



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 02:31 AM BST

PDB ID : 1A3W  
Title : PYRUVATE KINASE FROM SACCHAROMYCES CEREVISIAE COM-  
PLEXED WITH FBP, PG, MN2+ AND K+  
Authors : Jurica, M.S.; Mesecar, A.; Heath, P.J.; Shi, W.; Nowak, T.; Stoddard, B.L.  
Deposited on : 1998-01-26  
Resolution : 3.00 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

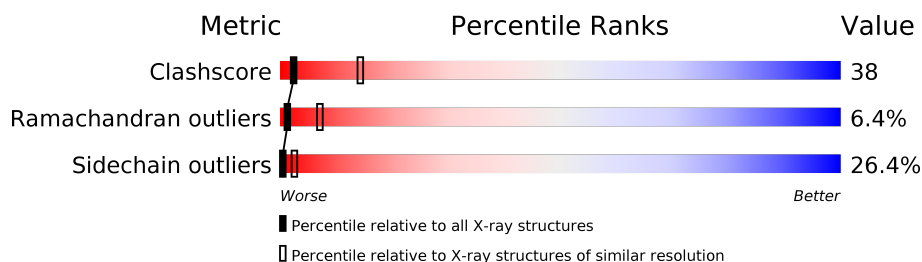
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	

## 2 Entry composition [i](#)

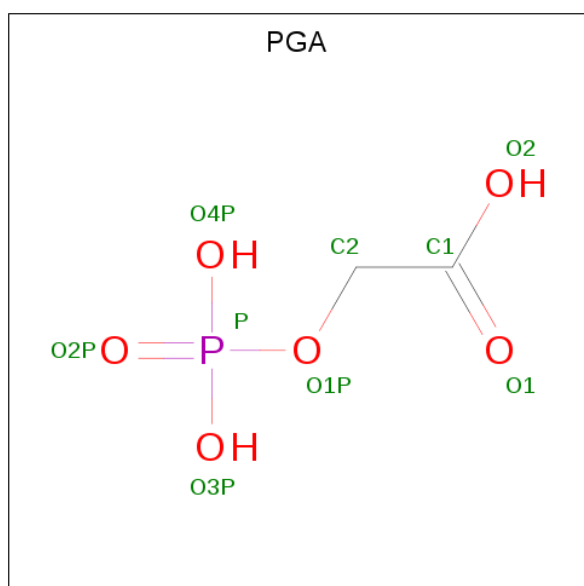
There are 5 unique types of molecules in this entry. The entry contains 7581 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

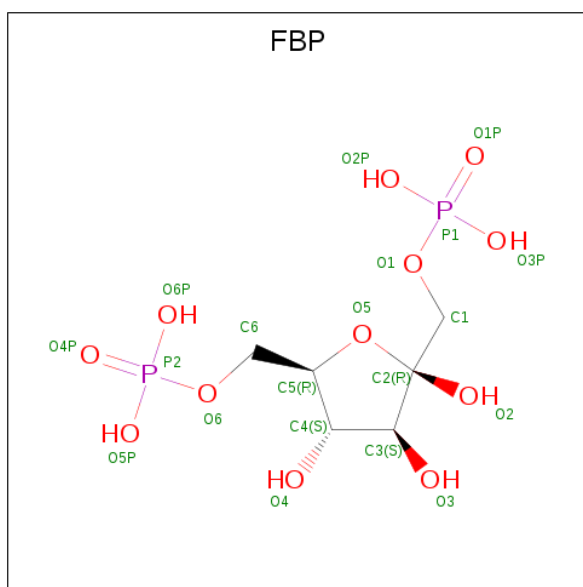
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3773	2380	650	726	17			
1	B	489	Total	C	N	O	S	0	0	0
			3746	2362	647	720	17			

- Molecule 2 is 2-PHOSPHOGLYCOLIC ACID (three-letter code: PGA) (formula:  $C_2H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			9	2	6	1		
2	B	1	Total	C	O	P	0	0
			9	2	6	1		

- Molecule 3 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
3	A	1	Total	C	O	P	0	0
			20	6	12	2		
3	B	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mn	0	0
			1	1		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

