Full wwPDB X-ray Structure Validation Report ⓘ

Jan 30, 2024 – 08:42 AM EST

PDB ID	:	1FPB
Title	:	CRYSTAL STRUCTURE OF THE NEUTRAL FORM OF FRUCTOSE 1,6-BISPHOSPHATASE COMPLEXED WITH REGULATORY INHIBITOR FRUCTOSE 2,6-BISPHOSPHATE AT 2.6-ANGSTROMS RESOLUTION
Authors	:	Liang, J.Y.; Huang, S.; Zhang, Y.; Ke, H.; Lipscomb, W.N.
Deposited on	:	1992-02-03
Resolution	:	2.60 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:

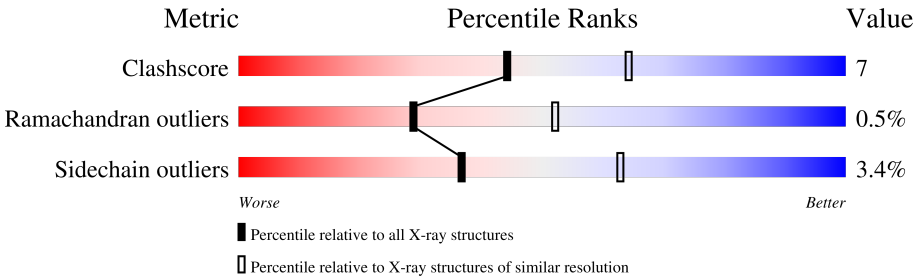
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	73% 19% • 6%
1	B	335	71% 21% •• 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5924 atoms, of which 1066 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.

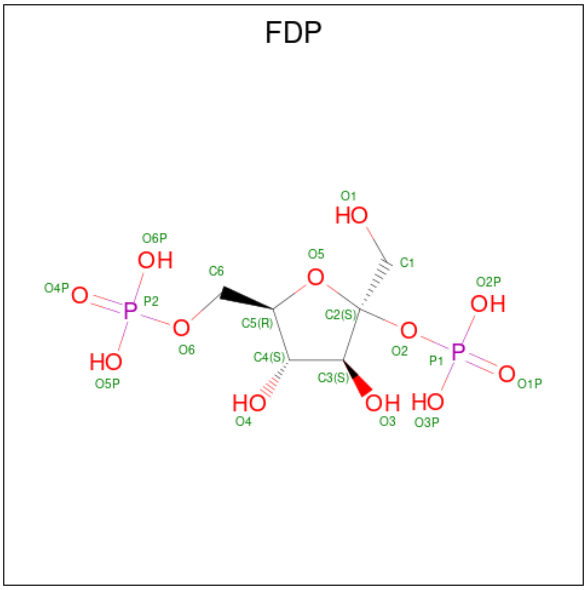
- Molecule 1 is a protein called FRUCTOSE 1,6-BISPHOSPHATASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	314	Total	C	H	N	O	S	0	0	1
			2926	1523	530	404	454	15			
1	B	314	Total	C	H	N	O	S	0	0	1
			2932	1529	530	404	454	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLN	GLU	conflict	UNP P00636
A	96	THR	SER	conflict	UNP P00636
A	199	ASN	ASP	conflict	UNP P00636
B	20	GLN	GLU	conflict	UNP P00636
B	96	THR	SER	conflict	UNP P00636
B	199	ASN	ASP	conflict	UNP P00636

- Molecule 2 is 2,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FDP) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	P	0	0
			22	6	2	12	2		
2	A	1	Total	C	H	O	P	0	0
			22	6	2	12	2		
2	B	1	Total	C	H	O	P	0	0
			22	6	2	12	2		

