WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Jun 12, 2024 – 11:02 PM EDT

PDB ID	:	1FDJ
Title	:	FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE FROM RABBIT LIVER
Authors	:	Blom, N.S.; White, A.; Sygusch, J.
Deposited on	:	2000-07-20
Resolution	:	2.10 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

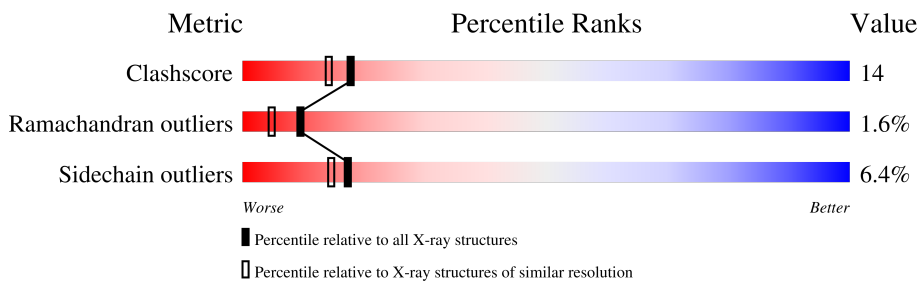|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.10 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		1.6%
Sidechain outliers		6.4%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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	363	76% 21% •
1	B	363	78% 19% ••
1	C	363	78% 19% •
1	D	363	76% 20% ••

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	2FP	A	5001	X	-	-	-
3	2FP	B	6001	X	-	-	-
4	13P	C	7001	-	-	X	-
4	13P	D	8002[A]	-	-	X	-
5	G3P	B	6003	X	-	-	-

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 15089 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 FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total 2820	C 1766	N 506	O 535	S 13	0	6	0
1	B	363	Total 2918	C 1834	N 517	O 554	S 13	0	18	0
1	C	363	Total 2914	C 1827	N 524	O 550	S 13	0	17	0
1	D	363	Total 2850	C 1787	N 506	O 544	S 13	0	9	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1051	SER	THR	CONFLICT	UNP P79226
B	2051	SER	THR	CONFLICT	UNP P79226
C	3051	SER	THR	CONFLICT	UNP P79226
D	4051	SER	THR	CONFLICT	UNP P79226

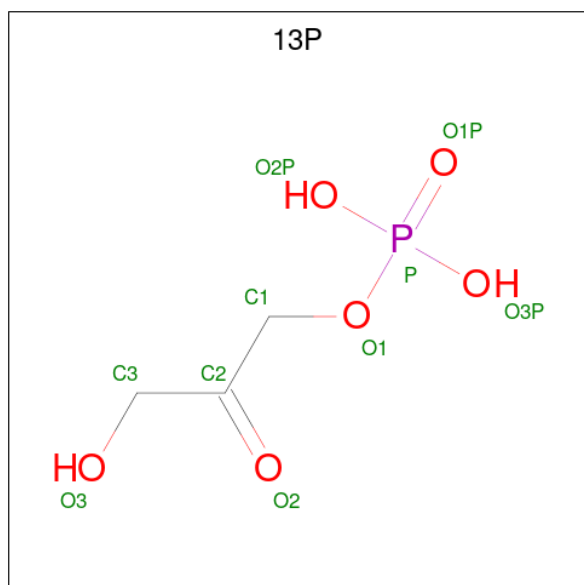- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

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

- Molecule 3 is 1,6-FRUCTOSE DIPHOSPHATE (LINEAR FORM) (three-letter code: 2FP) (formula: $C_6H_{14}O_{12}P_2$).