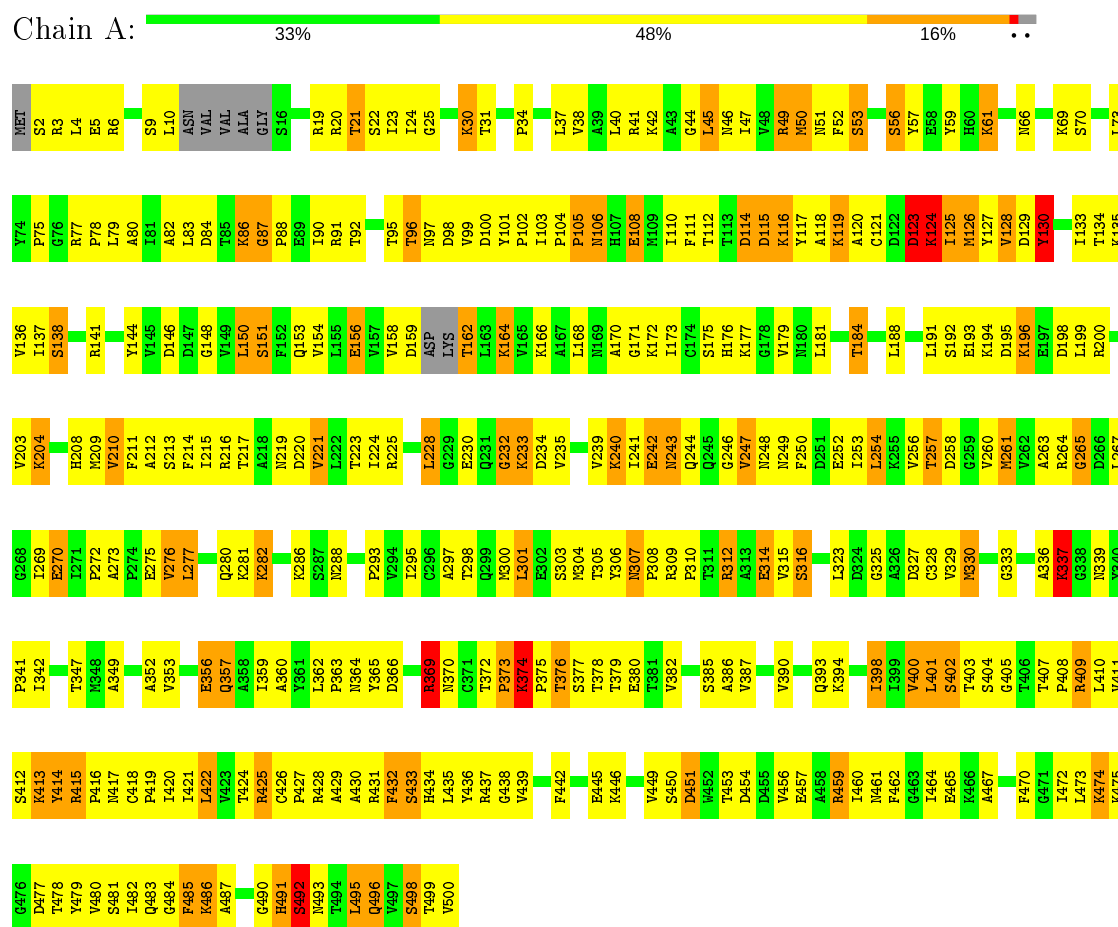
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	K	0	0
			1	1		
5	A	1	Total	K	0	0
			1	1		

