



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 5X1V / pdb_00005x1v
Title : PKM2 in complex with compound 2
Authors : Matsui, Y.; Hanzawa, H.
Deposited on : 2017-01-27
Resolution : 2.10 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

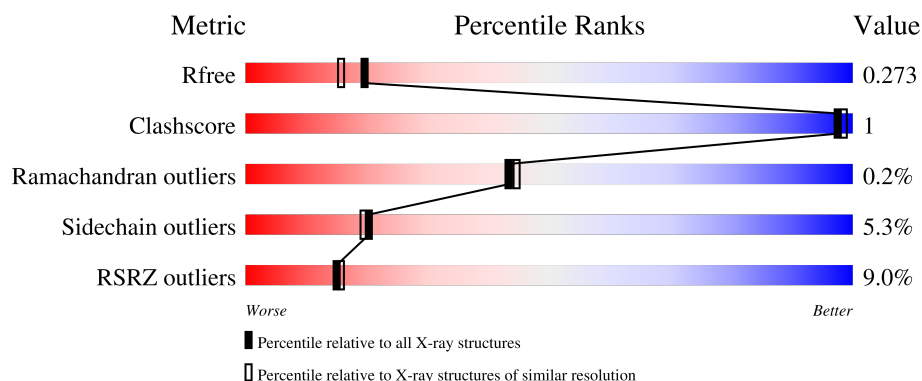
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 ≥ 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	550	13% 86% 7% 7%
1	B	550	8% 84% 8% 7%
1	C	550	3% 86% 8% 6%
1	D	550	10% 86% 6% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16367 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 PKM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3919	2463	696	735	25			
1	B	513	Total	C	N	O	S	0	0	0
			3935	2475	698	737	25			
1	C	518	Total	C	N	O	S	0	0	0
			3965	2492	704	744	25			
1	D	511	Total	C	N	O	S	0	0	0
			3919	2463	696	735	25			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-18	MET	-	expression tag	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618

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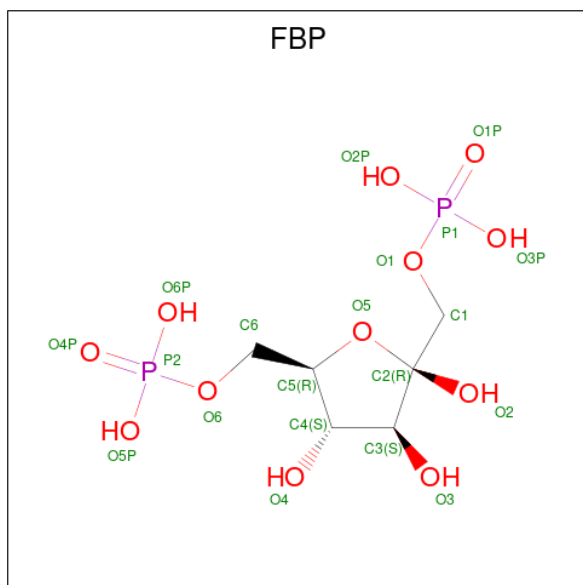
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-18	MET	-	expression tag	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-18	MET	-	expression tag	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618

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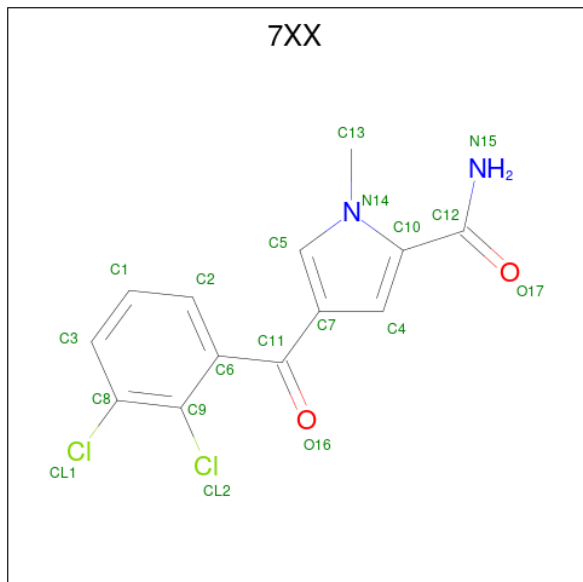
Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	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 (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 4-[2,3-bis(chloranyl)phenyl]carbonyl-1-methyl-pyrrole-2-carboxamide (CCD ID: 7XX) (formula: C₁₃H₁₀Cl₂N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	B	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	C	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		
3	D	1	Total	C	Cl	N	O	0	0
			19	13	2	2	2		

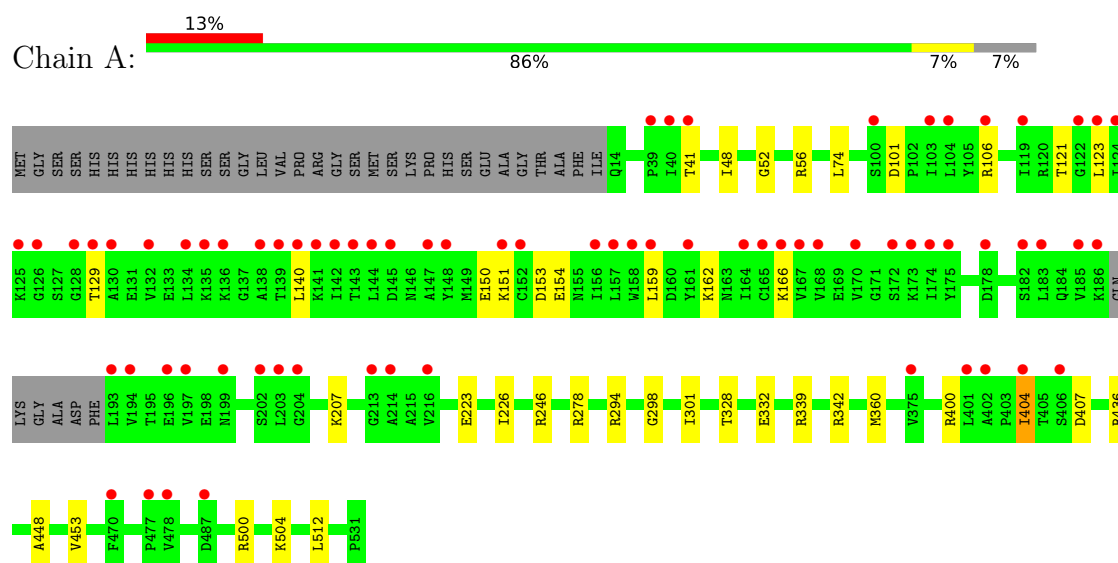
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	120	Total	O	0	0
			120	120		
4	C	127	Total	O	0	0
			127	127		
4	D	132	Total	O	0	0
			132	132		

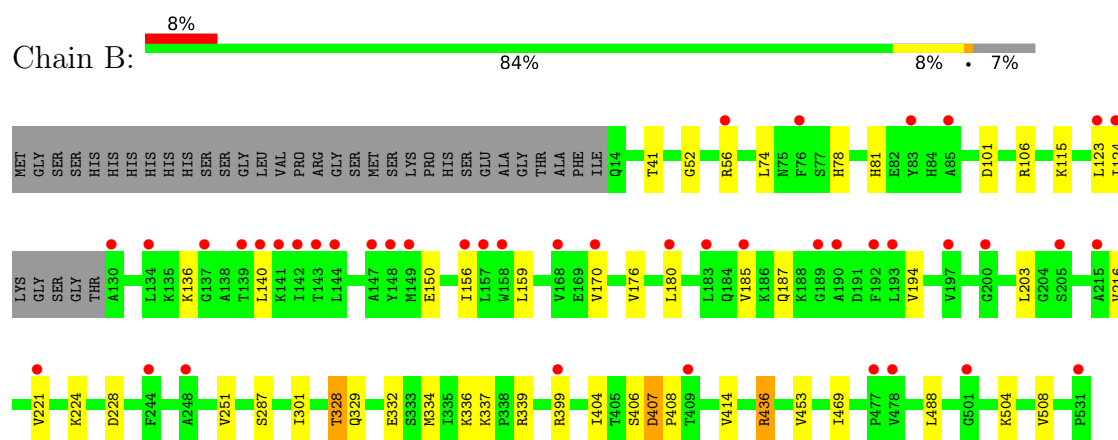
3 Residue-property plots [i](#)

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.