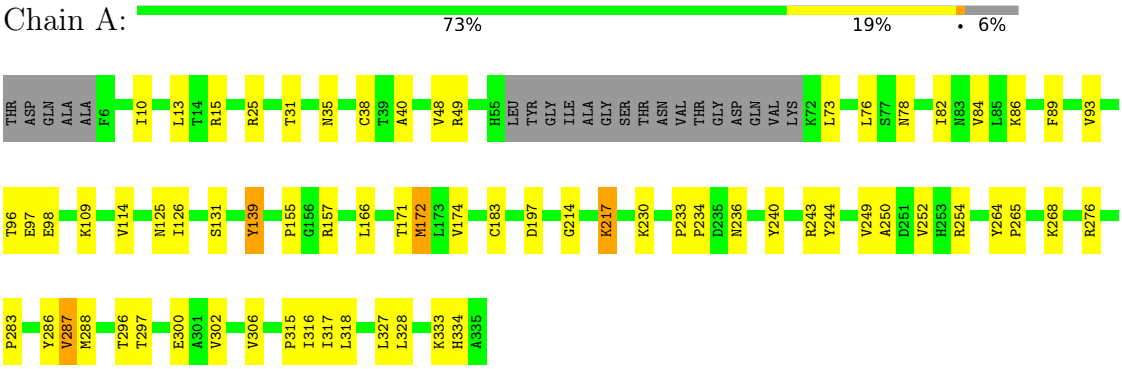
3 Residue-property plots (i)

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. 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.

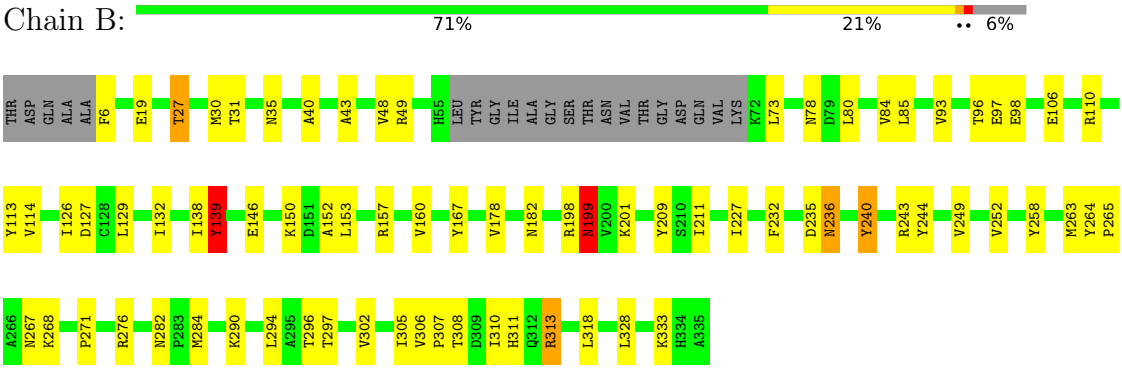
• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain A:



• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATASE

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	131.40Å 131.40Å 68.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5924	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FDP

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	0.69	0/2435	1.29	12/3293 (0.4%)
1	B	0.67	0/2442	1.37	16/3302 (0.5%)
All	All	0.68	0/4877	1.33	28/6595 (0.4%)

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	5
All	All	0	8

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	240	TYR	CB-CG-CD2	-8.75	115.75	121.00
1	B	313	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	B	243	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	217	LYS	CA-CB-CG	7.54	129.99	113.40
1	B	313	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	B	333	LYS	CA-CB-CG	6.83	128.42	113.40
1	A	48	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	B	249	VAL	CG1-CB-CG2	-6.44	100.60	110.90
1	B	263	MET	CA-CB-CG	6.39	124.17	113.30
1	A	15	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	157	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	27	THR	CA-C-N	-6.36	103.49	116.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	49	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	49	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	139	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	A	244	TYR	CB-CG-CD1	-5.86	117.48	121.00
1	B	236	ASN	CA-C-N	-5.74	104.58	117.20
1	B	27	THR	N-CA-C	5.54	125.96	111.00
1	A	172	MET	CA-CB-CG	5.43	122.54	113.30
1	A	139	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	48	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	A	157	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	209	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	A	287	VAL	CG1-CB-CG2	-5.17	102.63	110.90
1	A	76	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	333	LYS	CB-CG-CD	-5.15	98.20	111.60
1	A	243	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	286	TYR	CB-CG-CD1	-5.03	117.98	121.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	240	TYR	Sidechain
1	A	264	TYR	Sidechain
1	B	139	TYR	Sidechain
1	B	167	TYR	Sidechain
1	B	244	TYR	Sidechain
1	B	258	TYR	Sidechain
1	B	264	TYR	Sidechain

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	2396	530	2450	31	0
1	B	2402	530	2457	37	0
2	A	40	4	20	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	2	10	0	0
All	All	4858	1066	4937	65	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 7.

