



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:22 AM UTC

PDB ID : 6NN4 / pdb_00006nn4
Title : The structure of human liver pyruvate kinase, hLPYK-D499N, in complex with Fru-1,6-BP
Authors : McFarlane, J.S.; Ronnebaum, T.A.; Meneely, K.M.; Fenton, A.W.; Lamb, A.L.
Deposited on : 2019-01-14
Resolution : 2.15 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

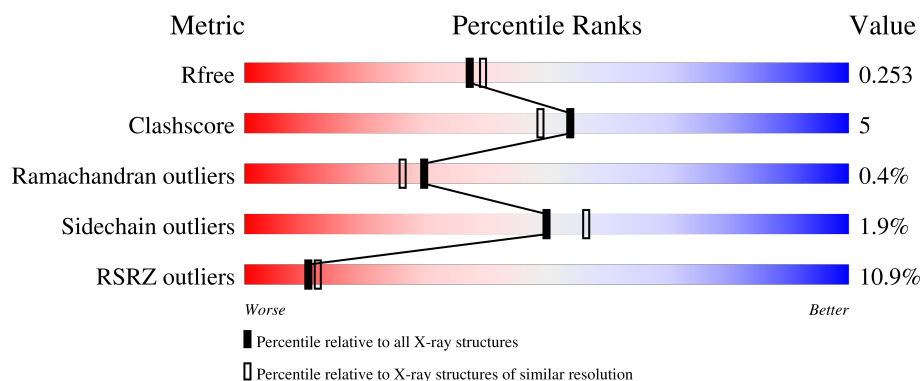
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	543	8% 68% 8% 23%
1	B	543	8% 67% 9% 24%
1	C	543	8% 67% 9% 23%
1	D	543	9% 67% 9% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26268 atoms, of which 13032 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.

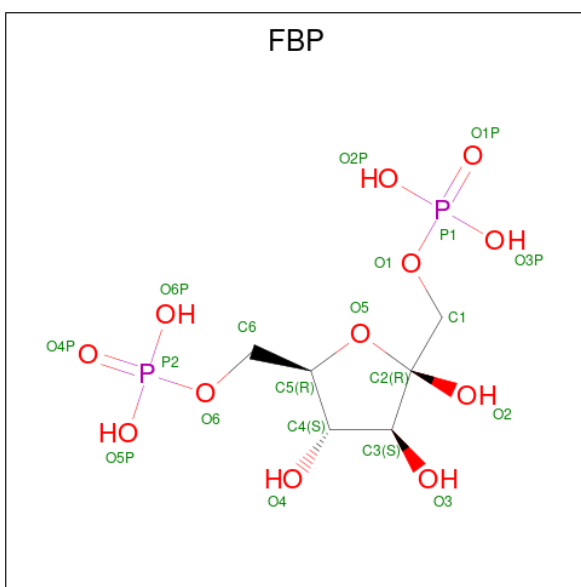
- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	H	N	O	S	0	1	0
			6436	2006	3242	580	590	18			
1	B	414	Total	C	H	N	O	S	0	0	0
			6373	1987	3211	575	582	18			
1	C	419	Total	C	H	N	O	S	0	0	0
			6467	2015	3260	582	592	18			
1	D	414	Total	C	H	N	O	S	0	0	0
			6401	1993	3229	578	583	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP P30613
A	2	GLU	-	expression tag	UNP P30613
A	499	ASN	ASP	engineered mutation	UNP P30613
B	1	MET	-	expression tag	UNP P30613
B	2	GLU	-	expression tag	UNP P30613
B	499	ASN	ASP	engineered mutation	UNP P30613
C	1	MET	-	expression tag	UNP P30613
C	2	GLU	-	expression tag	UNP P30613
C	499	ASN	ASP	engineered mutation	UNP P30613
D	1	MET	-	expression tag	UNP P30613
D	2	GLU	-	expression tag	UNP P30613
D	499	ASN	ASP	engineered mutation	UNP P30613

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



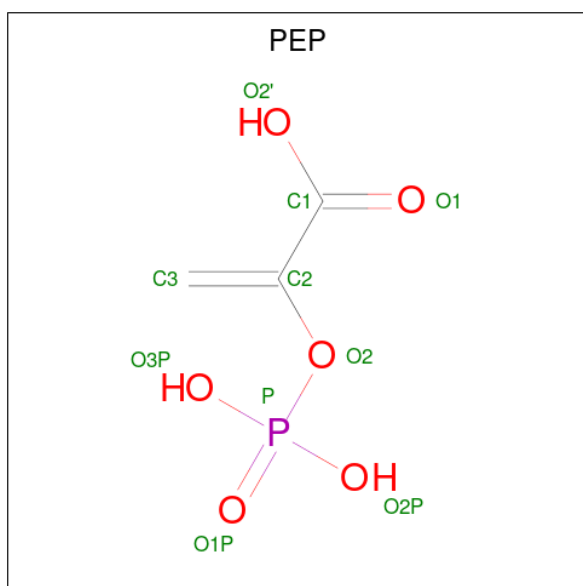
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			30	6	10	12	2		
2	B	1	Total	C	H	O	P	0	0
			30	6	10	12	2		
2	C	1	Total	C	H	O	P	0	0
			30	6	10	12	2		
2	D	1	Total	C	H	O	P	0	0
			30	6	10	12	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	C	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		
3	D	1	Total	C	H	O	0	0
			10	2	6	2		

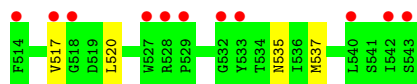
- Molecule 4 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	O	P	0	0
			12	3	2	6	1		
4	B	1	Total	C	H	O	P	0	0
			12	3	2	6	1		
4	C	1	Total	C	H	O	P	0	0
			12	3	2	6	1		
4	D	1	Total	C	H	O	P	0	0
			12	3	2	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	111	Total 111	O 111	0	0
5	B	94	Total 94	O 94	0	0
5	C	72	Total 72	O 72	0	0
5	D	76	Total 76	O 76	0	0



• Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.57Å 204.66Å 112.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.44 – 2.15 39.44 – 2.15	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.44-2.15) 98.6 (39.44-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.230 , 0.253 0.231 , 0.253	Depositor DCC
R_{free} test set	1994 reflections (1.32%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.910	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26268	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2346e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.54	0/3246	0.67	0/4388
1	B	0.53	0/3214	0.66	0/4344
1	C	0.50	0/3257	0.62	0/4402
1	D	0.53	0/3222	0.66	0/4352
All	All	0.52	0/12939	0.65	0/17486

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	3194	3242	3239	33	0
1	B	3162	3211	3211	36	0
1	C	3207	3260	3257	33	0
1	D	3172	3229	3225	32	0
2	A	20	10	10	1	0
2	B	20	10	10	0	0
2	C	20	10	10	0	0
2	D	20	10	10	0	0
3	A	8	12	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	6	6	0	0
3	C	4	6	6	1	0
3	D	12	18	17	1	0
4	A	10	2	2	1	0
4	B	10	2	2	3	0
4	C	10	2	2	1	0
4	D	10	2	2	0	0
5	A	111	0	0	4	0
5	B	94	0	0	1	0
5	C	72	0	0	0	0
5	D	76	0	0	1	0
All	All	13236	13032	13021	126	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 5.