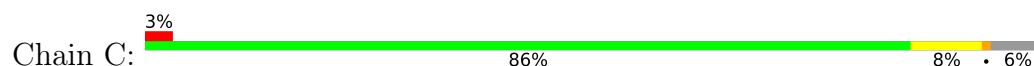
• Molecule 1: Pyruvate kinase PKM

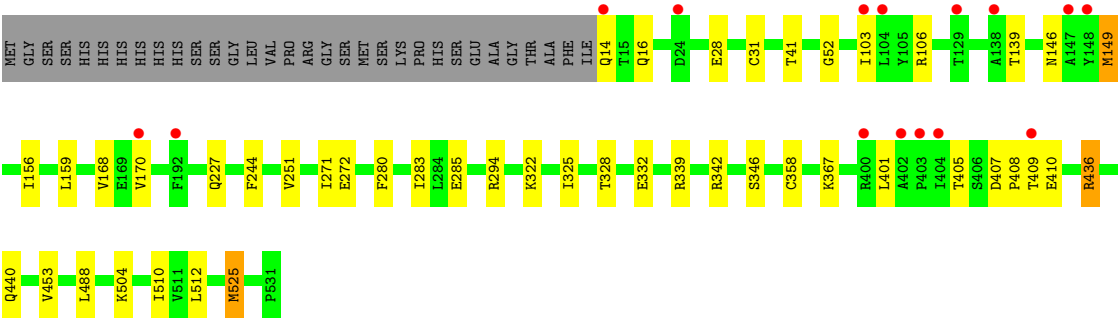


• Molecule 1: Pyruvate kinase PKM

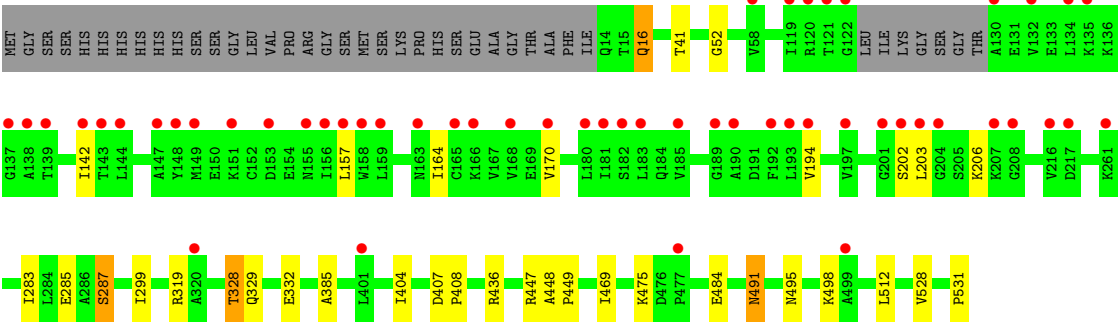
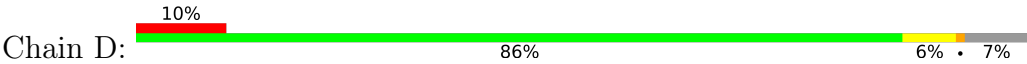


• Molecule 1: Pyruvate kinase PKM





● Molecule 1: Pyruvate kinase PKM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.47Å 151.66Å 92.08Å 90.00° 102.44° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.10) 97.9 (20.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.45 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.234 , 0.274 0.233 , 0.273	Depositor DCC
R_{free} test set	12248 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.448	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16367	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FBP, 7XX

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	0.72	0/3981	1.25	18/5376 (0.3%)
1	B	0.80	0/3998	1.29	14/5399 (0.3%)
1	C	0.74	0/4029	1.28	13/5441 (0.2%)
1	D	0.74	0/3982	1.29	9/5377 (0.2%)
All	All	0.75	0/15990	1.28	54/21593 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	332	GLU	N-CA-C	7.62	120.25	111.11
1	B	52	GLY	CA-C-N	6.73	126.69	119.28
1	B	52	GLY	C-N-CA	6.73	126.69	119.28
1	D	436	ARG	N-CA-C	6.67	118.55	111.28
1	B	101	ASP	CA-C-N	6.66	126.60	119.28
1	B	101	ASP	C-N-CA	6.66	126.60	119.28
1	C	280	PHE	N-CA-C	6.46	118.86	111.11
1	A	436	ARG	N-CA-C	6.43	118.82	111.11
1	B	221	VAL	CB-CA-C	6.38	119.64	110.33
1	A	56	ARG	N-CA-C	6.15	118.77	111.33
1	C	52	GLY	CA-C-N	6.08	125.97	119.28
1	C	52	GLY	C-N-CA	6.08	125.97	119.28
1	B	334	MET	N-CA-C	6.06	120.28	113.01
1	B	407	ASP	CA-C-N	6.06	125.94	119.28
1	B	407	ASP	C-N-CA	6.06	125.94	119.28
1	A	294	ARG	N-CA-C	6.04	118.66	111.71
1	C	339	ARG	CA-C-N	-6.03	114.33	120.85
1	C	339	ARG	C-N-CA	-6.03	114.33	120.85
1	D	332	GLU	N-CA-C	5.87	117.68	111.28
1	B	414	VAL	CA-C-N	5.85	126.47	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	VAL	C-N-CA	5.85	126.47	119.98
1	A	298	GLY	N-CA-C	5.85	121.10	114.67
1	C	436	ARG	N-CA-C	5.80	118.07	111.11
1	C	322	LYS	CA-C-N	5.73	125.75	119.90
1	C	322	LYS	C-N-CA	5.73	125.75	119.90
1	A	332	GLU	N-CA-C	5.63	118.14	111.33
1	D	16	GLN	N-CA-C	5.62	119.32	111.90
1	D	52	GLY	CA-C-N	5.61	125.97	119.47
1	D	52	GLY	C-N-CA	5.61	125.97	119.47
1	D	491	ASN	N-CA-C	5.54	117.32	111.28
1	C	332	GLU	N-CA-C	5.53	117.30	111.28
1	A	404	ILE	CB-CA-C	5.51	118.25	111.25
1	B	436	ARG	N-CA-C	5.40	118.67	111.75
1	C	244	PHE	N-CA-C	5.39	118.87	111.54
1	D	385	ALA	N-CA-C	5.37	118.05	111.82
1	C	294	ARG	N-CA-C	5.25	118.95	112.54
1	A	52	GLY	CA-C-N	5.22	125.28	119.32
1	A	52	GLY	C-N-CA	5.22	125.28	119.32
1	C	16	GLN	N-CA-C	5.16	118.71	111.90
1	C	31	CYS	N-CA-C	5.13	117.61	111.71
1	A	106	ARG	CA-C-N	5.12	125.36	119.83
1	A	106	ARG	C-N-CA	5.12	125.36	119.83
1	D	495	ASN	N-CA-C	5.12	116.86	111.28
1	A	448	ALA	CA-C-N	5.10	125.01	119.76
1	A	448	ALA	C-N-CA	5.10	125.01	119.76
1	A	101	ASP	CA-C-N	5.09	124.70	119.56
1	A	101	ASP	C-N-CA	5.09	124.70	119.56
1	D	299	ILE	N-CA-C	-5.09	106.71	111.45
1	A	407	ASP	CA-C-N	5.08	124.58	119.19
1	A	407	ASP	C-N-CA	5.08	124.58	119.19
1	B	337	LYS	CA-C-N	-5.07	114.75	120.89
1	B	337	LYS	C-N-CA	-5.07	114.75	120.89
1	A	339	ARG	CA-C-N	-5.04	115.17	120.66
1	A	339	ARG	C-N-CA	-5.04	115.17	120.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3919	0	4006	5	0
1	B	3935	0	4017	7	0
1	C	3965	0	4049	9	0
1	D	3919	0	3995	9	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	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	0	0
3	D	19	0	0	0	0
4	A	94	0	0	0	0
4	B	120	0	0	0	0
4	C	127	0	0	0	0
4	D	132	0	0	0	0
All	All	16367	0	16107	27	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 1.

All (27) 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:81:HIS:NE2	1:B:228:ASP:OD1	2.29	0.56
1:B:115:LYS:HD3	1:B:224:LYS:HE2	1.89	0.55
1:D:498:LYS:NZ	1:D:531:PRO:O	2.40	0.55
1:C:510:ILE:HG23	1:C:525:MET:HE3	1.88	0.54
1:C:342:ARG:HG2	1:D:329:GLN:HE21	1.74	0.52
1:C:325:ILE:HG12	1:C:358:CYS:HB2	1.93	0.51
1:D:328:THR:HG22	1:D:329:GLN:HG3	1.92	0.50
1:A:123:LEU:HD12	1:A:150:GLU:HG2	1.95	0.49
1:B:328:THR:HG22	1:B:329:GLN:HG3	1.96	0.47
1:B:123:LEU:HD13	1:B:150:GLU:HG2	1.97	0.46
1:A:48:ILE:HB	1:A:360:MET:HG3	2.00	0.44
1:A:121:THR:HG1	1:A:207:LYS:H	1.63	0.44
1:C:28:GLU:OE1	1:D:319:ARG:NH2	2.52	0.43
1:D:157:LEU:HD13	1:D:203:LEU:HD21	2.01	0.42
1:A:342:ARG:HG2	1:B:329:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ASP:HA	1:B:408:PRO:HD3	1.83	0.42
1:C:146:ASN:HB3	1:C:149:MET:HE2	2.02	0.42
1:C:407:ASP:OD1	1:C:409:THR:OG1	2.28	0.42
1:D:407:ASP:HA	1:D:408:PRO:HD3	1.92	0.41
1:C:407:ASP:HA	1:C:408:PRO:HD3	1.88	0.41
1:A:153:ASP:HB2	1:A:154:GLU:H	1.68	0.41
1:B:187:GLN:HB3	1:B:194:VAL:HB	2.02	0.41
1:C:410:GLU:HG2	1:C:440:GLN:HE21	1.85	0.41
1:D:283:ILE:O	1:D:287:SER:OG	2.35	0.40
1:D:448:ALA:HA	1:D:449:PRO:HD2	1.88	0.40
1:D:16:GLN:O	1:D:447:ARG:NH2	2.52	0.40
1:C:271:ILE:HD11	1:C:283:ILE:HG21	2.03	0.40

There are no symmetry-related clashes.

