



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2020 – 02:16 PM EDT

PDB ID : 6V74
Title : Crystal Structure of Human PKM2 in Complex with L-asparagine
Authors : Nandi, S.; Dey, M.
Deposited on : 2019-12-07
Resolution : 2.32 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 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 : 2.14.6
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) : 2.14.6

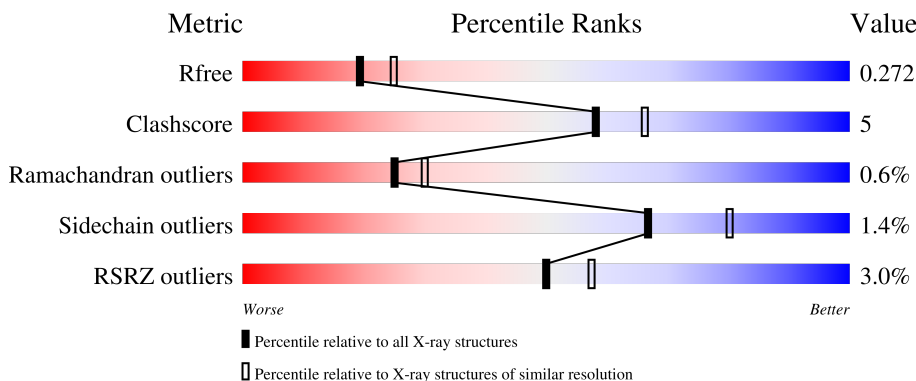
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 on 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	<div> <div>3%</div> <div>86%</div> <div>7%</div> <div>7%</div> </div>
1	B	550	<div> <div>2%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>
1	C	550	<div> <div>5%</div> <div>79%</div> <div>12%</div> <div>9%</div> </div>
1	D	550	<div> <div>0%</div> <div>67%</div> <div>10%</div> <div>22%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	613	-	-	X	-
4	OXL	C	614	-	-	X	-
4	OXL	D	602	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14426 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	513	Total	C	N	O	S	0	0	0
			3681	2320	653	684	24			
1	B	516	Total	C	N	O	S	0	0	0
			3712	2334	653	700	25			
1	C	499	Total	C	N	O	S	0	0	0
			3543	2220	635	665	23			
1	D	427	Total	C	N	O	S	0	0	0
			3101	1949	549	581	22			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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	-	initiating methionine	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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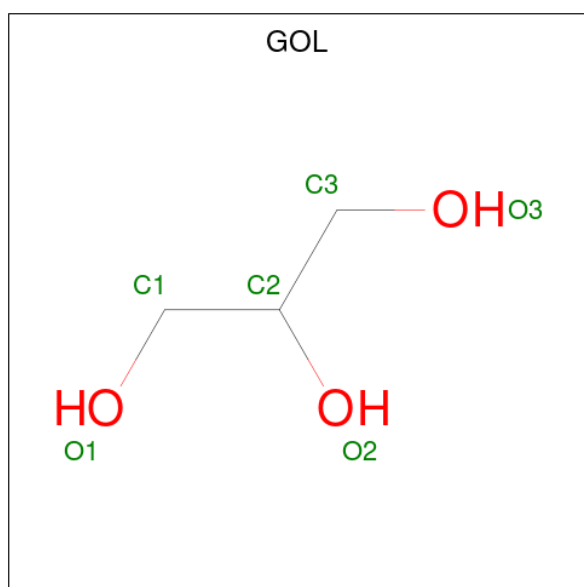
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression 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 POTASSIUM ION (three-letter code: K) (formula: K).

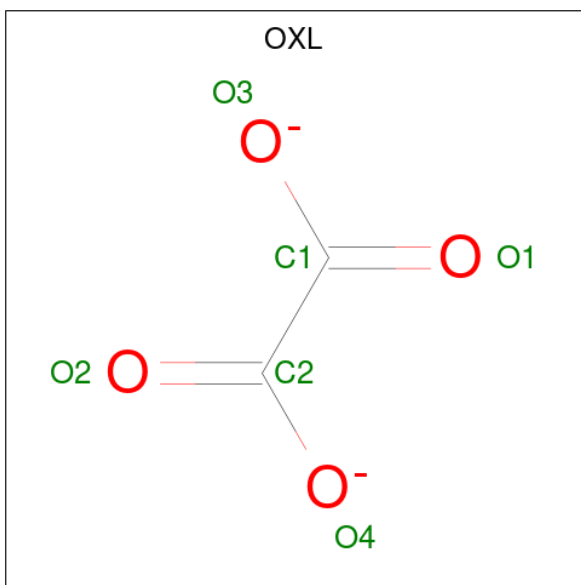
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total K 2 2	0	0
2	C	2	Total K 2 2	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



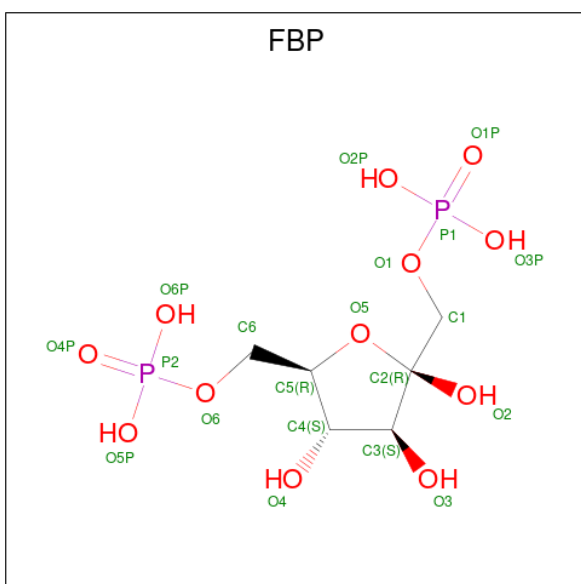
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0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

- Molecule 4 is OXALATE ION (three-letter code: OXL) (formula: C_2O_4).



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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			20	6	12	2		
5	B	1	Total	C	O	P	0	0
			20	6	12	2		
5	C	1	Total	C	O	P	0	0
			20	6	12	2		
5	D	1	Total	C	O	P	0	0
			20	6	12	2		

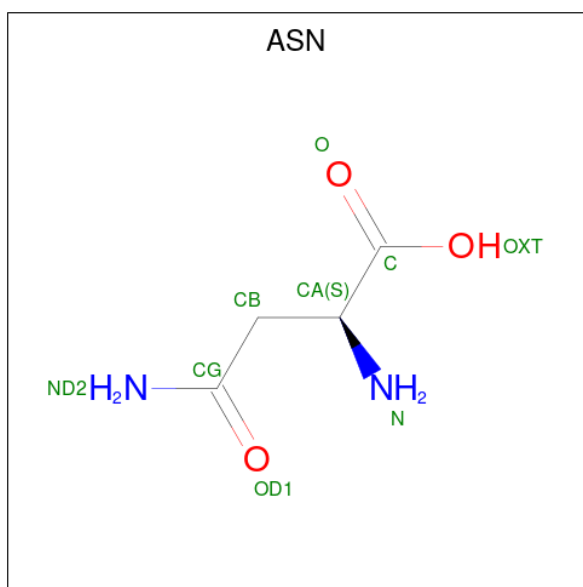
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	D	2	Total	Mg	0	0
			2	2		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

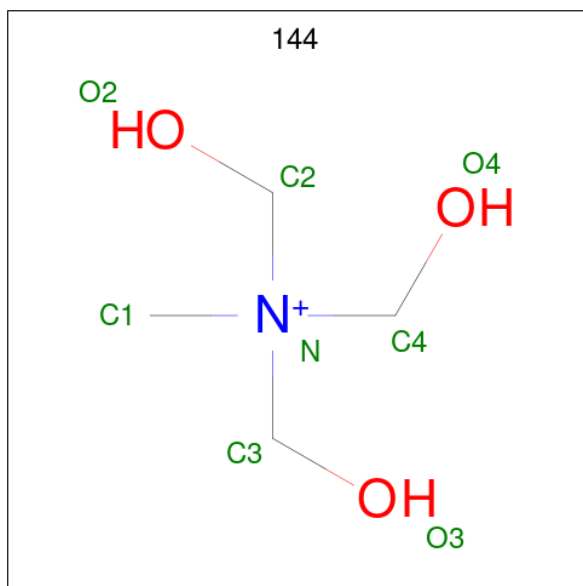
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ASPARAGINE (three-letter code: ASN) (formula: C₄H₈N₂O₃) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 9 is TRIS-HYDROXYMETHYL-METHYL-AMMONIUM (three-letter code: 144) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	0
			8	4	1	3		

