



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:34 am BST

PDB ID : 1ZAI  
Title : Fructose-1,6-bisphosphate Schiff base intermediate in FBP aldolase from rabbit muscle  
Authors : St-Jean, M.; Lafrance-Vanasse, J.; Liotard, B.; Sygusch, J.  
Deposited on : 2005-04-06  
Resolution : 1.76 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](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) : 1.13  
EDS : 2.11  
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) : 2.11

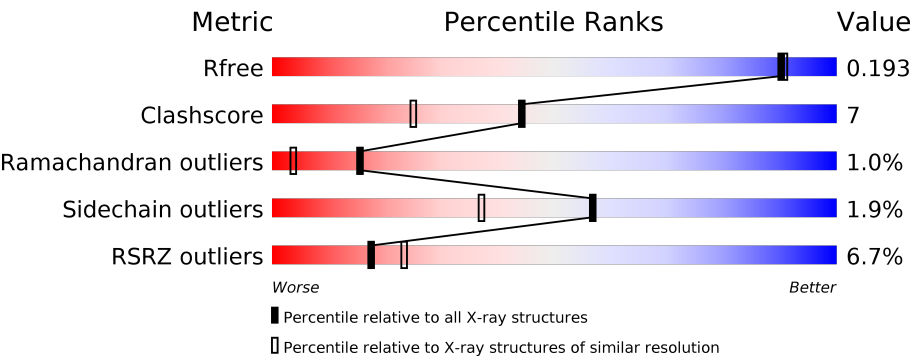
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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  $\leq 5\%$ . 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	363	<div><div>5%</div><div><div></div><div>85%</div><div>15%</div></div><div></div></div>
1	B	363	<div><div>6%</div><div><div></div><div>85%</div><div>14%</div></div><div></div></div>
1	C	363	<div><div>7%</div><div><div></div><div>84%</div><div>15%</div></div><div></div></div>
1	D	363	<div><div>9%</div><div><div></div><div>85%</div><div>15%</div></div><div></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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FP	A	3001	X	-	-	-
2	2FP	B	3002	X	-	-	-
2	2FP	C	3003	X	-	-	-
2	2FP	D	3004	X	-	-	-

## 2 Entry composition [i](#)

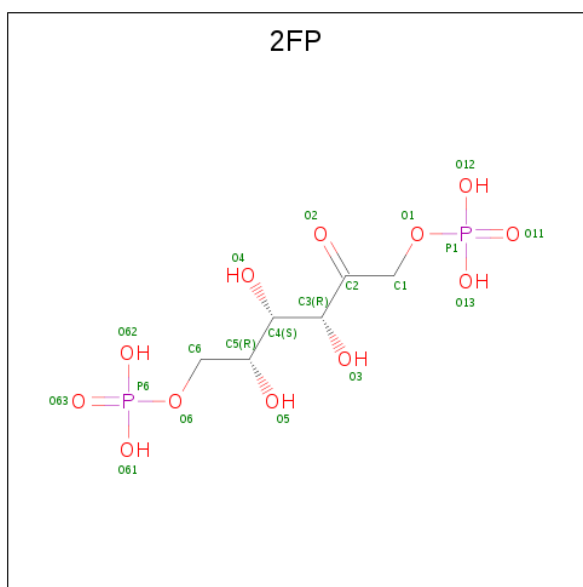
There are 3 unique types of molecules in this entry. The entry contains 13516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	B	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	C	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	D	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			

- Molecule 2 is 1,6-FRUCTOSE DIPHOSPHATE (LINEAR FORM) (three-letter code: 2FP) (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
			19	6	11	2		
2	B	1	Total	C	O	P	0	0
			19	6	11	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			19	6	11	2		
2	D	1	Total	C	O	P	0	0
			19	6	11	2		

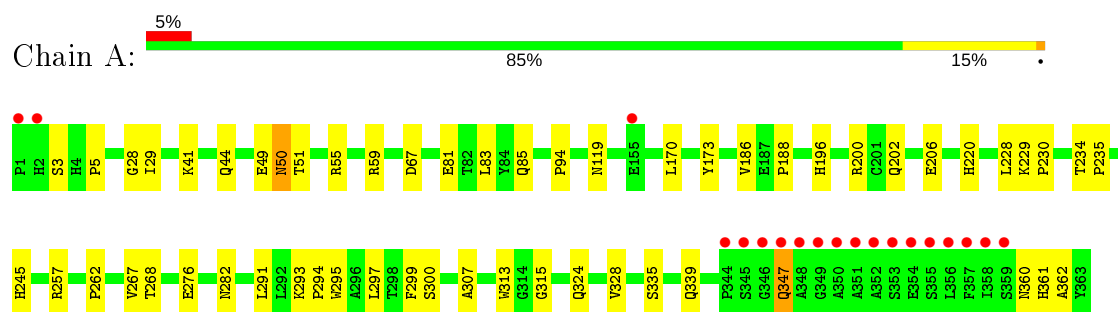
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	602	Total	O	0	0
			602	602		
3	B	610	Total	O	0	0
			610	610		
3	C	606	Total	O	0	0
			606	606		
3	D	590	Total	O	0	0
			590	590		