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	A	508/550 (92%)	495 (97%)	12 (2%)	1 (0%)	43	44
1	B	509/550 (92%)	496 (97%)	12 (2%)	1 (0%)	43	44
1	C	516/550 (94%)	504 (98%)	11 (2%)	1 (0%)	43	44
1	D	507/550 (92%)	495 (98%)	11 (2%)	1 (0%)	43	44
All	All	2040/2200 (93%)	1990 (98%)	46 (2%)	4 (0%)	43	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	B	328	THR

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Mol	Chain	Res	Type
1	D	328	THR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	422/452 (93%)	403 (96%)	19 (4%)	24	25
1	B	423/452 (94%)	393 (93%)	30 (7%)	13	11
1	C	426/452 (94%)	402 (94%)	24 (6%)	19	18
1	D	421/452 (93%)	405 (96%)	16 (4%)	29	32
All	All	1692/1808 (94%)	1603 (95%)	89 (5%)	20	19

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	74	LEU
1	A	129	THR
1	A	140	LEU
1	A	151	LYS
1	A	159	LEU
1	A	162	LYS
1	A	166	LYS
1	A	223	GLU
1	A	226	ILE
1	A	246	ARG
1	A	278	ARG
1	A	301	ILE
1	A	400	ARG
1	A	404	ILE
1	A	453	VAL
1	A	500	ARG
1	A	504	LYS
1	A	512	LEU
1	B	41	THR

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Mol	Chain	Res	Type
1	B	56	ARG
1	B	74	LEU
1	B	78	HIS
1	B	106	ARG
1	B	124	ILE
1	B	136	LYS
1	B	140	LEU
1	B	156	ILE
1	B	159	LEU
1	B	170	VAL
1	B	176	VAL
1	B	180	LEU
1	B	185	VAL
1	B	203	LEU
1	B	216	VAL
1	B	251	VAL
1	B	287	SER
1	B	301	ILE
1	B	336	LYS
1	B	339	ARG
1	B	399	ARG
1	B	404	ILE
1	B	406	SER
1	B	436	ARG
1	B	453	VAL
1	B	469	ILE
1	B	488	LEU
1	B	504	LYS
1	B	508	VAL
1	C	14	GLN
1	C	41	THR
1	C	103	ILE
1	C	106	ARG
1	C	139	THR
1	C	149	MET
1	C	156	ILE
1	C	159	LEU
1	C	168	VAL
1	C	170	VAL
1	C	227	GLN
1	C	251	VAL
1	C	272	GLU

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Mol	Chain	Res	Type
1	C	285	GLU
1	C	346	SER
1	C	367	LYS
1	C	401	LEU
1	C	405	THR
1	C	436	ARG
1	C	453	VAL
1	C	488	LEU
1	C	504	LYS
1	C	512	LEU
1	C	525	MET
1	D	41	THR
1	D	142	ILE
1	D	164	ILE
1	D	170	VAL
1	D	194	VAL
1	D	202	SER
1	D	206	LYS
1	D	285	GLU
1	D	287	SER
1	D	404	ILE
1	D	469	ILE
1	D	475	LYS
1	D	484	GLU
1	D	491	ASN
1	D	512	LEU
1	D	528	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	146	ASN
1	A	391	HIS
1	B	19	HIS
1	B	210	ASN
1	B	235	GLN
1	B	329	GLN
1	C	184	GLN
1	C	252	HIS
1	C	273	ASN
1	C	391	HIS

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Mol	Chain	Res	Type
1	C	393	GLN
1	C	458	GLN
1	D	44	ASN
1	D	78	HIS
1	D	199	ASN
1	D	235	GLN
1	D	252	HIS
1	D	329	GLN
1	D	393	GLN
1	D	440	GLN
1	D	458	GLN

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 oligosaccharides 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
2	FBP	D	601	-	18,20,20	0.84	1 (5%)	21,32,32	1.02	1 (4%)
3	7XX	C	602	-	20,20,20	0.91	1 (5%)	23,29,29	2.33	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	7XX	A	602	-	20,20,20	0.95	1 (5%)	23,29,29	2.37	10 (43%)
3	7XX	B	602	-	20,20,20	0.95	1 (5%)	23,29,29	2.52	13 (56%)
2	FBP	B	601	-	18,20,20	0.70	0	21,32,32	1.06	1 (4%)
2	FBP	A	601	-	18,20,20	0.69	0	21,32,32	1.04	2 (9%)
2	FBP	C	601	-	18,20,20	0.73	0	21,32,32	0.98	1 (4%)
3	7XX	D	602	-	20,20,20	0.86	0	23,29,29	2.21	6 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	D	601	-	-	2/13/32/32	0/1/1/1
3	7XX	C	602	-	-	2/12/12/12	0/2/2/2
3	7XX	A	602	-	-	2/12/12/12	0/2/2/2
3	7XX	B	602	-	-	2/12/12/12	0/2/2/2
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
2	FBP	A	601	-	-	3/13/32/32	0/1/1/1
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
3	7XX	D	602	-	-	4/12/12/12	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	7XX	C10-C12	-2.36	1.44	1.49
3	B	602	7XX	C10-C12	-2.31	1.44	1.49
3	C	602	7XX	C10-C12	-2.10	1.45	1.49
2	D	601	FBP	O2-C2	2.05	1.44	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	7XX	C12-C10-N14	7.32	130.67	122.79
3	B	602	7XX	C12-C10-N14	7.30	130.65	122.79
3	A	602	7XX	C12-C10-N14	7.10	130.43	122.79
3	D	602	7XX	C12-C10-N14	6.96	130.29	122.79
3	B	602	7XX	C6-C9-C8	-4.22	117.32	120.13
3	C	602	7XX	C6-C11-C7	3.87	126.45	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	7XX	C6-C11-C7	3.10	125.33	120.84
3	B	602	7XX	C13-N14-C5	-2.94	119.17	123.98
3	C	602	7XX	C13-N14-C5	-2.87	119.28	123.98
3	A	602	7XX	C13-N14-C5	-2.84	119.34	123.98
3	B	602	7XX	C6-C11-C7	2.83	124.95	120.84
3	B	602	7XX	C3-C8-C9	2.67	123.72	120.52
3	D	602	7XX	C13-N14-C5	-2.67	119.62	123.98
3	D	602	7XX	C6-C11-C7	2.65	124.69	120.84
3	B	602	7XX	C7-C4-C10	2.57	110.65	108.06
3	A	602	7XX	C7-C4-C10	2.53	110.61	108.06
3	A	602	7XX	C6-C9-CL2	2.50	123.68	120.11
2	A	601	FBP	O3P-P1-O2P	2.45	116.97	107.80
3	B	602	7XX	C13-N14-C10	2.44	130.56	127.70
3	C	602	7XX	C6-C9-C8	-2.43	118.51	120.13
2	D	601	FBP	O6P-P2-O5P	2.43	116.90	107.80
3	B	602	7XX	C6-C9-CL2	2.40	123.54	120.11
3	D	602	7XX	C1-C2-C6	2.38	124.09	119.80
3	A	602	7XX	C3-C8-C9	2.33	123.32	120.52
3	A	602	7XX	C4-C10-N14	-2.31	104.87	107.45
3	C	602	7XX	C13-N14-C10	2.27	130.36	127.70
3	B	602	7XX	C1-C2-C6	2.24	123.84	119.80
3	A	602	7XX	C1-C2-C6	2.21	123.79	119.80
3	B	602	7XX	O16-C11-C6	-2.21	114.77	120.41
3	B	602	7XX	C4-C10-N14	-2.18	105.01	107.45
3	A	602	7XX	C6-C9-C8	-2.18	118.68	120.13
2	A	601	FBP	O3P-P1-O1	-2.14	101.08	106.67
3	C	602	7XX	C4-C10-C12	-2.14	124.09	129.51
3	A	602	7XX	C13-N14-C10	2.12	130.18	127.70
3	B	602	7XX	C5-C7-C4	-2.12	104.28	106.35
3	D	602	7XX	C6-C9-CL2	2.11	123.12	120.11
2	B	601	FBP	O1-P1-O1P	-2.08	100.82	106.44
2	C	601	FBP	O1-P1-O1P	-2.05	100.90	106.44
3	B	602	7XX	C4-C10-C12	-2.04	124.34	129.51
3	D	602	7XX	C7-C4-C10	2.03	110.11	108.06
3	C	602	7XX	C1-C2-C6	2.03	123.46	119.80
3	C	602	7XX	C7-C4-C10	2.02	110.09	108.06
3	C	602	7XX	O16-C11-C6	-2.01	115.27	120.41

There are no chirality outliers.

All (19) torsion outliers are listed below:

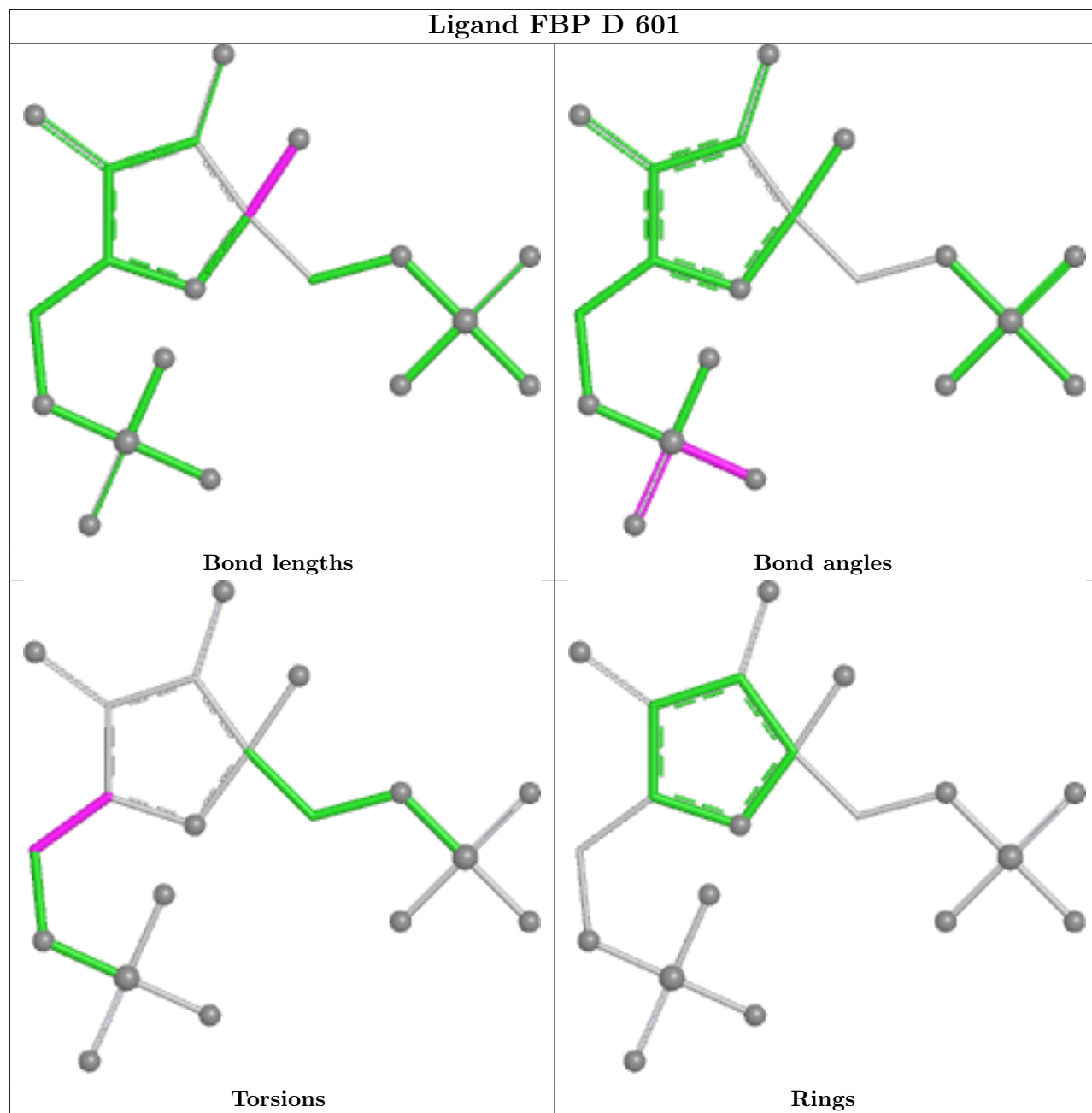
Mol	Chain	Res	Type	Atoms
3	A	602	7XX	O16-C11-C7-C4
3	B	602	7XX	O16-C11-C7-C4
3	C	602	7XX	O16-C11-C7-C4
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6
2	D	601	FBP	O5-C5-C6-O6
3	D	602	7XX	O16-C11-C7-C5
2	A	601	FBP	O5-C5-C6-O6
3	D	602	7XX	O16-C11-C7-C4
2	A	601	FBP	C6-O6-P2-O4P
3	A	602	7XX	O16-C11-C7-C5
3	B	602	7XX	O16-C11-C7-C5
3	C	602	7XX	O16-C11-C7-C5
3	D	602	7XX	C4-C10-C12-N15
3	D	602	7XX	C4-C10-C12-O17

There are no ring outliers.

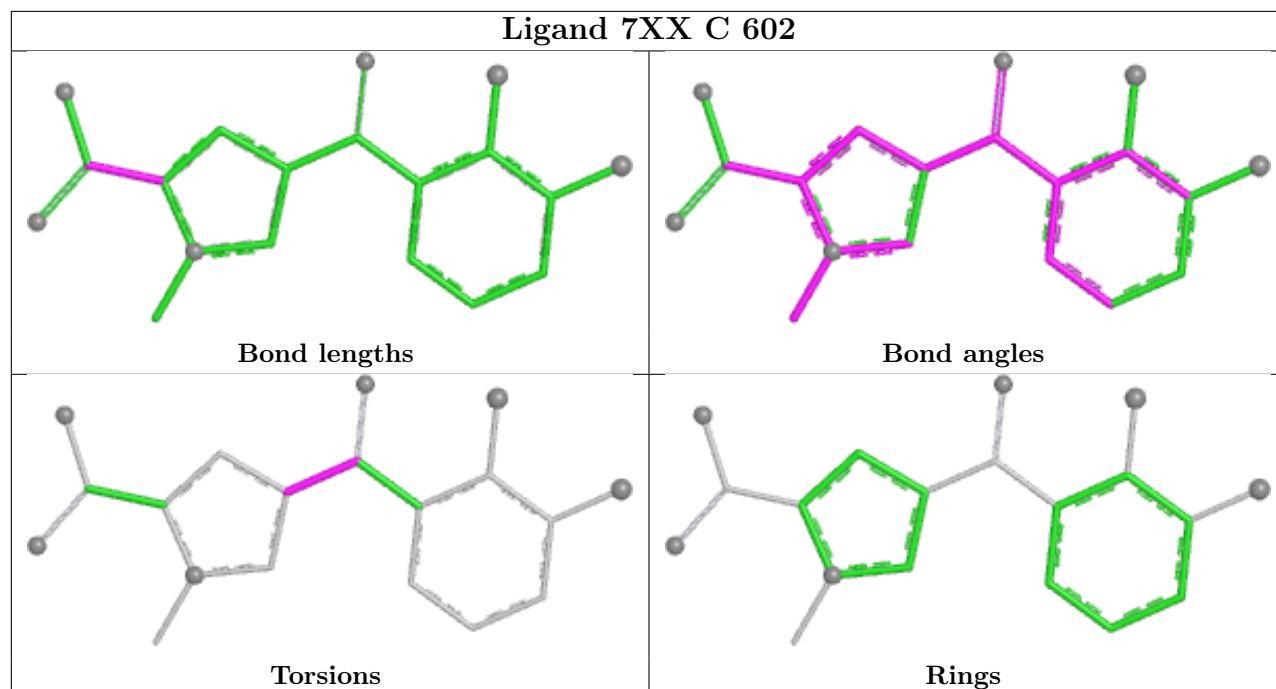
No monomer is involved in short contacts.