All (65) 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:78:ASN:OD1	1:B:96:THR:HG21	1.82	0.79
1:B:182:ASN:HD22	1:B:198:ARG:HA	1.50	0.77
1:A:96:THR:HG22	1:A:98:GLU:H	1.53	0.72
1:B:126:ILE:HG12	1:B:132:ILE:HD13	1.73	0.69
1:B:182:ASN:ND2	1:B:198:ARG:HA	2.09	0.68
1:A:217:LYS:HB3	1:B:232:PHE:CE1	2.33	0.64
1:A:155:PRO:HG3	1:A:306:VAL:HG22	1.79	0.62
1:B:294:LEU:O	1:B:318:LEU:HA	1.99	0.62
1:A:297:THR:HB	1:A:315:PRO:HG2	1.82	0.61
1:B:43:ALA:HB3	1:B:80:LEU:HD21	1.82	0.60
1:A:73:LEU:HD23	1:A:126:ILE:HD13	1.83	0.60
1:A:31:THR:O	1:A:35:ASN:HB2	2.04	0.58
1:B:40:ALA:HB2	1:B:84:VAL:HG21	1.86	0.58
1:A:166:LEU:HD13	1:A:249:VAL:HG12	1.86	0.58
1:B:31:THR:O	1:B:35:ASN:HB2	2.04	0.57
1:B:282:ASN:ND2	1:B:302:VAL:HG12	2.19	0.56
1:A:166:LEU:HD23	1:B:129:LEU:HD12	1.87	0.55
1:A:13:LEU:HD22	1:A:38:CYS:SG	2.48	0.54
1:B:138:ILE:O	1:B:160:VAL:HG22	2.09	0.53
1:B:297:THR:HG21	1:B:305:ILE:HD11	1.91	0.53
1:B:114:VAL:HG11	1:B:152:ALA:HA	1.90	0.52
1:B:252:VAL:HG11	1:B:284:MET:SD	2.49	0.52
1:B:96:THR:HG22	1:B:98:GLU:H	1.74	0.52
1:B:178:VAL:HA	1:B:290:LYS:HE2	1.92	0.52
1:A:78:ASN:OD1	1:A:96:THR:HG21	2.11	0.50
1:B:150:LYS:HD3	1:B:153:LEU:HD12	1.94	0.49
1:A:296:THR:HG21	1:A:328:LEU:HD21	1.94	0.48
1:B:182:ASN:HD21	1:B:198:ARG:HG2	1.79	0.48
1:A:252:VAL:HG22	1:A:318:LEU:HD11	1.96	0.47
1:B:310:ILE:HG13	1:B:311:HIS:CD2	2.49	0.47
1:A:283:PRO:O	1:A:287:VAL:HG23	2.15	0.46
1:A:96:THR:HG22	1:A:97:GLU:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG21	1:A:316:ILE:HD13	1.97	0.46
1:A:93:VAL:HB	1:A:114:VAL:HG13	1.97	0.46
1:B:96:THR:HG22	1:B:97:GLU:N	2.30	0.46
1:B:182:ASN:HD21	1:B:199:ASN:H	1.64	0.46
1:B:276:ARG:HD3	1:B:313:ARG:HG2	1.96	0.46
1:A:288:MET:HG3	1:A:318:LEU:HB2	1.97	0.45
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.98	0.45
1:B:114:VAL:HB	1:B:139:TYR:HB2	1.98	0.44
1:A:82:ILE:O	1:A:86:LYS:HG3	2.18	0.44
1:B:211:ILE:HD13	1:B:227:ILE:HD11	1.99	0.44
1:B:267:ASN:O	1:B:271:PRO:HA	2.17	0.44
1:A:166:LEU:O	1:A:171:THR:HA	2.18	0.43
1:B:306:VAL:HA	1:B:307:PRO:HD3	1.79	0.43
1:B:27:THR:HB	1:B:30:MET:H	1.83	0.43
1:A:40:ALA:HB2	1:A:84:VAL:HG21	2.00	0.43
1:A:317:ILE:HG21	1:A:327:LEU:HD23	2.00	0.43
1:A:288:MET:HE2	1:A:288:MET:HB3	1.83	0.42
1:A:131:SER:HB2	1:A:250:ALA:HB2	1.99	0.42
1:A:172:MET:SD	1:A:183:CYS:HB3	2.59	0.42
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.84	0.42
1:A:233:PRO:HA	1:A:234:PRO:HD2	1.76	0.42
1:B:296:THR:HG21	1:B:328:LEU:HD21	2.00	0.42
1:B:27:THR:HG21	1:B:113:TYR:OH	2.20	0.41
1:B:182:ASN:ND2	1:B:199:ASN:H	2.17	0.41
1:B:93:VAL:HB	1:B:114:VAL:HG22	2.02	0.41
1:A:13:LEU:CD2	1:A:38:CYS:SG	3.08	0.41
1:A:214:GLY:HA3	1:B:240:TYR:O	2.21	0.41
1:B:199:ASN:HD22	1:B:201:LYS:HZ3	1.68	0.41
1:A:174:VAL:HG22	1:A:183:CYS:SG	2.60	0.41
1:A:333:LYS:HG3	1:A:334:HIS:N	2.35	0.41
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.79	0.41
1:A:254:ARG:HH11	1:A:254:ARG:HD3	1.78	0.40
1:B:106:GLU:O	1:B:110:ARG:HG3	2.21	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	310/335 (92%)	298 (96%)	11 (4%)	1 (0%)	41 64
1	B	310/335 (92%)	289 (93%)	19 (6%)	2 (1%)	25 47
All	All	620/670 (92%)	587 (95%)	30 (5%)	3 (0%)	29 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	B	236	ASN
1	B	199	ASN