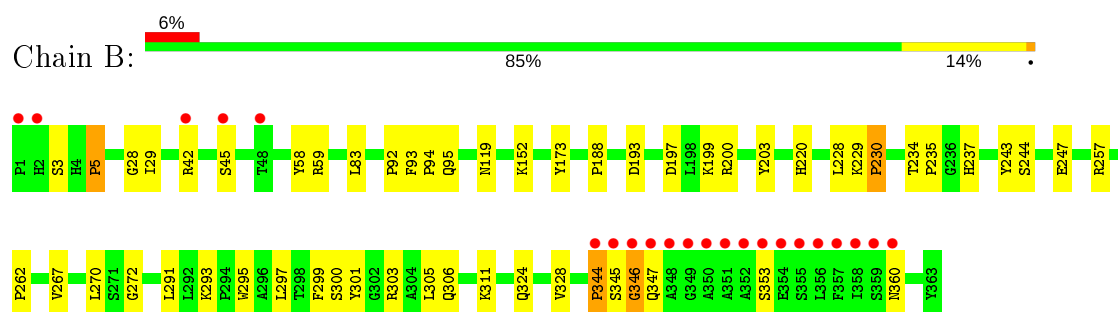
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

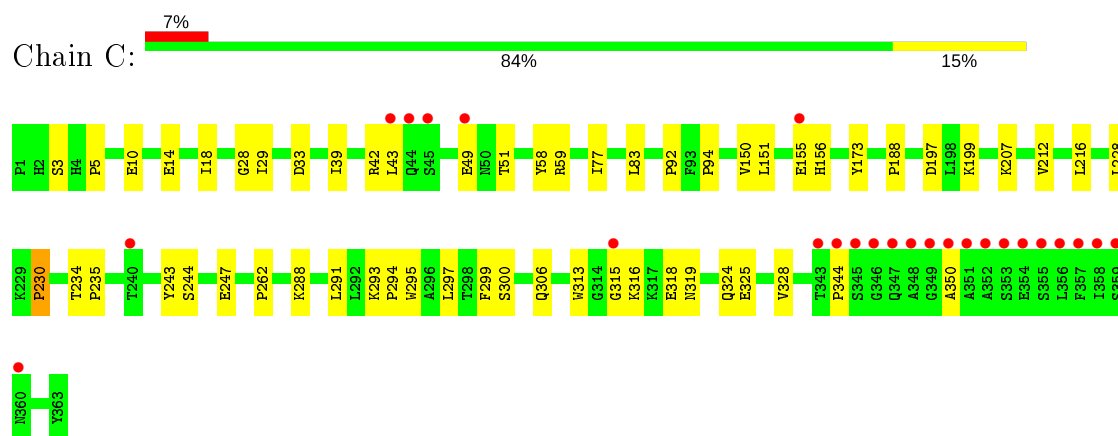
- Molecule 1: Fructose-bisphosphate aldolase A



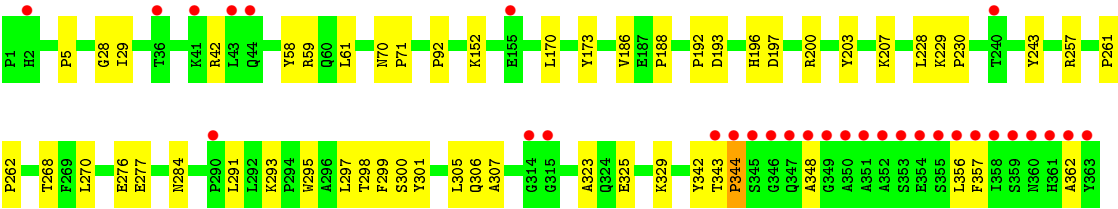
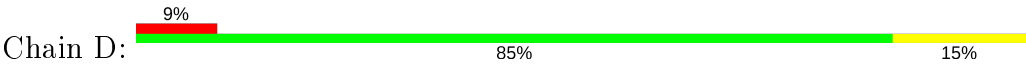
- Molecule 1: Fructose-bisphosphate aldolase A



- Molecule 1: Fructose-bisphosphate aldolase A



- Molecule 1: Fructose-bisphosphate aldolase A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.00Å 103.23Å 84.31Å 90.00° 98.77° 90.00°	Depositor
Resolution (Å)	50.00 – 1.76 43.88 – 1.63	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-1.76) 82.7 (43.88-1.63)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 1.63Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.155 , 0.190 0.159 , 0.193	Depositor DCC
$R_{free}$ test set	15431 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.4	Xtriage
Anisotropy	0.444	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 68.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: 2FP

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	0.28	0/2812	0.58	0/3810
1	B	0.29	0/2812	0.59	0/3810
1	C	0.29	0/2812	0.58	0/3810
1	D	0.28	0/2812	0.57	0/3810
All	All	0.29	0/11248	0.58	0/15240

There are no bond length outliers.

There are no bond angle outliers.

