



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:08 PM UTC

PDB ID : 6ECK / pdb\_00006eck  
Title : Pyruvate Kinase Isoform L-type with phosphorylated Ser113 (pS113) in complex with FBP  
Authors : Padyana, A.; Tong, S.  
Deposited on : 2018-08-08  
Resolution : 2.36 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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)  
Xtrriage (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

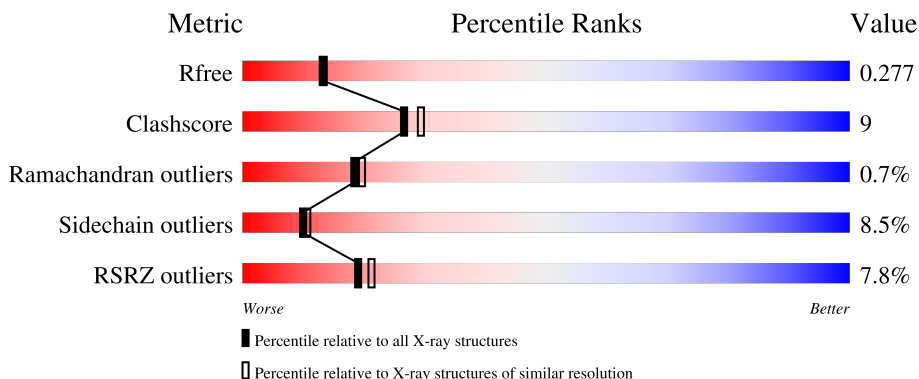
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

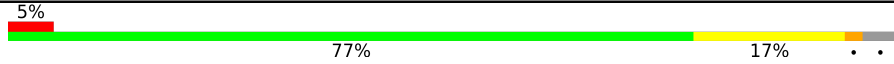
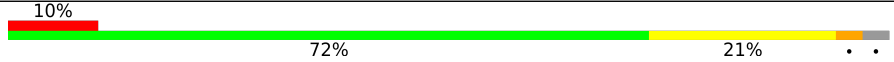
The reported resolution of this entry is 2.36 Å.

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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	550	
1	B	550	

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	B	602	-	X	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8633 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.

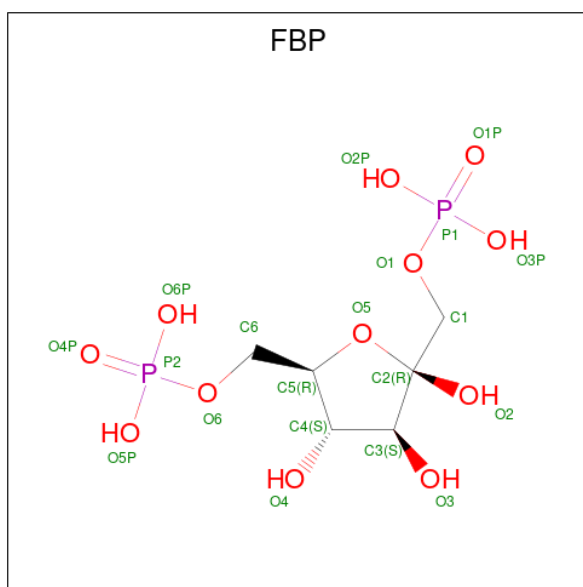
- Molecule 1 is a protein called Pyruvate kinase PKLR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	529	4054	2547	725	762	1	19	0	2	0
1	B	532	4085	2563	734	768	1	19	0	3	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P12928
A	544	HIS	-	expression tag	UNP P12928
A	546	HIS	-	expression tag	UNP P12928
A	547	HIS	-	expression tag	UNP P12928
A	548	HIS	-	expression tag	UNP P12928
A	549	HIS	-	expression tag	UNP P12928
A	550	HIS	-	expression tag	UNP P12928
B	0	HIS	-	expression tag	UNP P12928
B	544	HIS	-	expression tag	UNP P12928
B	545	HIS	-	expression tag	UNP P12928
B	546	HIS	-	expression tag	UNP P12928
B	547	HIS	-	expression tag	UNP P12928
B	548	HIS	-	expression tag	UNP P12928
B	549	HIS	-	expression tag	UNP P12928

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (CCD ID: FBP) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>12</sub>P<sub>2</sub>).