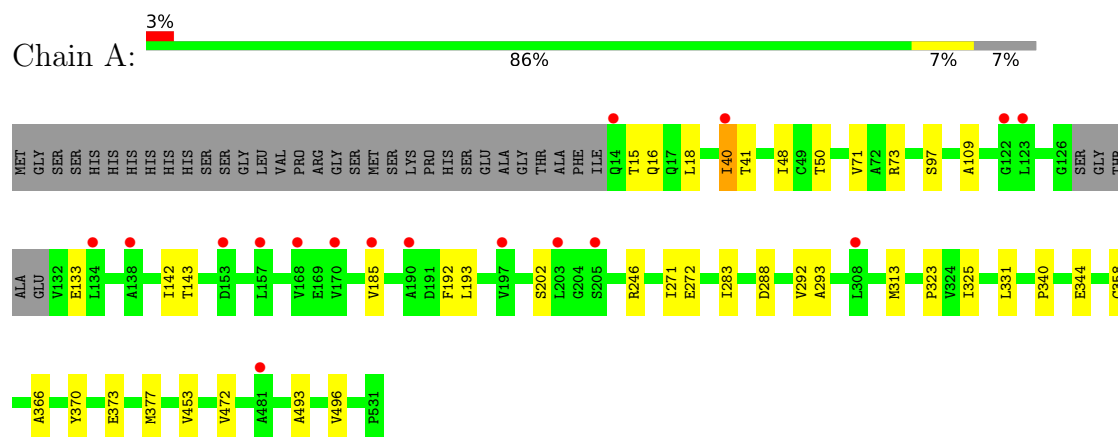
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	61	Total 61	O 61	0	0
10	B	31	Total 31	O 31	0	0
10	C	41	Total 41	O 41	0	0
10	D	23	Total 23	O 23	0	0

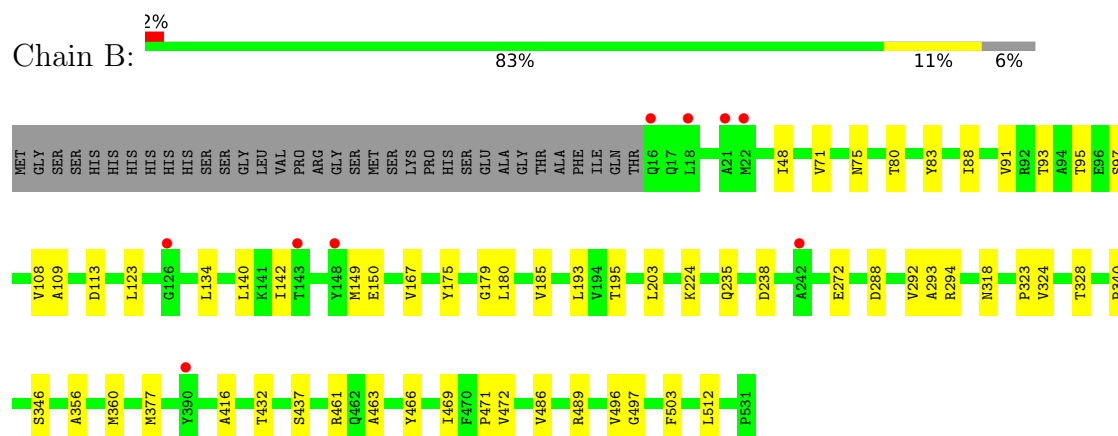
3 Residue-property plots [i](#)

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.

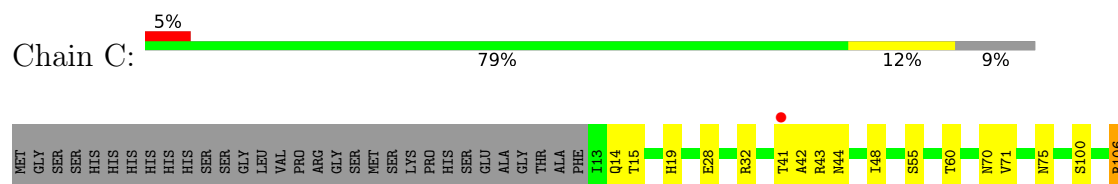
• Molecule 1: Pyruvate kinase PKM

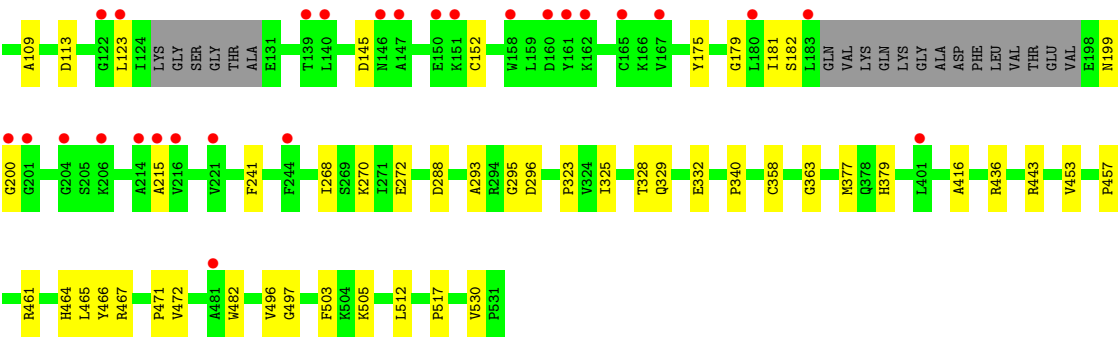


• Molecule 1: Pyruvate kinase PKM

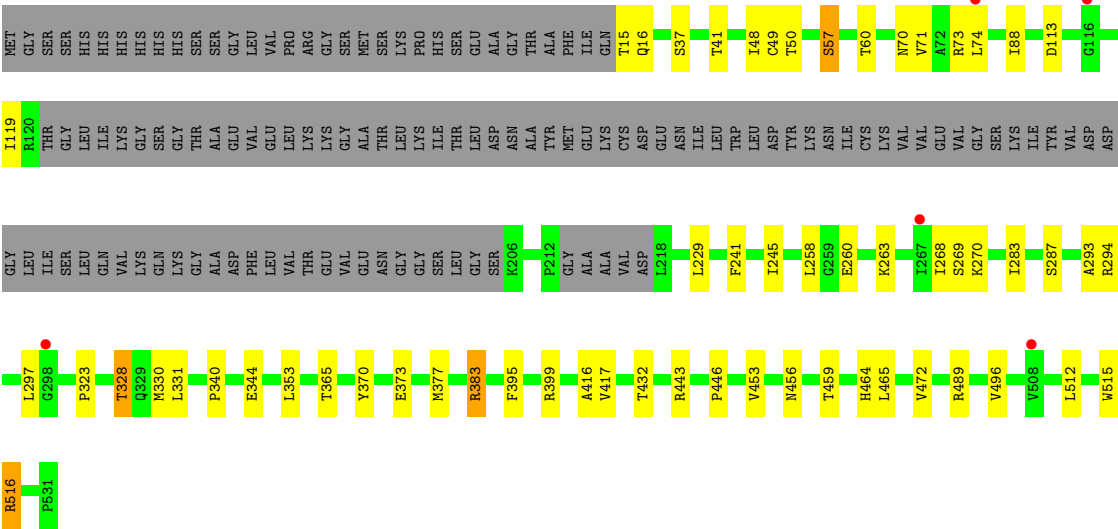


• Molecule 1: Pyruvate kinase PKM





● 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	80.99Å 154.58Å 92.15Å 90.00° 102.54° 90.00°	Depositor
Resolution (Å)	58.62 – 2.32 77.75 – 2.32	Depositor EDS
% Data completeness (in resolution range)	97.0 (58.62-2.32) 97.1 (77.75-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.233 , 0.275 0.231 , 0.272	Depositor DCC
R_{free} test set	4613 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14426	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, FBP, CL, K, 144, OXL

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	0.26	0/3742	0.43	0/5084
1	B	0.24	0/3774	0.42	0/5135
1	C	0.45	5/3601 (0.1%)	0.48	2/4898 (0.0%)
1	D	0.24	0/3155	0.42	0/4290
All	All	0.31	5/14272 (0.0%)	0.44	2/19407 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	70	ASN	C-O	-11.92	1.00	1.23
1	C	70	ASN	C-N	8.82	1.54	1.34
1	C	70	ASN	CG-OD1	-8.10	1.06	1.24
1	C	70	ASN	CG-ND2	-7.08	1.15	1.32
1	C	70	ASN	CB-CG	-5.04	1.39	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	ASN	O-C-N	-9.82	106.99	122.70
1	C	70	ASN	CA-C-N	5.30	128.87	117.20