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	261/278 (94%)	252 (97%)	9 (3%)	37 63
1	B	262/278 (94%)	253 (97%)	9 (3%)	37 63
All	All	523/556 (94%)	505 (97%)	18 (3%)	37 63

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	25	ARG
1	A	125	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	197	ASP
1	A	230	LYS
1	A	265	PRO
1	A	268	LYS
1	A	276	ARG
1	A	300	GLU
1	B	6	PHE
1	B	19	GLU
1	B	127	ASP
1	B	146	GLU
1	B	199	ASN
1	B	235	ASP
1	B	265	PRO
1	B	268	LYS
1	B	308	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	154	GLN
1	A	158	ASN
1	A	182	ASN
1	A	282	ASN
1	B	154	GLN
1	B	182	ASN
1	B	199	ASN
1	B	267	ASN
1	B	282	ASN
1	B	334	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	FDP	B	336	-	19,20,20	0.49	0	30,32,32	1.04	2 (6%)
2	FDP	A	336	-	19,20,20	0.51	0	30,32,32	0.84	0
2	FDP	A	337	-	19,20,20	0.61	0	30,32,32	0.93	1 (3%)

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	FDP	B	336	-	-	5/12/34/34	0/1/1/1
2	FDP	A	336	-	-	7/12/34/34	0/1/1/1
2	FDP	A	337	-	-	5/12/34/34	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	337	FDP	O5-C2-C1	2.19	113.36	108.03
2	B	336	FDP	O5P-P2-O6	2.10	112.31	106.73
2	B	336	FDP	O3P-P1-O2	2.01	114.99	105.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