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		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



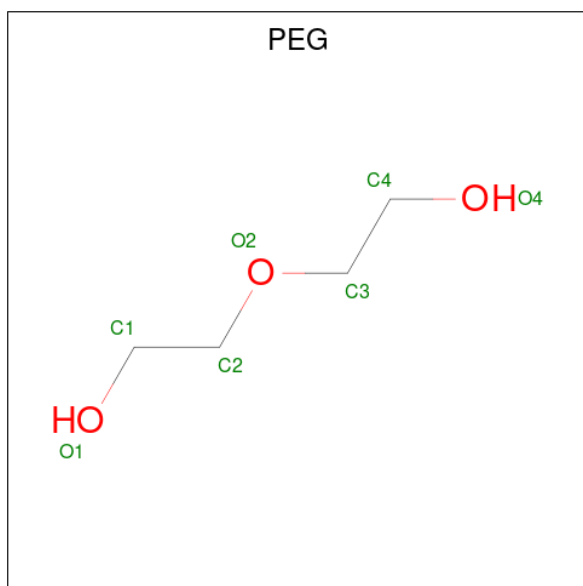
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



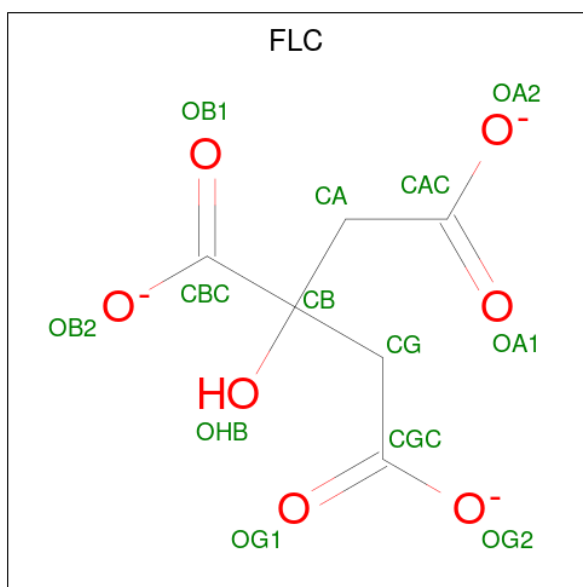
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	7	4	3	0	0
4	B	1	7	4	3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula:  $C_2H_6O_2$ ).



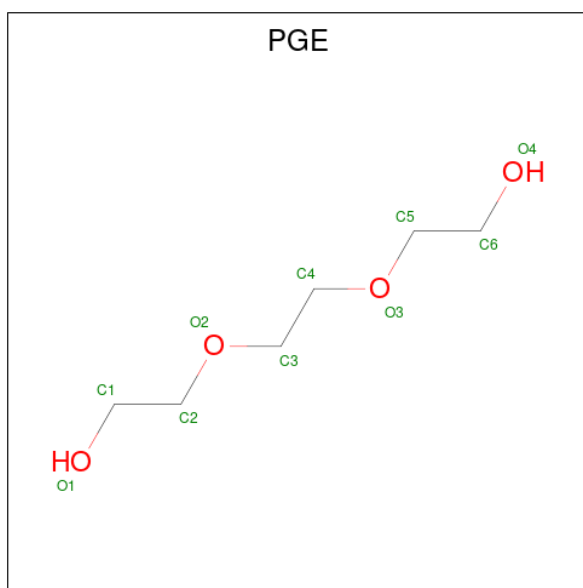
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is CITRATE ANION (CCD ID: FLC) (formula:  $C_6H_5O_7^-$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	C O	0	0
			10	6 4		