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

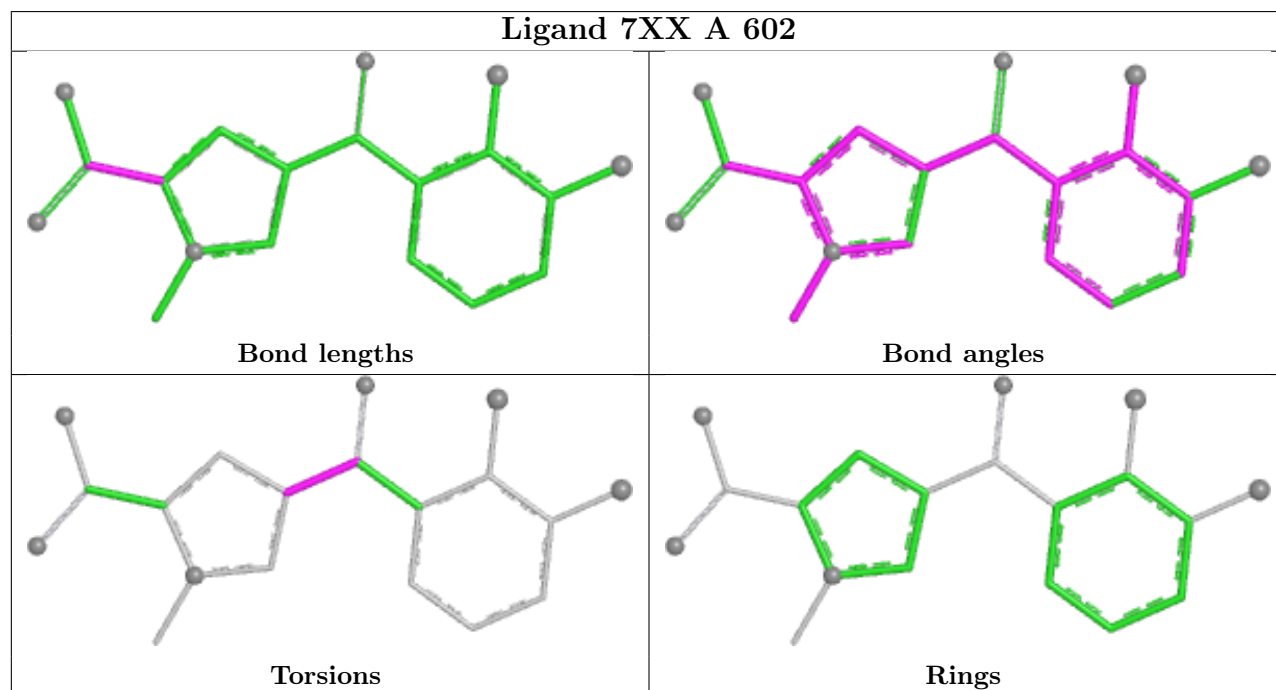
Ligand FBP D 601

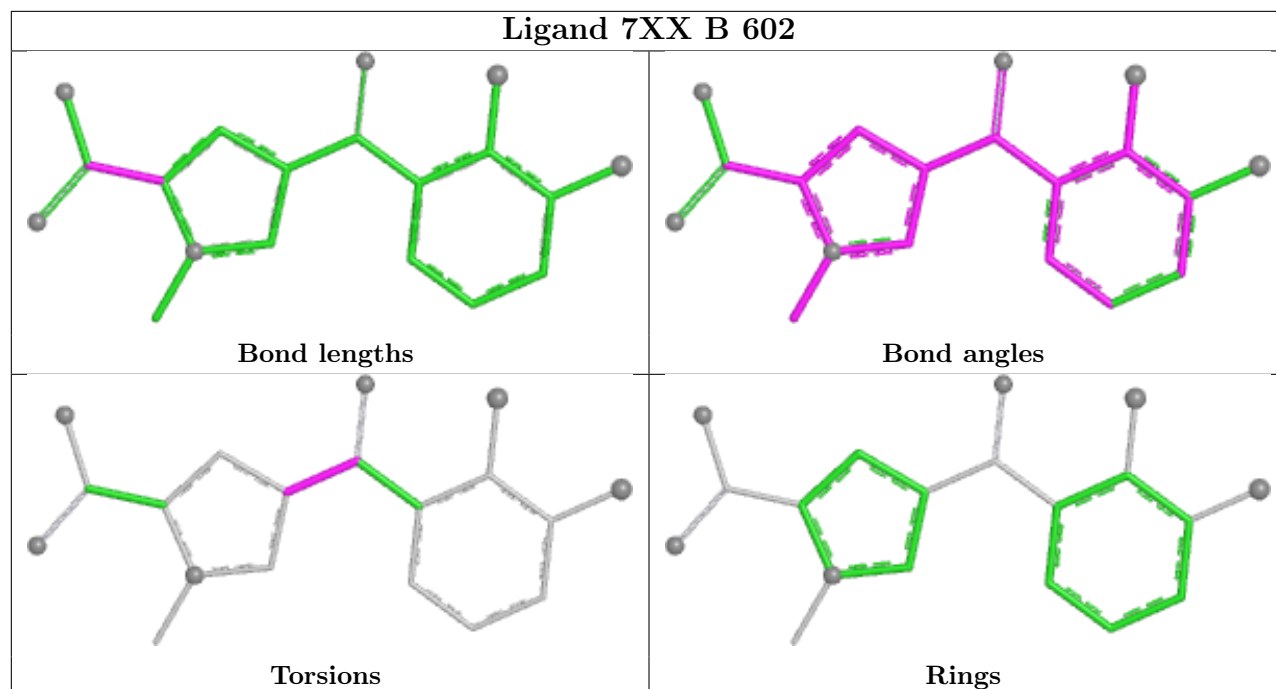


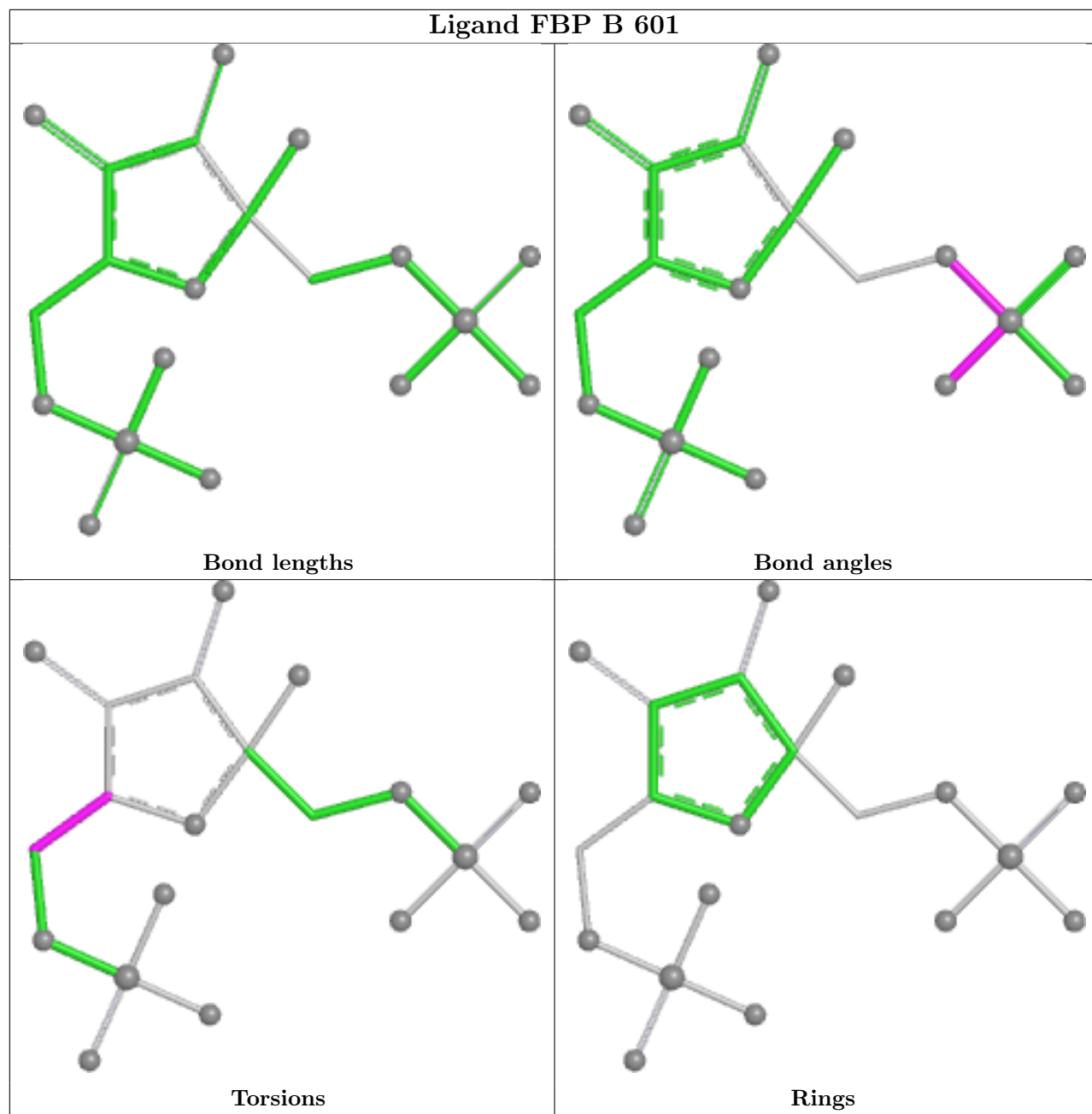
Ligand 7XX C 602

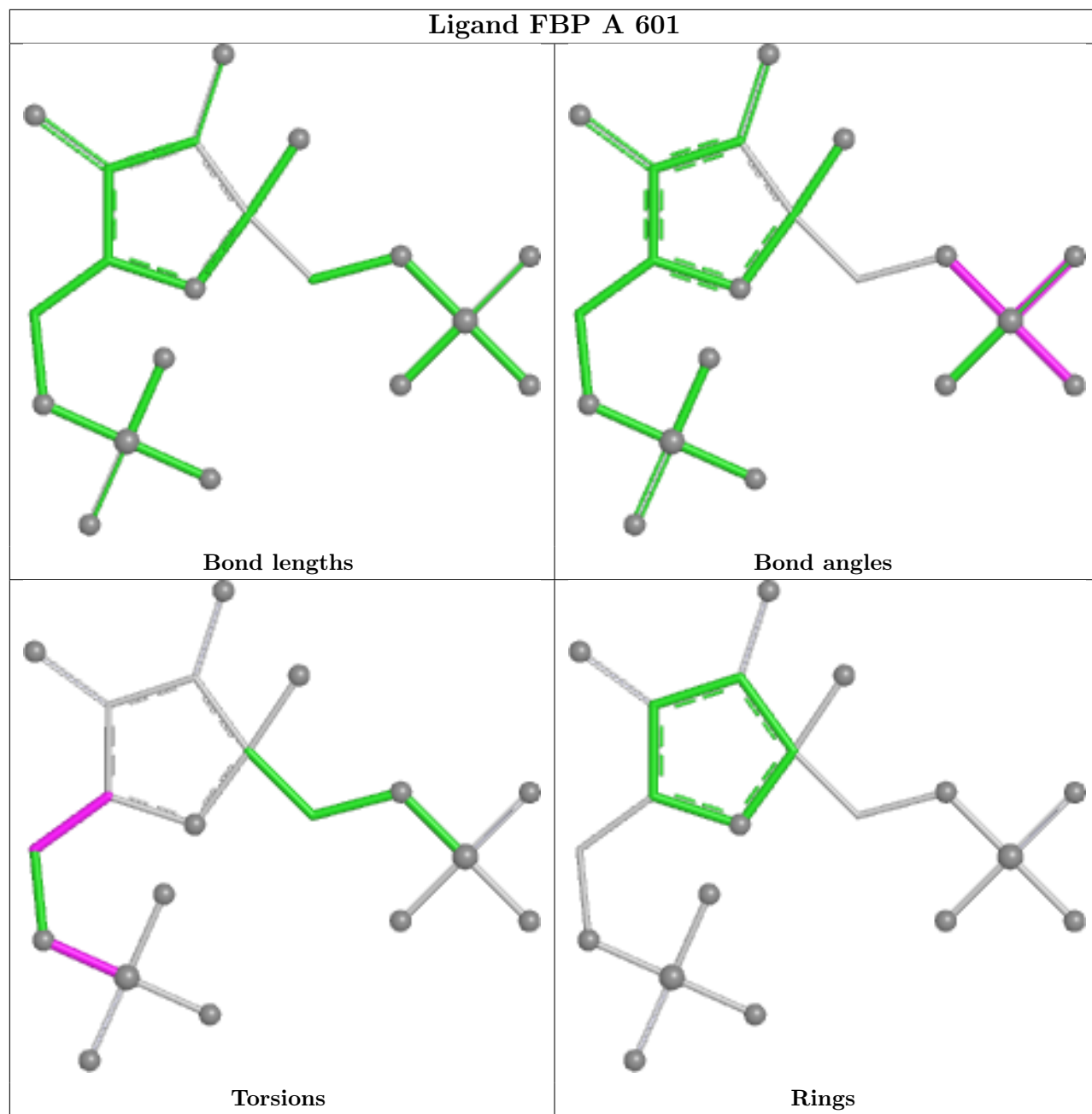


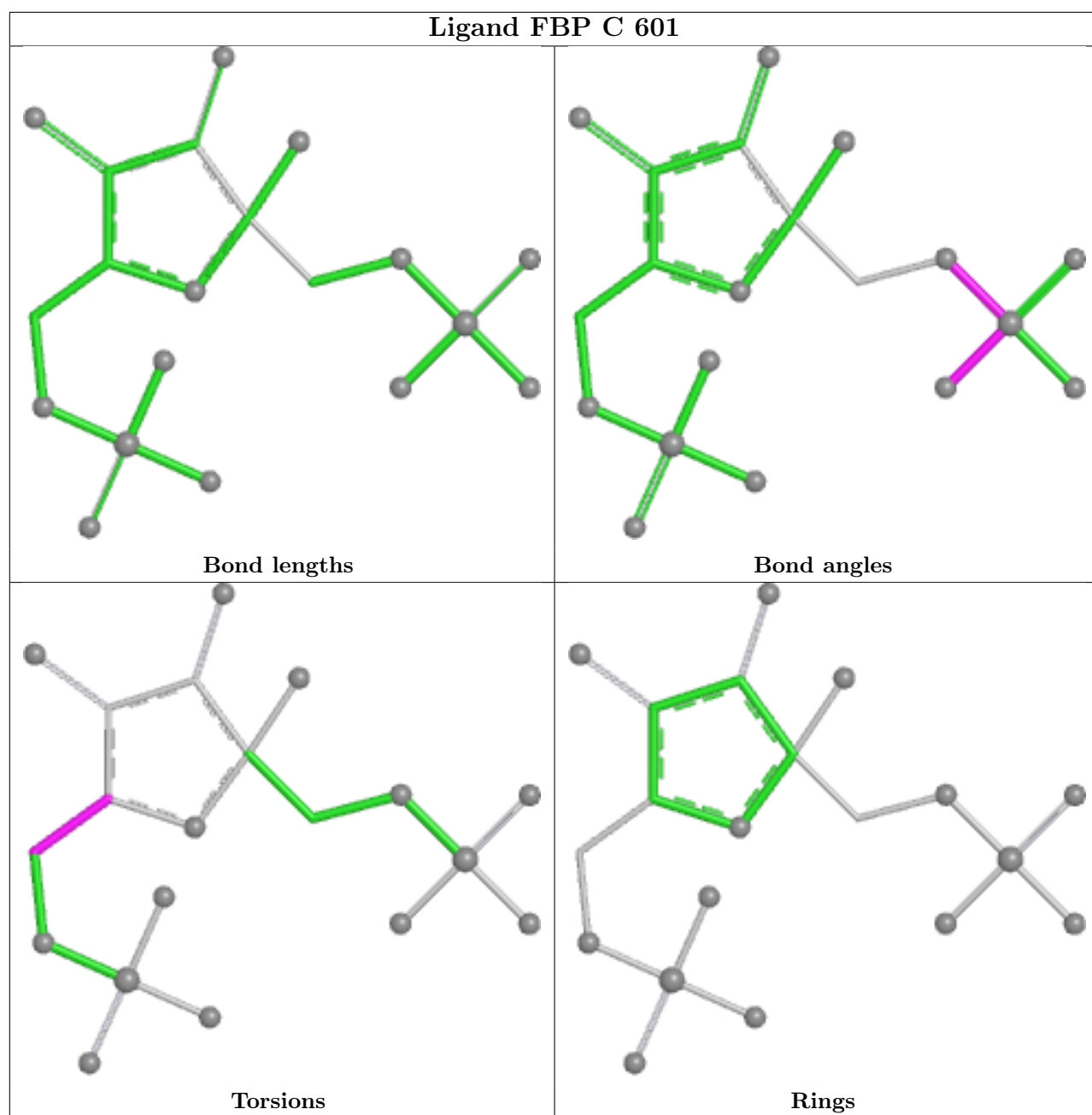
Ligand 7XX A 602

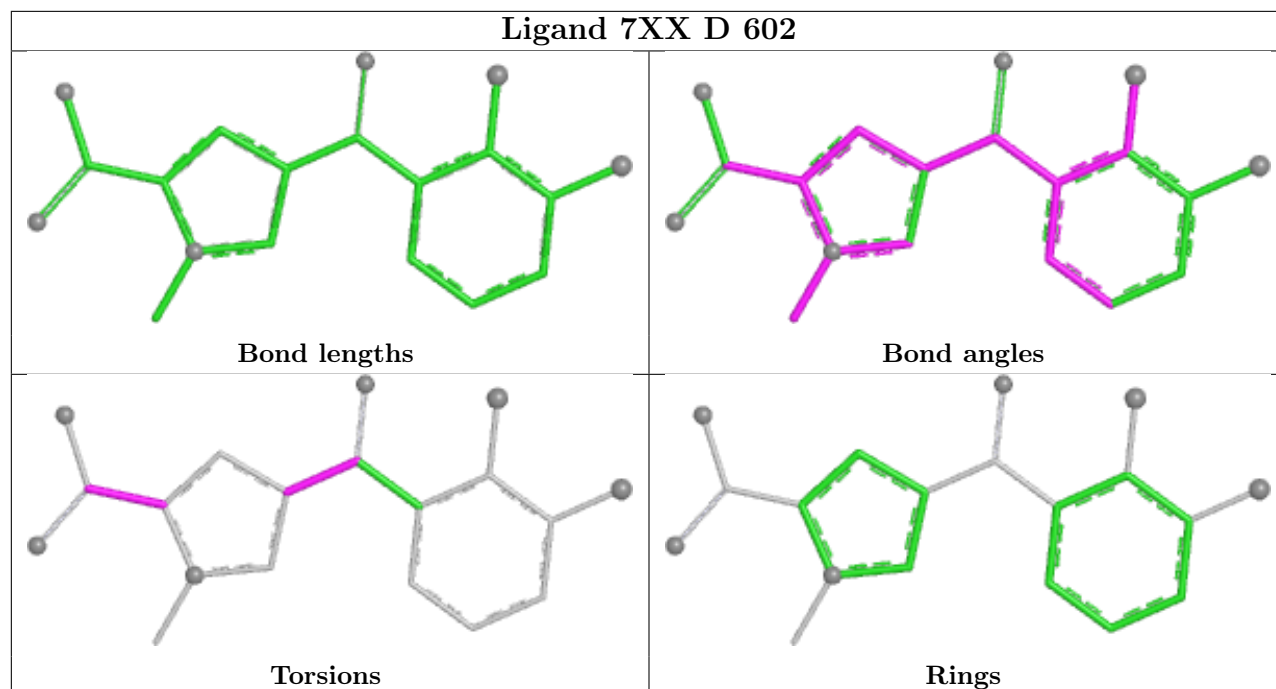












5.7 Other polymers [i](#)

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, 95th 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 ²)	Q<0.9
1	A	512/550 (93%)	0.89	72 (14%) 6 6	19, 42, 95, 108	0
1	B	513/550 (93%)	0.73	43 (8%) 17 18	22, 37, 82, 103	1 (0%)
1	C	518/550 (94%)	0.36	15 (2%) 53 56	23, 36, 55, 69	0
1	D	511/550 (92%)	0.60	54 (10%) 11 12	24, 36, 80, 97	0
All	All	2054/2200 (93%)	0.65	184 (8%) 15 16	19, 38, 81, 108	1 (0%)