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	3681	0	3486	23	0
1	B	3712	0	3524	30	0
1	C	3543	0	3291	43	0
1	D	3101	0	2961	35	0
2	A	2	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	16	2	0
3	B	30	0	40	1	0
3	C	54	0	72	10	0
3	D	6	0	8	0	0
4	A	6	0	0	1	0
4	B	6	0	0	1	0
4	C	6	0	0	3	0
4	D	6	0	0	2	0
5	A	20	0	10	0	0
5	B	20	0	10	2	0
5	C	20	0	10	0	0
5	D	20	0	10	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	D	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	C	9	0	5	3	0
9	D	8	0	12	3	0
10	A	61	0	0	0	0
10	B	31	0	0	0	0
10	C	41	0	0	0	0
10	D	23	0	0	0	0
All	All	14426	0	13455	133	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 (133) 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:43:ARG:H	3:C:613:GOL:H31	1.50	0.77
1:C:379:HIS:HE1	3:C:613:GOL:H32	1.51	0.75
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:O	1:C:467:ARG:HD3	1.90	0.70
1:C:464:HIS:HD1	8:C:604:ASN:N	1.89	0.69
1:A:16:GLN:HB3	1:A:18:LEU:HG	1.74	0.68
1:C:175:TYR:HB3	1:C:179:GLY:HA2	1.73	0.68
1:B:272:GLU:HG2	1:B:293:ALA:HB3	1.74	0.68
1:C:466:TYR:O	8:C:604:ASN:ND2	2.26	0.68
1:C:272:GLU:HG2	1:C:293:ALA:HB3	1.76	0.67
1:B:88:ILE:HD13	1:B:235:GLN:HG2	1.77	0.66
1:C:363:GLY:H	3:C:607:GOL:H11	1.63	0.64
1:C:472:VAL:HG11	1:C:496:VAL:HG11	1.82	0.61
1:B:71:VAL:HG22	1:B:109:ALA:HB3	1.81	0.60
1:A:40:ILE:H	1:A:40:ILE:HD12	1.65	0.60
1:C:461:ARG:NH1	3:C:606:GOL:O1	2.34	0.60
1:D:241:PHE:HE1	1:D:268:ILE:HD11	1.68	0.59
1:D:241:PHE:CE1	1:D:268:ILE:HD11	2.38	0.59
1:A:340:PRO:HG3	1:A:377:MET:HG2	1.85	0.59
1:A:142:ILE:O	1:A:193:LEU:N	2.36	0.58
1:C:464:HIS:ND1	8:C:604:ASN:N	2.51	0.58
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.85	0.58
1:D:15:THR:HG22	1:D:16:GLN:HG2	1.85	0.57
1:B:80:THR:HG23	1:B:83:TYR:H	1.69	0.56
1:D:113:ASP:HA	1:D:241:PHE:HB2	1.88	0.56
1:B:142:ILE:HB	1:B:193:LEU:HB2	1.88	0.55
1:D:283:ILE:O	1:D:287:SER:OG	2.22	0.55
1:B:175:TYR:HB3	1:B:179:GLY:HA2	1.89	0.55
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.89	0.55
1:C:71:VAL:HG22	1:C:109:ALA:HB3	1.88	0.54
1:A:133:GLU:HA	1:A:202:SER:HA	1.90	0.54
1:B:95:THR:HG21	1:B:108:VAL:HB	1.90	0.54
1:D:353:LEU:HD13	9:D:606:144:H32	1.90	0.53
1:D:48:ILE:HG12	1:D:71:VAL:HB	1.89	0.53
1:D:229:LEU:HD22	1:D:258:LEU:HD21	1.89	0.53
1:A:16:GLN:HG3	1:A:40:ILE:HG13	1.90	0.53
1:B:91:VAL:O	1:B:95:THR:HG23	2.08	0.53
1:B:134:LEU:HD11	1:B:203:LEU:HD22	1.91	0.53
1:B:140:LEU:O	1:B:195:THR:OG1	2.26	0.53
1:C:48:ILE:HG12	1:C:71:VAL:HB	1.91	0.52
1:B:293:ALA:HB1	4:B:607:OXL:C1	2.40	0.52
1:D:74:LEU:HD11	1:D:88:ILE:HG13	1.92	0.52
1:A:143:THR:HA	1:A:192:PHE:HA	1.91	0.52
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PRO:HG3	1:C:377:MET:HG2	1.91	0.51
1:D:50:THR:OG1	1:D:73:ARG:NH1	2.38	0.51
1:D:340:PRO:HG3	1:D:377:MET:HG2	1.93	0.50
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.93	0.50
1:D:57:SER:OG	1:D:60:THR:HG23	2.12	0.50
9:D:606:144:HO4	9:D:606:144:HO2	1.59	0.50
1:C:329:GLN:HG3	3:C:607:GOL:H31	1.94	0.50
1:A:71:VAL:HG22	1:A:109:ALA:HB3	1.94	0.49
1:B:340:PRO:HG3	1:B:377:MET:HG2	1.93	0.49
1:C:181:ILE:HA	1:C:200:GLY:HA2	1.94	0.49
1:C:482:TRP:CD1	1:C:517:PRO:HG3	2.46	0.49
1:D:49:CYS:HB3	1:D:365:THR:HG21	1.94	0.49
1:B:432:THR:HA	5:B:608:FBP:H61	1.94	0.49
1:D:245:ILE:HG13	1:D:269:SER:HB3	1.95	0.49
1:A:48:ILE:HG12	1:A:71:VAL:HB	1.94	0.48
1:C:293:ALA:HB1	4:C:614:OXL:C2	2.43	0.48
1:C:43:ARG:N	3:C:613:GOL:H31	2.25	0.48
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.94	0.48
1:B:432:THR:HB	1:B:437:SER:HB2	1.94	0.48
1:A:325:ILE:HG12	1:A:358:CYS:HB2	1.96	0.48
1:A:370:TYR:HB3	1:A:373:GLU:HB2	1.97	0.47
1:A:292:VAL:HG22	1:A:313:MET:HE2	1.96	0.47
1:A:366:ALA:HB3	3:A:603:GOL:H11	1.95	0.47
1:D:328:THR:HG21	4:D:602:OXL:O4	2.15	0.47
1:D:293:ALA:HB1	4:D:602:OXL:C2	2.45	0.47
1:D:515:TRP:CD2	1:D:516:ARG:HG2	2.50	0.47
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.97	0.47
1:C:332:GLU:OE1	3:C:607:GOL:H12	2.15	0.46
1:B:48:ILE:HB	1:B:360:MET:HG3	1.97	0.46
1:A:142:ILE:N	1:A:193:LEU:O	2.37	0.46
1:C:75:ASN:HA	1:C:113:ASP:HB3	1.98	0.46
1:D:456:ASN:HB3	1:D:459:THR:HB	1.98	0.46
1:A:50:THR:OG1	1:A:73:ARG:HD3	2.16	0.45
1:C:379:HIS:CE1	3:C:613:GOL:H32	2.42	0.45
1:D:417:VAL:HG13	1:D:446:PRO:HB3	1.98	0.45
1:B:472:VAL:HG21	1:B:496:VAL:HG11	1.99	0.45
1:C:75:ASN:HD22	3:C:605:GOL:H11	1.81	0.45
1:D:395:PHE:CE1	1:D:399:ARG:HD2	2.52	0.45
1:A:271:ILE:HD11	1:A:283:ILE:HG21	1.98	0.45
1:B:489:ARG:NH1	5:B:608:FBP:O3P	2.43	0.45
1:C:241:PHE:HD1	1:C:268:ILE:HB	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:SER:HA	1:C:60:THR:HG21	1.99	0.45
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.51	0.45
9:D:606:144:O4	9:D:606:144:O2	2.29	0.44
1:B:123:LEU:HD13	1:B:150:GLU:HG2	1.99	0.44
1:D:119:ILE:H	1:D:119:ILE:HD12	1.81	0.44
1:D:453:VAL:HG11	1:D:489:ARG:HB3	1.99	0.44
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.52	0.44
1:C:270:LYS:NZ	4:C:614:OXL:O3	2.33	0.44
1:D:15:THR:N	1:D:37:SER:HG	2.15	0.44
1:D:515:TRP:CE2	1:D:516:ARG:HG2	2.53	0.44
1:D:323:PRO:HB3	1:D:465:LEU:O	2.18	0.43
1:B:463:ALA:HB3	1:B:471:PRO:HB3	1.99	0.43
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.99	0.43
1:A:293:ALA:HB1	4:A:605:OXL:C1	2.48	0.43
1:B:75:ASN:HA	1:B:113:ASP:HB3	2.01	0.43
1:D:70:ASN:HB3	1:D:464:HIS:CG	2.52	0.43
1:B:288:ASP:O	1:B:323:PRO:HD2	2.19	0.43
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.43
1:C:28:GLU:O	1:C:32:ARG:HG3	2.19	0.43
1:C:295:GLY:HA3	1:C:328:THR:HG21	2.00	0.43
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.01	0.43
1:C:457:PRO:HB3	3:C:606:GOL:H2	2.01	0.43
1:D:370:TYR:HB3	1:D:373:GLU:HB2	2.01	0.43
1:C:453:VAL:HA	1:C:472:VAL:HG23	2.02	0.42
1:C:106:ARG:NE	1:C:106:ARG:HA	2.34	0.42
1:B:486:VAL:HG11	3:B:605:GOL:H32	2.01	0.42
1:C:106:ARG:HH12	1:C:471:PRO:HD2	1.84	0.42
1:D:294:ARG:NH2	1:D:330:MET:HG2	2.35	0.42
1:D:432:THR:HA	5:D:603:FBP:H61	2.00	0.42
1:A:246:ARG:NH2	3:A:604:GOL:H31	2.34	0.42
1:C:416:ALA:HB2	1:C:512:LEU:HD21	2.02	0.42
1:C:328:THR:OG1	4:C:614:OXL:O2	2.30	0.42
1:C:182:SER:N	1:C:199:ASN:O	2.50	0.42
1:B:292:VAL:HG12	1:B:294:ARG:HG2	2.01	0.41
1:B:93:THR:O	1:B:97:SER:OG	2.37	0.41
1:C:323:PRO:HB3	1:C:465:LEU:O	2.20	0.41
1:D:241:PHE:HB3	1:D:270:LYS:HD2	2.01	0.41
1:B:180:LEU:HA	1:B:180:LEU:HD23	1.90	0.41
1:C:106:ARG:HE	1:C:106:ARG:HA	1.85	0.41
1:C:288:ASP:O	1:C:323:PRO:HD2	2.21	0.41
1:B:238:ASP:OD1	1:B:461:ARG:NE	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ASP:O	1:A:323:PRO:HD2	2.21	0.41
1:C:123:LEU:O	1:C:152:CYS:HB2	2.21	0.41
1:C:19:HIS:NE2	1:C:32:ARG:HD2	2.36	0.41
1:B:324:VAL:HG13	1:B:356:ALA:HA	2.02	0.40
1:C:505:LYS:HA	1:C:530:VAL:HG23	2.02	0.40
1:D:260:GLU:HA	1:D:263:LYS:HB3	2.03	0.40
1:D:41:THR:HA	1:D:383:ARG:HH21	1.86	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	509/550 (92%)	490 (96%)	15 (3%)	4 (1%)	19	23
1	B	514/550 (94%)	499 (97%)	12 (2%)	3 (1%)	25	30
1	C	493/550 (90%)	467 (95%)	22 (4%)	4 (1%)	19	23
1	D	421/550 (76%)	407 (97%)	13 (3%)	1 (0%)	47	58
All	All	1937/2200 (88%)	1863 (96%)	62 (3%)	12 (1%)	25	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	40	ILE
1	A	41	THR
1	C	41	THR
1	C	215	ALA
1	C	14	GLN
1	B	167	VAL
1	C	42	ALA