All (126) 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:C:459:ARG:NH2	3:C:602:EDO:O2	1.98	0.95
1:B:67:SER:HB2	1:B:76:MET:HE1	1.54	0.88
1:D:260:ALA:O	1:D:263:VAL:HG12	1.76	0.85
1:B:67:SER:CB	1:B:76:MET:HE1	2.12	0.79
1:D:263:VAL:HG11	1:D:298:VAL:CG2	2.16	0.76
1:A:67:SER:CB	1:A:76:MET:HE1	2.18	0.73
1:B:418:ARG:NH2	1:C:20:LEU:HD21	2.04	0.72
1:C:331:LEU:O	1:C:455:ARG:NH2	2.23	0.72
1:C:408:GLU:OE1	1:C:411:ARG:NH2	2.22	0.71
1:D:263:VAL:HG11	1:D:298:VAL:HG23	1.73	0.69
1:A:435:CYS:O	1:D:418:ARG:NH1	2.26	0.69
1:A:528:ARG:NH1	1:A:529:PRO:O	2.26	0.68
1:A:491:GLU:OE2	1:A:500:ARG:NH1	2.27	0.67
2:A:601:FBP:O4P	5:A:701:HOH:O	2.13	0.65
1:B:339:ALA:HB1	1:B:372:MET:HE2	1.78	0.65
1:B:331:LEU:HD11	1:B:413:ALA:CB	2.29	0.63
1:A:67:SER:HB2	1:A:76:MET:HE1	1.81	0.62
1:B:331:LEU:HD11	1:B:413:ALA:HB1	1.80	0.62
1:C:421:THR:HG22	1:C:452:LEU:HD12	1.82	0.61
3:A:602:EDO:O1	5:A:702:HOH:O	2.16	0.60
1:A:331:LEU:HD13	1:C:39:LEU:HD21	1.83	0.60
1:D:418:ARG:HG2	1:D:418:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HG2	1:A:426:ILE:HD11	1.85	0.59
1:C:507:GLU:O	1:C:511:LEU:HG	2.04	0.57
1:D:422:GLU:HG2	1:D:452:LEU:HD13	1.87	0.56
1:D:127:LYS:O	1:D:130:GLU:HG3	2.06	0.56
1:A:79:ALA:HB1	1:A:388:LYS:HG3	1.88	0.56
1:D:317:LYS:NZ	5:D:702:HOH:O	2.39	0.55
1:A:68:ARG:HD2	1:A:95:TYR:CZ	2.41	0.55
1:B:241:LEU:O	1:B:245:VAL:HG23	2.07	0.55
1:D:94:GLU:OE1	1:D:98:GLU:OE2	2.25	0.55
1:B:68:ARG:NH1	1:B:98:GLU:OE1	2.40	0.55
1:C:494:TRP:O	1:C:497:ASP:N	2.39	0.55
1:A:67:SER:CA	1:A:76:MET:HE1	2.37	0.55
1:B:537:MET:HE3	1:C:537:MET:HE3	1.89	0.55
1:A:267:ARG:HD2	5:A:805:HOH:O	2.08	0.53
1:D:331:LEU:O	1:D:455:ARG:NH2	2.42	0.52
1:B:124:LEU:C	1:B:124:LEU:HD23	2.34	0.52
1:D:133:THR:O	1:D:133:THR:HG22	2.09	0.51
1:A:418:ARG:NH1	1:D:520:LEU:HD12	2.27	0.50
1:A:124:LEU:C	1:A:124:LEU:HD23	2.37	0.50
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.94	0.50
1:B:520:LEU:HD12	1:C:418:ARG:HG2	1.94	0.49
1:A:284:GLU:OE2	4:A:604:PEP:H31	2.13	0.49
1:B:232:GLY:HA2	1:B:258:ARG:HH22	1.78	0.49
1:B:243:PHE:CE2	1:B:247:HIS:CE1	3.00	0.49
1:C:493:ILE:HB	1:C:496:ASP:OD2	2.13	0.49
1:B:305:ALA:HB1	4:B:603:PEP:C1	2.43	0.48
1:B:253:PHE:HD1	1:B:280:ILE:HB	1.78	0.48
1:B:491:GLU:OE2	1:B:500:ARG:NH1	2.43	0.48
4:B:603:PEP:C3	4:B:603:PEP:O3P	2.58	0.48
1:B:267:ARG:NH2	1:B:274:GLY:O	2.47	0.48
1:D:415:PRO:O	1:D:416:LEU:C	2.55	0.48
1:B:418:ARG:CZ	1:C:20:LEU:HD21	2.44	0.48
1:A:267:ARG:NH2	1:A:274:GLY:O	2.46	0.47
1:C:528:ARG:HG2	1:C:529:PRO:N	2.29	0.47
1:C:16:LEU:HB3	1:C:20:LEU:HD12	1.97	0.47
1:C:469:ALA:HA	1:C:485:LEU:HD13	1.96	0.47
1:D:263:VAL:HG11	1:D:298:VAL:HG21	1.93	0.47
1:A:339:ALA:O	1:A:340:THR:HB	2.15	0.47
1:C:337:VAL:HG22	1:C:370:CYS:HB2	1.97	0.47
1:D:83:ILE:HG12	1:D:121:ALA:HB3	1.97	0.47
1:D:24:PHE:HD2	1:D:25:PHE:CD2	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:CZ	1:A:529:PRO:O	2.62	0.46
1:C:94:GLU:OE1	1:C:98:GLU:OE2	2.32	0.46
1:A:532:GLY:O	5:A:703:HOH:O	2.20	0.46
1:B:418:ARG:NE	1:C:19:GLU:HG2	2.30	0.46
1:A:67:SER:HA	1:A:76:MET:HE1	1.97	0.46
1:C:17:THR:HG23	1:C:22:THR:HA	1.97	0.46
1:D:527:TRP:CZ3	1:D:528:ARG:HB2	2.50	0.45
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.97	0.45
1:B:28:GLN:HA	5:B:735:HOH:O	2.16	0.45
1:B:68:ARG:HD2	1:B:95:TYR:CZ	2.51	0.45
1:B:25:PHE:HD1	1:B:30:LEU:HD13	1.81	0.45
1:A:233:LEU:HD21	1:A:266:VAL:HG22	1.98	0.44
1:B:428:ALA:HA	1:B:537:MET:HE2	2.00	0.44
1:A:253:PHE:HD1	1:A:280:ILE:HB	1.83	0.44
1:D:119:PRO:HG2	1:D:483:PRO:HG2	2.00	0.44
1:B:308:ASP:OD2	4:B:603:PEP:H31	2.17	0.43
1:C:428:ALA:HA	1:C:537:MET:HE2	2.00	0.43
1:C:339:ALA:O	1:C:340:THR:HB	2.17	0.43
1:D:74:LYS:HE2	1:D:109:SER:OG	2.17	0.43
1:D:454:SER:OG	3:D:603:EDO:H11	2.17	0.43
1:C:23:ALA:O	1:C:24:PHE:C	2.62	0.43
1:C:510:LYS:HE3	1:C:542:ILE:CG2	2.48	0.43
1:C:308:ASP:N	4:C:603:PEP:O2'	2.32	0.43
1:C:69:SER:HB2	1:C:72:ARG:H	1.84	0.43
1:D:523:VAL:O	1:D:537:MET:HA	2.19	0.43
1:A:72:ARG:HB3	1:A:76:MET:CE	2.49	0.42
1:B:423:VAL:HG21	1:C:435:CYS:HB3	2.00	0.42
1:D:56:SER:HB2	1:D:480:GLY:HA2	2.00	0.42
1:D:235:GLU:O	1:D:239:ARG:HG3	2.19	0.42
1:D:527:TRP:CE3	1:D:528:ARG:HB2	2.54	0.42
1:D:429:VAL:HG11	1:D:456:TYR:HB3	2.01	0.42
1:A:233:LEU:HD22	1:A:237:ASP:HB3	2.01	0.42
1:B:339:ALA:O	1:B:340:THR:HB	2.20	0.42
1:A:25:PHE:O	1:A:31:PRO:HD3	2.19	0.42
1:D:284:GLU:HG2	1:D:305:ALA:HB3	2.00	0.42
1:C:272:PRO:HA	1:C:275:HIS:HD1	1.85	0.42
1:D:253:PHE:HD1	1:D:280:ILE:HB	1.85	0.42
1:A:230:LEU:HB3	1:A:231:PRO:HD2	2.02	0.42
1:C:253:PHE:HD1	1:C:280:ILE:HB	1.85	0.42
1:A:335:PRO:HB3	1:A:477:LEU:O	2.20	0.42
1:A:527:TRP:CH2	1:A:528:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLU:O	1:B:312:GLU:HG3	2.18	0.42
1:A:331:LEU:CD1	1:C:39:LEU:HD21	2.50	0.41
1:A:493:ILE:HB	1:A:496:ASP:OD2	2.20	0.41
1:B:306:ARG:HD3	1:B:322:GLN:OE1	2.20	0.41
1:D:28:GLN:OE1	1:D:459:ARG:HD3	2.20	0.41
1:D:419:ASP:HB3	1:D:422:GLU:HG3	2.03	0.41
1:C:17:THR:CG2	1:C:22:THR:HG22	2.50	0.41
1:C:429:VAL:HG21	1:C:456:TYR:HB2	2.02	0.41
1:D:124:LEU:HD23	1:D:124:LEU:C	2.45	0.41
1:A:436:CYS:SG	1:D:416:LEU:HD13	2.61	0.41
1:C:272:PRO:HA	1:C:275:HIS:ND1	2.36	0.41
1:A:30:LEU:O	1:A:34:MET:HG2	2.21	0.40
1:B:336:VAL:HG13	1:B:368:ALA:HA	2.03	0.40
1:B:489:PRO:O	1:B:490:PRO:C	2.64	0.40
1:B:488:GLU:HB3	1:B:489:PRO:HD2	2.03	0.40
1:C:68:ARG:O	1:C:69:SER:C	2.65	0.40
1:A:235:GLU:O	1:A:239:ARG:HG3	2.21	0.40
1:B:284:GLU:OE2	1:B:308:ASP:OD2	2.39	0.40
1:B:284:GLU:HB3	1:B:308:ASP:HB2	2.02	0.40
1:B:284:GLU:HG2	1:B:305:ALA:HB3	2.03	0.40
1:B:314:PRO:HD2	1:B:317:LYS:HD2	2.01	0.40
1:D:429:VAL:HG21	1:D:456:TYR:HB2	2.04	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	413/543 (76%)	400 (97%)	11 (3%)	2 (0%)	24	20
1	B	408/543 (75%)	393 (96%)	13 (3%)	2 (0%)	24	20
1	C	411/543 (76%)	403 (98%)	7 (2%)	1 (0%)	43	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	406/543 (75%)	395 (97%)	10 (2%)	1 (0%)	43	44
All	All	1638/2172 (75%)	1591 (97%)	41 (2%)	6 (0%)	30	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	340	THR
1	A	340	THR
1	A	535	ASN
1	B	340	THR
1	B	535	ASN
1	D	340	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	333/433 (77%)	329 (99%)	4 (1%)	63	70
1	B	331/433 (76%)	327 (99%)	4 (1%)	63	70
1	C	336/433 (78%)	326 (97%)	10 (3%)	36	38
1	D	332/433 (77%)	325 (98%)	7 (2%)	47	52
All	All	1332/1732 (77%)	1307 (98%)	25 (2%)	50	56