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ASN	5.8
1	A	140	LEU	5.2
1	A	170	VAL	5.0
1	A	147	ALA	4.5
1	B	130	ALA	4.4
1	B	142	ILE	4.4
1	A	132	VAL	4.3
1	A	138	ALA	4.2
1	A	126	GLY	4.0
1	A	143	THR	4.0
1	A	151	LYS	4.0
1	D	130	ALA	3.9
1	D	156	ILE	3.9
1	D	134	LEU	3.9
1	D	168	VAL	3.9
1	D	207	LYS	3.9
1	A	41	THR	3.9
1	A	159	LEU	3.9
1	A	167	VAL	3.8
1	B	140	LEU	3.8
1	A	145	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	403	PRO	3.7
1	B	170	VAL	3.7
1	D	204	GLY	3.7
1	D	170	VAL	3.7
1	A	130	ALA	3.7
1	D	190	ALA	3.7
1	A	144	LEU	3.6
1	D	147	ALA	3.6
1	A	158	TRP	3.5
1	A	185	VAL	3.5
1	B	409	THR	3.5
1	D	192	PHE	3.5
1	B	134	LEU	3.5
1	D	149	MET	3.5
1	A	404	ILE	3.4
1	A	401	LEU	3.4
1	A	152	CYS	3.4
1	A	470	PHE	3.4
1	A	197	VAL	3.4
1	D	208	GLY	3.3
1	B	143	THR	3.3
1	A	40	ILE	3.2
1	A	193	LEU	3.2
1	B	478	VAL	3.2
1	B	190	ALA	3.2
1	C	402	ALA	3.2
1	D	194	VAL	3.1
1	A	156	ILE	3.1
1	A	148	TYR	3.1
1	A	123	LEU	3.1
1	B	144	LEU	3.1
1	D	157	LEU	3.1
1	A	100	SER	3.1
1	D	181	ILE	3.1
1	A	164	ILE	3.1
1	A	157	LEU	3.0
1	D	137	GLY	3.0
1	D	158	TRP	3.0
1	B	197	VAL	3.0
1	A	122	GLY	3.0
1	A	124	ILE	3.0
1	B	124	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	142	ILE	3.0
1	A	129	THR	3.0
1	B	192	PHE	3.0
1	D	203	LEU	2.9
1	D	499	ALA	2.9
1	A	136	LYS	2.9
1	C	409	THR	2.9
1	D	139	THR	2.9
1	D	193	LEU	2.8
1	B	156	ILE	2.8
1	D	201	GLY	2.8
1	A	134	LEU	2.8
1	C	129	THR	2.8
1	C	148	TYR	2.8
1	D	143	THR	2.8
1	A	166	LYS	2.8
1	C	404	ILE	2.8
1	A	178	ASP	2.7
1	A	139	THR	2.7
1	C	138	ALA	2.7
1	A	199	ASN	2.7
1	D	216	VAL	2.7
1	B	215	ALA	2.7
1	B	244	PHE	2.7
1	D	180	LEU	2.7
1	B	185	VAL	2.7
1	C	170	VAL	2.7
1	A	402	ALA	2.6
1	B	149	MET	2.6
1	A	214	ALA	2.6
1	B	183	LEU	2.6
1	D	58	VAL	2.6
1	A	173	LYS	2.6
1	A	203	LEU	2.6
1	A	406	SER	2.6
1	B	168	VAL	2.6
1	B	123	LEU	2.6
1	C	192	PHE	2.5
1	D	148	TYR	2.5
1	D	163	ASN	2.5
1	D	121	THR	2.5
1	D	189	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	125	LYS	2.5
1	A	196	GLU	2.5
1	B	147	ALA	2.5
1	A	183	LEU	2.5
1	A	103	ILE	2.5
1	B	85	ALA	2.5
1	A	168	VAL	2.4
1	D	197	VAL	2.4
1	A	204	GLY	2.4
1	B	180	LEU	2.4
1	D	144	LEU	2.4
1	D	183	LEU	2.4
1	C	103	ILE	2.4
1	D	135	LYS	2.4
1	D	119	ILE	2.4
1	B	205	SER	2.4
1	D	151	LYS	2.4
1	D	182	SER	2.4
1	D	261	LYS	2.4
1	D	165	CYS	2.4
1	D	138	ALA	2.3
1	B	148	TYR	2.3
1	D	122	GLY	2.3
1	A	194	VAL	2.3
1	A	478	VAL	2.3
1	A	104	LEU	2.3
1	A	175	TYR	2.3
1	D	132	VAL	2.3
1	A	186	LYS	2.3
1	C	24	ASP	2.3
1	B	189	GLY	2.3
1	B	158	TRP	2.3
1	B	221	VAL	2.2
1	C	400	ARG	2.2
1	A	213	GLY	2.2
1	B	501	GLY	2.2
1	A	182	SER	2.2
1	D	202	SER	2.2
1	A	141	LYS	2.2
1	B	137	GLY	2.2
1	B	248	ALA	2.2
1	C	104	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	172	SER	2.2
1	A	477	PRO	2.2
1	B	531	PRO	2.2
1	D	153	ASP	2.2
1	D	185	VAL	2.2
1	D	320	ALA	2.2
1	B	56	ARG	2.2
1	B	399	ARG	2.2
1	A	135	LYS	2.2
1	A	375	VAL	2.1
1	B	157	LEU	2.1
1	D	120	ARG	2.1
1	D	159	LEU	2.1
1	A	202	SER	2.1
1	D	166	LYS	2.1
1	A	128	GLY	2.1
1	B	141	LYS	2.1
1	A	487	ASP	2.1
1	A	161	TYR	2.1
1	B	193	LEU	2.1
1	D	217	ASP	2.1
1	C	14	GLN	2.1
1	B	83	TYR	2.1
1	B	200	GLY	2.1
1	A	119	ILE	2.1
1	A	216	VAL	2.1
1	B	76	PHE	2.1
1	C	147	ALA	2.1
1	D	401	LEU	2.0
1	A	106	ARG	2.0
1	A	39	PRO	2.0
1	A	142	ILE	2.0
1	A	174	ILE	2.0
1	A	165	CYS	2.0
1	B	139	THR	2.0
1	B	477	PRO	2.0
1	D	477	PRO	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

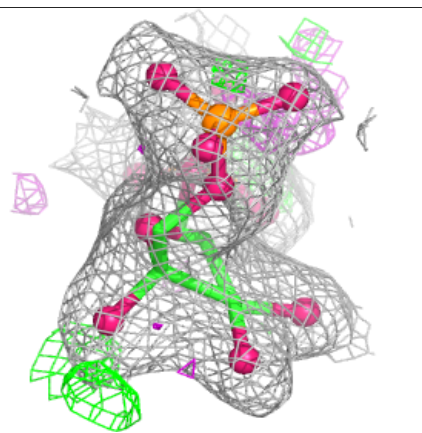
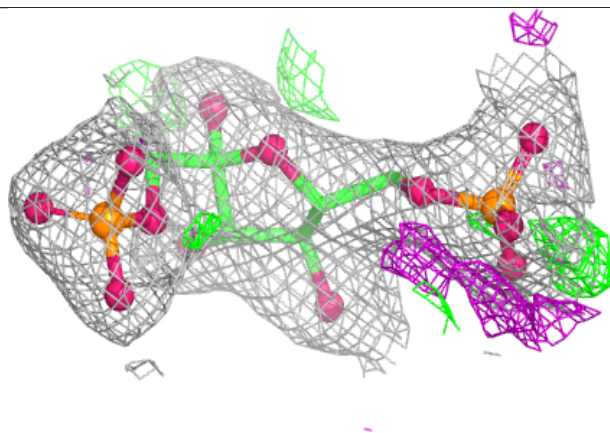
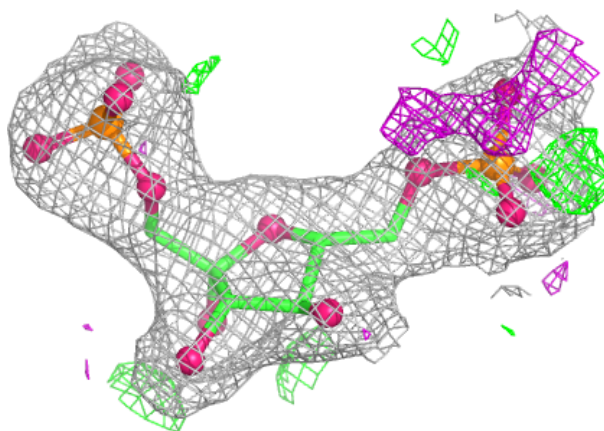
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	FBP	B	601	20/20	0.92	0.11	33,39,44,45	0
3	7XX	C	602	19/19	0.92	0.09	35,40,44,45	0
2	FBP	C	601	20/20	0.93	0.10	39,44,49,49	0
2	FBP	A	601	20/20	0.93	0.10	41,46,52,53	0
3	7XX	D	602	19/19	0.93	0.09	37,39,41,43	0
3	7XX	A	602	19/19	0.95	0.08	37,41,48,52	0
2	FBP	D	601	20/20	0.96	0.08	31,32,39,40	0
3	7XX	B	602	19/19	0.96	0.07	35,38,39,40	0

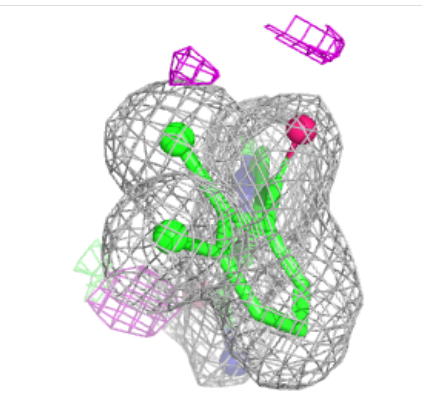
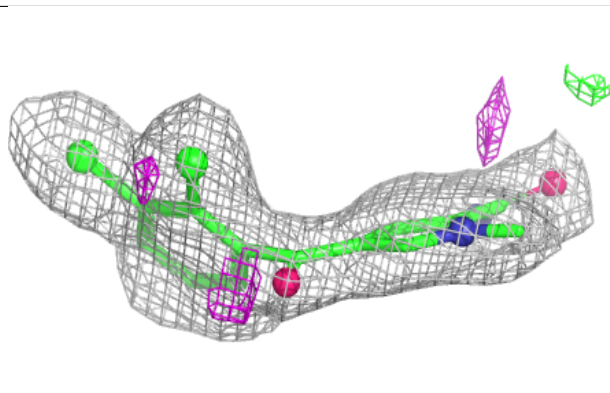
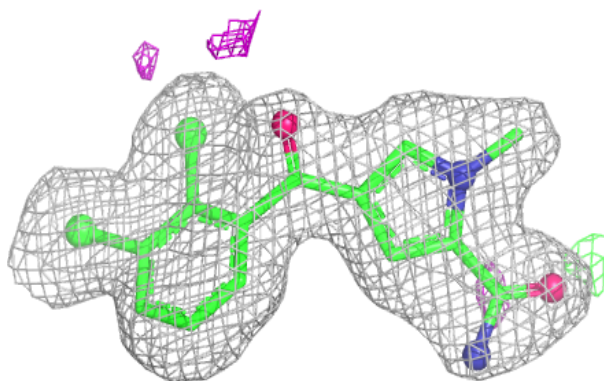
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

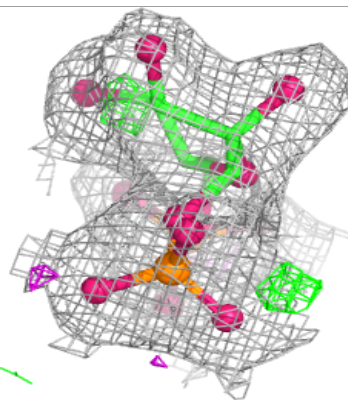
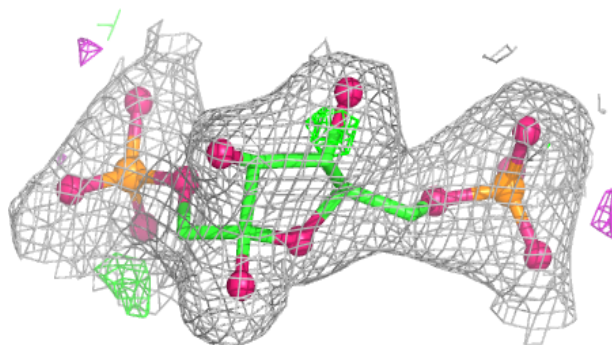
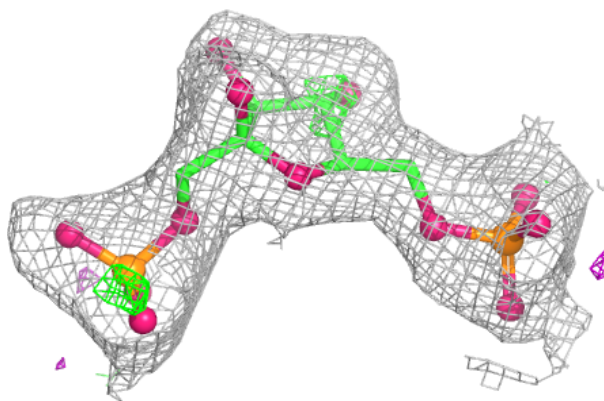
**Electron density around 7XX C 602:**

