B]	1OX	C9-C14-N20	3.66	120.15	116.85
3	D	602[B]	1OX	C1-C3-C6	-2.94	115.85	120.08
3	D	602[A]	1OX	C1-C3-C6	-2.89	115.92	120.08
3	B	602[B]	1OX	N20-C14-N18	-2.86	119.84	122.96
3	B	602[A]	1OX	N20-C14-N18	-2.76	119.94	122.96
3	B	602[A]	1OX	C1-C3-C6	-2.71	116.18	120.08
3	B	602[A]	1OX	C2-C4-C7	-2.70	114.26	119.44
3	B	602[B]	1OX	C2-C4-C7	-2.62	114.43	119.44
3	D	602[A]	1OX	C2-C4-C7	-2.58	114.50	119.44
3	D	602[B]	1OX	C2-C4-C7	-2.57	114.52	119.44
2	D	601	FBP	O3P-P1-O1	-2.54	99.98	106.73
3	B	602[B]	1OX	C1-C3-C6	-2.51	116.47	120.08
3	D	602[B]	1OX	N20-C14-N18	-2.46	120.27	122.96
3	D	602[A]	1OX	N20-C14-N18	-2.38	120.36	122.96
3	B	602[A]	1OX	C14-N18-C13	2.29	119.96	118.00
2	B	601	FBP	P2-O6-C6	2.26	124.52	118.30
3	B	602[B]	1OX	C14-N18-C13	2.24	119.92	118.00
3	B	602[B]	1OX	O21-C15-C11	-2.23	120.01	125.72
3	B	602[A]	1OX	C1-C2-C4	2.09	123.38	120.44
2	A	601	FBP	O5-C5-C6	2.06	114.00	109.45

There are no chirality outliers.

All (8) torsion outliers are listed below:

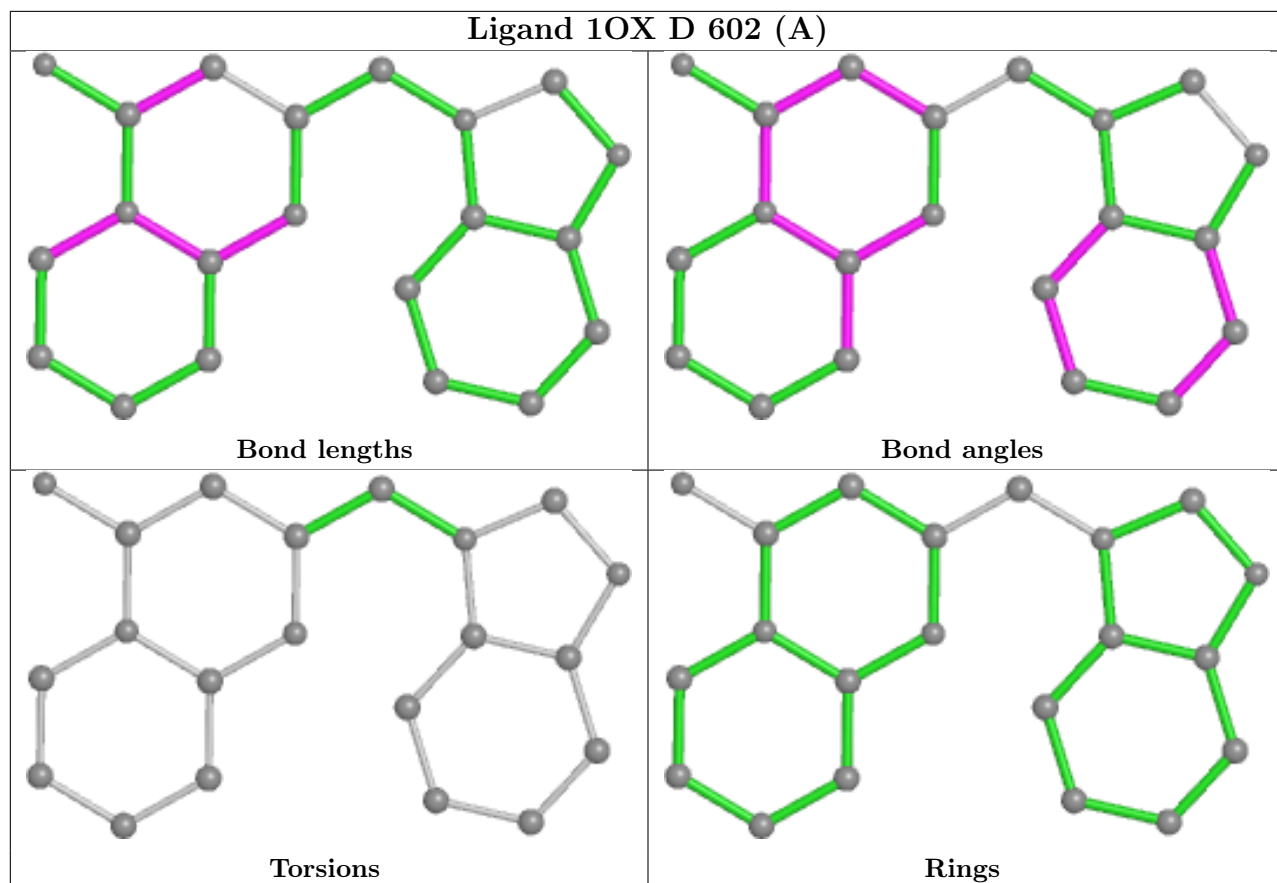
Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6