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	2758	0	2774	38	0
1	B	2758	0	2773	37	0
1	C	2758	0	2774	37	0
1	D	2758	0	2774	45	0
2	A	19	0	10	0	0
2	B	19	0	10	0	0
2	C	19	0	10	0	0
2	D	19	0	10	0	0
3	A	602	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	610	0	0	10	0
3	C	606	0	0	7	0
3	D	590	0	0	9	0
All	All	13516	0	11135	147	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 (147) 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:344:PRO:HG3	3:D:3347:HOH:O	1.82	0.78
1:A:347:GLN:H	1:A:347:GLN:NE2	1.87	0.72
1:C:42:ARG:HH11	1:C:42:ARG:HG2	1.53	0.72
1:D:42:ARG:HG2	1:D:42:ARG:HH11	1.56	0.71
1:C:49:GLU:HG2	1:C:51:THR:HG23	1.73	0.70
1:D:284:ASN:ND2	1:D:342:TYR:H	1.92	0.67
1:B:92:PRO:HD2	1:B:95:GLN:HE21	1.60	0.67
1:C:344:PRO:HD3	3:C:3398:HOH:O	1.97	0.64
1:B:200:ARG:HD2	3:C:3409:HOH:O	1.97	0.64
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.80	0.63
1:C:199:LYS:HG3	3:C:3164:HOH:O	1.97	0.63
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.81	0.62
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.81	0.62
1:A:200:ARG:HD2	3:D:3387:HOH:O	2.03	0.59
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.85	0.58
1:A:50:ASN:ND2	1:A:55:ARG:HH11	2.02	0.57
1:A:361:HIS:HB2	3:A:3132:HOH:O	2.05	0.57
1:B:92:PRO:HD2	1:B:95:GLN:NE2	2.19	0.57
1:C:350:ALA:HA	3:C:3208:HOH:O	2.04	0.56
1:A:293:LYS:HG2	1:A:297:LEU:HD11	1.87	0.55
1:B:42:ARG:NH2	3:B:3312:HOH:O	2.36	0.55
1:B:257:ARG:HA	1:C:262:PRO:HG2	1.89	0.54
3:A:3140:HOH:O	1:D:200:ARG:HD2	2.08	0.53
1:B:344:PRO:HG2	1:B:345:SER:H	1.74	0.53
1:B:152:LYS:HE2	3:B:3253:HOH:O	2.06	0.53
1:D:192:PRO:HG2	1:D:357:PHE:HE2	1.74	0.53
1:C:10:GLU:HG2	3:C:3273:HOH:O	2.09	0.53
1:B:220:HIS:HD2	1:C:207:LYS:NZ	2.07	0.53
1:B:291:LEU:O	1:B:293:LYS:HE2	2.10	0.52
1:D:61:LEU:HD11	1:D:323:ALA:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:GLU:O	1:D:329:LYS:HG3	2.08	0.52
1:C:151:LEU:N	1:C:151:LEU:HD12	2.25	0.52
1:C:316:LYS:HB3	1:C:318:GLU:OE1	2.10	0.52
1:B:42:ARG:NH1	3:B:3428:HOH:O	2.43	0.52
1:D:29:ILE:HB	1:D:300:SER:HA	1.91	0.52
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.45	0.51
1:A:220:HIS:HD2	1:D:207:LYS:NZ	2.08	0.51
1:C:150:VAL:C	1:C:151:LEU:HD12	2.31	0.51
1:A:360:ASN:HB2	3:A:3439:HOH:O	2.10	0.51
1:A:291:LEU:O	1:A:293:LYS:HD3	2.11	0.51
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.46	0.50
1:C:324:GLN:O	1:C:328:VAL:HG23	2.11	0.50
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.46	0.50
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.32	0.50
1:A:3:SER:HB2	1:D:203:TYR:CG	2.46	0.50
1:A:347:GLN:HG3	3:A:3337:HOH:O	2.12	0.49
1:B:324:GLN:O	1:B:328:VAL:HG23	2.13	0.49
1:D:356:LEU:HD22	3:D:3433:HOH:O	2.11	0.49
1:D:92:PRO:HB3	3:D:3483:HOH:O	2.12	0.49
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.94	0.49
1:C:288:LYS:HB3	1:C:288:LYS:NZ	2.28	0.49
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.48	0.49
1:B:42:ARG:NE	3:B:3312:HOH:O	2.43	0.48
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.48	0.48
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.95	0.48
1:C:155:GLU:HG2	1:C:156:HIS:CD2	2.49	0.48
1:A:81:GLU:O	1:A:85:GLN:HG3	2.13	0.48
1:C:325:GLU:HG2	3:C:3383:HOH:O	2.14	0.48
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.95	0.48
1:D:344:PRO:CG	3:D:3347:HOH:O	2.51	0.47
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.14	0.47
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.50	0.47
1:B:344:PRO:HD3	3:B:3010:HOH:O	2.15	0.47
1:B:262:PRO:CG	1:C:294:PRO:HG3	2.45	0.47
1:C:39:ILE:O	1:C:43:LEU:HG	2.15	0.47