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Mol	Chain	Res	Type
1	A	185	VAL
1	D	328	THR
1	B	328	THR
1	B	185	VAL

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	342/452 (76%)	341 (100%)	1 (0%)	92	96
1	B	351/452 (78%)	347 (99%)	4 (1%)	73	85
1	C	323/452 (72%)	316 (98%)	7 (2%)	52	68
1	D	299/452 (66%)	294 (98%)	5 (2%)	60	75
All	All	1315/1808 (73%)	1298 (99%)	17 (1%)	67	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	B	149	MET
1	B	224	LYS
1	B	318	ASN
1	B	346	SER
1	C	15	THR
1	C	100	SER
1	C	106	ARG
1	C	145	ASP
1	C	296	ASP
1	C	436	ARG
1	C	443	ARG
1	D	57	SER
1	D	297	LEU
1	D	383	ARG
1	D	443	ARG
1	D	516	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 37 ligands modelled in this entry, 10 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	C	609	-	5,5,5	0.91	0	5,5,5	0.98	0
5	FBP	D	603	-	18,20,20	0.95	1 (5%)	23,32,32	0.70	0
3	GOL	B	606	-	5,5,5	0.87	0	5,5,5	1.00	0
3	GOL	A	604	-	5,5,5	0.91	0	5,5,5	1.01	0
4	OXL	C	614	2	0,5,5	0.00	-	0,6,6	0.00	-
3	GOL	B	603	-	5,5,5	0.86	0	5,5,5	1.02	0
3	GOL	C	613	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	B	604	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	C	611	-	5,5,5	0.90	0	5,5,5	0.98	0
3	GOL	A	603	-	5,5,5	0.84	0	5,5,5	1.07	0
5	FBP	A	606	-	18,20,20	0.92	1 (5%)	23,32,32	0.69	0
3	GOL	C	607	-	5,5,5	0.96	0	5,5,5	0.87	0
3	GOL	C	610	-	5,5,5	0.91	0	5,5,5	0.98	0
9	144	D	606	-	1,7,7	0.80	0	3,9,9	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	602	-	5,5,5	0.93	0	5,5,5	1.00	0
3	GOL	C	612	-	5,5,5	0.90	0	5,5,5	0.99	0
3	GOL	C	608	-	5,5,5	0.91	0	5,5,5	1.01	0
3	GOL	D	601	-	5,5,5	0.90	0	5,5,5	0.99	0
8	ASN	C	604	-	5,8,8	0.19	0	5,10,10	0.19	0
3	GOL	C	605	-	5,5,5	0.97	0	5,5,5	0.94	0
4	OXL	D	602	6	0,5,5	0.00	-	0,6,6	0.00	-
3	GOL	B	605	-	5,5,5	0.89	0	5,5,5	1.00	0
5	FBP	C	615	-	18,20,20	0.92	1 (5%)	23,32,32	0.68	0
4	OXL	A	605	6	0,5,5	0.00	-	0,6,6	0.00	-
4	OXL	B	607	6	0,5,5	0.00	-	0,6,6	0.00	-
3	GOL	C	606	-	5,5,5	0.94	0	5,5,5	0.99	0
5	FBP	B	608	-	18,20,20	0.92	1 (5%)	23,32,32	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	609	-	-	4/4/4/4	-
5	FBP	D	603	-	-	5/13/32/32	0/1/1/1
3	GOL	B	606	-	-	0/4/4/4	-
3	GOL	A	604	-	-	2/4/4/4	-
4	OXL	C	614	2	-	0/0/4/4	-
3	GOL	B	603	-	-	2/4/4/4	-
3	GOL	C	613	-	-	0/4/4/4	-
3	GOL	B	604	-	-	2/4/4/4	-
3	GOL	C	611	-	-	4/4/4/4	-
3	GOL	A	603	-	-	0/4/4/4	-
5	FBP	A	606	-	-	2/13/32/32	0/1/1/1
3	GOL	C	607	-	-	4/4/4/4	-
3	GOL	C	610	-	-	0/4/4/4	-
9	144	D	606	-	-	0/0/9/9	-
3	GOL	B	602	-	-	0/4/4/4	-
3	GOL	C	612	-	-	2/4/4/4	-
3	GOL	C	608	-	-	1/4/4/4	-
3	GOL	D	601	-	-	2/4/4/4	-
8	ASN	C	604	-	-	1/4/8/8	-
3	GOL	C	605	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OXL	D	602	6	-	0/0/4/4	-
3	GOL	B	605	-	-	3/4/4/4	-
5	FBP	C	615	-	-	4/13/32/32	0/1/1/1
4	OXL	A	605	6	-	0/0/4/4	-
4	OXL	B	607	6	-	0/0/4/4	-
3	GOL	C	606	-	-	0/4/4/4	-
5	FBP	B	608	-	-	4/13/32/32	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	603	FBP	O2-C2	2.85	1.45	1.40
5	C	615	FBP	O2-C2	2.72	1.45	1.40
5	A	606	FBP	O2-C2	2.71	1.45	1.40
5	B	608	FBP	O2-C2	2.70	1.45	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	609	GOL	C1-C2-C3-O3
3	C	609	GOL	O2-C2-C3-O3
5	D	603	FBP	O1-C1-C2-O2
5	D	603	FBP	O1-C1-C2-C3
5	D	603	FBP	O1-C1-C2-O5
5	D	603	FBP	C4-C5-C6-O6
3	A	604	GOL	O1-C1-C2-C3
3	B	603	GOL	C1-C2-C3-O3
3	B	604	GOL	O1-C1-C2-O2
3	B	604	GOL	O1-C1-C2-C3
3	C	611	GOL	O1-C1-C2-C3
5	A	606	FBP	C4-C5-C6-O6
3	C	612	GOL	C1-C2-C3-O3
3	D	601	GOL	C1-C2-C3-O3
8	C	604	ASN	N-CA-CB-CG
3	B	605	GOL	O1-C1-C2-C3
5	C	615	FBP	C1-O1-P1-O2P
5	C	615	FBP	C1-O1-P1-O3P
5	C	615	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	608	FBP	C4-C5-C6-O6
5	D	603	FBP	O5-C5-C6-O6
5	B	608	FBP	O5-C5-C6-O6
5	C	615	FBP	O5-C5-C6-O6
3	C	609	GOL	O1-C1-C2-C3
3	C	611	GOL	C1-C2-C3-O3
3	C	607	GOL	O1-C1-C2-C3
3	C	605	GOL	O1-C1-C2-C3
3	B	605	GOL	C1-C2-C3-O3
3	A	604	GOL	O1-C1-C2-O2
3	B	603	GOL	O2-C2-C3-O3
3	C	611	GOL	O2-C2-C3-O3
3	D	601	GOL	O2-C2-C3-O3
3	B	605	GOL	O1-C1-C2-O2
5	A	606	FBP	O5-C5-C6-O6
3	C	607	GOL	O1-C1-C2-O2
3	C	605	GOL	O1-C1-C2-O2
5	B	608	FBP	C6-O6-P2-O4P
3	C	605	GOL	O2-C2-C3-O3
3	C	609	GOL	O1-C1-C2-O2
3	C	607	GOL	C1-C2-C3-O3
3	C	611	GOL	O1-C1-C2-O2
3	C	612	GOL	O2-C2-C3-O3
3	C	608	GOL	O1-C1-C2-C3
5	B	608	FBP	C6-O6-P2-O5P
3	C	605	GOL	C1-C2-C3-O3
3	C	607	GOL	O2-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	603	FBP	1	0
3	A	604	GOL	1	0
4	C	614	OXL	3	0
3	C	613	GOL	4	0
3	A	603	GOL	1	0
3	C	607	GOL	3	0
9	D	606	144	3	0
8	C	604	ASN	3	0
3	C	605	GOL	1	0
4	D	602	OXL	2	0