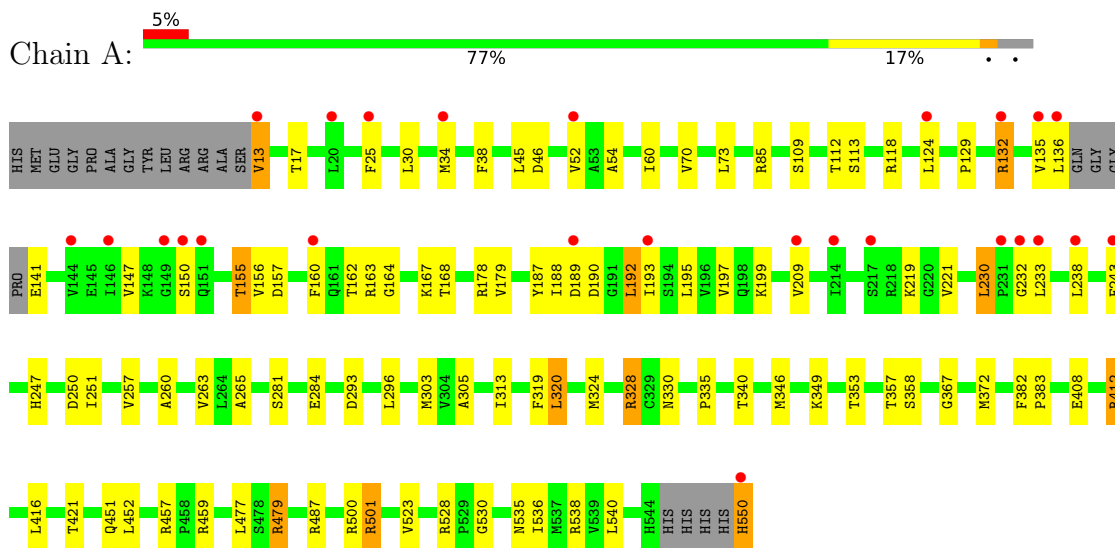
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	229	Total	O	0	0
			229	229		
8	B	158	Total	O	0	0
			158	158		

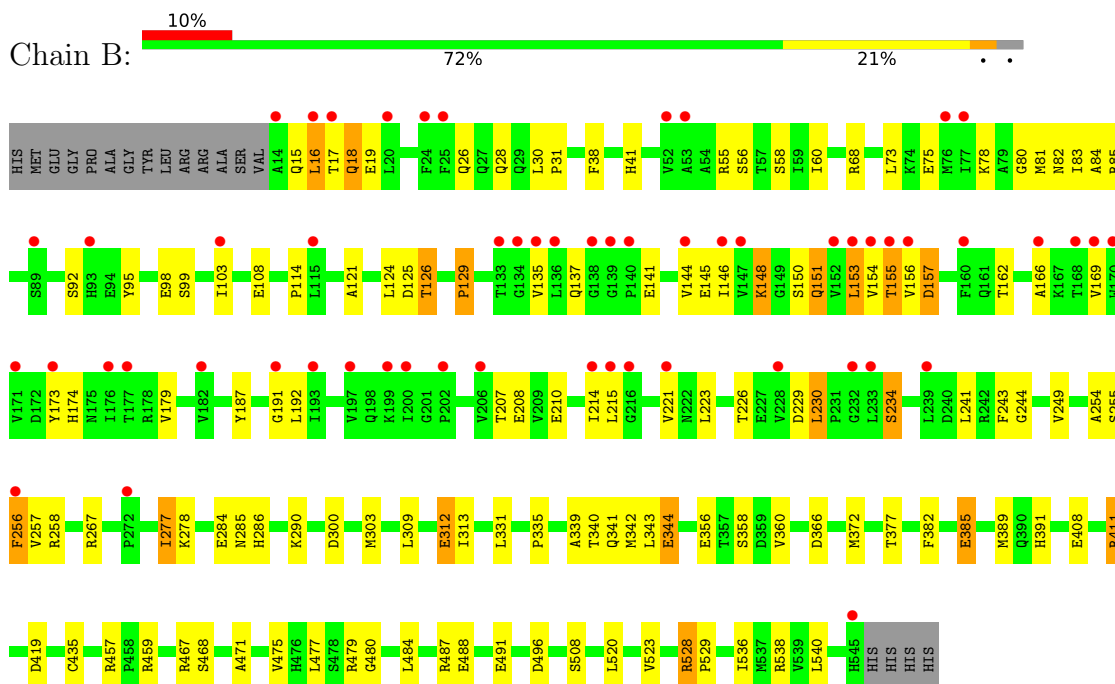
### 3 Residue-property plots [i](#)