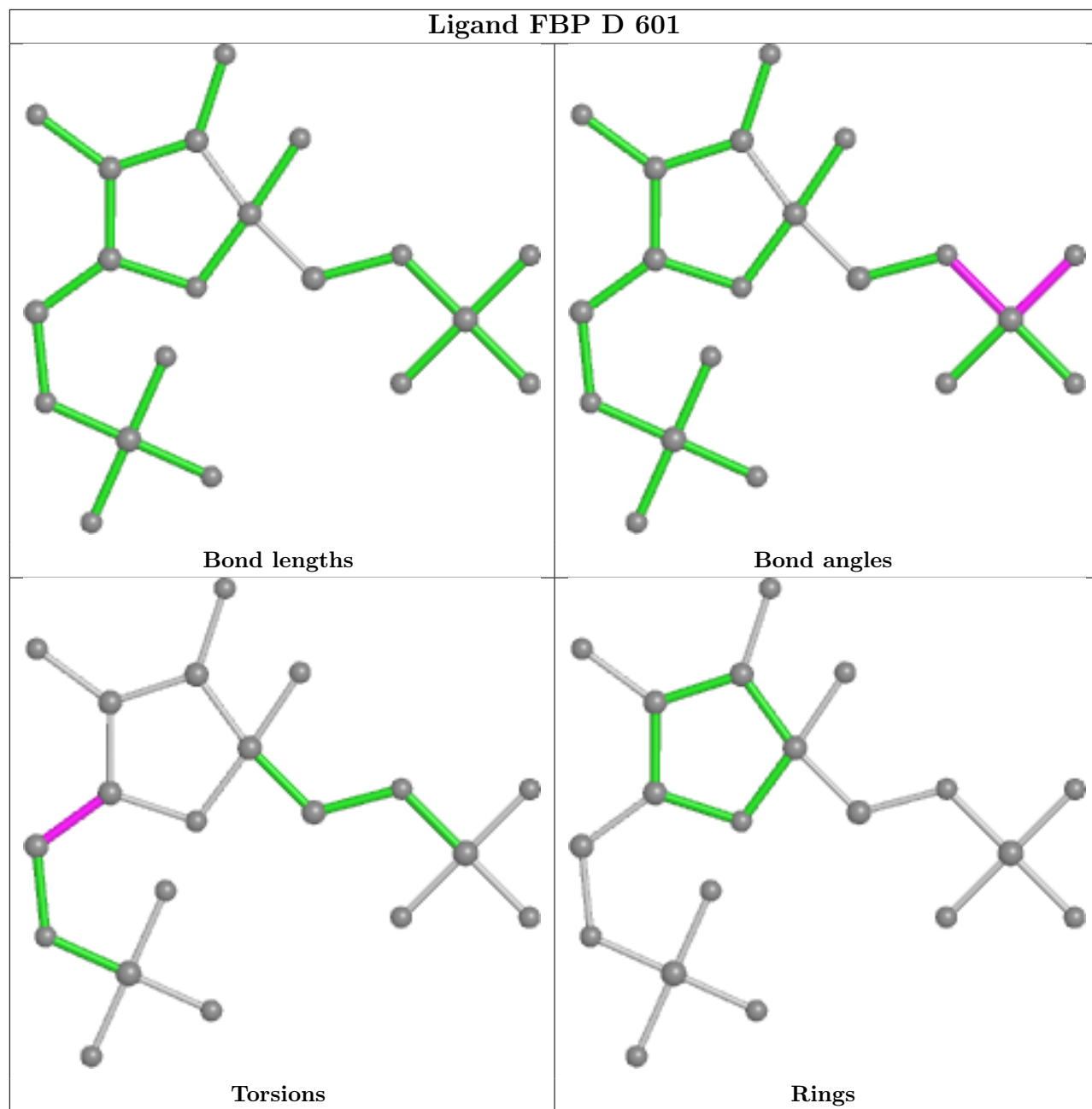
There are no ring outliers.

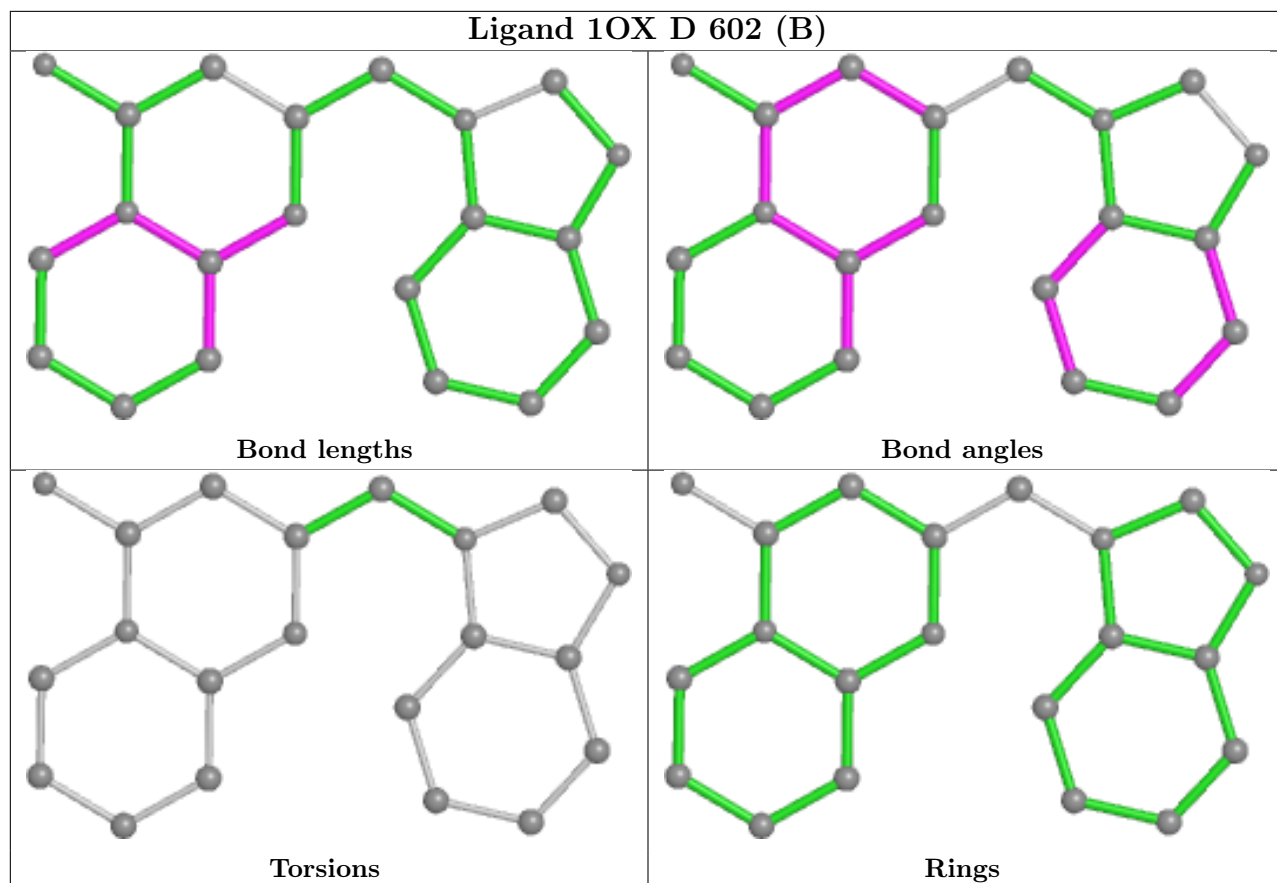
4 monomers are involved in 6 short contacts:

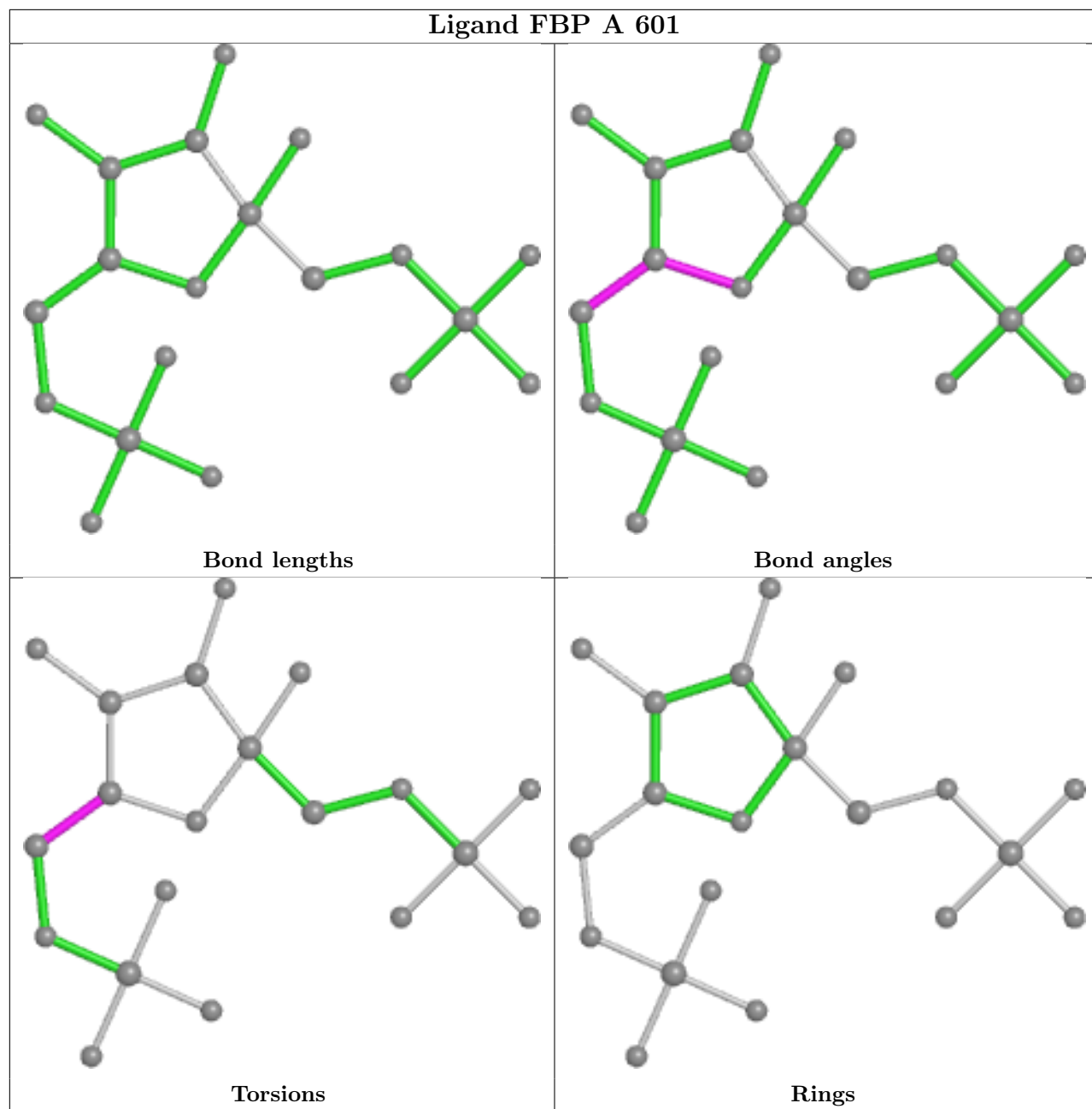
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602[A]	1OX	1	0
3	D	602[B]	1OX	2	0
3	B	602[A]	1OX	2	0
3	B	602[B]	1OX	1	0

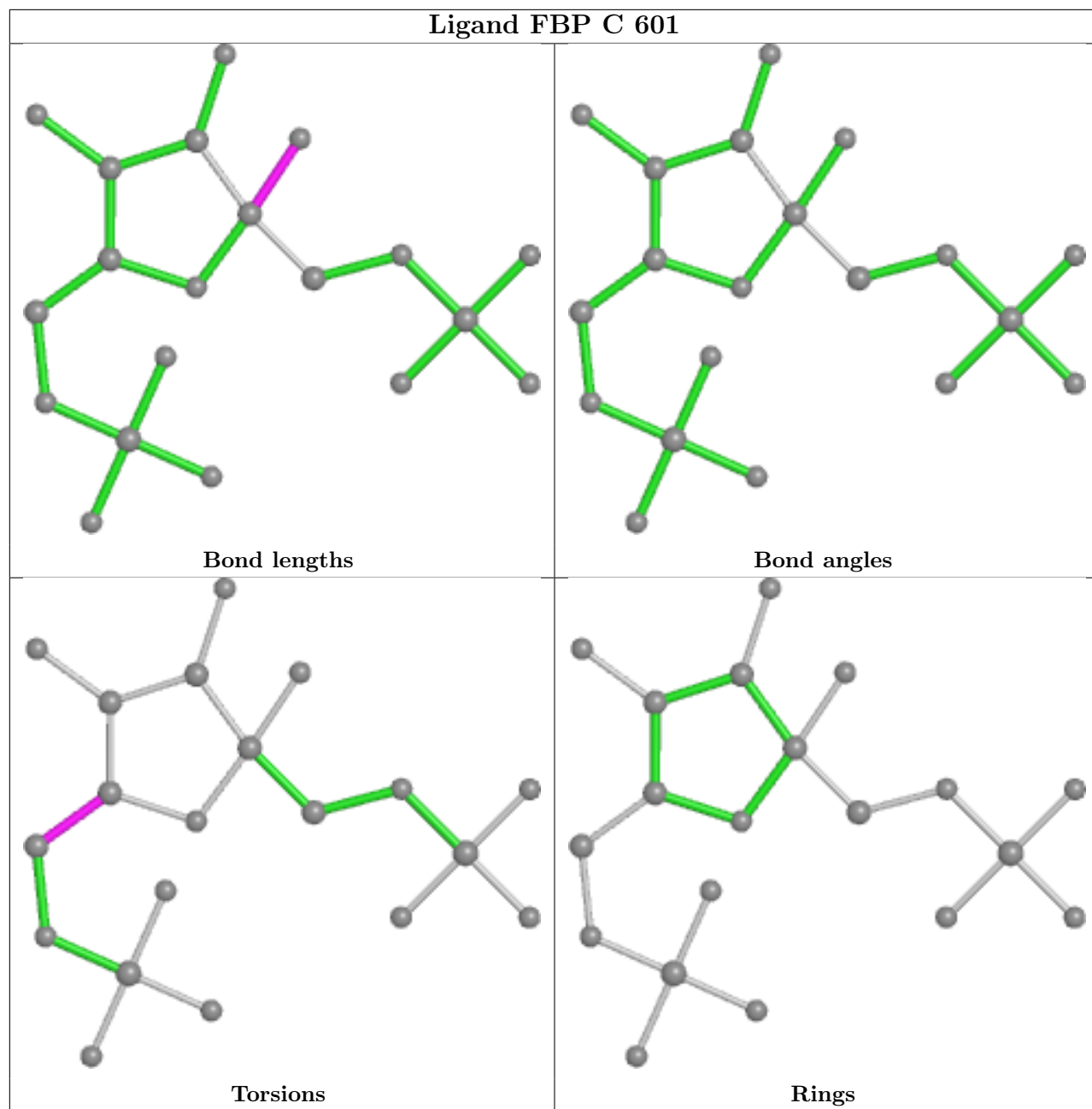
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