### 3 Residue-property plots

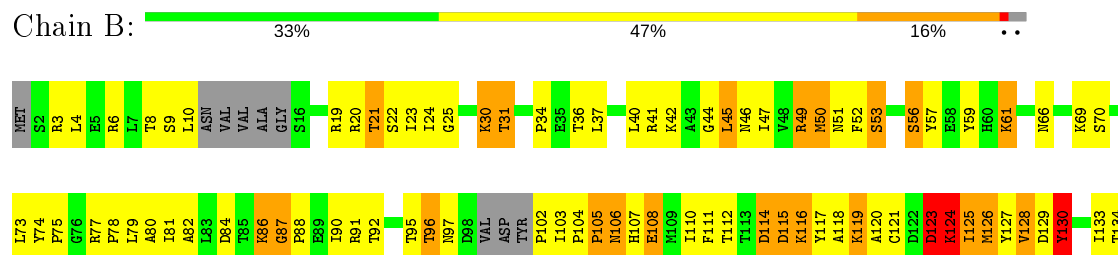
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: PYRUVATE KINASE



#### • Molecule 1: PYRUVATE KINASE



S481	N417	T347	I269	K204	K135
I482	C418	P348	E270	H208	V136
Q483	P419	A349	I271	M209	I137
G484	I420	P272	P272	V210	S138
F485	I421	A352	A273	F211	
K486	I422	V353	P274	A212	R141
A487	V423		E275	S213	
	T424		V276	F214	Y144
G490	R425	E356	L277	I215	V145
H491		Q357		R216	D146
S492	R428	A358		T217	G148
N493	A429	I359	Q280	A218	V149
T494	A430	A360	K281	N219	L150
L495	A431	Y361	K282	D220	S151
Q496	P432	L362		V221	F152
S498	S433	P363		L222	Q153
T499	H434	N364		T223	V154
V500	L435	D366		I224	L155
	Y436			R225	E156
	R437	R369			V157
	G438	N370			D158
	V439	T372			D159
		P373			ASP
	F442	K374			LYS
		P375			T162
	E445	T376			L163
	K446	S377			K164
		T378			V165
V449	S450	T379			K166
D451	D451	E360			A167
I452		T381			L168
T453		V382			R169
D454					A170
D455		S385			G171
V456		A386			K172
E457		V387			I173
A458					G174
R459		Q393			S175
I460		K394			H176
N461					K177
F462		I398			G178
G463		I399			V179
I464		V400			R180
E465		L401			L181
K466		S402			T184
A467		T403			
K468		S404			L191
E469		G405			S192
F470		T406			E193
G471		T407			K194
I472		P408			D195
L473		R409			K196
K474		L410			E197
K475		V411			D198
G476		S412			L199
D477		K413			R200
T478		Y414			
Y479		R415			V203
V480		P416			
					G204
					H208
					M209
					V210
					F211
					A212
					S213
					F214
					I215
					R216
					T217
					G148
					V149
					L150
					S151
					F152
					Q153
					V154
					L155
					E156
					V157
					D158
					D159
					ASP
					LYS
					T162
					L163
					K164
					V165
					K166
					A167
					L168
					R169
					A170
					G171
					K172
					I173
					G174
					S175
					H176
					K177
					G178
					V179
					R180
					L181
					T184
					L191
					S192
					E193
					K194
					D195
					K196
					E197
					D198
					L199
					R200
					G204
					H208
					M209
					V210
					F211
					A212
					S213
					F214
					I215
					R216
					T217
					G148
					V149
					L150
					S151
					F152
					Q153
					V154
					L155
					E156
					V157
					D158
					D159
					ASP
					LYS
					T162
					L163
					K164
					V165
					K166
					A167
					L168
					R169
					A170
					G171
					K172
					I173
					G174
					S175
					H176
					K177
					G178
					V179
					R180
					L181
					T184
					L191
					S192
					E193
					K194
					D195
					K196
					E197
					D198
					L199
					R200
					G204
					H208
					M209
					V210
					F211
					A212
					S213
					F214
					I215
					R216
					T217
					G148
					V149
					L150
					S151
					F152
					Q153
					V154
					L155
					E156
					V157
					D158
					D159
					ASP
					LYS
					T162
					L163
					K164
					V165
					K166
					A167
					L168
					R169
					A170
					G171
					K172
					I173
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					S175
					H176
					K177
					G178
					V179
					R180
					L181
					T184
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					K194
					D195
					K196
					E197
					D198
					L199
					R200
					G204
					H208
					M209
					V210
					F211
					A212
					S213
					F214
					I215
					R216
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					V149
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					L163
					K164
					V165
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					A170
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					K172
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					R180
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					K194
					D195
					K196
					E197
					D198
					L199
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					H208
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					S175
					H176
					K177
					G178
					V179
					R180
					L181
					T184
					L191
					S192
					E193
					K194
					D195