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 PKLR



- 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, $\alpha$ , $\beta$ , $\gamma$	97.77Å 111.84Å 127.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.59 – 2.36 48.59 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.6 (48.59-2.36) 97.6 (48.59-2.36)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.37Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, $R_{free}$	0.203 , 0.275 0.209 , 0.277	Depositor DCC
$R_{free}$ test set	2815 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtrriage
Anisotropy	0.072	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8633	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, FLC, GOL, SEP, PEG, EDO, FBP

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	1.00	4/4109 (0.1%)	1.12	4/5560 (0.1%)
1	B	0.95	0/4140	1.16	3/5604 (0.1%)
All	All	0.98	4/8249 (0.0%)	1.14	7/11164 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	PHE	N-CA	-6.63	1.38	1.46
1	A	179	VAL	N-CA	5.79	1.51	1.46
1	A	353	THR	C-O	-5.57	1.16	1.23
1	A	451	GLN	C-O	-5.09	1.18	1.24

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ASP	CA-CB-CG	6.46	119.06	112.60
1	A	293	ASP	CA-CB-CG	5.62	118.22	112.60
1	A	530	GLY	CA-C-N	5.47	128.48	120.71
1	A	530	GLY	C-N-CA	5.47	128.48	120.71
1	B	377	THR	CA-CB-OG1	5.10	117.25	109.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	A	412	ARG	Sidechain
1	A	528	ARG	Sidechain
1	B	339	ALA	Peptide
1	B	467	ARG	Sidechain

## 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	4054	0	4123	69	0
1	B	4085	0	4149	90	0
2	A	20	0	10	2	0
2	B	20	0	10	0	0
3	A	12	0	16	1	0
3	B	6	0	8	12	0
4	A	7	0	10	3	0
4	B	7	0	10	3	0
5	A	12	0	18	1	0
6	B	13	0	5	2	0
7	B	10	0	14	0	0
8	A	229	0	0	7	0
8	B	158	0	0	3	0
All	All	8633	0	8373	155	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 9.

The worst 5 of 155 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:A:188:ILE:HD12	1:A:193:ILE:HD11	1.54	0.89
1:B:58:SER:OG	3:B:602:GOL:H12	1.83	0.79
1:B:303:MET:CE	1:B:372:MET:HE1	2.14	0.78

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:ARG:HD3	1:B:391:HIS:ND1	2.00	0.77
1:B:303:MET:HE2	1:B:372:MET:HE1	1.72	0.72

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	525/550 (96%)	500 (95%)	23 (4%)	2 (0%)	30	34
1	B	532/550 (97%)	490 (92%)	37 (7%)	5 (1%)	14	14
All	All	1057/1100 (96%)	990 (94%)	60 (6%)	7 (1%)	18	20

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	17	THR
1	B	340	THR
1	A	129	PRO
1	A	340	THR
1	B	234	SER

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/446 (97%)	404 (93%)	29 (7%)	15	17
1	B	435/446 (98%)	391 (90%)	44 (10%)	7	6
All	All	868/892 (97%)	795 (92%)	73 (8%)	10	11

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	230	LEU
1	B	491	GLU
1	B	256	PHE
1	B	358	SER
1	A	416	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	236	GLN
1	B	535	ASN
1	B	15	GLN
1	B	18	GLN
1	B	26	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](#)

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	SEP	A	113	1	8,9,10	0.70	0	7,12,14	2.05	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	SEP	B	113	1	8,9,10	0.68	0	7,12,14	1.21	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
1	SEP	A	113	1	-	5/6/8/10	-
1	SEP	B	113	1	-	1/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	113	SEP	O3P-P-O2P	3.39	120.52	107.80
1	A	113	SEP	O2P-P-OG	-3.38	97.86	106.67