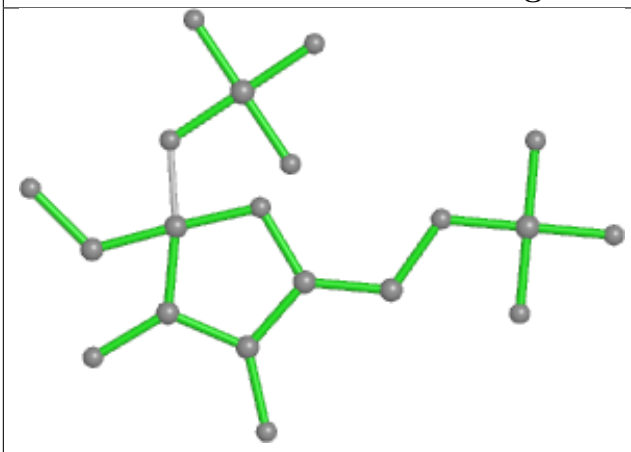
Mol	Chain	Res	Type	Atoms
2	A	336	FDP	C6-O6-P2-O6P
2	A	337	FDP	C6-O6-P2-O4P
2	A	337	FDP	C6-O6-P2-O5P
2	A	337	FDP	C6-O6-P2-O6P
2	B	336	FDP	C6-O6-P2-O4P
2	B	336	FDP	C6-O6-P2-O5P
2	B	336	FDP	C6-O6-P2-O6P
2	A	336	FDP	O1-C1-C2-O5
2	B	336	FDP	C4-C5-C6-O6
2	B	336	FDP	O5-C5-C6-O6
2	A	336	FDP	C6-O6-P2-O4P
2	A	336	FDP	O1-C1-C2-C3
2	A	336	FDP	O1-C1-C2-O2
2	A	336	FDP	C6-O6-P2-O5P
2	A	337	FDP	O5-C5-C6-O6
2	A	336	FDP	C2-O2-P1-O3P
2	A	337	FDP	C2-O2-P1-O2P

There are no ring outliers.

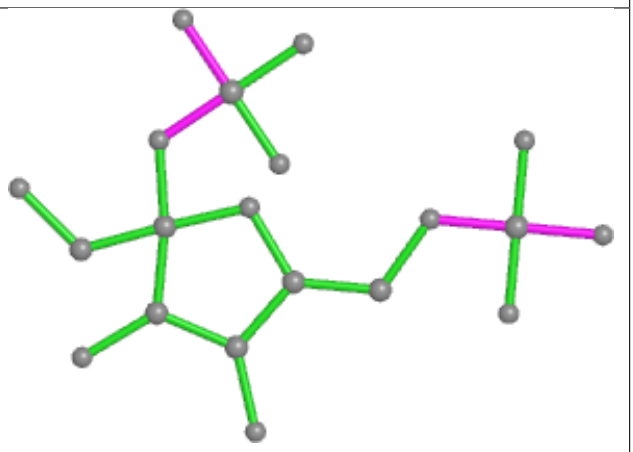
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