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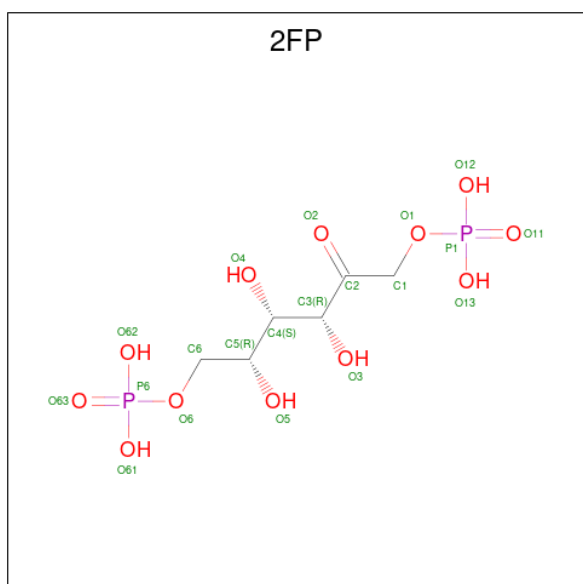
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 20	C 6	O 12	P 2	0	0
3	B	1	Total 20	C 6	O 12	P 2	0	0

- Molecule 4 is 1,3-DIHYDROXYACETONEPHOSPHATE (three-letter code: 13P) (formula: $C_3H_7O_6P$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 10	C 3	O 6	P 1	0	0
4	C	1	Total 10	C 3	O 6	P 1	0	0
4	D	1	Total 10	C 3	O 6	P 1	0	1
4	D	1	Total 10	C 3	O 6	P 1	0	1

- Molecule 5 is SN-GLYCEROL-3-PHOSPHATE (three-letter code: G3P) (formula: $C_3H_9O_6P$).

G3P
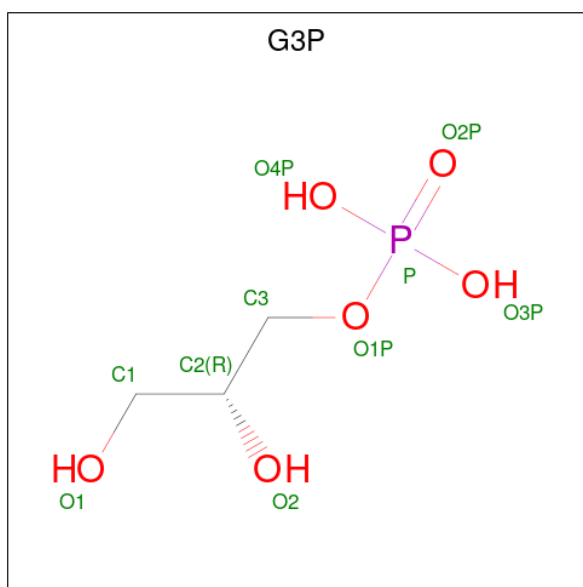
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 10	C 3	O 6	P 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	775	Total 775	O 775	0	0
6	B	858	Total 858	O 858	0	0
6	C	917	Total 917	O 917	0	0
6	D	927	Total 927	O 927	0	0