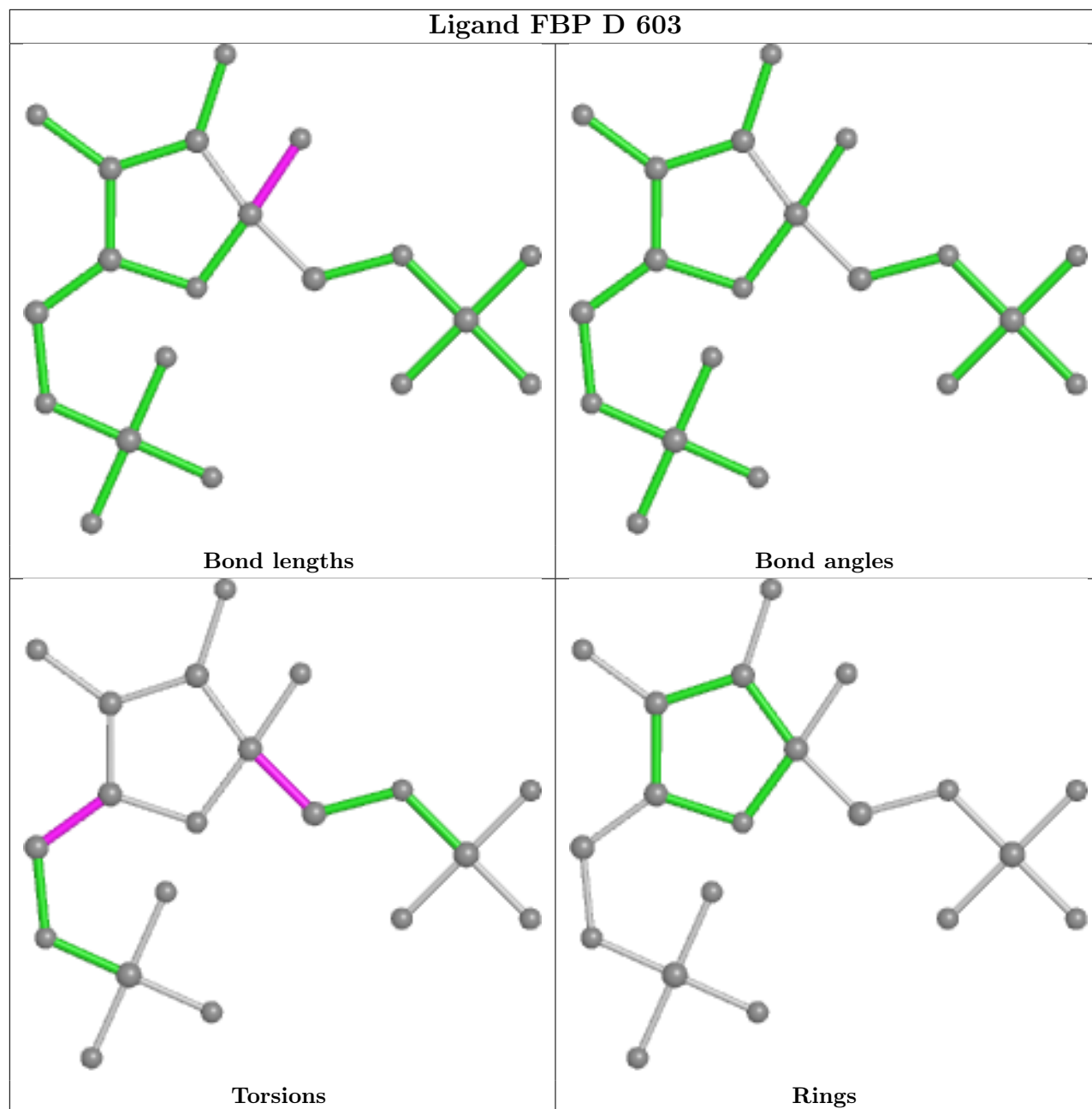
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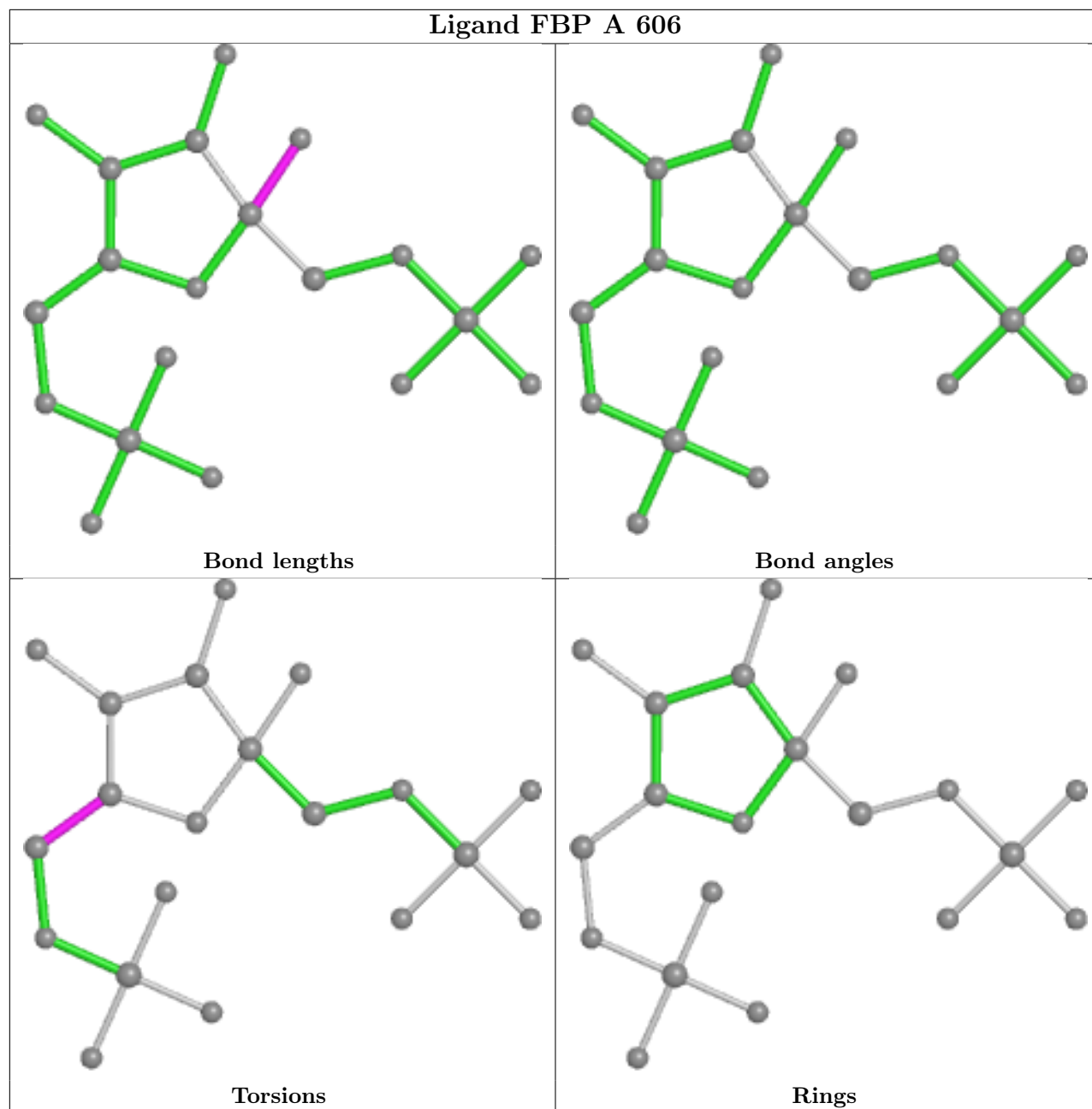
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	605	GOL	1	0
4	A	605	OXL	1	0
4	B	607	OXL	1	0
3	C	606	GOL	2	0
5	B	608	FBP	2	0