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.40 Å   102.70 Å   110.90 Å 90.00°   112.30°   90.00°	Depositor
Resolution (Å)	100.00 – 3.00	Depositor
% Data completeness (in resolution range)	75.9 (100.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.218 , 0.323	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7581	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

## 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: K, FBP, PGA, MN

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	0.29	0/3834	0.63	7/5196 (0.1%)
1	B	0.31	0/3805	0.65	8/5153 (0.2%)
All	All	0.30	0/7639	0.64	15/10349 (0.1%)

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	369	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	B	369	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	A	369	ARG	NE-CZ-NH2	-10.79	114.91	120.30
1	A	369	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	B	409	ARG	NE-CZ-NH2	-10.42	115.09	120.30

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	3773	0	3844	296	0
1	B	3746	0	3822	298	0
2	A	9	0	2	1	0
2	B	9	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	20	0	10	3	0
3	B	20	0	10	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	7581	0	7690	579	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 38.

The worst 5 of 579 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LYS:H	1:B:375:PRO:HA	1.16	1.11
1:A:374:LYS:H	1:A:375:PRO:HA	1.19	1.05
1:B:398:ILE:HD11	1:B:482:ILE:HD11	1.43	1.01
1:A:242:GLU:HG3	1:A:263:ALA:CB	1.95	0.96
1:B:242:GLU:HG3	1:B:263:ALA:CB	1.97	0.95

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	486/500 (97%)	398 (82%)	56 (12%)	32 (7%)	1	6
1	B	481/500 (96%)	394 (82%)	57 (12%)	30 (6%)	1	8
All	All	967/1000 (97%)	792 (82%)	113 (12%)	62 (6%)	1	7

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	99	VAL
1	A	106	ASN
1	A	170	ALA
1	A	337	LYS

### 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	417/423 (99%)	307 (74%)	110 (26%)	0	2
1	B	414/423 (98%)	305 (74%)	109 (26%)	0	2
All	All	831/846 (98%)	612 (74%)	219 (26%)	0	2

5 of 219 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	451	ASP
1	B	50	MET
1	B	422	LEU
1	A	461	ASN
1	B	4	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	434	HIS
1	B	106	ASN
1	B	434	HIS
1	A	483	GLN
1	B	46	ASN

### 5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	FBP	B	1008	-	18,20,20	1.08	1 (5%)	23,32,32	0.83	0
3	FBP	A	1007	-	18,20,20	1.04	0	23,32,32	0.68	0
2	PGA	A	1005	5,4	5,8,8	2.50	3 (60%)	6,11,11	3.73	3 (50%)
2	PGA	B	1006	5,4	5,8,8	2.44	2 (40%)	6,11,11	3.56	4 (66%)

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	FBP	B	1008	-	-	1/13/32/32	0/1/1/1
3	FBP	A	1007	-	-	2/13/32/32	0/1/1/1
2	PGA	A	1005	5,4	-	0/4/6/6	-
2	PGA	B	1006	5,4	-	1/4/6/6	-

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	PGA	P-O3P	4.16	1.70	1.54
2	A	1005	PGA	P-O3P	4.05	1.70	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1006	PGA	P-O2P	2.56	1.58	1.50
2	A	1005	PGA	P-O2P	2.47	1.58	1.50
3	B	1008	FBP	O5-C2	2.34	1.46	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1005	PGA	O1P-P-O2P	7.74	128.19	106.47
2	B	1006	PGA	O1P-P-O2P	7.30	126.95	106.47
2	B	1006	PGA	O3P-P-O1P	3.09	114.94	106.73
2	A	1005	PGA	O3P-P-O1P	2.97	114.64	106.73
2	A	1005	PGA	O4P-P-O1P	-2.41	100.32	106.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1007	FBP	O5-C5-C6-O6
3	A	1007	FBP	C4-C5-C6-O6
3	B	1008	FBP	C4-C5-C6-O6
2	B	1006	PGA	C2-O1P-P-O3P