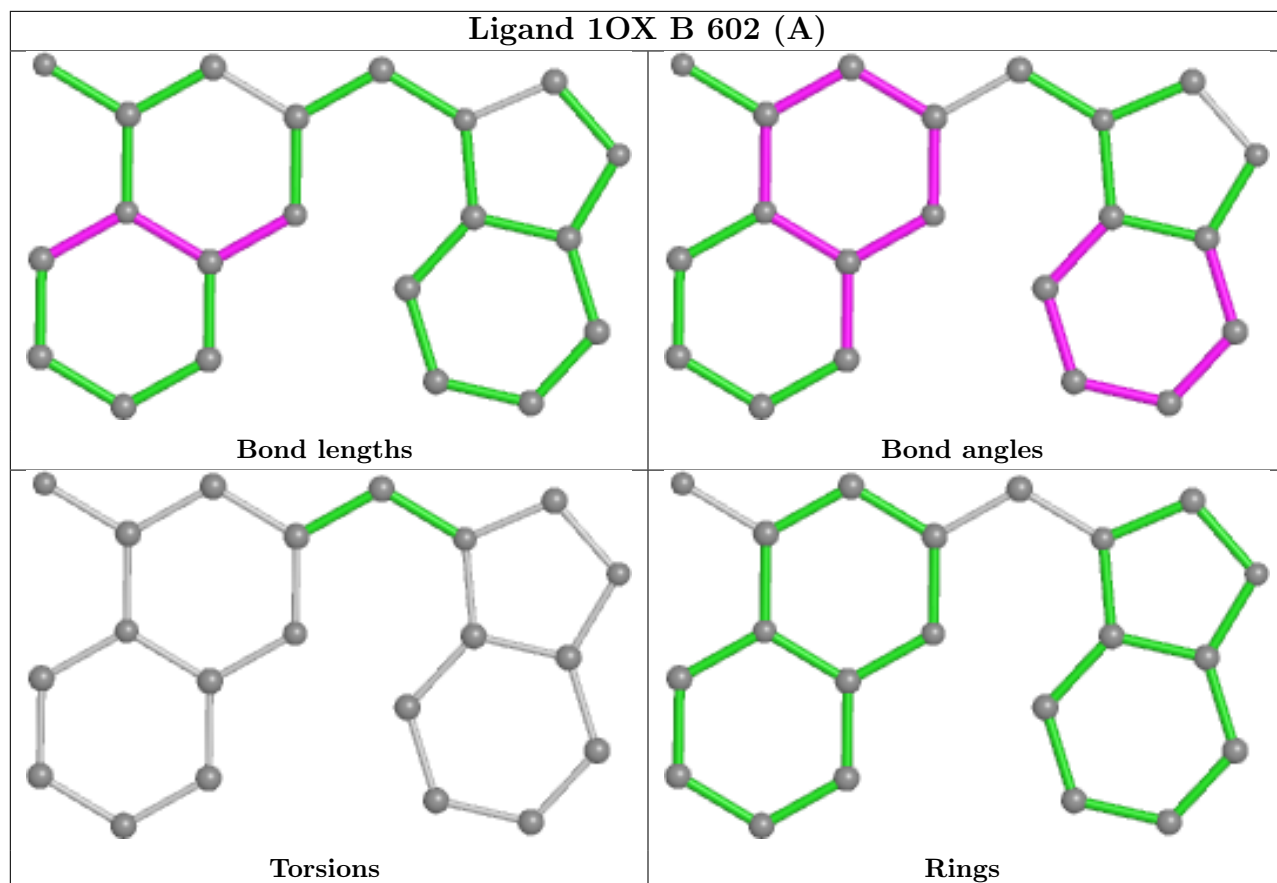


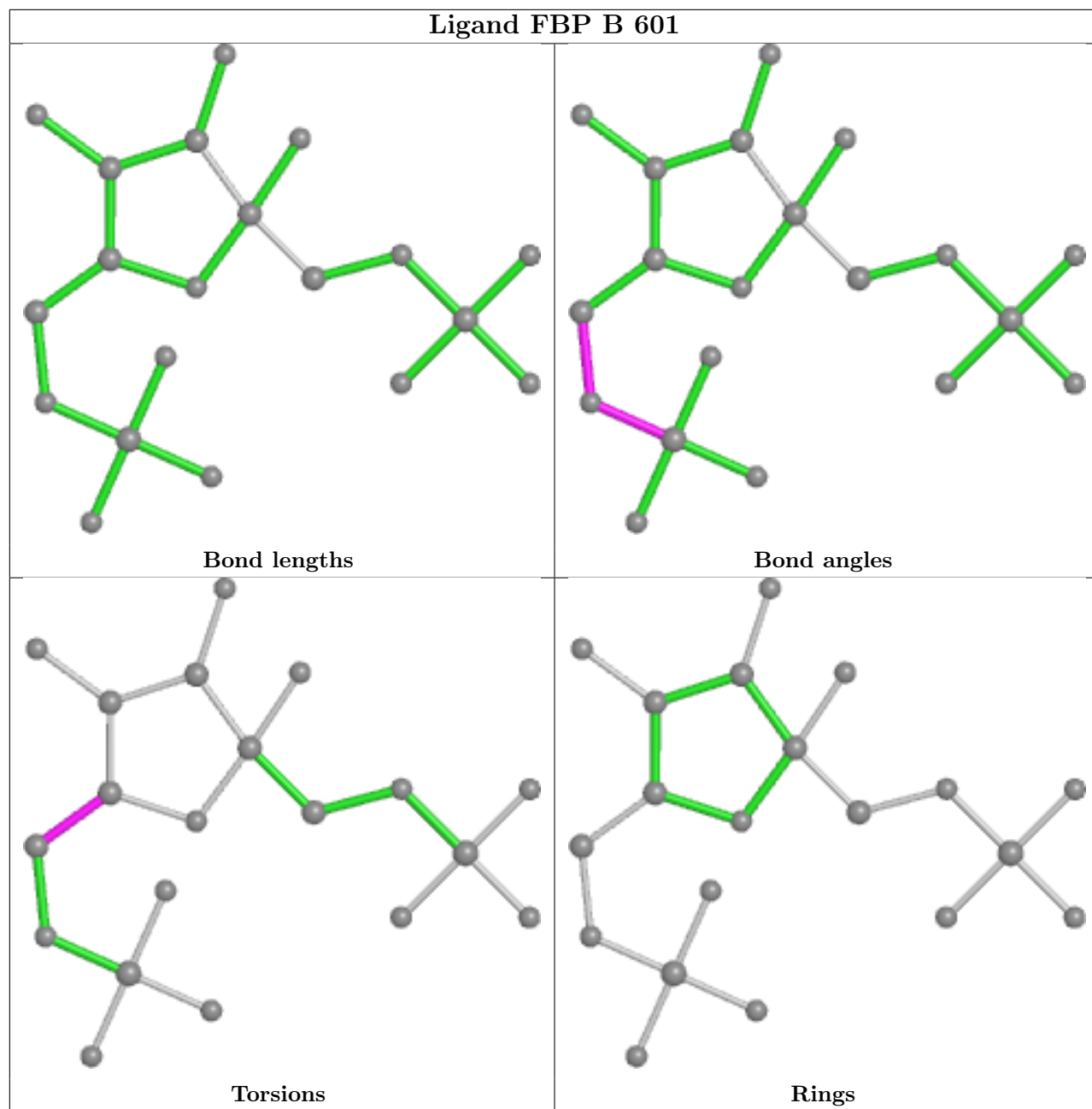


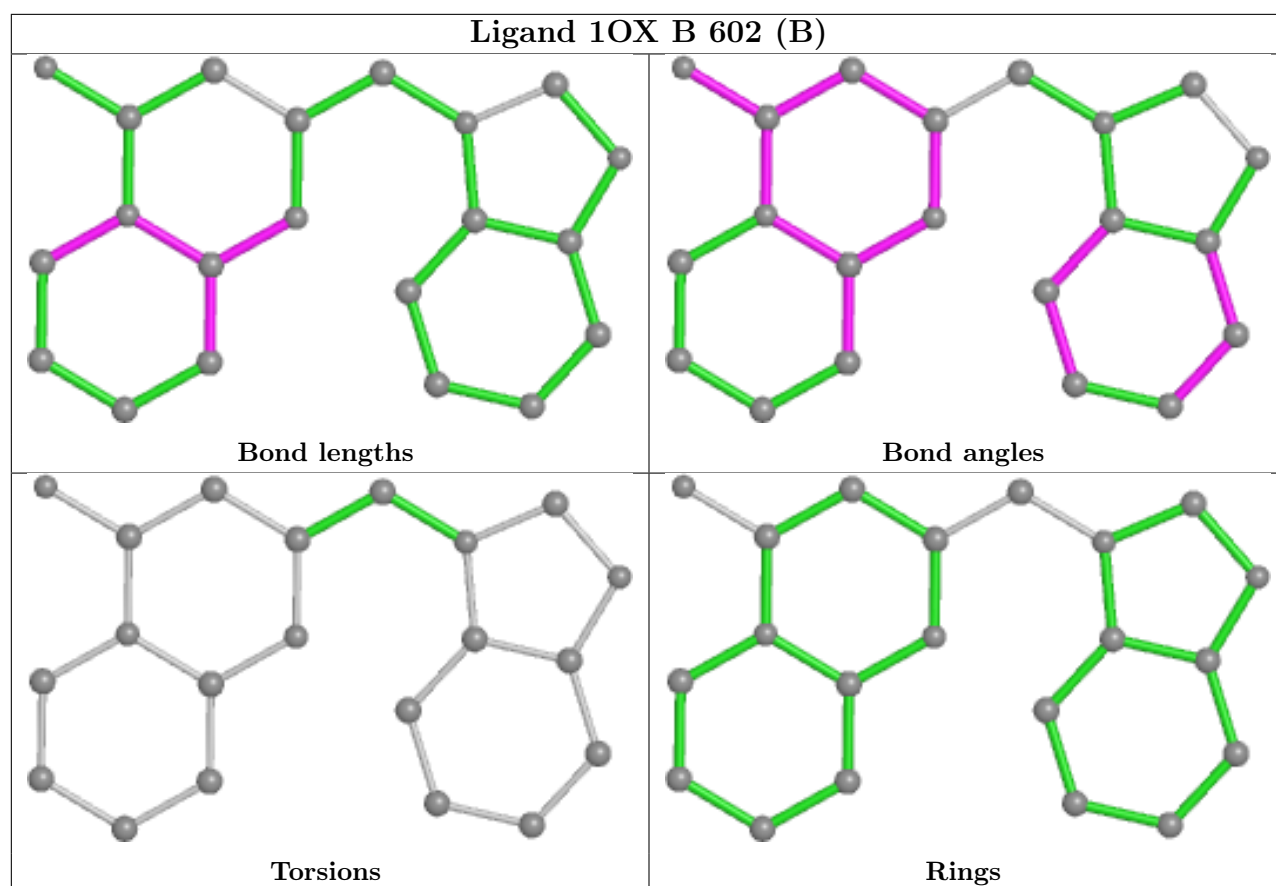












## 5.7 Other polymers [i](#)

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

### 6.1 Protein, DNA and RNA chains

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	519/556 (93%)	0.01	20 (3%) 39 50	33, 46, 85, 106	0
1	B	510/556 (91%)	0.13	35 (6%) 16 24	35, 48, 100, 113	0
1	C	518/556 (93%)	-0.04	11 (2%) 63 73	36, 50, 74, 94	0
1	D	512/556 (92%)	0.25	40 (7%) 13 19	37, 50, 107, 125	0
All	All	2059/2224 (92%)	0.09	106 (5%) 28 39	33, 49, 92, 125	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	192	PHE	6.7
1	B	197	VAL	6.7
1	B	123	LEU	6.0
1	D	148	TYR	5.7
1	D	203	LEU	5.7
1	D	168	VAL	5.7
1	D	159	LEU	5.2
1	D	139	THR	5.2
1	B	192	PHE	5.1
1	D	144	LEU	4.8
1	D	138	ALA	4.6
1	B	193	LEU	4.5
1	D	158	TRP	4.5
1	B	140	LEU	4.5
1	B	122	GLY	4.4
1	A	124	ILE	4.4
1	D	194	VAL	4.3
1	D	152	CYS	4.3
1	D	145	ASP	4.3
1	A	132	VAL	4.2
1	B	170	VAL	4.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	183	LEU	4.2