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	LYS
1	A	507	GLU
1	A	528	ARG
1	A	537	MET
1	B	68	ARG
1	B	436	CYS
1	B	512	ARG
1	B	517	VAL

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Mol	Chain	Res	Type
1	C	19	GLU
1	C	26	GLN
1	C	52	VAL
1	C	118	ARG
1	C	263	VAL
1	C	331	LEU
1	C	459	ARG
1	C	534	THR
1	C	537	MET
1	C	538	ARG
1	D	52	VAL
1	D	412	ARG
1	D	418	ARG
1	D	454	SER
1	D	508	SER
1	D	534	THR
1	D	543	SER

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

Mol	Chain	Res	Type
1	C	403	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 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	C	601	-	18,20,20	3.77	6 (33%)	21,32,32	0.86	0
3	EDO	C	602	-	3,3,3	0.44	0	2,2,2	0.47	0
2	FBP	A	601	-	18,20,20	3.76	5 (27%)	21,32,32	0.82	0
3	EDO	B	602	-	3,3,3	0.44	0	2,2,2	0.35	0
4	PEP	B	603	-	9,9,9	2.03	3 (33%)	11,13,13	1.33	2 (18%)
2	FBP	D	601	-	18,20,20	3.91	7 (38%)	21,32,32	0.85	0
4	PEP	D	605	-	9,9,9	1.23	1 (11%)	11,13,13	2.23	3 (27%)
2	FBP	B	601	-	18,20,20	3.82	7 (38%)	21,32,32	0.91	0
3	EDO	D	604	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	D	602	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	A	602	-	3,3,3	0.43	0	2,2,2	0.60	0
3	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.73	0
4	PEP	A	604	-	9,9,9	1.26	1 (11%)	11,13,13	2.91	3 (27%)
4	PEP	C	603	-	9,9,9	2.00	4 (44%)	11,13,13	2.74	3 (27%)
3	EDO	D	603	-	3,3,3	0.90	0	2,2,2	1.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	C	601	-	-	5/13/32/32	0/1/1/1
3	EDO	C	602	-	-	1/1/1/1	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
3	EDO	B	602	-	-	1/1/1/1	-
4	PEP	B	603	-	-	2/9/9/9	-
2	FBP	D	601	-	-	8/13/32/32	0/1/1/1
4	PEP	D	605	-	-	4/9/9/9	-
2	FBP	B	601	-	-	6/13/32/32	0/1/1/1
3	EDO	D	604	-	-	1/1/1/1	-
3	EDO	D	602	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
4	PEP	A	604	-	-	0/9/9/9	-
4	PEP	C	603	-	-	4/9/9/9	-
3	EDO	D	603	-	-	0/1/1/1	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	FBP	O5-C2	-10.11	1.27	1.43
2	A	601	FBP	O5-C2	-9.72	1.28	1.43
2	B	601	FBP	O5-C2	-9.72	1.28	1.43
2	C	601	FBP	O5-C2	-9.46	1.28	1.43
2	D	601	FBP	O5-C5	8.52	1.62	1.43
2	B	601	FBP	O5-C5	8.46	1.62	1.43
2	C	601	FBP	O5-C5	8.38	1.62	1.43
2	A	601	FBP	O5-C5	8.36	1.62	1.43
2	D	601	FBP	C4-C5	-7.34	1.34	1.53
2	C	601	FBP	C4-C5	-7.27	1.34	1.53
2	A	601	FBP	C4-C5	-7.08	1.35	1.53
2	B	601	FBP	C4-C5	-7.04	1.35	1.53
4	B	603	PEP	C2-C1	4.47	1.53	1.49
4	C	603	PEP	C2-C1	4.38	1.53	1.49
2	C	601	FBP	O4-C4	3.98	1.52	1.43
2	D	601	FBP	O4-C4	3.69	1.52	1.43
2	A	601	FBP	O4-C4	3.66	1.52	1.43
2	B	601	FBP	O4-C4	3.62	1.51	1.43
2	B	601	FBP	O2-C2	3.18	1.46	1.40
2	C	601	FBP	O2-C2	2.93	1.45	1.40
2	D	601	FBP	O3-C3	-2.86	1.37	1.42
2	A	601	FBP	O2-C2	2.80	1.45	1.40
4	C	603	PEP	P-O2	2.54	1.64	1.59
4	B	603	PEP	O2'-C1	-2.50	1.23	1.30
4	B	603	PEP	P-O2	2.49	1.64	1.59
4	A	604	PEP	C2-C1	2.48	1.51	1.49
2	D	601	FBP	O2-C2	2.48	1.45	1.40
2	B	601	FBP	O3-C3	-2.45	1.37	1.42
2	D	601	FBP	P2-O6	2.40	1.67	1.60
2	C	601	FBP	O3-C3	-2.37	1.38	1.42
2	B	601	FBP	P2-O6	2.24	1.67	1.60
4	C	603	PEP	O2'-C1	-2.22	1.24	1.30
4	D	605	PEP	C2-C1	2.13	1.51	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	603	PEP	O1-C1	2.07	1.27	1.22