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	113	SEP	N-CA-CB-OG
1	A	113	SEP	C-CA-CB-OG
1	A	113	SEP	CB-OG-P-O2P
1	A	113	SEP	CB-OG-P-O3P
1	B	113	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	GOL	A	602	-	5,5,5	1.13	0	5,5,5	1.26	1 (20%)
5	EDO	A	605	-	3,3,3	0.43	0	2,2,2	0.34	0
3	GOL	A	603	-	5,5,5	0.64	0	5,5,5	0.40	0
2	FBP	B	601	-	18,20,20	1.05	1 (5%)	21,32,32	1.79	7 (33%)
4	PEG	A	604	-	6,6,6	1.00	0	5,5,5	1.17	0
5	EDO	A	606	-	3,3,3	0.67	0	2,2,2	0.26	0
7	PGE	B	605	-	9,9,9	0.66	0	8,8,8	0.67	0
2	FBP	A	601	-	18,20,20	1.08	2 (11%)	21,32,32	1.85	7 (33%)
3	GOL	B	602	-	5,5,5	1.36	1 (20%)	5,5,5	2.18	3 (60%)
6	FLC	B	603	-	12,12,12	1.43	1 (8%)	17,17,17	1.64	3 (17%)
5	EDO	A	607	-	3,3,3	0.57	0	2,2,2	0.28	0
4	PEG	B	604	-	6,6,6	0.61	0	5,5,5	0.84	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	A	602	-	-	4/4/4/4	-
5	EDO	A	605	-	-	0/1/1/1	-
3	GOL	A	603	-	-	2/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
4	PEG	A	604	-	-	1/4/4/4	-
5	EDO	A	606	-	-	0/1/1/1	-
7	PGE	B	605	-	-	5/7/7/7	-
2	FBP	A	601	-	-	1/13/32/32	0/1/1/1
3	GOL	B	602	-	-	3/4/4/4	-
6	FLC	B	603	-	-	9/16/16/16	-
5	EDO	A	607	-	-	1/1/1/1	-
4	PEG	B	604	-	-	1/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	603	FLC	CB-CBC	2.83	1.56	1.53
2	A	601	FBP	C4-C5	-2.41	1.46	1.53
2	A	601	FBP	P1-O2P	-2.37	1.46	1.54
2	B	601	FBP	O5-C5	2.25	1.48	1.43
3	B	602	GOL	O2-C2	2.20	1.49	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	603	FLC	OB2-CBC-CB	5.19	123.10	113.14
2	B	601	FBP	O6P-P2-O5P	4.06	123.01	107.80
2	A	601	FBP	O3P-P1-O1	-3.41	97.77	106.67
2	A	601	FBP	O5-C5-C6	3.19	117.00	109.50
3	B	602	GOL	O1-C1-C2	3.12	124.43	110.38

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-O2
3	A	602	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	B	602	GOL	C1-C2-C3-O3
3	B	602	GOL	O2-C2-C3-O3