1	B	134	LEU	4.1
1	A	189	GLY	4.0
1	A	203	LEU	4.0
1	B	195	THR	3.9
1	A	194	VAL	3.9
1	D	197	VAL	3.9
1	D	140	LEU	3.8
1	B	174	ILE	3.8
1	B	198	GLU	3.8
1	A	170	VAL	3.7
1	D	123	LEU	3.7
1	B	156	ILE	3.6
1	B	167	VAL	3.6
1	B	143	THR	3.6
1	B	185	VAL	3.5
1	B	194	VAL	3.5
1	A	13	ILE	3.5
1	B	147	ALA	3.5
1	B	139	THR	3.4
1	B	196	GLU	3.4
1	A	139	THR	3.4
1	D	193	LEU	3.4
1	D	186	LYS	3.3
1	B	149	MET	3.3
1	B	13	ILE	3.3
1	A	214	ALA	3.3
1	A	148	TYR	3.3
1	B	157	LEU	3.3
1	D	170	VAL	3.2
1	A	134	LEU	3.2
1	D	121	THR	3.1
1	C	194	VAL	3.1
1	D	155	ASN	3.1
1	C	192	PHE	3.1
1	C	132	VAL	3.1
1	D	156	ILE	3.1
1	A	157	LEU	3.0
1	A	158	TRP	3.0
1	A	168	VAL	3.0
1	D	165	CYS	2.9
1	A	167	VAL	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	192	PHE	2.9
1	D	157	LEU	2.9
1	C	193	LEU	2.8
1	D	130	ALA	2.8
1	B	155	ASN	2.8
1	C	147	ALA	2.8
1	D	171	GLY	2.8
1	B	158	TRP	2.8
1	B	121	THR	2.8
1	B	161	TYR	2.8
1	D	119	ILE	2.7
1	C	190	ALA	2.7
1	D	134	LEU	2.6
1	A	156	ILE	2.6
1	D	202	SER	2.6
1	D	167	VAL	2.6
1	B	215	ALA	2.6
1	D	151	LYS	2.6