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	603	PEP	O1-C1-C2	6.98	132.32	121.79
4	A	604	PEP	O2'-C1-C2	6.93	125.73	113.91
4	A	604	PEP	O1-C1-C2	-5.58	113.38	121.79
4	D	605	PEP	O2'-C1-C2	4.89	122.26	113.91
4	D	605	PEP	O1-C1-C2	-4.38	115.19	121.79
4	C	603	PEP	O2-C2-C3	-3.58	118.01	124.85
4	C	603	PEP	O2'-C1-C2	-3.44	108.04	113.91
4	B	603	PEP	O2-C2-C3	-2.53	120.02	124.85
4	A	604	PEP	O2P-P-O2	2.28	111.95	105.32
4	D	605	PEP	C3-C2-C1	-2.03	118.98	122.73
4	B	603	PEP	O3P-P-O2P	2.01	115.33	107.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	FBP	C1-O1-P1-O3P
2	B	601	FBP	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-O5
2	C	601	FBP	C1-O1-P1-O2P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	C6-O6-P2-O5P
2	C	601	FBP	C6-O6-P2-O6P
2	D	601	FBP	C1-O1-P1-O1P
2	D	601	FBP	C1-O1-P1-O2P
2	D	601	FBP	C1-O1-P1-O3P
2	D	601	FBP	O1-C1-C2-O2
2	D	601	FBP	O1-C1-C2-C3
2	D	601	FBP	O1-C1-C2-O5
4	C	603	PEP	O1-C1-C2-C3
4	C	603	PEP	O1-C1-C2-O2
4	C	603	PEP	O2'-C1-C2-C3
4	C	603	PEP	O2'-C1-C2-O2
4	D	605	PEP	O2'-C1-C2-O2
2	D	601	FBP	C4-C5-C6-O6
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6

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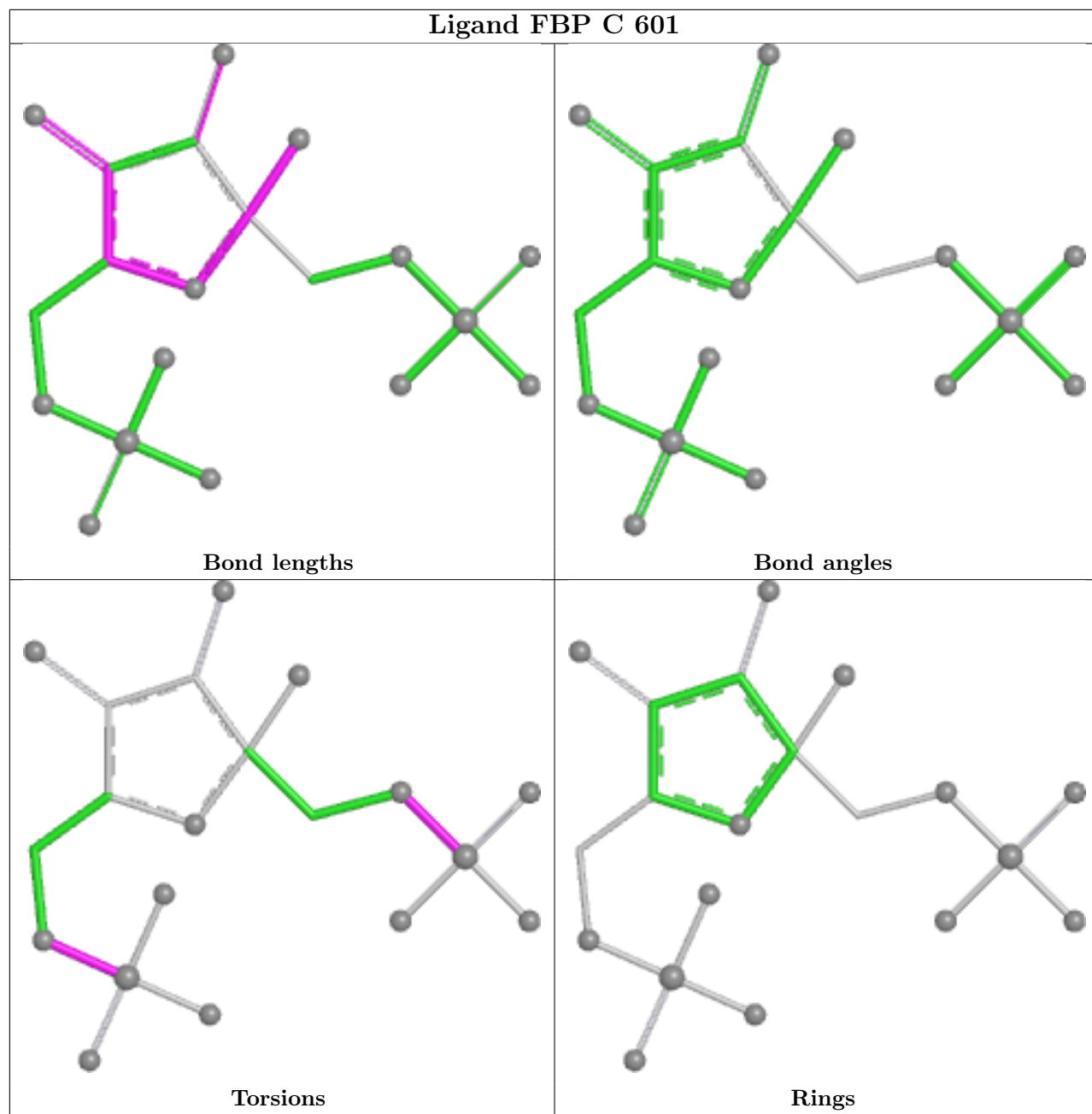
Mol	Chain	Res	Type	Atoms
3	C	602	EDO	O1-C1-C2-O2
2	D	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	601	FBP	O5-C5-C6-O6
2	C	601	FBP	C1-O1-P1-O1P
3	D	604	EDO	O1-C1-C2-O2
4	D	605	PEP	O1-C1-C2-O2
3	B	602	EDO	O1-C1-C2-O2
4	D	605	PEP	O1-C1-C2-C3
3	D	602	EDO	O1-C1-C2-O2
2	B	601	FBP	O1-C1-C2-C3
4	B	603	PEP	C2-O2-P-O2P
4	B	603	PEP	C2-O2-P-O1P
3	A	602	EDO	O1-C1-C2-O2
4	D	605	PEP	O2'-C1-C2-C3