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

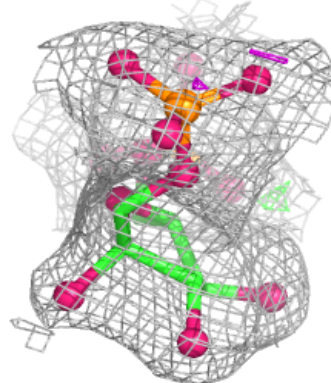
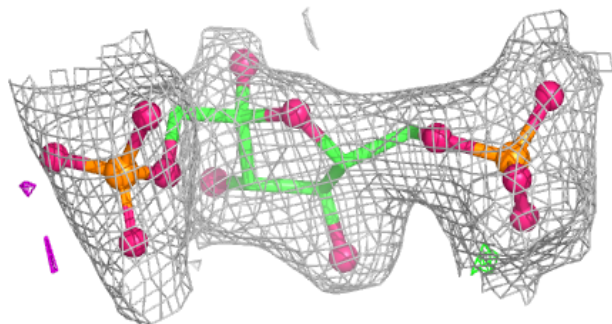
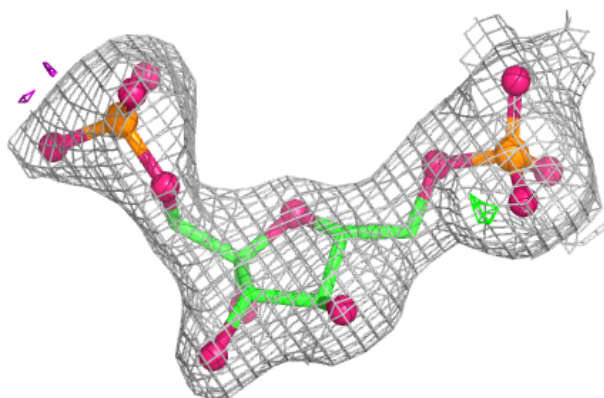


Electron density around FBP C 601:

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

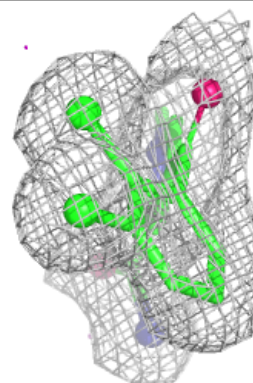
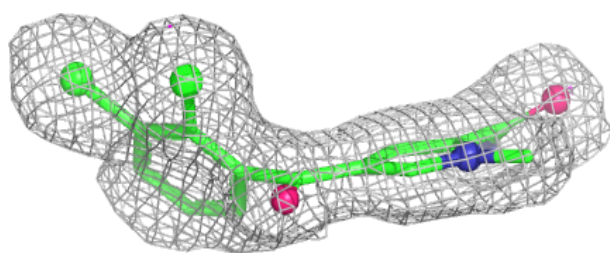
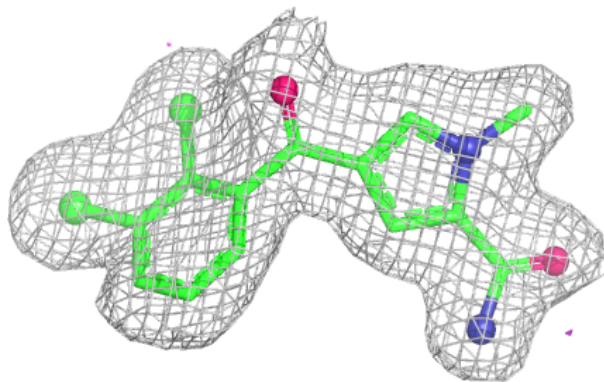
**Electron density around FBP A 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

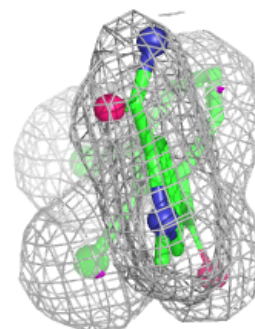
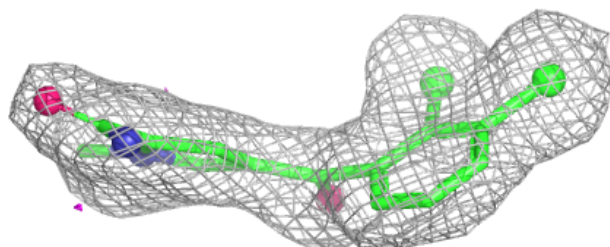
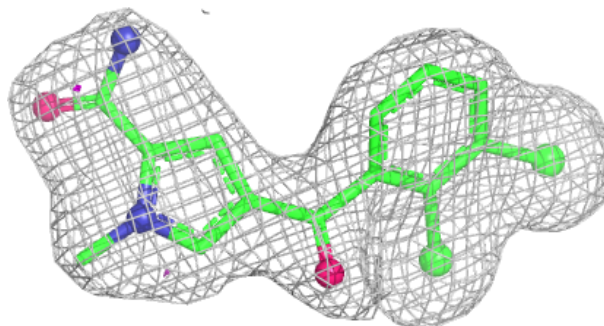


Electron density around 7XX D 602:

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

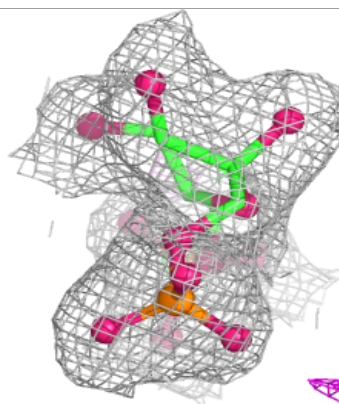
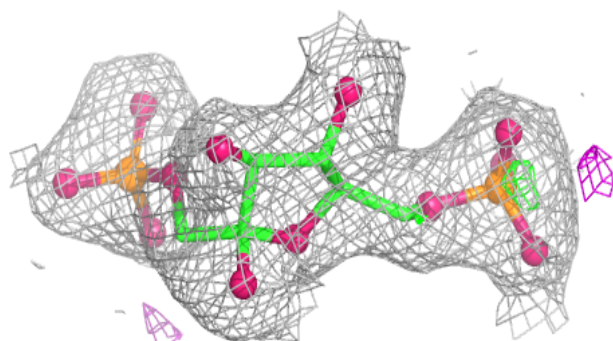
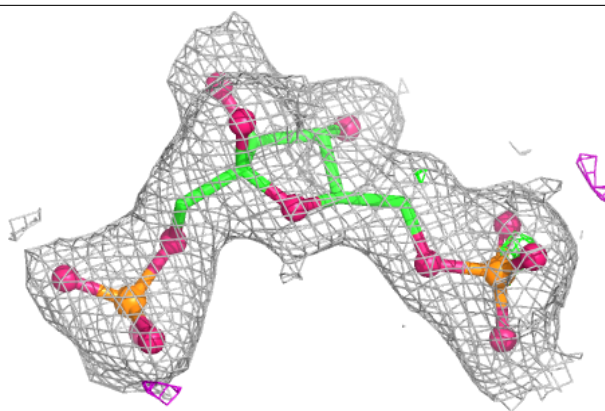
**Electron density around 7XX A 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

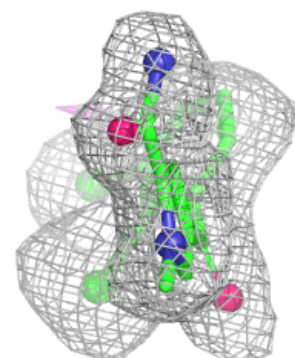
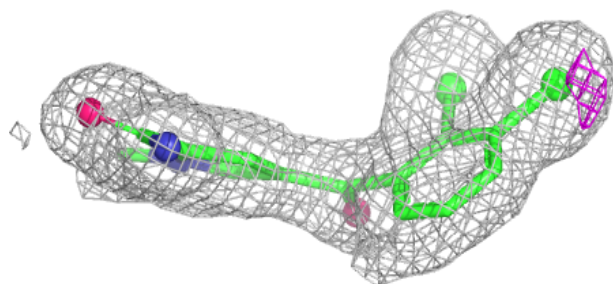
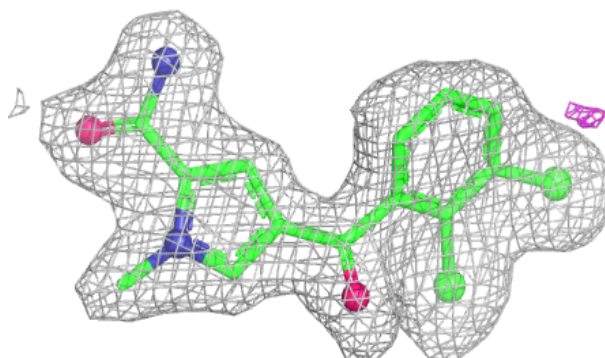


Electron density around FBP D 601:

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

**Electron density around 7XX B 602:**

$2mF_o-DF_c$ (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.