3 Residue-property plots ⓘ

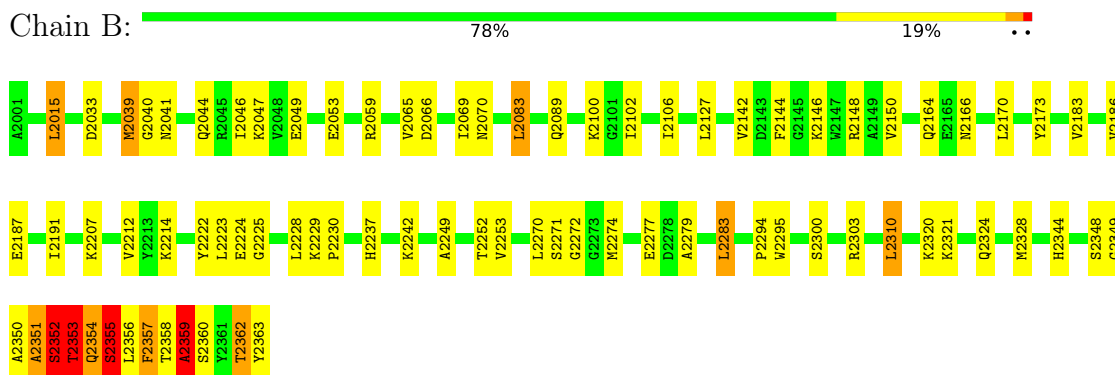These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.
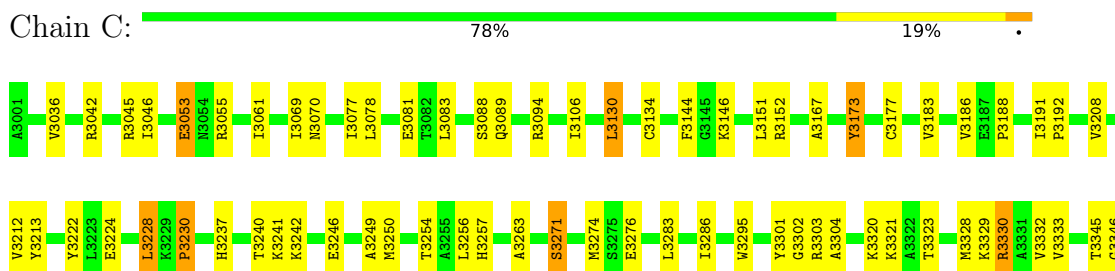
Note EDS was not executed.

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain A:

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain B:

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain C:

G3349 A3350 A3351 S3352 T3353 Q3354 S3355 L3356 F3357 T3358 A3359 S3360 Y3361 T3362 Y3363

• Molecule 1: FRUCTOSE 1,6-BISPHOSPHATE ALDOLASE

Chain D:

76%
20%

A4001 L4007 I4018 R4021 I4022 L4030 E4034 T4038 M4039 G4040 N4041 R4042 L4043 Q4044 R4045 I4046 K4047 D4066 N4067 S4068 I4069 N4070 Q4071 S4072 I4073 V4076 F4079 H4080 E4081 T4082 E4099 K4100 G4101 I4102 I4106 K4107 L4108 K4120 I4124 L4127 L4130 S4131 Q4136

V4142 R4148 A4149 V4150 L4151 R4152 Q4156 L4161 N4168 R4172 Y4173 C4177 V4186 E4187 P4188 I4191 Q4202 Y4203 V4204 T4205 E4206 K4207 V4208 K4214 H4219 L4228 K4229 P4230 V4233 H4237 K4241 K4242 T4254 R4258 V4264 P4265 C4268 S4271 T4280

L4281 W4295 K4296 L4297 Y4301 G4302 R4303 A4304 L4310 V4333 A4350 A4351 S4352 T4353 Q4354 S4355 L4356 F4357 S4360 Y4361 T4362 Y4363

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	377.25Å 130.54Å 80.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10	Depositor
% Data completeness (in resolution range)	8.0 (12.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.171 , 0.214	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15089	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: 2FP, 13P, G3P, SO4

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	0.35	0/2869	0.64	0/3880
1	B	0.44	1/2973 (0.0%)	0.73	7/4023 (0.2%)
1	C	0.33	0/2966	0.62	0/4010
1	D	0.41	0/2900	0.69	2/3922 (0.1%)
All	All	0.38	1/11708 (0.0%)	0.67	9/15835 (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	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	2352	SER	N-CA	-6.02	1.34	1.46

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	2353	THR	N-CA-C	7.00	129.89	111.00
1	B	2352	SER	CA-C-N	-6.77	102.30	117.20
1	B	2354	GLN	N-CA-C	-6.73	92.84	111.00
1	B	2353	THR	CA-C-N	-6.60	102.68	117.20
1	D	4042[A]	ARG	NE-CZ-NH2	6.33	123.46	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1213	TYR	Sidechain
1	B	2353	THR	Mainchain

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	2820	0	2831	60	0
1	B	2918	0	2912	89	0
1	C	2914	0	2928	68	0
1	D	2850	0	2853	92	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	10	2	0
3	B	20	0	8	5	0
4	B	10	0	1	1	0
4	C	10	0	5	6	0
4	D	20	0	10	7	0
5	B	10	0	4	3	0
6	A	775	0	0	12	0
6	B	858	0	0	33	0
6	C	917	0	0	24	0
6	D	927	0	0	32	0
All	All	15089	0	11562	315	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 14.