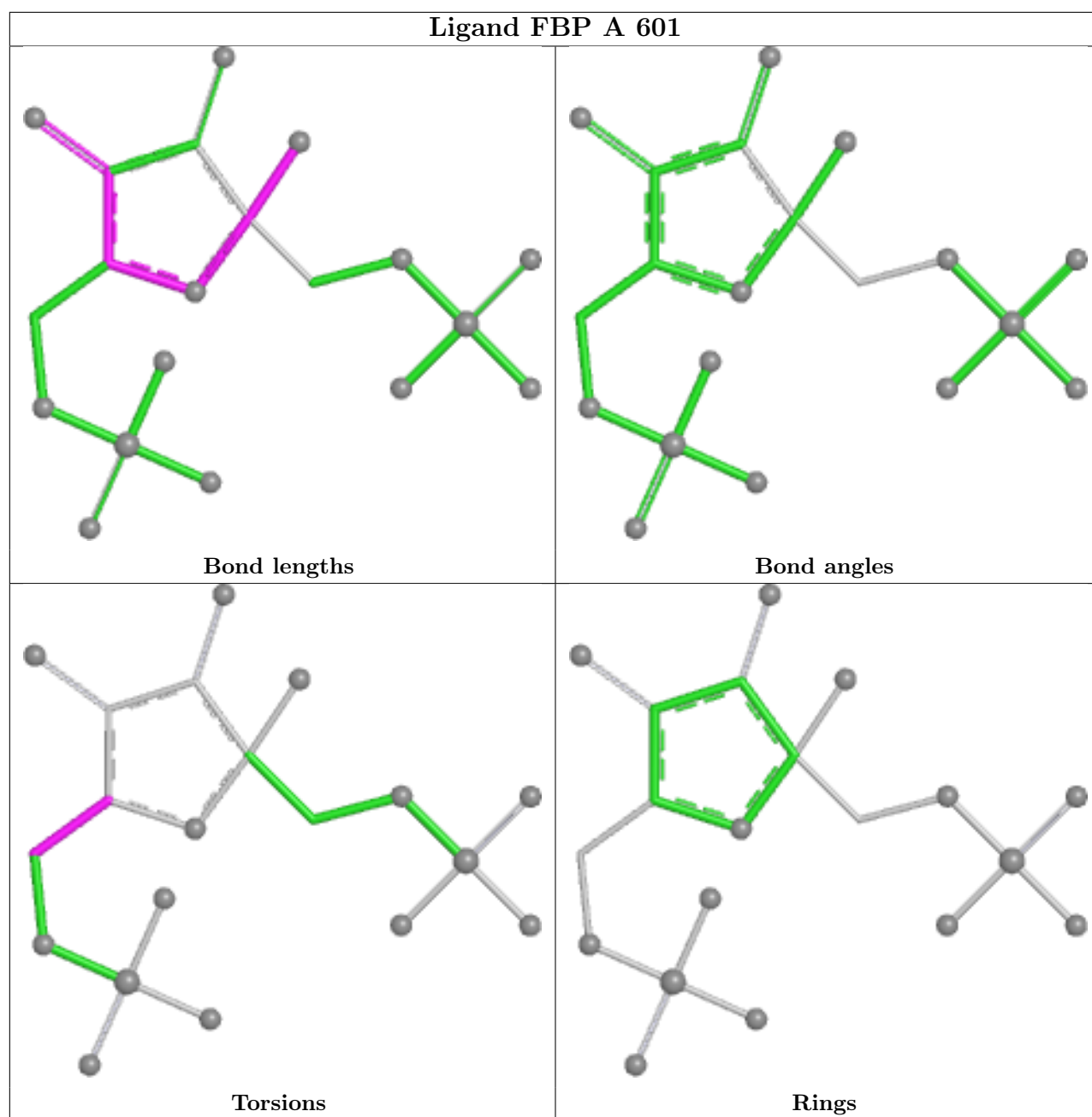
There are no ring outliers.

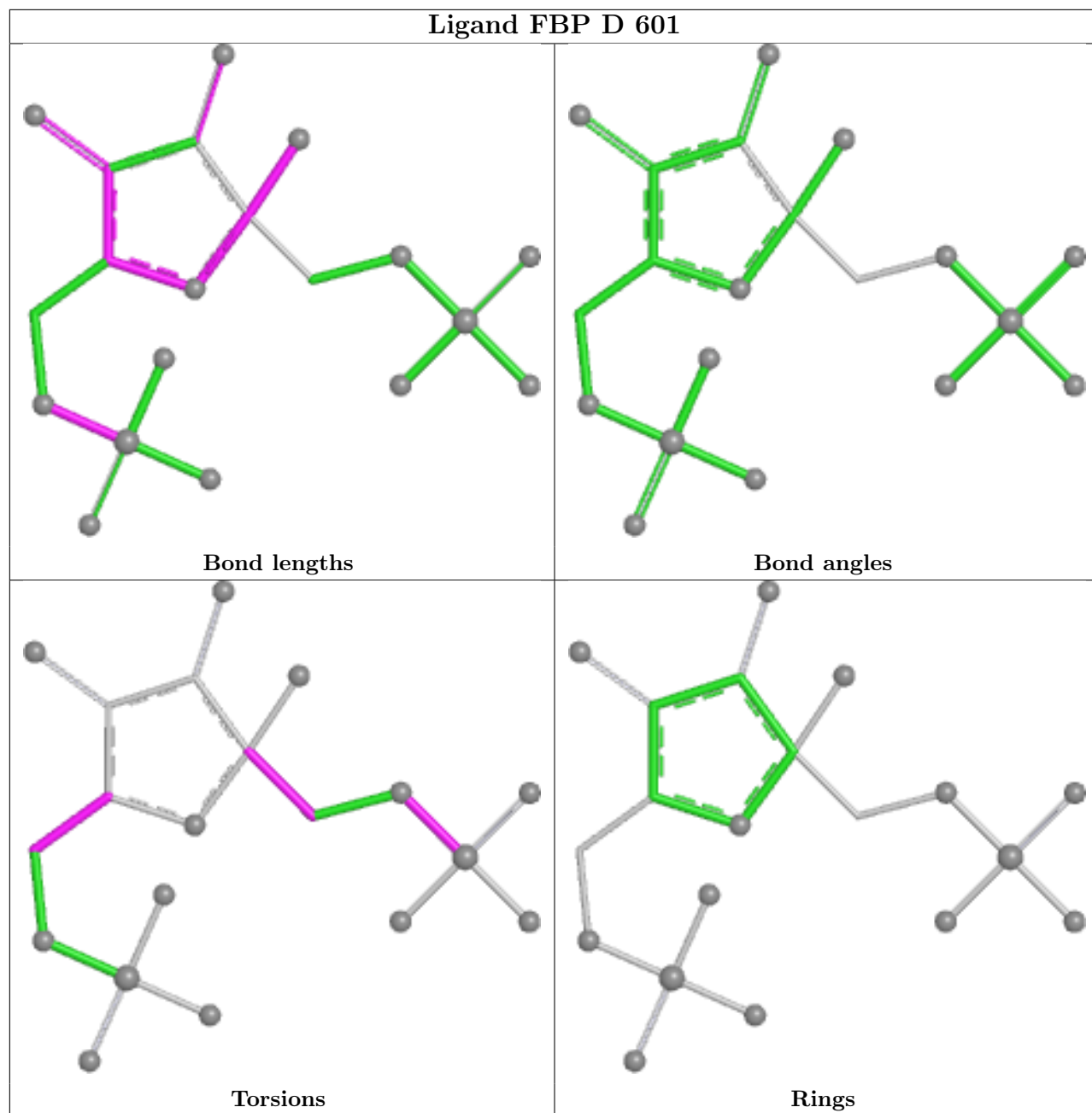
7 monomers are involved in 9 short contacts:

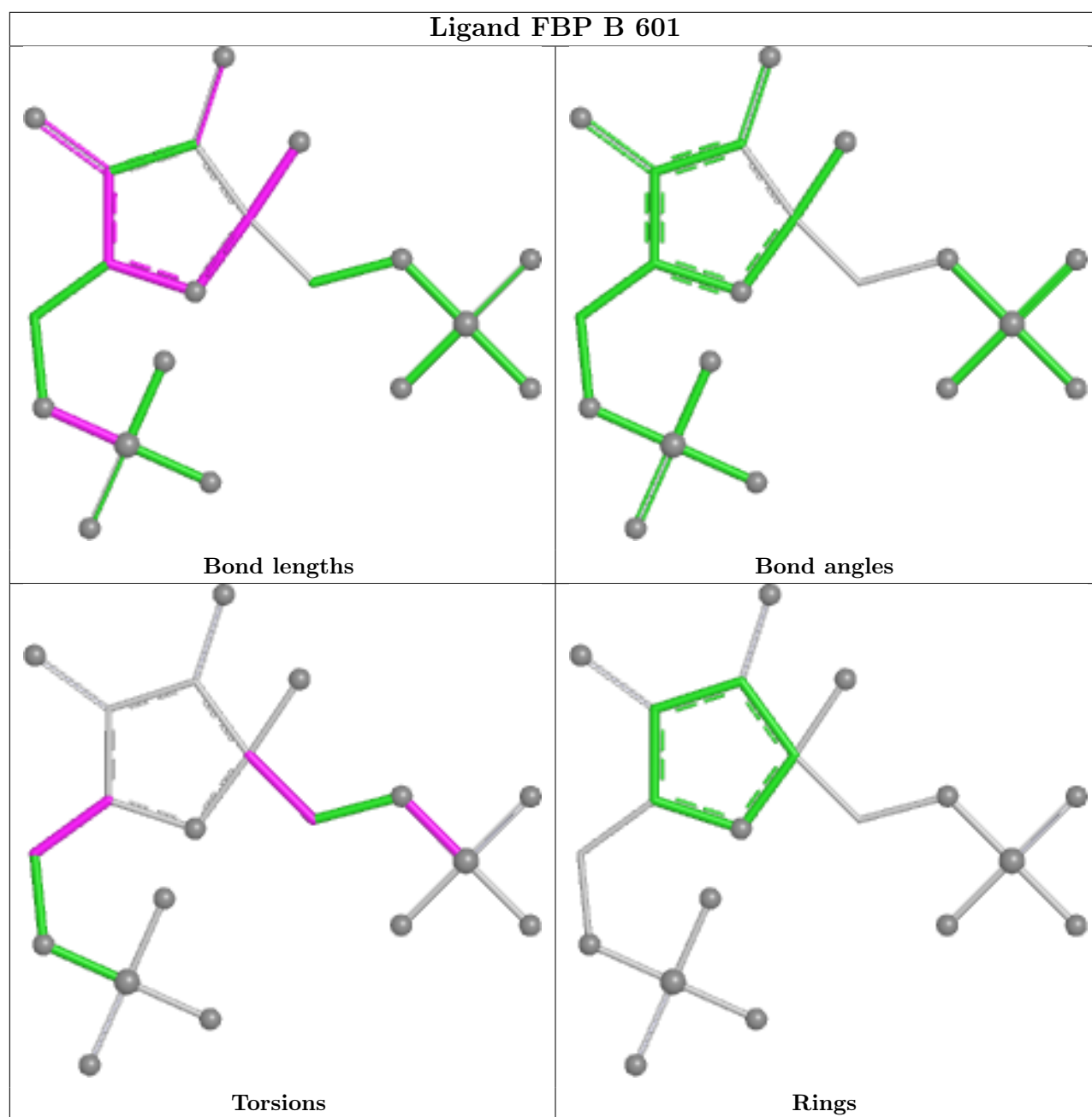
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	EDO	1	0
2	A	601	FBP	1	0
4	B	603	PEP	3	0
3	A	602	EDO	1	0
4	A	604	PEP	1	0
4	C	603	PEP	1	0
3	D	603	EDO	1	0