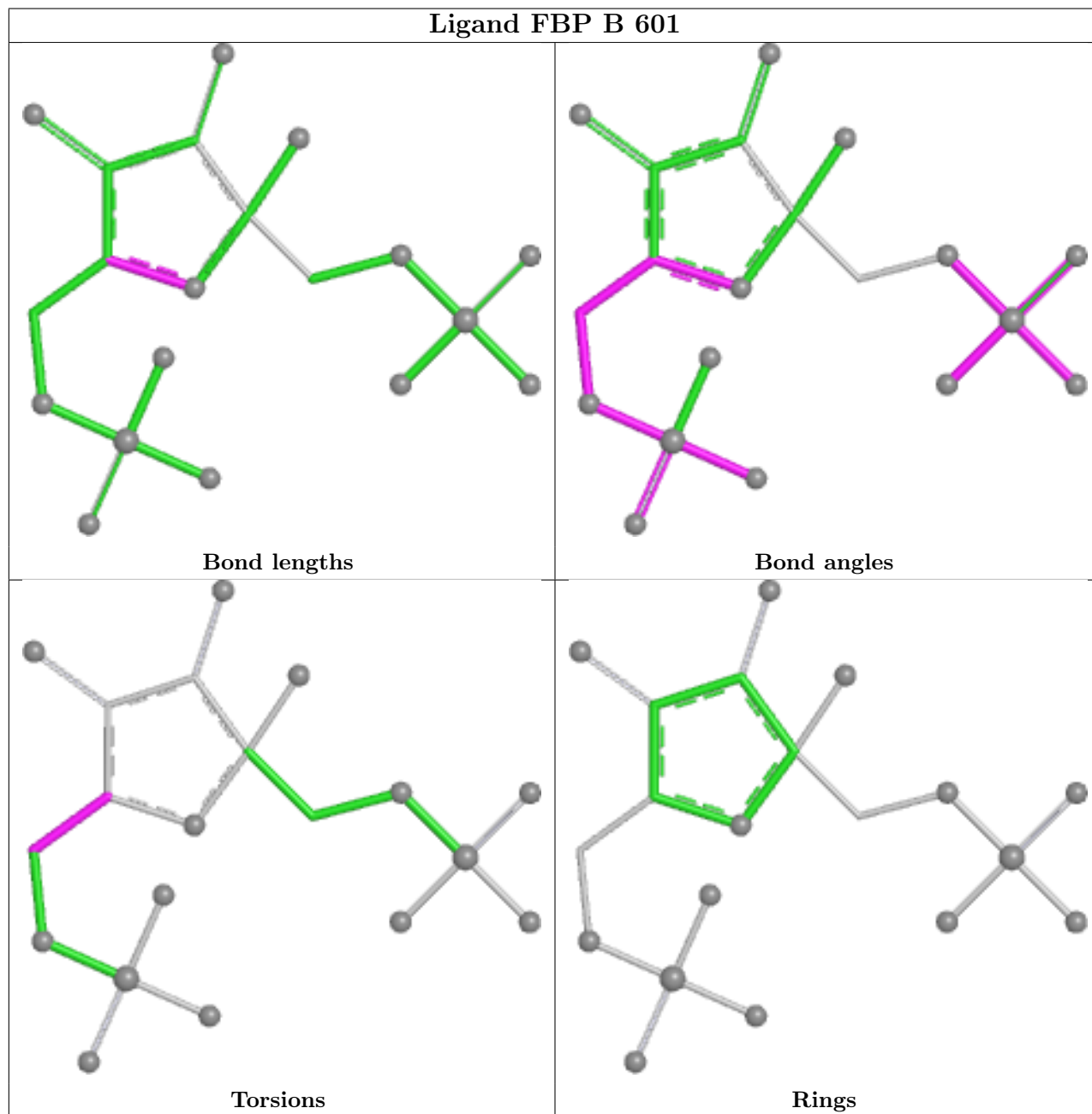
There are no ring outliers.