1	D	153	ASP	2.5
1	D	136	LYS	2.5
1	B	172	SER	2.4
1	A	153	ASP	2.4
1	B	159	LEU	2.4
1	C	215	ALA	2.4
1	D	187	GLN	2.3
1	D	149	MET	2.3
1	C	170	VAL	2.3
1	B	199	ASN	2.3
1	D	132	VAL	2.3
1	B	181	ILE	2.3
1	B	164	ILE	2.2
1	D	182	SER	2.2
1	C	488	LEU	2.1
1	C	148	TYR	2.1
1	D	122	GLY	2.1
1	B	142	ILE	2.1
1	A	138	ALA	2.1
1	D	147	ALA	2.1
1	B	144	LEU	2.0
1	C	165	CYS	2.0
1	A	144	LEU	2.0
1	D	181	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	129	THR	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](#)

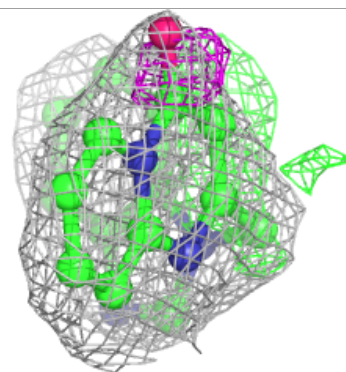
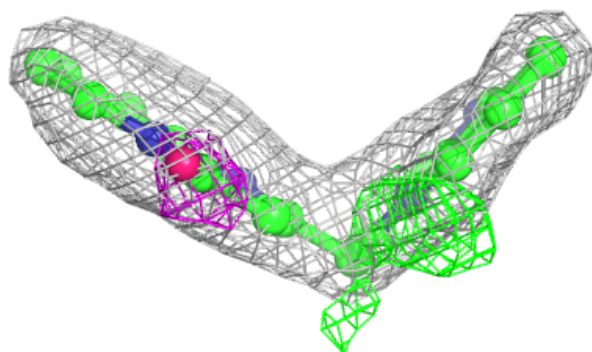
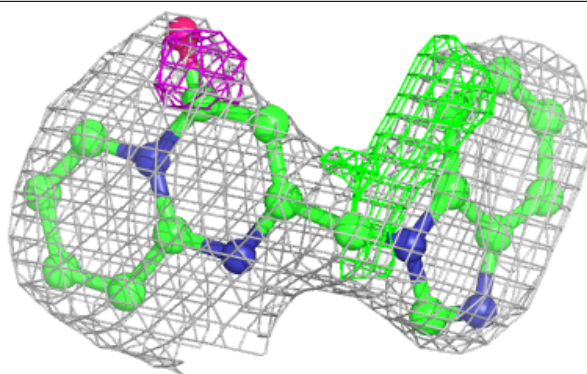
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	1OX	D	602[A]	21/21	0.88	0.29	22,30,37,40	21
3	1OX	D	602[B]	21/21	0.88	0.29	21,40,51,52	21
3	1OX	B	602[A]	21/21	0.92	0.24	23,29,39,41	21
3	1OX	B	602[B]	21/21	0.92	0.24	20,30,43,44	21
2	FBP	A	601	20/20	0.98	0.10	41,49,52,54	0
2	FBP	B	601	20/20	0.98	0.11	36,40,54,56	0
2	FBP	C	601	20/20	0.98	0.09	45,53,61,62	0
2	FBP	D	601	20/20	0.98	0.10	41,44,52,54	0