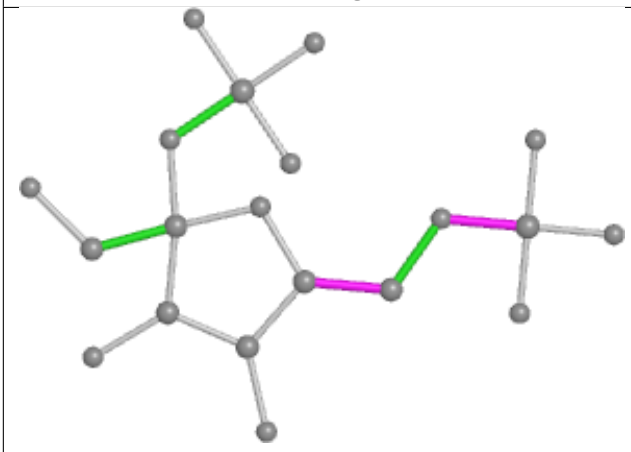
Ligand FDP B 336



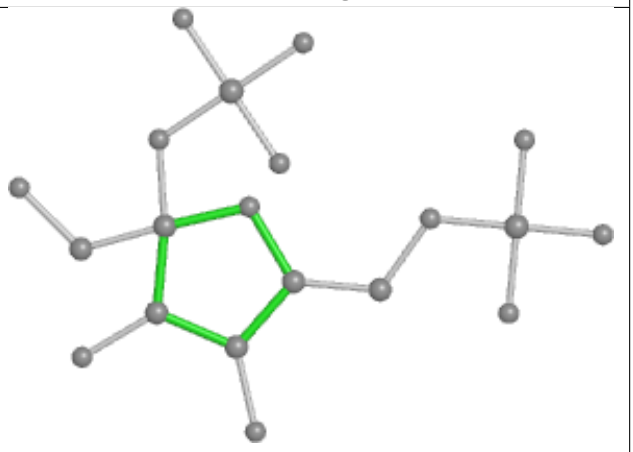
Bond lengths



Bond angles

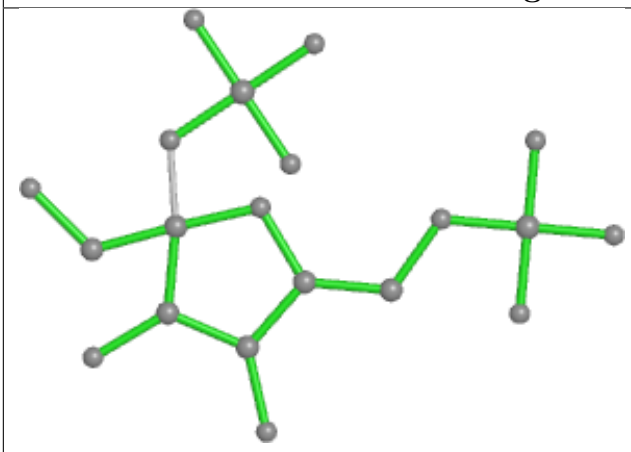


Torsions

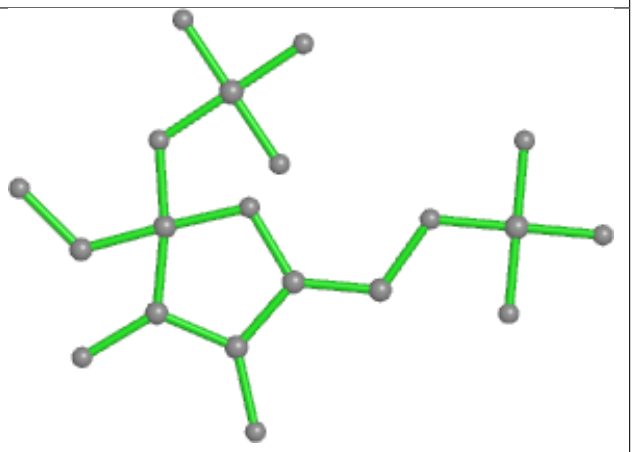


Rings