The worst 5 of 315 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:D:4363[B]:TYR:CD2	6:D:8916:HOH:O	1.72	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4042[A]:ARG:HH11	1:D:4042[A]:ARG:HG3	0.97	1.10
1:D:4363[B]:TYR:OH	6:D:8918:HOH:O	1.74	1.04
1:D:4042[A]:ARG:HG3	1:D:4042[A]:ARG:NH1	1.74	0.98
1:D:4363[B]:TYR:CE1	6:D:8917:HOH:O	2.16	0.98

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	367/363 (101%)	337 (92%)	22 (6%)	8 (2%)	6	2
1	B	379/363 (104%)	352 (93%)	20 (5%)	7 (2%)	8	4
1	C	378/363 (104%)	356 (94%)	17 (4%)	5 (1%)	12	7
1	D	369/363 (102%)	343 (93%)	22 (6%)	4 (1%)	14	9
All	All	1493/1452 (103%)	1388 (93%)	81 (5%)	24 (2%)	9	5

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1344	HIS
1	A	1353	THR
1	A	1361	TYR
1	B	2357	PHE
1	B	2359	ALA

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	297/293 (101%)	280 (94%)	17 (6%)	20	18
1	B	307/293 (105%)	293 (95%)	14 (5%)	27	26
1	C	307/293 (105%)	287 (94%)	20 (6%)	17	14
1	D	301/293 (103%)	273 (91%)	28 (9%)	9	6
All	All	1212/1172 (103%)	1133 (94%)	79 (6%)	17	14

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4070	ASN
1	D	4242	LYS
1	D	4108	LEU
1	D	4152	ARG
1	D	4333	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2354	GLN
1	D	4070	ASN
1	C	3089	GLN
1	D	4095	ASN
1	A	1202	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 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	2FP	B	6001	5,1,4	18,19,19	1.05	1 (5%)	21,28,28	2.05	9 (42%)
5	G3P	B	6003	3	9,9,9	2.08	2 (22%)	11,12,12	1.14	1 (9%)
2	SO4	C	7000	-	4,4,4	0.54	0	6,6,6	0.25	0
4	13P	D	8002[A]	-	9,9,9	1.06	1 (11%)	10,12,12	1.46	2 (20%)
3	2FP	A	5001	-	18,19,19	1.18	2 (11%)	21,28,28	1.56	6 (28%)
4	13P	C	7001	-	9,9,9	1.14	1 (11%)	10,12,12	1.51	2 (20%)
4	13P	B	6002	3	9,9,9	1.09	1 (11%)	10,12,12	1.21	1 (10%)
4	13P	D	8001[B]	-	9,9,9	1.13	1 (11%)	10,12,12	1.41	2 (20%)
2	SO4	A	5000	-	4,4,4	0.45	0	6,6,6	0.15	0
2	SO4	D	8000	-	4,4,4	0.65	0	6,6,6	0.25	0
2	SO4	B	6000	-	4,4,4	0.59	0	6,6,6	0.28	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	2FP	B	6001	5,1,4	2/2/6/6	16/24/24/24	-
5	G3P	B	6003	3	1/1/2/2	4/8/8/8	-
3	2FP	A	5001	-	2/2/6/6	15/24/24/24	-
4	13P	C	7001	-	-	2/7/8/8	-
4	13P	B	6002	3	-	2/7/8/8	-
4	13P	D	8001[B]	-	-	6/7/8/8	-
4	13P	D	8002[A]	-	-	7/7/8/8	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	6003	G3P	O1-C1	-4.95	1.21	1.42
5	B	6003	G3P	P-O2P	2.94	1.60	1.50
4	D	8001[B]	13P	P-O1P	2.80	1.59	1.50
4	B	6002	13P	P-O1P	2.50	1.58	1.50
3	A	5001	2FP	O2-C2	2.47	1.25	1.21