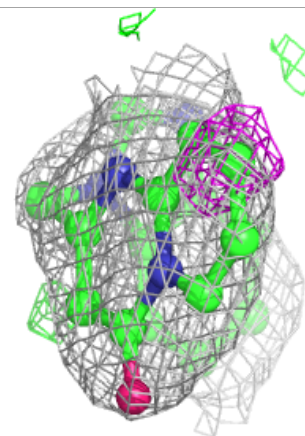
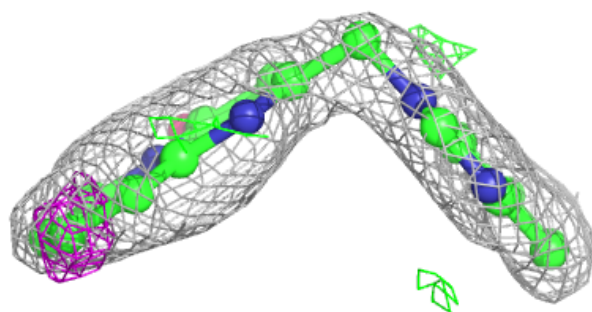
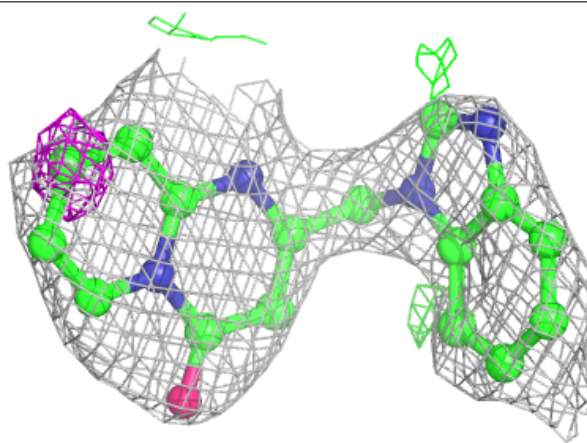
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around 1OX D 602 (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 1OX D 602 (B):**

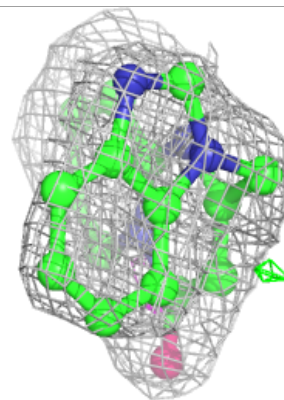
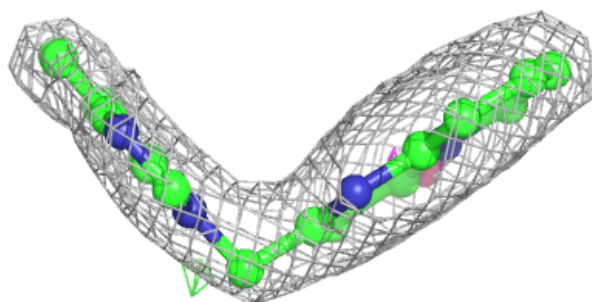
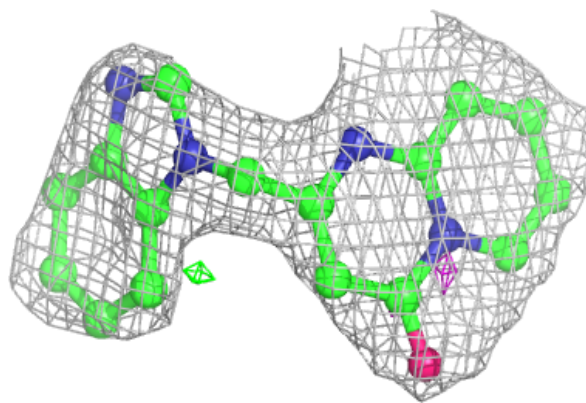
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



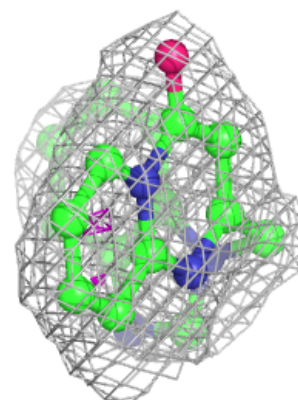
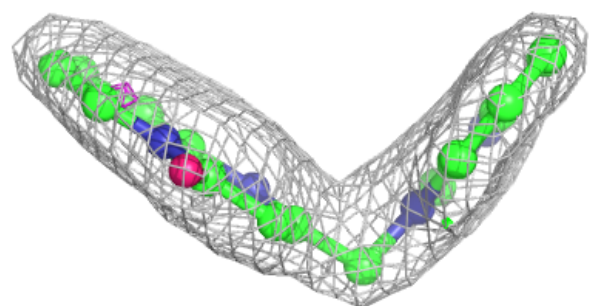
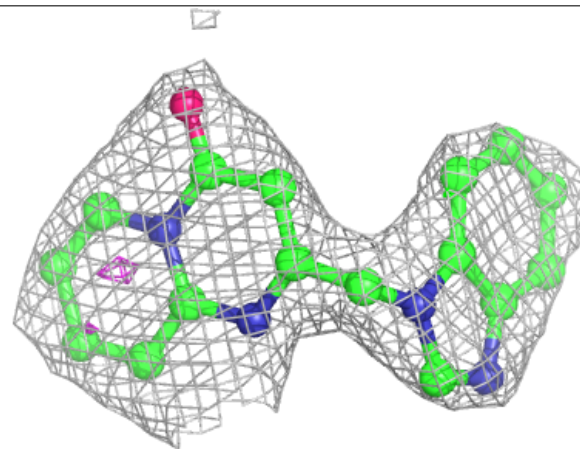


**Electron density around 1OX B 602 (A):**

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

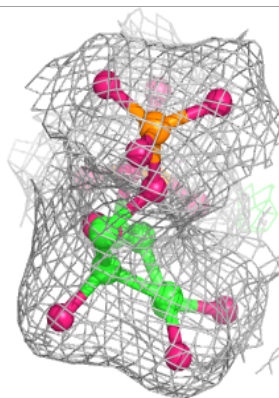
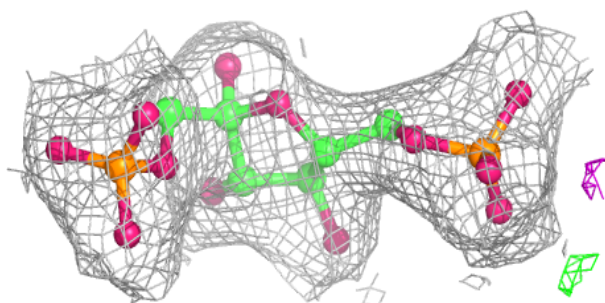
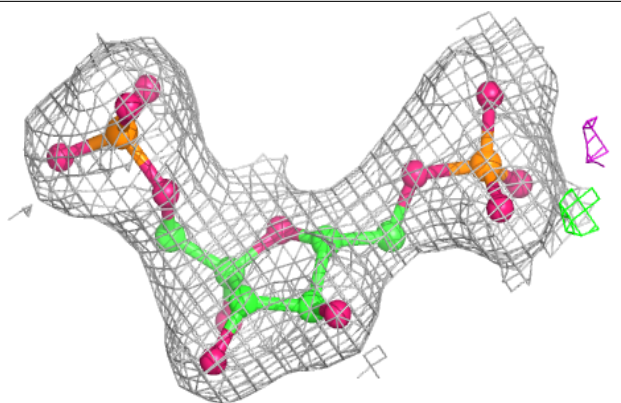
**Electron density around 1OX B 602 (B):**