1:A:202:GLN:O	1:A:206:GLU:HG3	2.15	0.47
1:D:42:ARG:HG2	1:D:42:ARG:NH1	2.27	0.47
1:A:324:GLN:O	1:A:328:VAL:HG23	2.15	0.47
1:C:42:ARG:NH1	1:C:42:ARG:HG2	2.25	0.47
1:A:262:PRO:HD2	1:D:257:ARG:O	2.15	0.47
1:D:58:TYR:OH	1:D:306:GLN:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.15	0.46
1:D:42:ARG:HH11	1:D:42:ARG:CG	2.26	0.46
1:B:220:HIS:HD2	1:C:207:LYS:HZ1	1.64	0.46
1:D:348:ALA:HB3	3:D:3316:HOH:O	2.14	0.46
1:C:83:LEU:HD12	1:C:94:PRO:HG3	1.97	0.46
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.15	0.46
1:A:245:HIS:HD2	1:A:282:ASN:OD1	1.98	0.46
1:B:229:LYS:HE2	1:B:270:LEU:HB3	1.98	0.46
1:D:42:ARG:HD3	3:D:3235:HOH:O	2.16	0.46
1:D:196:HIS:HB2	1:D:200:ARG:HG2	1.98	0.45
1:D:229:LYS:HE2	1:D:270:LEU:HB3	1.98	0.45
1:D:268:THR:HB	1:D:300:SER:HB2	1.99	0.45
1:A:29:ILE:HB	1:A:300:SER:HA	1.97	0.45
1:C:234:THR:HB	1:C:235:PRO:HD2	1.97	0.45
1:D:301:TYR:HB2	1:D:305:LEU:HG	1.98	0.45
1:D:343:THR:O	1:D:344:PRO:C	2.55	0.45
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.31	0.45
1:A:234:THR:HB	1:A:235:PRO:HD2	1.99	0.44
1:A:335:SER:O	1:A:339:GLN:HG3	2.18	0.44
1:B:311:LYS:HD3	3:B:3335:HOH:O	2.17	0.44
1:D:277:GLU:HG2	3:D:3249:HOH:O	2.17	0.44
1:B:234:THR:HB	1:B:235:PRO:HD2	2.00	0.43
1:B:237:HIS:HB3	3:B:3217:HOH:O	2.18	0.43
1:B:346:GLY:O	1:B:347:GLN:HB2	2.19	0.43
1:D:61:LEU:HD11	1:D:323:ALA:CB	2.49	0.43
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.53	0.43
1:D:61:LEU:HD23	1:D:61:LEU:C	2.38	0.43
1:A:268:THR:HB	1:A:300:SER:HB2	2.01	0.43
1:C:58:TYR:OH	1:C:306:GLN:HB3	2.19	0.43
1:B:244:SER:OG	1:B:247:GLU:HG3	2.19	0.43
1:A:276:GLU:CD	1:A:307:ALA:HB3	2.39	0.42
1:A:313:TRP:CE2	1:A:315:GLY:HA2	2.54	0.42
1:D:152:LYS:HE2	3:D:3455:HOH:O	2.18	0.42
1:A:294:PRO:HG3	1:D:262:PRO:HG3	2.01	0.42
1:A:83:LEU:HD12	1:A:94:PRO:HG3	2.01	0.42
1:B:267:VAL:HB	1:B:297:LEU:HD23	2.00	0.42
1:D:42:ARG:NH1	1:D:42:ARG:CG	2.82	0.42
1:A:257:ARG:O	1:D:262:PRO:HD2	2.19	0.42
1:A:267:VAL:HB	1:A:297:LEU:HD23	2.02	0.42
1:B:203:TYR:CG	1:C:3:SER:HB2	2.54	0.42
1:B:360:ASN:HB2	3:B:3439:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:SER:OG	1:C:247:GLU:HG3	2.19	0.42
1:D:170:LEU:HD22	1:D:186:VAL:HG13	2.01	0.42
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.94	0.42
3:A:3087:HOH:O	1:B:220:HIS:HE1	2.02	0.42
1:C:92:PRO:HB3	3:C:3435:HOH:O	2.19	0.42
1:B:3:SER:HB3	3:B:3058:HOH:O	2.20	0.42
1:C:291:LEU:O	1:C:293:LYS:HE2	2.19	0.41
1:B:272:GLY:HA2	1:B:303:ARG:NH2	2.35	0.41
1:C:293:LYS:HD2	1:C:297:LEU:HD12	2.00	0.41
1:C:33:ASP:HB3	1:C:77:ILE:HG22	2.02	0.41
1:D:229:LYS:HG3	1:D:268:THR:O	2.21	0.41
1:A:347:GLN:HG2	3:A:3547:HOH:O	2.20	0.41
1:C:29:ILE:HB	1:C:300:SER:HA	2.01	0.41
1:A:196:HIS:HB2	1:A:200:ARG:HG2	2.03	0.41
1:A:41:LYS:HA	1:A:44:GLN:HG2	2.01	0.41
1:D:298:THR:OG1	1:D:299:PHE:N	2.54	0.41
1:D:277:GLU:OE2	1:D:344:PRO:HB3	2.20	0.41
1:B:93:PHE:N	1:B:94:PRO:CD	2.84	0.41
1:C:212:VAL:O	1:C:216:LEU:HG	2.21	0.41
1:D:291:LEU:O	1:D:293:LYS:HE2	2.20	0.41
1:A:28:GLY:HA3	1:A:299:PHE:CE1	2.55	0.41
1:A:362:ALA:HB2	3:A:3455:HOH:O	2.19	0.41
1:B:29:ILE:HB	1:B:300:SER:HA	2.02	0.41
1:A:229:LYS:HG3	1:A:268:THR:O	2.20	0.41
1:A:50:ASN:HD21	1:A:55:ARG:HD3	1.86	0.41
1:C:14:GLU:O	1:C:18:ILE:HG13	2.21	0.41
1:C:313:TRP:CE2	1:C:315:GLY:HA2	2.56	0.41
1:A:170:LEU:HD22	1:A:186:VAL:HG13	2.03	0.40
1:B:301:TYR:HB2	1:B:305:LEU:HG	2.03	0.40
1:B:199:LYS:HG3	3:B:3105:HOH:O	2.20	0.40
1:D:293:LYS:HD2	1:D:297:LEU:HD12	2.03	0.40
1:D:284:ASN:HD21	1:D:342:TYR:H	1.68	0.40
1:B:58:TYR:OH	1:B:306:GLN:HB3	2.21	0.40
1:A:313:TRP:CZ2	1:A:315:GLY:HA2	2.57	0.40
1:A:50:ASN:HD21	1:A:55:ARG:HH11	1.68	0.40