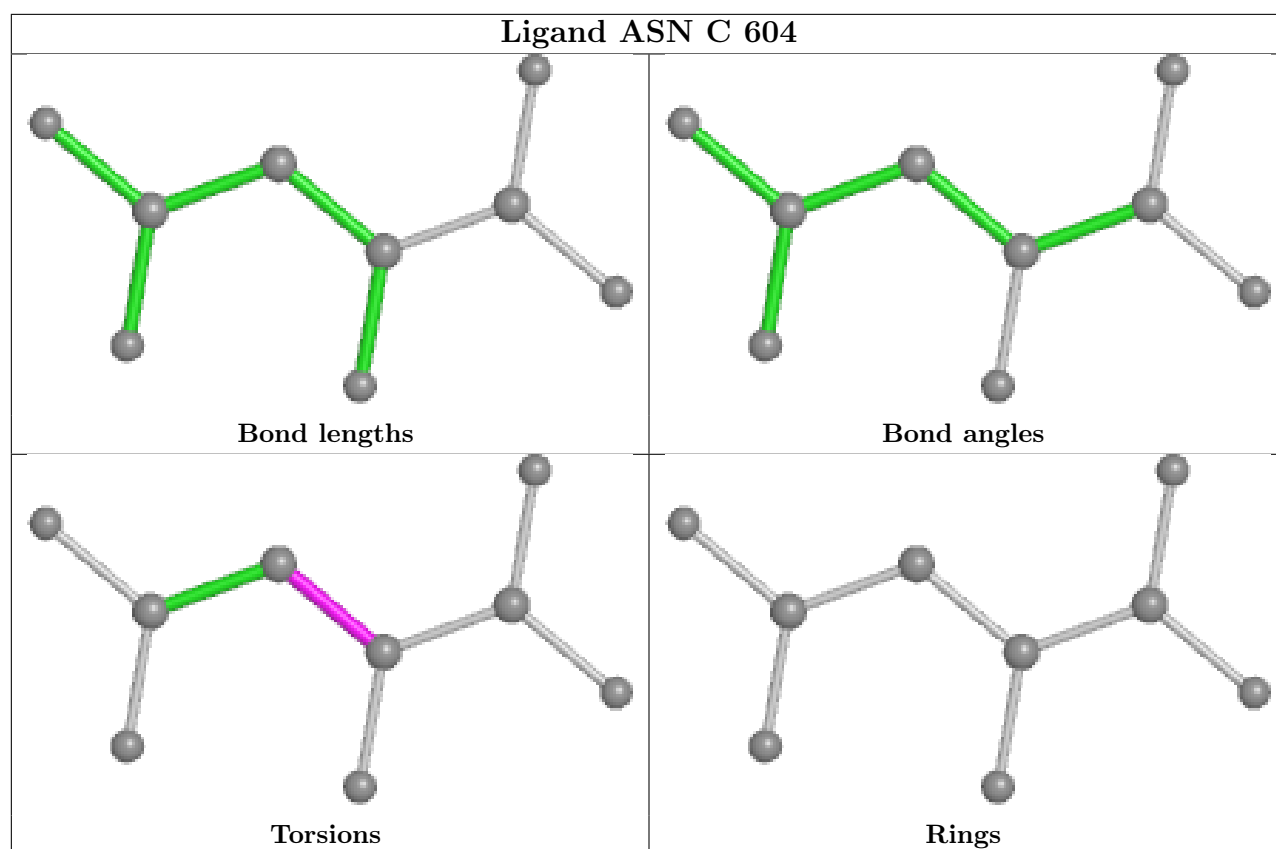
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