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

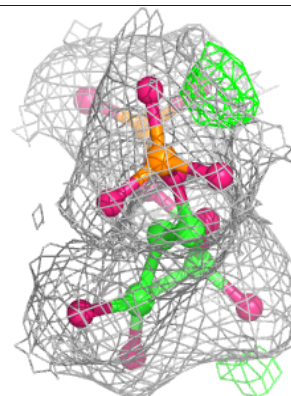
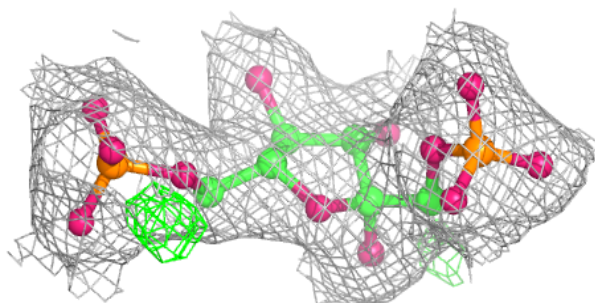
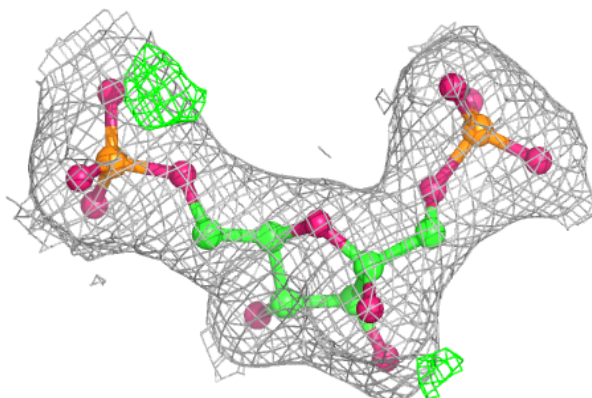


**Electron density around FBP A 601:**

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

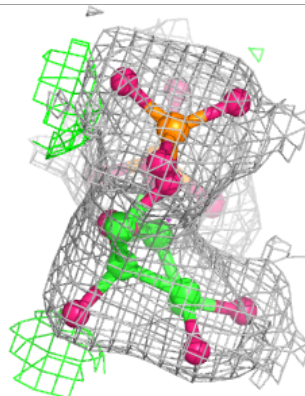
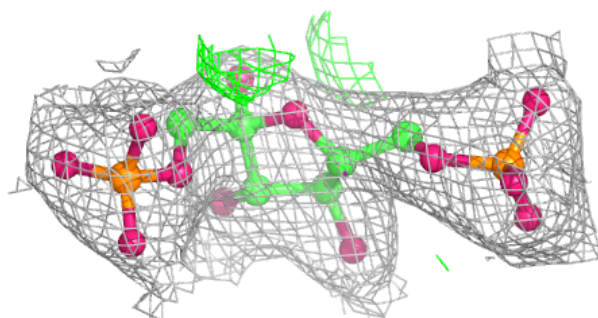
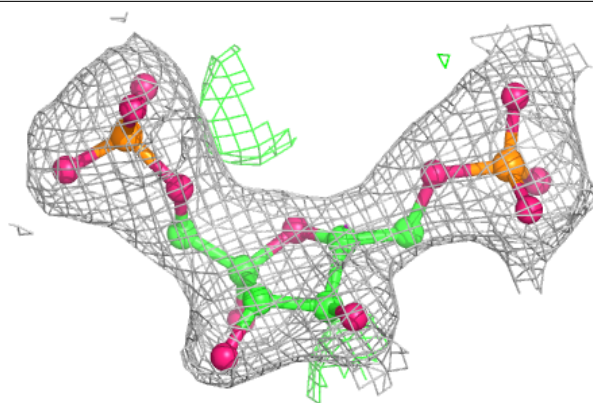
**Electron density around FBP B 601:**

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

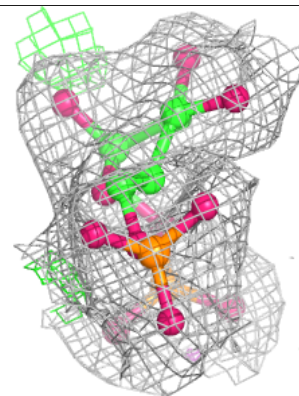
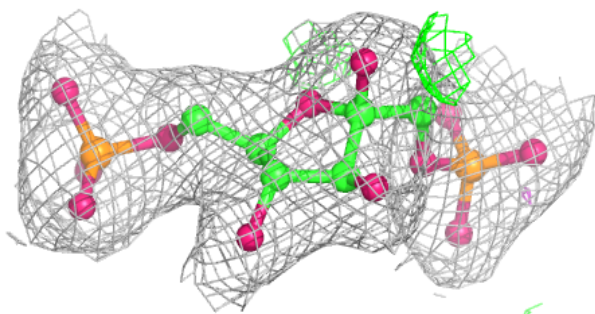
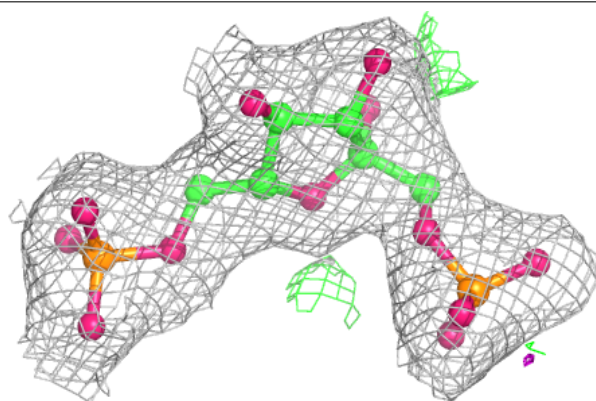


**Electron density around FBP C 601:**

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

**Electron density around FBP D 601:**

$2mF_o-DF_c$  (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.