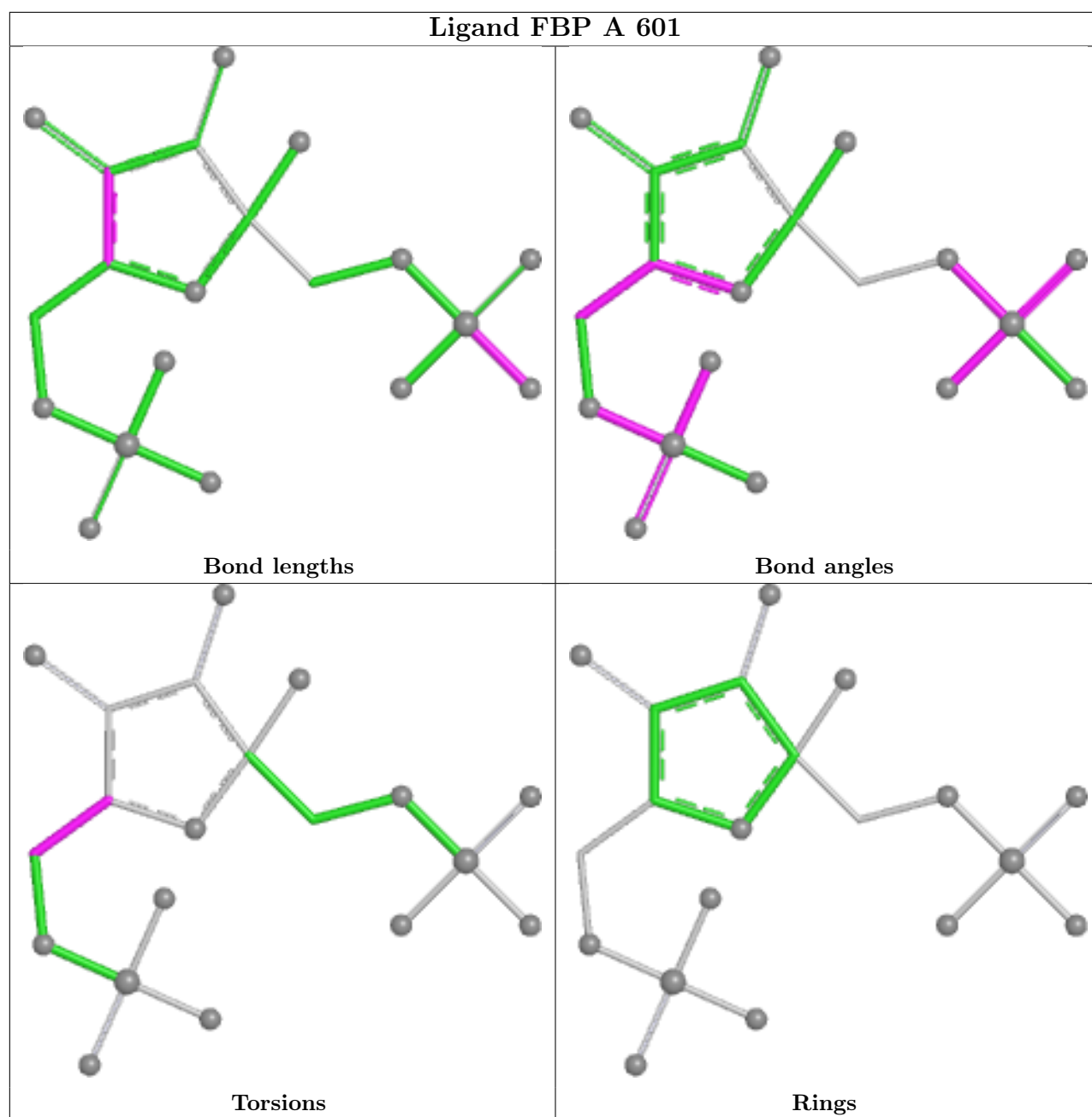
7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	GOL	1	0
4	A	604	PEG	3	0
5	A	606	EDO	1	0
2	A	601	FBP	2	0
3	B	602	GOL	12	0
6	B	603	FLC	2	0
4	B	604	PEG	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	528/550 (96%)	0.28	26 (4%) 35 41	20, 48, 96, 135	2 (0%)
1	B	531/550 (96%)	0.69	57 (10%) 11 13	18, 56, 136, 206	3 (0%)
All	All	1059/1100 (96%)	0.48	83 (7%) 19 21	18, 53, 126, 206	5 (0%)

The worst 5 of 83 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	ILE	5.4
1	B	545	HIS	4.7
1	A	13	VAL	4.6
1	A	136	LEU	4.4
1	B	215	LEU	4.2

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	SEP	B	113	10/11	0.77	0.10	81,88,111,130	0
1	SEP	A	113	10/11	0.93	0.07	57,69,84,84	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands