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, 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	418/543 (76%)	0.60	44 (10%) 11 13	21, 44, 75, 96	1 (0%)
1	B	414/543 (76%)	0.65	42 (10%) 12 14	31, 45, 79, 119	0
1	C	419/543 (77%)	0.77	46 (10%) 10 12	32, 48, 82, 119	0
1	D	414/543 (76%)	0.72	50 (12%) 8 9	32, 47, 78, 107	0
All	All	1665/2172 (76%)	0.68	182 (10%) 10 12	21, 46, 79, 119	1 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PHE	8.4
1	B	231	PRO	8.2
1	C	511	LEU	6.1
1	B	24	PHE	5.9
1	A	232	GLY	5.4
1	B	232	GLY	5.2
1	A	25	PHE	5.1
1	C	532	GLY	5.1
1	D	530	GLY	5.1
1	C	527	TRP	5.0
1	C	15	GLN	4.9
1	C	533	TYR	4.8
1	B	511	LEU	4.8
1	D	24	PHE	4.7
1	A	490	PRO	4.6
1	D	415	PRO	4.6
1	C	543	SER	4.5
1	B	528	ARG	4.4
1	D	412	ARG	4.4
1	D	527	TRP	4.4
1	B	489	PRO	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	529	PRO	4.4
1	B	233	LEU	4.3
1	D	118	ARG	4.2
1	A	527	TRP	4.2
1	D	529	PRO	4.1
1	C	24	PHE	4.0
1	A	130	GLU	4.0
1	C	20	LEU	3.9
1	B	527	TRP	3.9
1	A	272	PRO	3.9
1	D	489	PRO	3.9
1	A	493	ILE	3.9
1	A	23	ALA	3.9
1	D	275	HIS	3.8
1	C	412	ARG	3.8
1	D	494	TRP	3.7
1	C	275	HIS	3.7
1	C	110	PHE	3.7
1	A	129	PRO	3.6
1	B	490	PRO	3.6
1	B	275	HIS	3.6
1	D	110	PHE	3.6
1	B	256	PHE	3.6
1	B	493	ILE	3.6
1	D	133	THR	3.6
1	A	111	ALA	3.6
1	A	489	PRO	3.6
1	C	489	PRO	3.6
1	C	130	GLU	3.5
1	B	492	ALA	3.5
1	B	529	PRO	3.5
1	D	533	TYR	3.5
1	D	411	ARG	3.4
1	C	528	ARG	3.4
1	D	117	TYR	3.4
1	A	411	ARG	3.4
1	B	26	GLN	3.3
1	D	493	ILE	3.3
1	C	490	PRO	3.2
1	D	108	GLU	3.2
1	D	131	ILE	3.2
1	B	36	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	414	ALA	3.1
1	D	263	VAL	3.1
1	C	17	THR	3.1
1	C	25	PHE	3.1
1	D	528	ARG	3.1
1	B	436	CYS	3.1
1	A	531	SER	3.1
1	A	229	ASP	3.0
1	A	492	ALA	3.0
1	A	52	VAL	3.0
1	C	411	ARG	3.0
1	A	24	PHE	3.0
1	A	511	LEU	3.0
1	B	30	LEU	3.0
1	C	118	ARG	2.9
1	D	422	GLU	2.9
1	C	26	GLN	2.9
1	B	412	ARG	2.9
1	B	512	ARG	2.9
1	B	494	TRP	2.9
1	B	411	ARG	2.8
1	B	540	LEU	2.8
1	A	543	SER	2.8
1	D	508	SER	2.8
1	A	275	HIS	2.8
1	B	413	ALA	2.8
1	B	487	ARG	2.8
1	B	130	GLU	2.7
1	C	16	LEU	2.7
1	D	511	LEU	2.7
1	B	415	PRO	2.7
1	D	26	GLN	2.7
1	D	490	PRO	2.7
1	B	543	SER	2.7
1	C	494	TRP	2.7
1	A	230	LEU	2.7
1	A	117	TYR	2.7
1	D	418	ARG	2.7
1	A	71	GLU	2.6
1	D	513	GLY	2.6
1	C	351	ARG	2.6
1	A	533	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	246	GLU	2.6
1	A	487	ARG	2.6
1	D	25	PHE	2.5
1	D	34	MET	2.5
1	C	129	PRO	2.5
1	A	233	LEU	2.5
1	C	19	GLU	2.5
1	D	532	GLY	2.5
1	B	52	VAL	2.5
1	D	423	VAL	2.5
1	A	529	PRO	2.5
1	D	272	PRO	2.5
1	D	492	ALA	2.5
1	A	26	GLN	2.4
1	B	517	VAL	2.4
1	B	129	PRO	2.4
1	D	290	LYS	2.4
1	D	410	LEU	2.4
1	A	494	TRP	2.4
1	A	507	GLU	2.3
1	D	413	ALA	2.3
1	C	90	HIS	2.3
1	D	273	GLU	2.3
1	C	413	ALA	2.3
1	C	492	ALA	2.3
1	C	21	GLY	2.3
1	C	487	ARG	2.3
1	C	233	LEU	2.3
1	D	408	GLU	2.3
1	B	542	ILE	2.3
1	C	493	ILE	2.3
1	A	436	CYS	2.3
1	D	512	ARG	2.3
1	D	469	ALA	2.3
1	B	518	GLY	2.3
1	D	44	LEU	2.3
1	B	117	TYR	2.3
1	A	256	PHE	2.2
1	C	22	THR	2.2
1	D	498	VAL	2.2
1	D	534	THR	2.2
1	C	23	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	30	LEU	2.2
1	B	110	PHE	2.2
1	D	487	ARG	2.2
1	A	542	ILE	2.2
1	B	532	GLY	2.2
1	C	540	LEU	2.2
1	B	514	PHE	2.2
1	C	517	VAL	2.2
1	A	518	GLY	2.2
1	A	530	GLY	2.2
1	C	513	GLY	2.2
1	A	416	LEU	2.2
1	B	533	TYR	2.2
1	C	534	THR	2.2
1	C	407	PHE	2.1
1	C	430	GLU	2.1
1	A	413	ALA	2.1
1	A	36	ASP	2.1
1	A	231	PRO	2.1
1	D	517	VAL	2.1
1	C	18	GLN	2.1
1	A	242	ARG	2.1
1	B	242	ARG	2.1
1	A	514	PHE	2.1
1	C	331	LEU	2.1
1	D	518	GLY	2.1
1	C	290	LYS	2.1
1	A	504	PHE	2.1
1	D	52	VAL	2.1
1	B	507	GLU	2.0
1	D	132	ARG	2.0
1	D	351	ARG	2.0
1	A	541	SER	2.0
1	C	512	ARG	2.0
1	D	267	ARG	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](#)

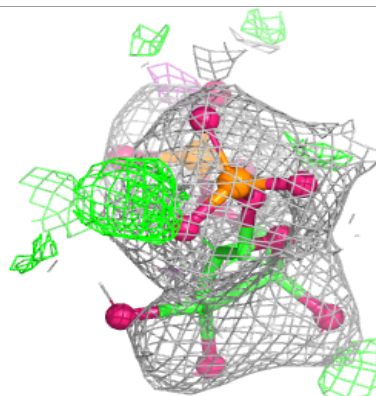
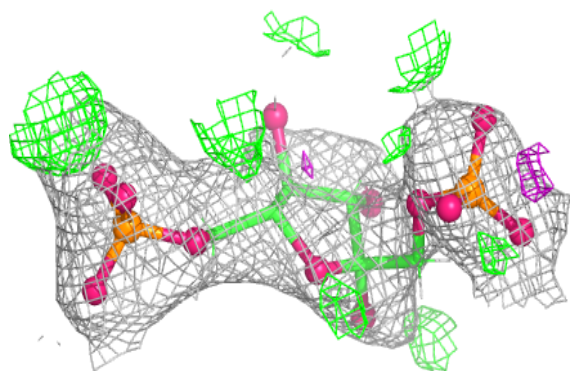
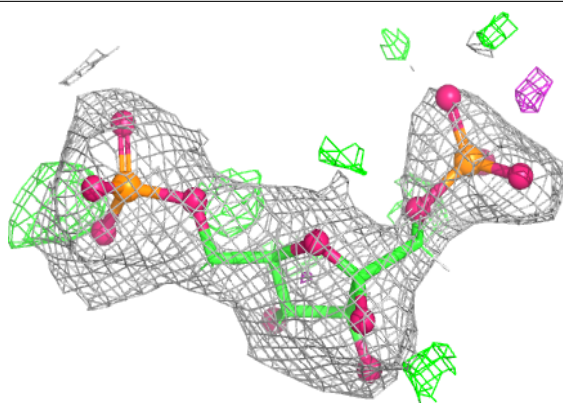
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	EDO	A	602	4/4	0.61	0.30	60,72,80,83	0
3	EDO	A	603	4/4	0.64	0.23	56,68,81,92	0
3	EDO	D	602	4/4	0.67	0.25	51,65,78,78	0
3	EDO	B	602	4/4	0.72	0.23	57,69,73,73	0
4	PEP	D	605	10/10	0.76	0.21	43,56,67,83	12
4	PEP	A	604	10/10	0.77	0.18	36,50,64,69	12
4	PEP	B	603	10/10	0.78	0.17	37,49,58,78	0
4	PEP	C	603	10/10	0.80	0.20	40,48,62,76	12
2	FBP	C	601	20/20	0.82	0.17	49,80,98,106	0
2	FBP	D	601	20/20	0.87	0.14	44,73,90,93	0
2	FBP	A	601	20/20	0.89	0.13	39,60,71,76	30
3	EDO	C	602	4/4	0.90	0.26	64,108,153,153	0
2	FBP	B	601	20/20	0.90	0.12	42,72,92,110	0
3	EDO	D	603	4/4	0.93	0.11	37,44,53,53	0
3	EDO	D	604	4/4	0.93	0.19	61,90,141,141	0