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	361/363 (99%)	342 (95%)	16 (4%)	3 (1%)	19	6
1	B	361/363 (99%)	341 (94%)	15 (4%)	5 (1%)	11	2
1	C	361/363 (99%)	343 (95%)	16 (4%)	2 (1%)	25	10
1	D	361/363 (99%)	346 (96%)	11 (3%)	4 (1%)	14	3
All	All	1444/1452 (99%)	1372 (95%)	58 (4%)	14 (1%)	15	4

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	PRO
1	D	362	ALA
1	A	67	ASP
1	B	5	PRO
1	B	353	SER
1	C	5	PRO
1	D	5	PRO
1	A	5	PRO
1	A	188	PRO
1	B	188	PRO
1	B	346	GLY
1	C	188	PRO
1	D	188	PRO
1	D	344	PRO

### 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	291/291 (100%)	285 (98%)	6 (2%)	53	31
1	B	291/291 (100%)	283 (97%)	8 (3%)	44	22
1	C	291/291 (100%)	287 (99%)	4 (1%)	67	52
1	D	291/291 (100%)	287 (99%)	4 (1%)	67	52
All	All	1164/1164 (100%)	1142 (98%)	22 (2%)	57	37

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	59	ARG
1	A	119	ASN
1	A	173	TYR
1	A	295	TRP
1	A	347	GLN
1	B	5	PRO
1	B	45	SER
1	B	59	ARG
1	B	119	ASN
1	B	173	TYR
1	B	193	ASP
1	B	230	PRO
1	B	295	TRP
1	C	59	ARG
1	C	173	TYR
1	C	230	PRO
1	C	295	TRP
1	D	59	ARG
1	D	173	TYR
1	D	193	ASP
1	D	295	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	119	ASN
1	A	220	HIS
1	A	237	HIS
1	A	241	GLN

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Mol	Chain	Res	Type
1	A	245	HIS
1	A	319	ASN
1	A	347	GLN
1	B	95	GLN
1	B	119	ASN
1	B	220	HIS
1	C	237	HIS
1	C	241	GLN
1	C	245	HIS
1	C	319	ASN
1	C	347	GLN
1	D	85	GLN
1	D	180	ASN
1	D	241	GLN
1	D	284	ASN
1	D	319	ASN

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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	2FP	D	3004	1	18,18,19	1.21	1 (5%)	24,26,28	0.86	2 (8%)
2	2FP	C	3003	1	18,18,19	1.21	1 (5%)	24,26,28	0.84	1 (4%)
2	2FP	A	3001	1	18,18,19	1.21	1 (5%)	24,26,28	0.83	2 (8%)
2	2FP	B	3002	1	18,18,19	1.21	1 (5%)	24,26,28	0.86	2 (8%)

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	2FP	D	3004	1	2/2/5/6	1/21/21/24	-
2	2FP	C	3003	1	2/2/5/6	2/21/21/24	-
2	2FP	A	3001	1	2/2/5/6	1/21/21/24	-
2	2FP	B	3002	1	2/2/5/6	3/21/21/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3003	2FP	P6-O63	3.39	1.61	1.50
2	D	3004	2FP	P6-O63	3.38	1.61	1.50
2	B	3002	2FP	P6-O63	3.37	1.61	1.50
2	A	3001	2FP	P6-O63	3.36	1.61	1.50

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3002	2FP	O61-P6-O6	2.36	113.01	106.73
2	C	3003	2FP	O61-P6-O6	2.27	112.77	106.73
2	D	3004	2FP	O61-P6-O6	2.23	112.66	106.73
2	A	3001	2FP	O61-P6-O6	2.13	112.41	106.73
2	D	3004	2FP	O1-P1-O11	2.12	112.42	106.47
2	B	3002	2FP	O1-P1-O11	2.10	112.35	106.47
2	A	3001	2FP	O1-P1-O11	2.07	112.27	106.47

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	3004	2FP	C3
2	D	3004	2FP	C4

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Mol	Chain	Res	Type	Atom
2	C	3003	2FP	C3
2	C	3003	2FP	C4
2	B	3002	2FP	C3
2	B	3002	2FP	C4
2	A	3001	2FP	C3
2	A	3001	2FP	C4