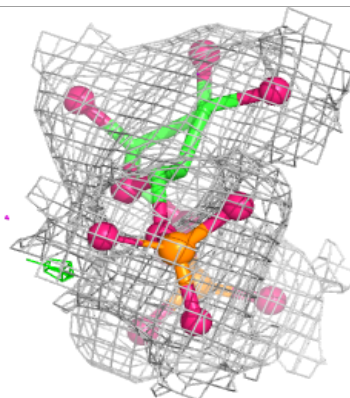
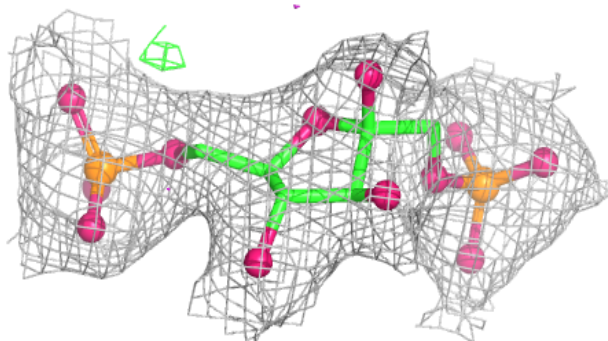
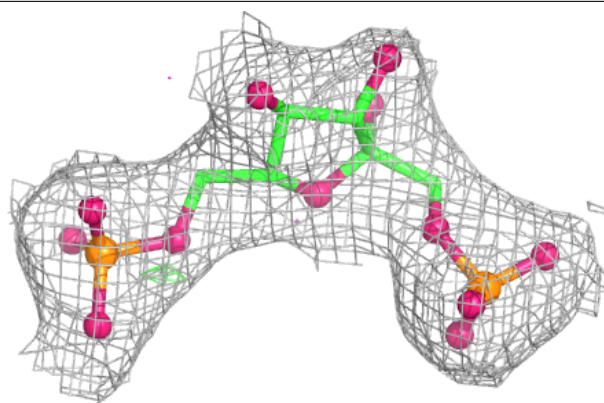
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	EDO	A	606	4/4	0.70	0.24	76,77,81,81	0
5	EDO	A	605	4/4	0.79	0.18	72,79,80,83	0
5	EDO	A	607	4/4	0.83	0.21	68,70,74,80	0
6	FLC	B	603	13/13	0.85	0.13	67,77,84,95	0
4	PEG	B	604	7/7	0.87	0.20	66,75,82,85	0
4	PEG	A	604	7/7	0.88	0.15	62,70,80,83	0
3	GOL	A	602	6/6	0.90	0.16	62,73,74,77	0
3	GOL	A	603	6/6	0.90	0.14	61,70,75,78	0
7	PGE	B	605	10/10	0.90	0.17	67,73,76,77	0
3	GOL	B	602	6/6	0.92	0.11	44,45,52,52	0
2	FBP	A	601	20/20	0.98	0.05	28,33,42,44	0
2	FBP	B	601	20/20	0.98	0.05	30,36,43,43	0

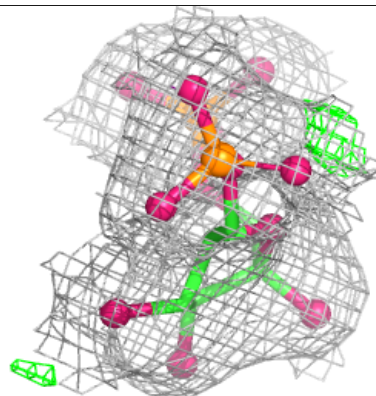
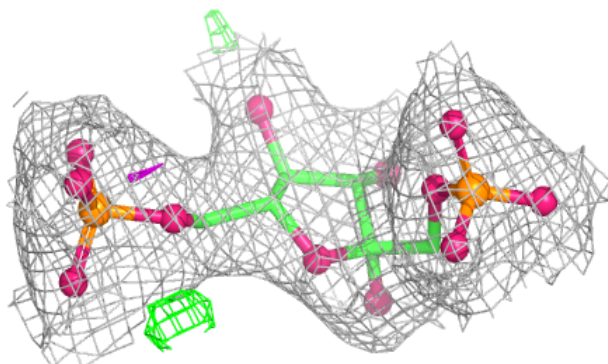
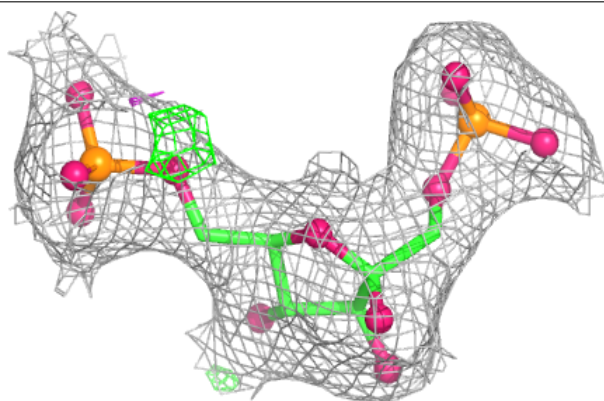
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FBP 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

There are no such residues in this entry.