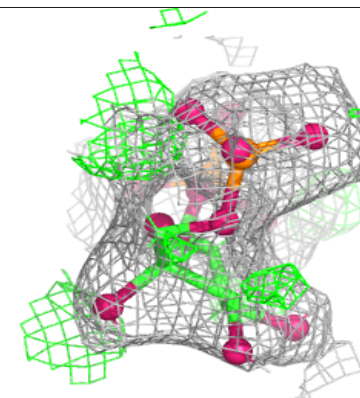
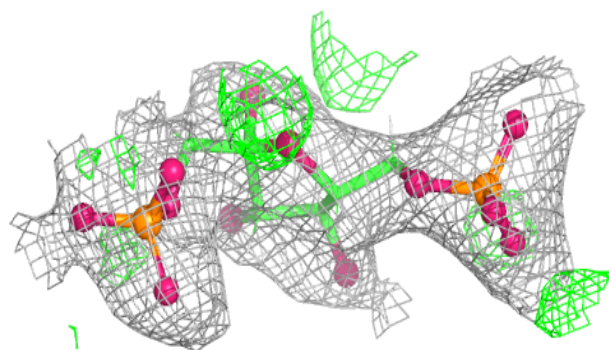
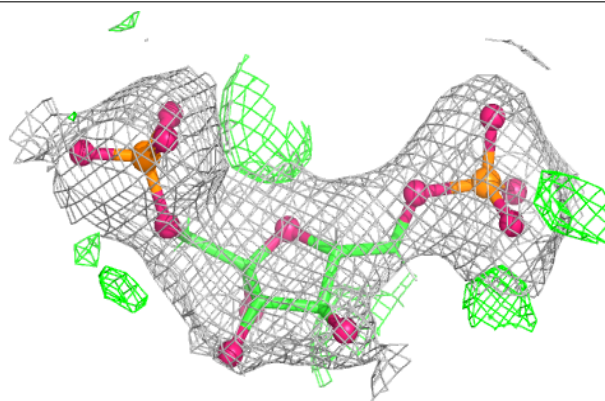
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FBP 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)

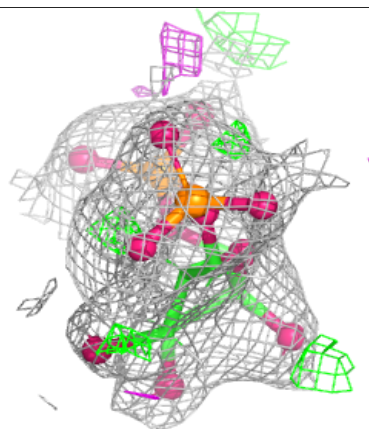
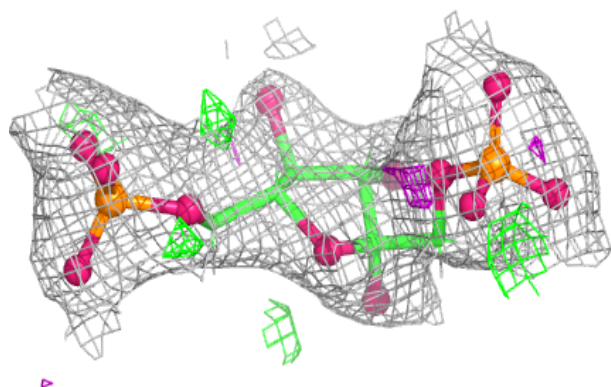
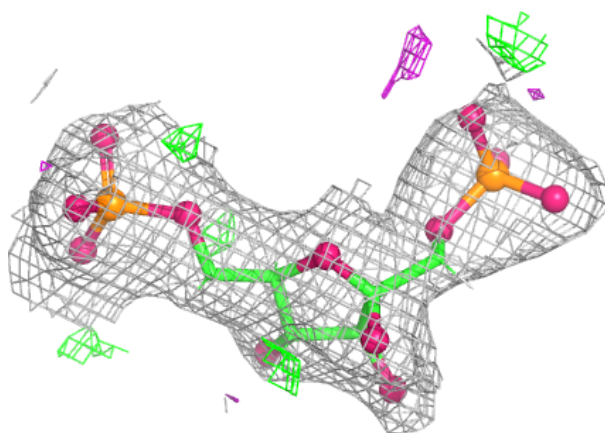
**Electron density around FBP D 601:**

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



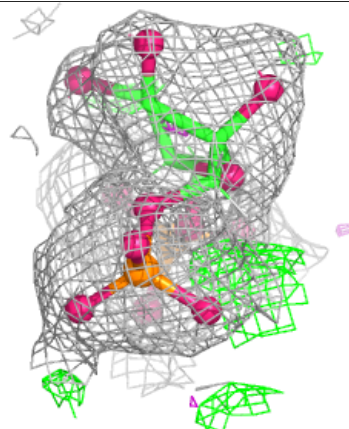
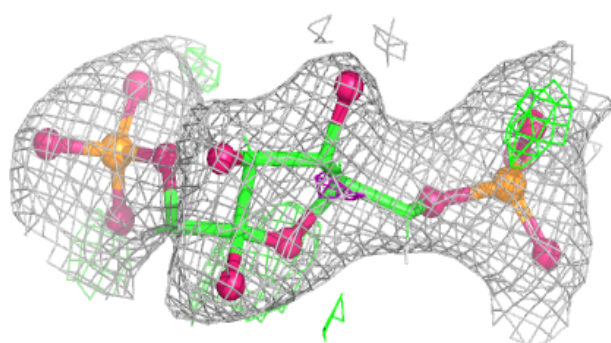
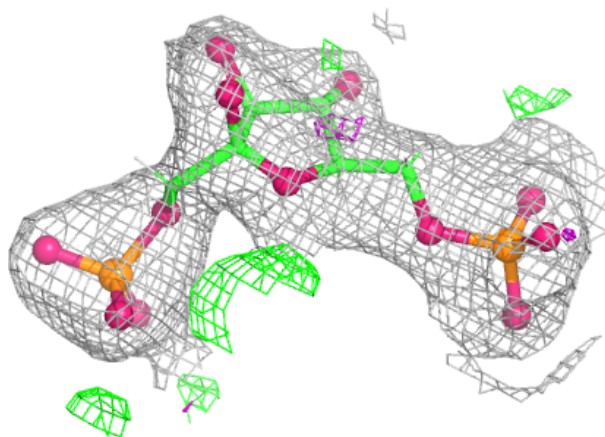
Electron density around FBP A 601:

$2mF_o - DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.