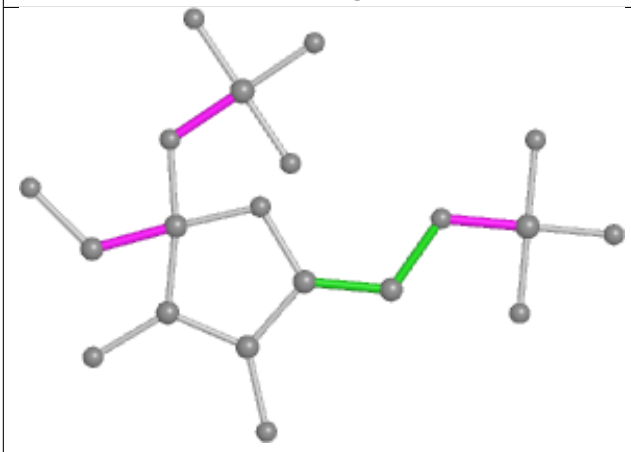
Ligand FDP A 336



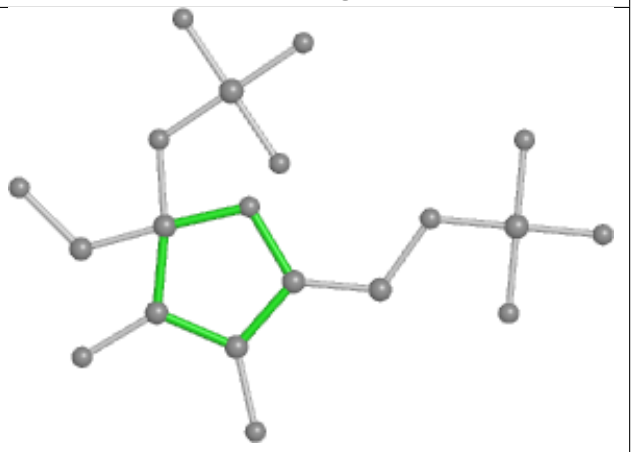
Bond lengths



Bond angles

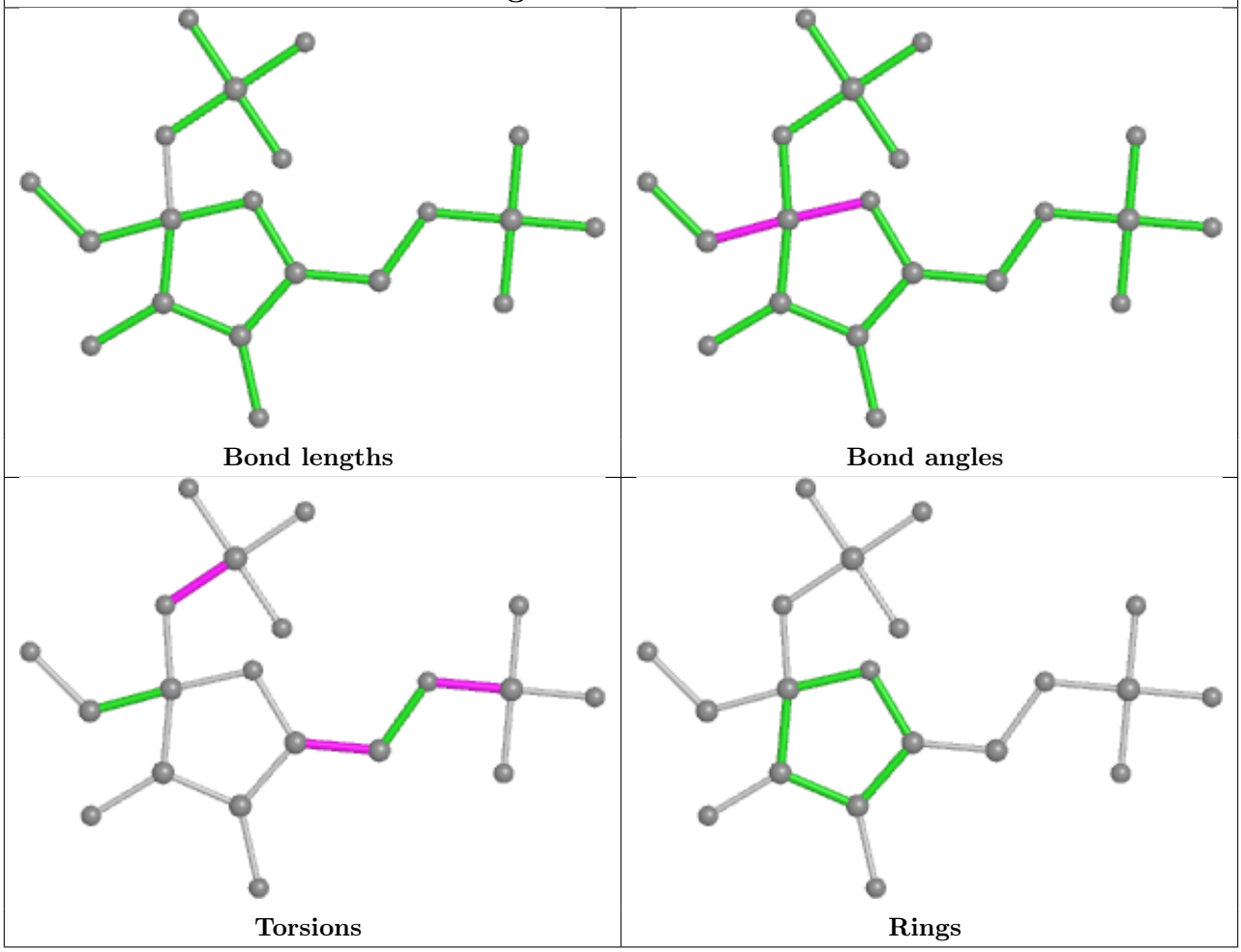


Torsions



Rings

Ligand FDP A 337



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.