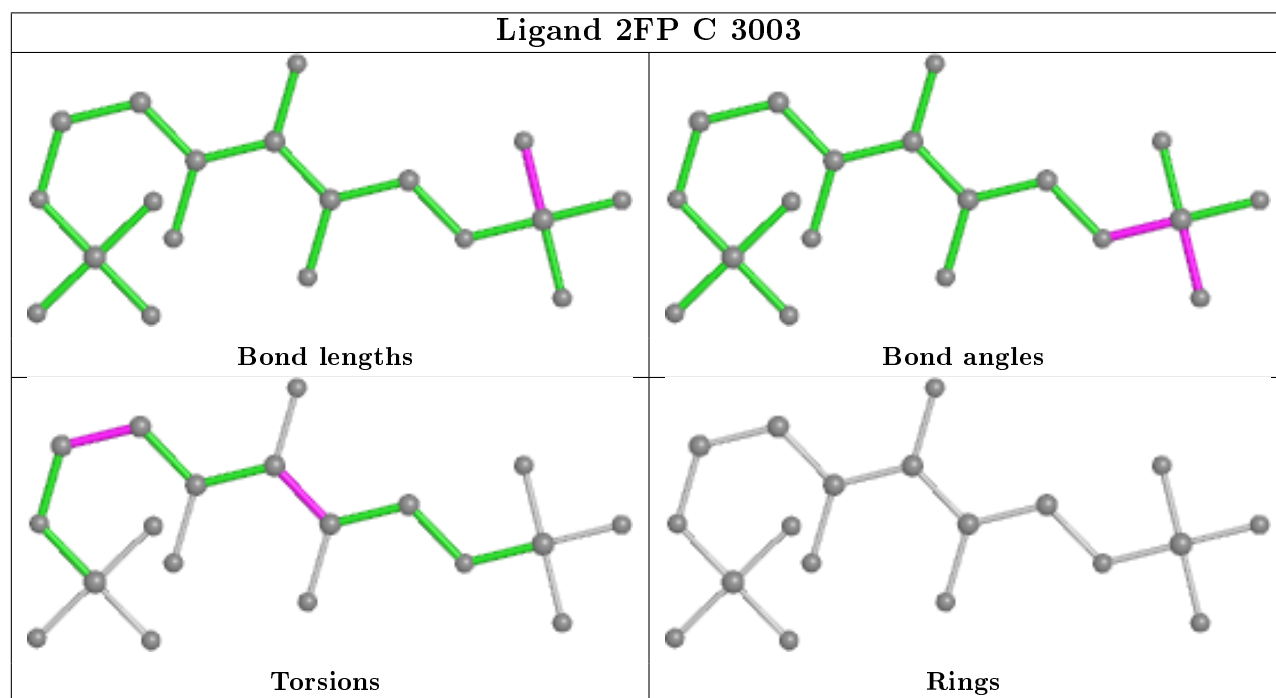
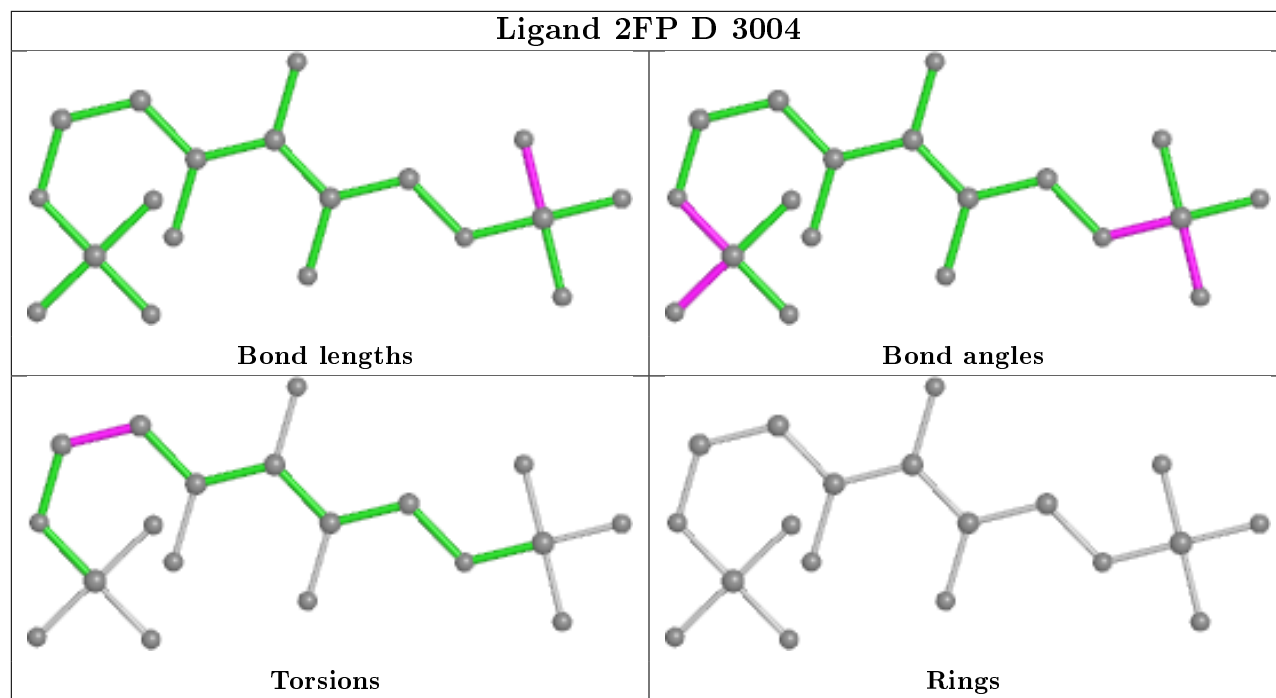
All (7) torsion outliers are listed below:

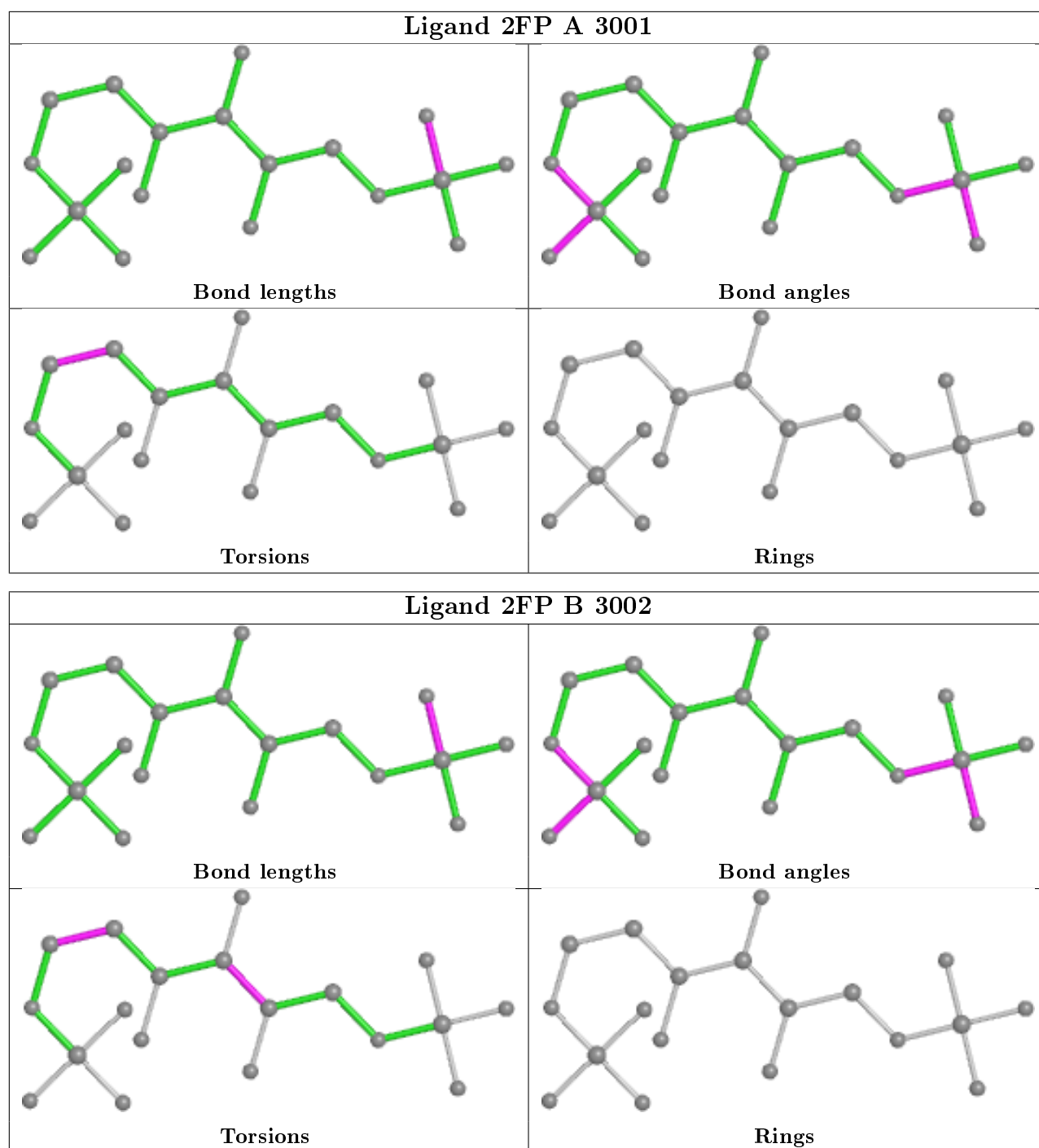
Mol	Chain	Res	Type	Atoms
2	D	3004	2FP	O1-C1-C2-C3
2	C	3003	2FP	O1-C1-C2-C3
2	B	3002	2FP	O1-C1-C2-C3
2	A	3001	2FP	O1-C1-C2-C3
2	B	3002	2FP	O4-C4-C5-C6
2	C	3003	2FP	O4-C4-C5-C6
2	B	3002	2FP	O4-C4-C5-O5

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 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

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	363/363 (100%)	0.23	19 (5%)	27 33	11, 18, 44, 73	15 (4%)
1	B	363/363 (100%)	0.32	22 (6%)	21 26	10, 18, 47, 82	15 (4%)
1	C	363/363 (100%)	0.44	25 (6%)	16 22	11, 19, 44, 76	15 (4%)
1	D	363/363 (100%)	0.36	31 (8%)	10 14	11, 21, 60, 106	3 (0%)
All	All	1452/1452 (100%)	0.34	97 (6%)	17 23	10, 19, 49, 106	48 (3%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	356	LEU	31.4
1	C	358	ILE	28.9
1	C	350	ALA	28.6
1	C	357	PHE	23.2
1	B	358	ILE	22.7
1	D	361	HIS	20.2
1	D	363	TYR	20.0
1	B	351	ALA	18.7
1	B	356	LEU	17.7
1	A	355	SER	17.3
1	B	357	PHE	17.3
1	C	353	SER	16.1
1	C	356	LEU	15.7
1	A	350	ALA	15.6
1	B	355	SER	15.1
1	A	357	PHE	14.6
1	A	352	ALA	13.8
1	D	362	ALA	13.1
1	A	351	ALA	12.8
1	C	354	GLU	12.5
1	A	349	GLY	12.3