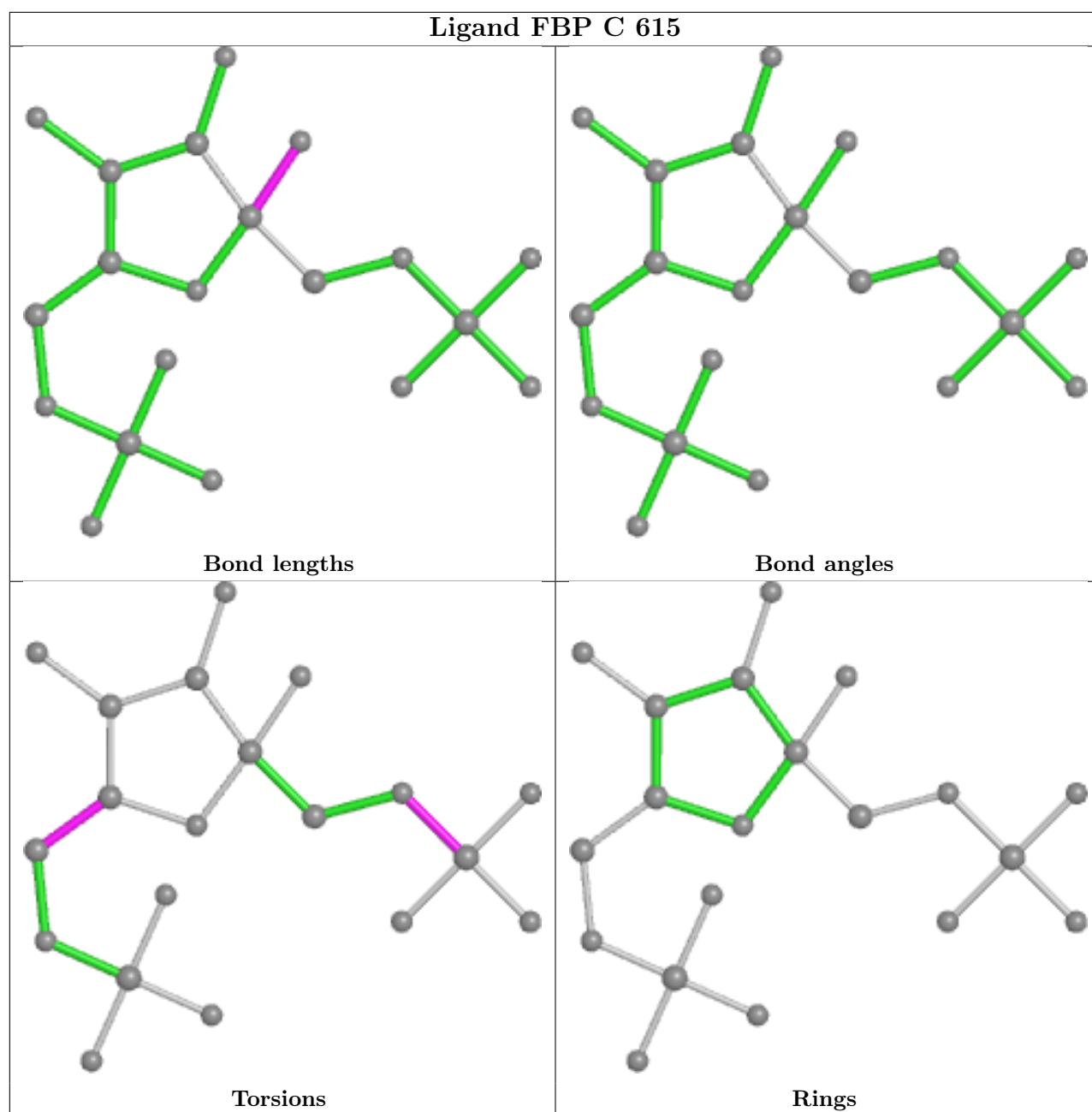
Ligand FBP D 603

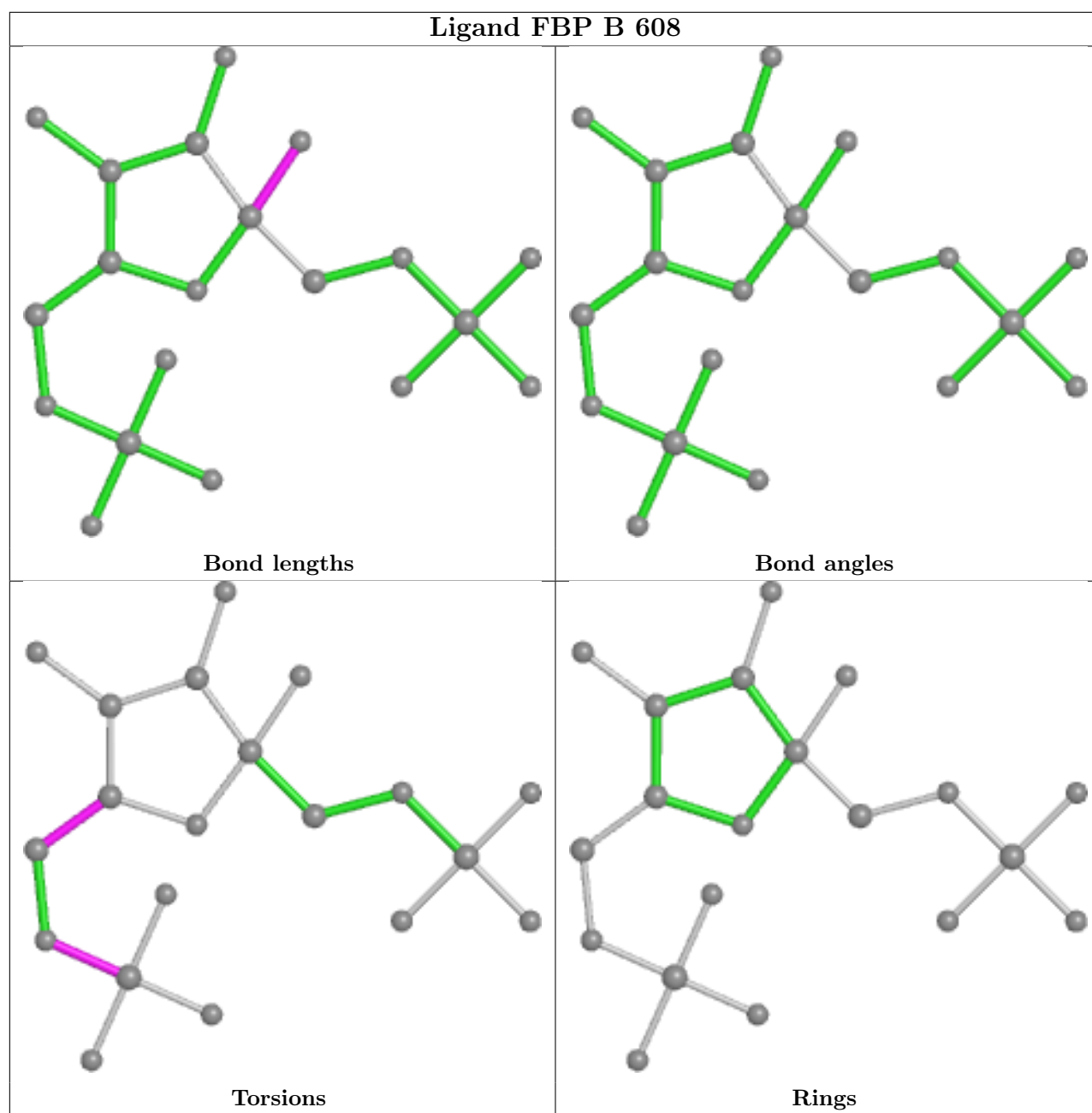


Ligand FBP A 606









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	513/550 (93%)	0.43	17 (3%) 46 53	31, 43, 82, 92	0
1	B	516/550 (93%)	0.43	9 (1%) 70 76	36, 51, 70, 87	0
1	C	499/550 (90%)	0.58	28 (5%) 24 31	30, 46, 95, 105	0
1	D	427/550 (77%)	0.40	5 (1%) 79 83	36, 48, 66, 98	0
All	All	1955/2200 (88%)	0.46	59 (3%) 50 57	30, 47, 82, 105	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	140	LEU	5.4
1	C	162	LYS	4.7
1	C	123	LEU	4.6
1	C	158	TRP	3.9
1	C	161	TYR	3.9
1	C	214	ALA	3.7
1	A	134	LEU	3.6
1	B	16	GLN	3.6
1	B	21	ALA	3.5
1	A	157	LEU	3.3
1	A	122	GLY	3.2
1	C	122	GLY	3.2
1	C	221	VAL	3.0
1	C	244	PHE	3.0
1	C	139	THR	2.9
1	A	168	VAL	2.9
1	A	14	GLN	2.9
1	A	190	ALA	2.8
1	A	153	ASP	2.8
1	B	143	THR	2.8
1	D	508	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	242	ALA	2.6
1	B	18	LEU	2.5
1	B	22	MET	2.5
1	C	215	ALA	2.5
1	C	180	LEU	2.5
1	C	160	ASP	2.5
1	B	390	TYR	2.4
1	D	267	ILE	2.4
1	C	165	CYS	2.4
1	A	481	ALA	2.3
1	C	41	THR	2.3
1	C	216	VAL	2.3
1	C	146	ASN	2.3
1	C	481	ALA	2.3
1	C	201	GLY	2.3
1	C	167	VAL	2.3
1	A	205	SER	2.2
1	C	147	ALA	2.2
1	D	116	GLY	2.2
1	D	74	LEU	2.2
1	A	197	VAL	2.2
1	D	298	GLY	2.2
1	C	151	LYS	2.2
1	C	206	LYS	2.1
1	A	138	ALA	2.1
1	C	200	GLY	2.1
1	A	308	LEU	2.1
1	C	150	GLU	2.1
1	A	203	LEU	2.1
1	A	123	LEU	2.1
1	B	126	GLY	2.1
1	A	185	VAL	2.0
1	C	183	LEU	2.0
1	C	401	LEU	2.0
1	C	204	GLY	2.0
1	A	170	VAL	2.0
1	B	148	TYR	2.0
1	A	40	ILE	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 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, 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(\AA^2)	Q<0.9
3	GOL	C	607	6/6	0.63	0.28	48,54,56,61	0
9	144	D	606	8/8	0.69	0.26	49,64,66,68	0
3	GOL	B	606	6/6	0.78	0.25	63,65,66,69	0
3	GOL	C	610	6/6	0.79	0.34	38,46,57,57	0
2	K	C	601	1/1	0.80	0.15	69,69,69,69	0
3	GOL	C	613	6/6	0.82	0.26	44,49,63,76	0
3	GOL	C	611	6/6	0.82	0.26	48,58,60,65	0
3	GOL	A	603	6/6	0.82	0.23	28,45,52,56	0
3	GOL	B	605	6/6	0.84	0.17	49,56,59,66	0
3	GOL	C	609	6/6	0.85	0.27	56,59,62,63	0
3	GOL	C	612	6/6	0.85	0.18	54,61,67,71	0
2	K	C	602	1/1	0.85	0.23	73,73,73,73	0
6	MG	A	607	1/1	0.85	0.25	42,42,42,42	0
3	GOL	D	601	6/6	0.86	0.17	46,56,58,64	0
6	MG	D	605	1/1	0.87	0.22	62,62,62,62	0
3	GOL	C	608	6/6	0.88	0.23	50,53,59,67	0
3	GOL	B	604	6/6	0.88	0.23	47,56,59,63	0
4	OXL	D	602	6/6	0.89	0.14	54,59,62,64	0
3	GOL	B	603	6/6	0.89	0.19	46,51,59,62	0
3	GOL	C	605	6/6	0.89	0.24	46,55,64,66	0
4	OXL	C	614	6/6	0.90	0.20	47,52,56,59	0
6	MG	B	609	1/1	0.91	0.18	50,50,50,50	0
3	GOL	C	606	6/6	0.91	0.24	47,55,57,58	0
3	GOL	A	604	6/6	0.92	0.20	48,53,56,59	0
8	ASN	C	604	9/9	0.93	0.15	48,51,54,62	0
4	OXL	B	607	6/6	0.93	0.15	40,43,47,47	0
3	GOL	B	602	6/6	0.93	0.12	47,51,52,62	0
6	MG	D	604	1/1	0.94	0.14	57,57,57,57	0
4	OXL	A	605	6/6	0.95	0.13	38,42,45,45	0
5	FBP	D	603	20/20	0.95	0.14	39,48,60,63	0
2	K	A	602	1/1	0.95	0.10	53,53,53,53	0
5	FBP	C	615	20/20	0.96	0.14	39,44,56,61	0

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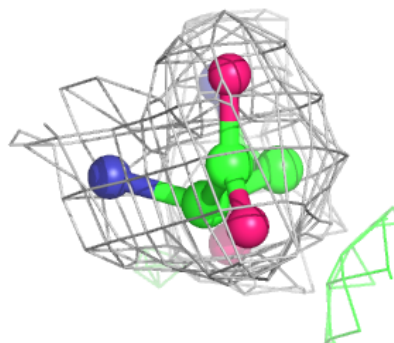
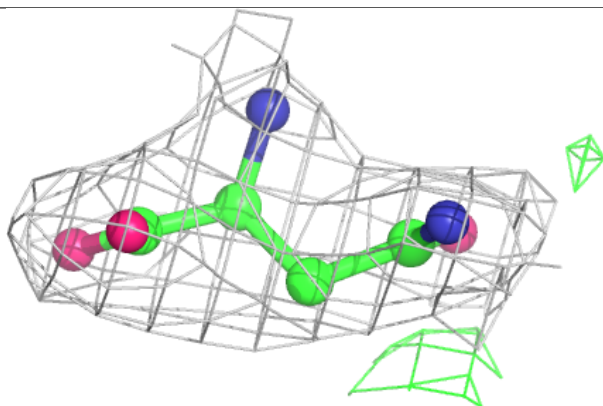
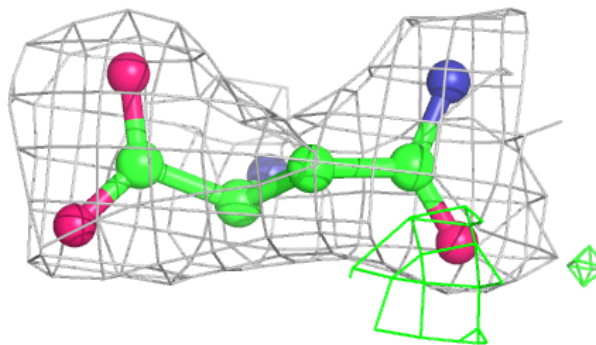
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	K	A	601	1/1	0.96	0.11	56,56,56,56	0
5	FBP	B	608	20/20	0.96	0.14	43,48,55,57	0
5	FBP	A	606	20/20	0.97	0.14	33,46,49,52	0
7	CL	B	601	1/1	0.97	0.13	56,56,56,56	0
7	CL	C	603	1/1	0.98	0.15	37,37,37,37	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.