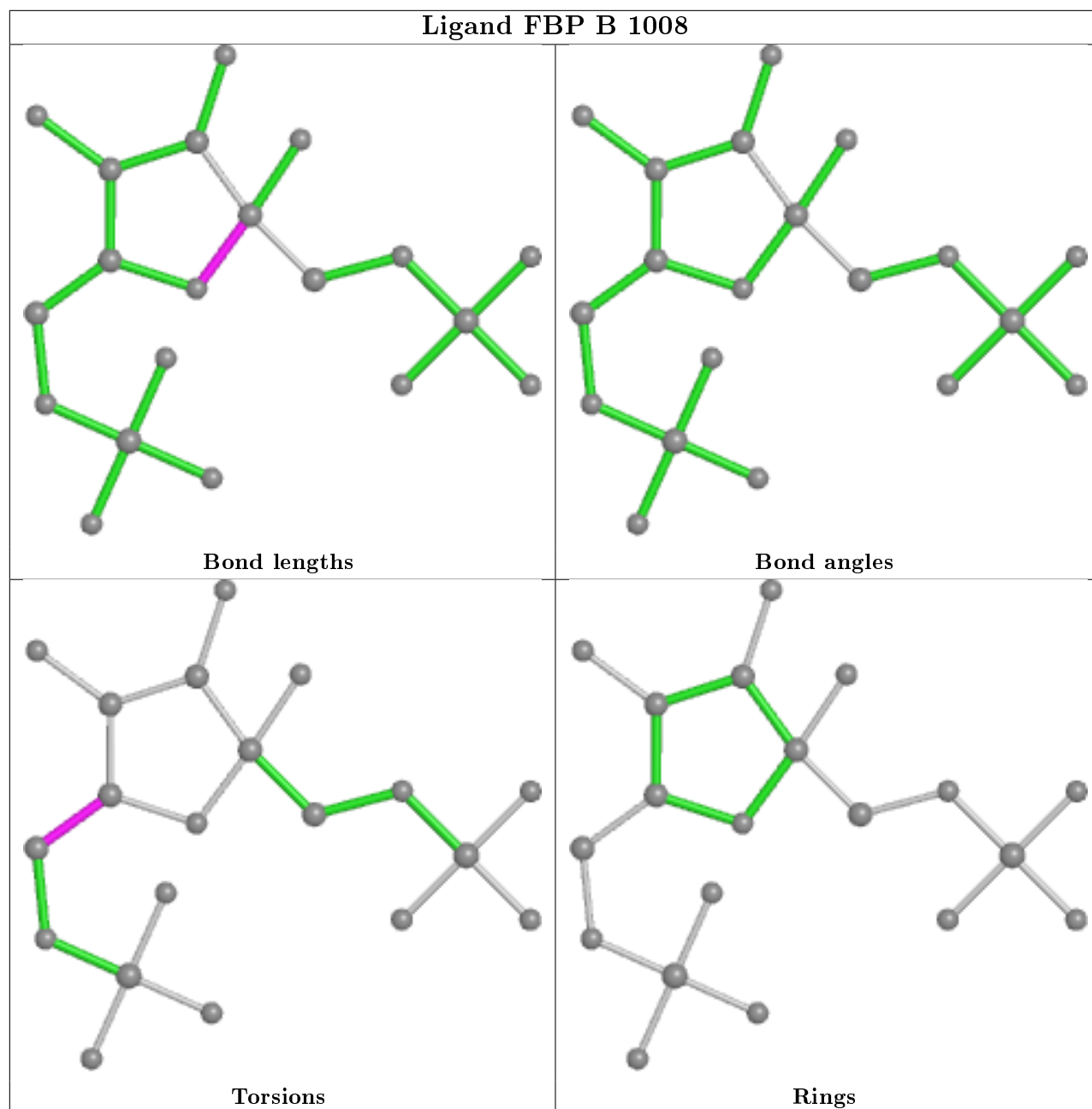
There are no ring outliers.