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6001	2FP	O13-P1-O1	3.87	117.04	106.73
3	B	6001	2FP	O12-P1-O11	-3.85	95.59	110.68
3	B	6001	2FP	O6-P6-O63	3.39	115.98	106.47
5	B	6003	G3P	O1-C1-C2	3.22	125.63	110.20
3	A	5001	2FP	O4-C4-C3	3.08	114.82	109.21

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	5001	2FP	C4
3	A	5001	2FP	C3
3	B	6001	2FP	C4
3	B	6001	2FP	C3
5	B	6003	G3P	C2

5 of 52 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	5001	2FP	O5-C5-C6-O6
3	A	5001	2FP	C4-C5-C6-O6
3	A	5001	2FP	O4-C4-C5-C6
3	A	5001	2FP	O4-C4-C5-O5
3	A	5001	2FP	C3-C4-C5-O5

There are no ring outliers.

7 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6001	2FP	5	0
5	B	6003	G3P	3	0
4	D	8002[A]	13P	5	0
3	A	5001	2FP	2	0
4	C	7001	13P	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	6002	13P	1	0
4	D	8001[B]	13P	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 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 2FP B 6001

Bond lengths

Bond angles

Torsions

Rings

Ligand 2FP A 5001

Bond lengths

Bond angles

Torsions

Rings
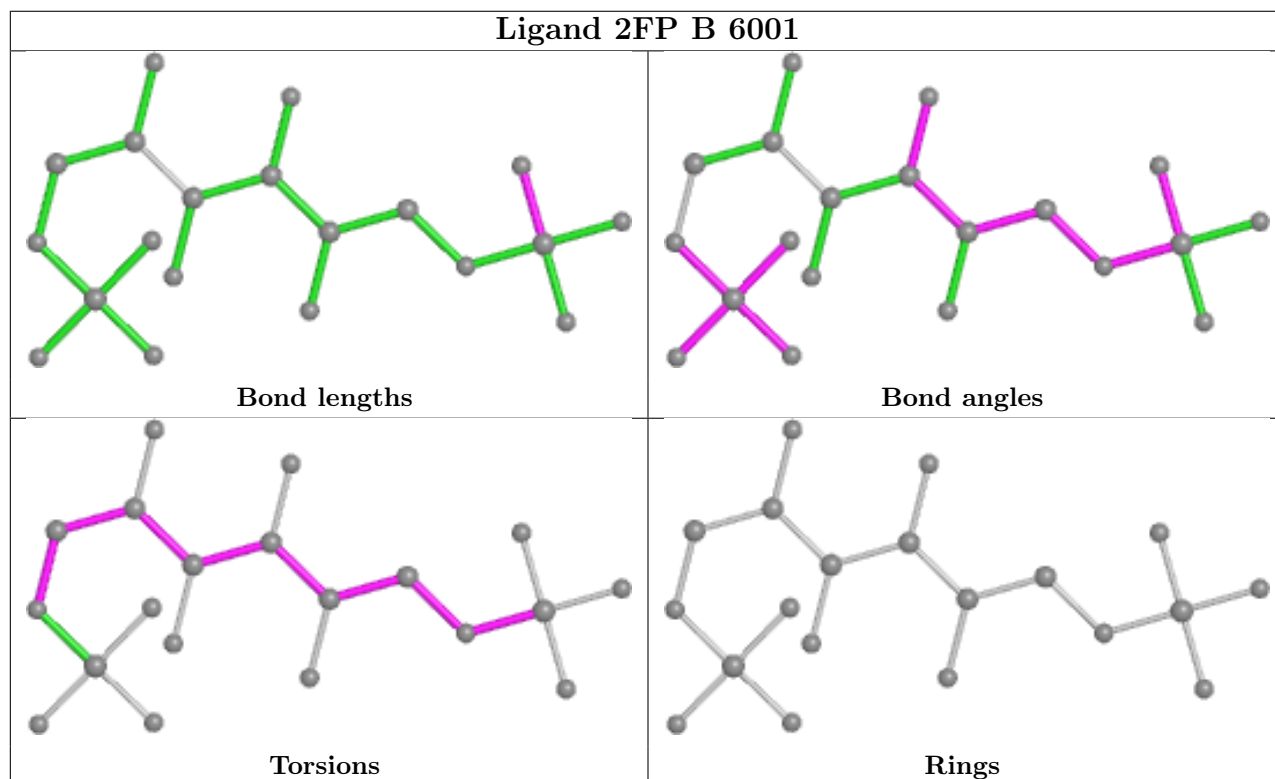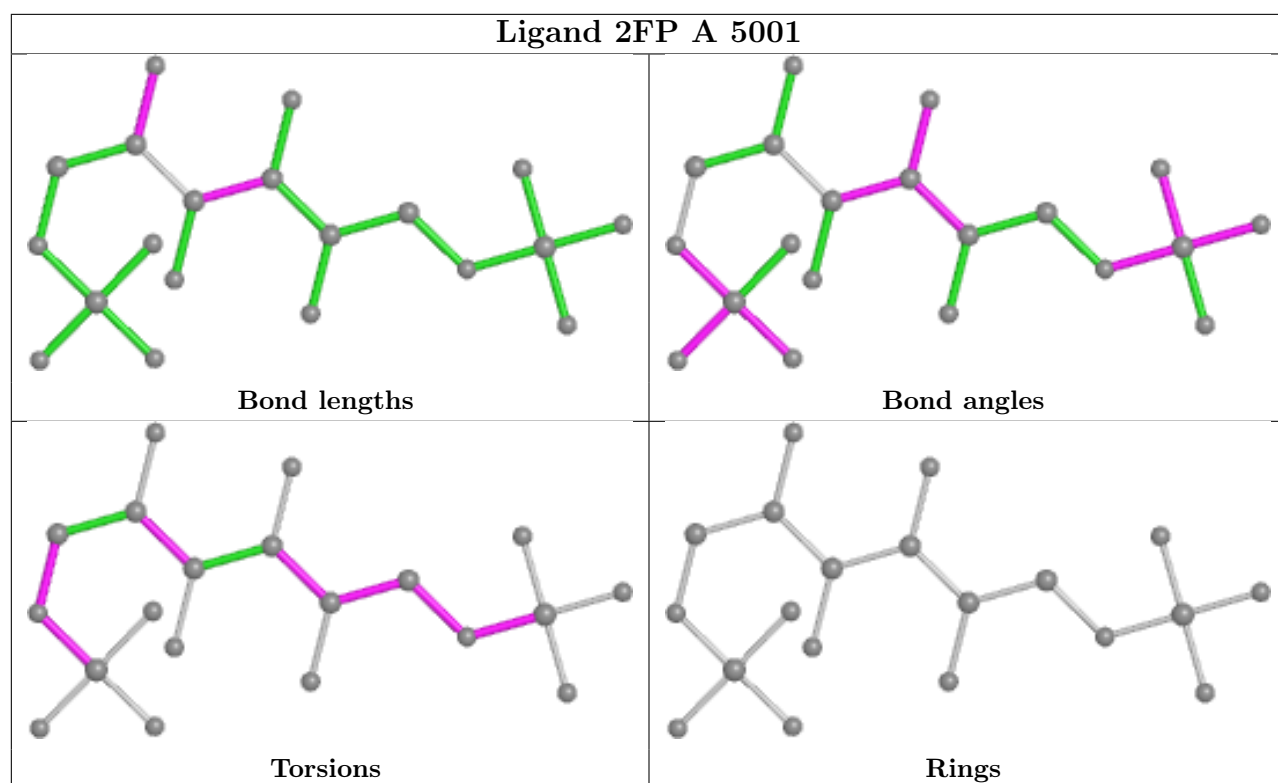
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.