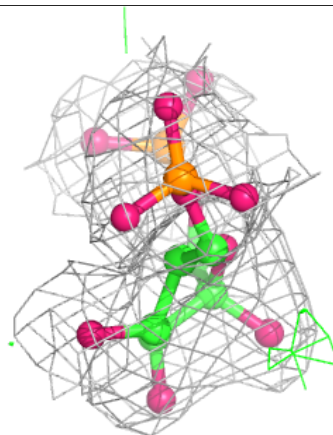
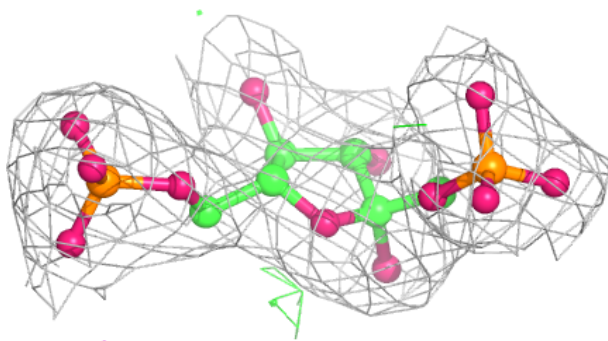
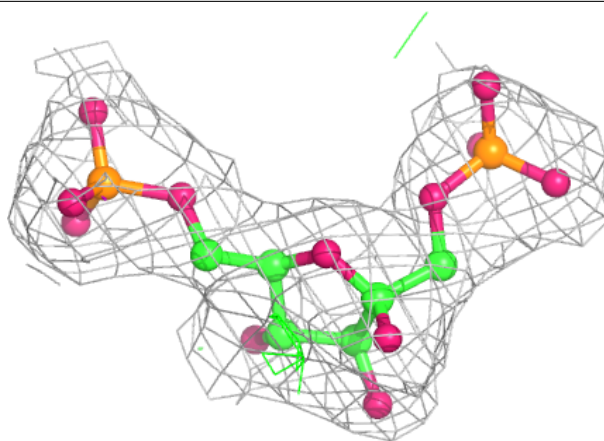
Electron density around ASN C 604:

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



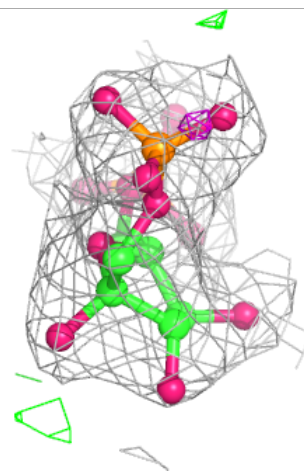
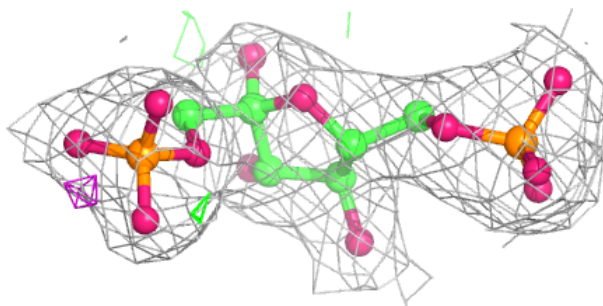
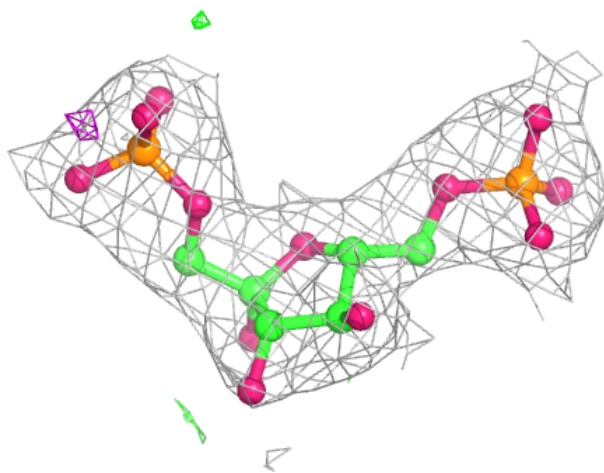
Electron density around FBP D 603:

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



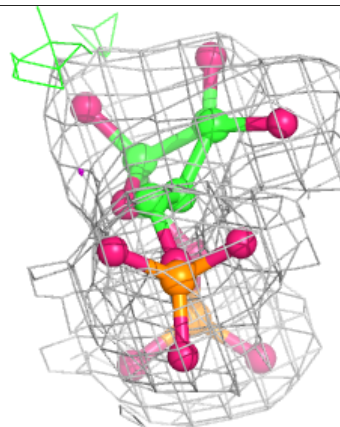
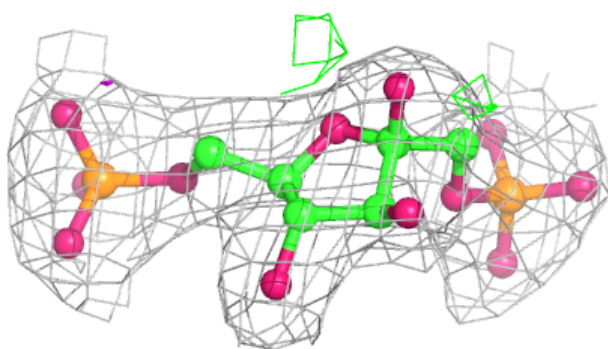
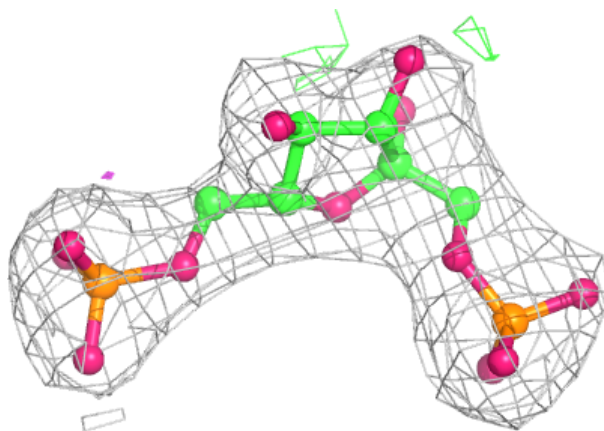
Electron density around FBP C 615:

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

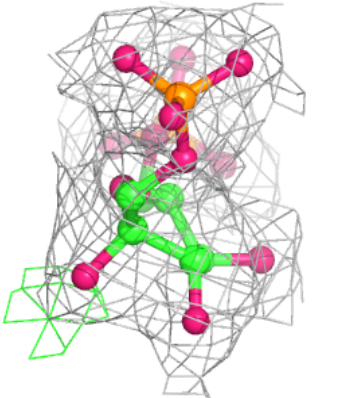
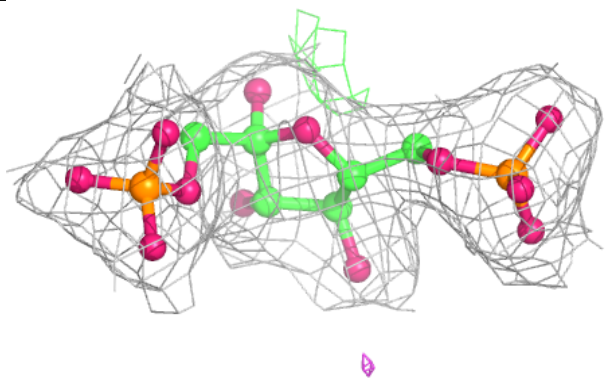
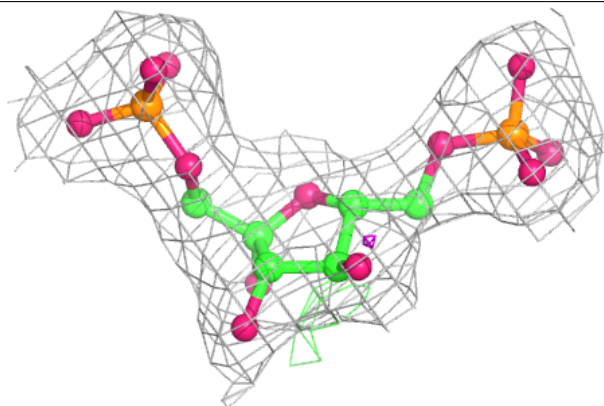


Electron density around FBP B 608:

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

**Electron density around FBP A 606:**

$2mF_o - DF_c$ (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.