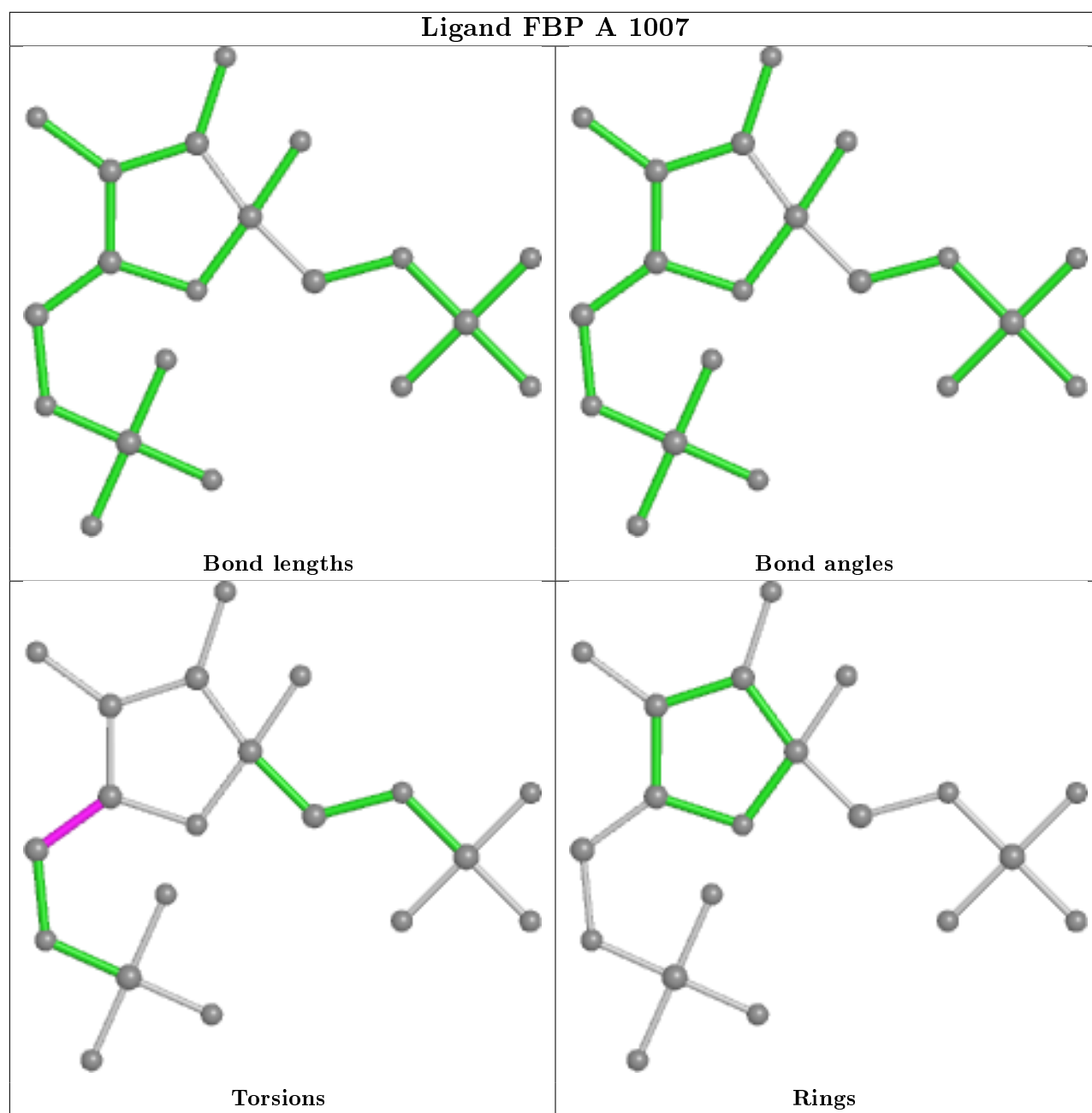
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1008	FBP	2	0
3	A	1007	FBP	3	0
2	A	1005	PGA	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 ⓘ

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.