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Mol	Chain	Res	Type	RSRZ
1	B	350	ALA	12.3
1	B	345	SER	12.2
1	B	348	ALA	11.9
1	A	346	GLY	11.9
1	B	349	GLY	11.5
1	C	351	ALA	11.0
1	C	352	ALA	10.9
1	A	358	ILE	9.8
1	B	346	GLY	9.6
1	B	353	SER	9.3
1	D	360	ASN	9.1
1	A	348	ALA	9.0
1	A	353	SER	8.9
1	D	348	ALA	8.9
1	B	347	GLN	8.5
1	D	346	GLY	8.2
1	A	345	SER	8.2
1	B	352	ALA	8.0
1	C	349	GLY	8.0
1	D	358	ILE	7.9
1	C	345	SER	7.9
1	A	354	GLU	7.7
1	C	348	ALA	7.5
1	C	355	SER	7.2
1	A	347	GLN	6.7
1	B	354	GLU	6.6
1	C	344	PRO	6.6
1	D	345	SER	6.6
1	C	347	GLN	6.4
1	D	357	PHE	6.2
1	D	359	SER	5.9
1	D	352	ALA	5.8
1	D	351	ALA	5.7
1	C	359	SER	5.3
1	D	353	SER	5.3
1	D	347	GLN	5.1
1	D	355	SER	5.0
1	D	350	ALA	4.9
1	B	344	PRO	4.5
1	C	44	GLN	4.4
1	C	346	GLY	4.2
1	D	356	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	359	SER	3.8
1	A	359	SER	3.7
1	D	349	GLY	3.4
1	A	344	PRO	3.2
1	C	49	GLU	2.9
1	D	44	GLN	2.8
1	C	45	SER	2.7
1	C	360	ASN	2.7
1	D	344	PRO	2.7
1	C	155	GLU	2.7
1	D	343	THR	2.7
1	D	354	GLU	2.6
1	A	155	GLU	2.6
1	C	43	LEU	2.5
1	C	315	GLY	2.5
1	B	1	PRO	2.4
1	A	2	HIS	2.4
1	D	290	PRO	2.4
1	D	43	LEU	2.4
1	D	155	GLU	2.3
1	C	240	THR	2.3
1	D	314	GLY	2.3
1	D	240	THR	2.3
1	B	2	HIS	2.2
1	D	2	HIS	2.2
1	B	42	ARG	2.1
1	D	315	GLY	2.1
1	B	48	THR	2.1
1	C	343	THR	2.1
1	B	360	ASN	2.1
1	A	1	PRO	2.1
1	B	45	SER	2.1
1	D	41	LYS	2.0
1	D	36	THR	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](#)

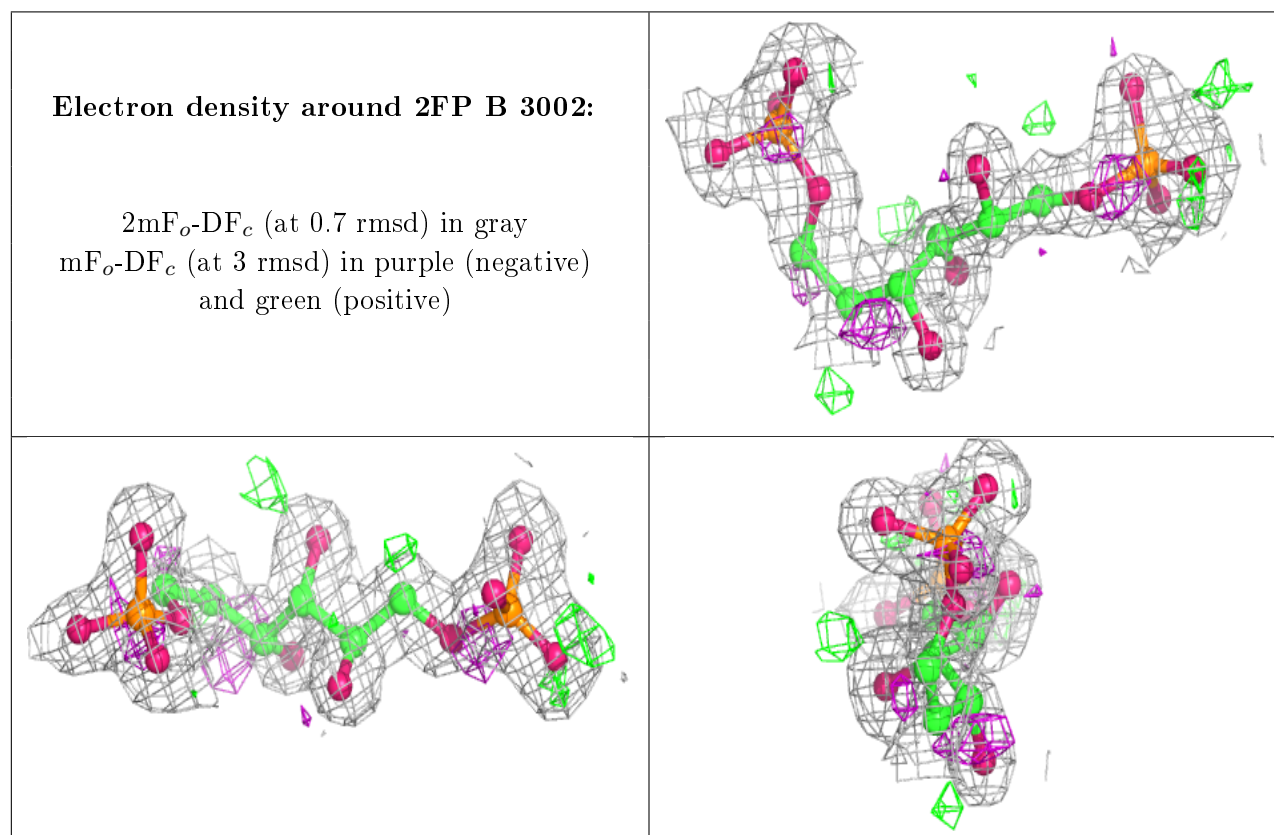
There are no carbohydrates in this entry.

## 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, 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( $\text{\AA}^2$ )	Q<0.9
2	2FP	B	3002	19/20	0.93	0.14	22,25,30,31	0
2	2FP	C	3003	19/20	0.94	0.14	19,25,28,28	0
2	2FP	A	3001	19/20	0.95	0.11	19,23,24,26	0
2	2FP	D	3004	19/20	0.96	0.11	23,26,29,29	0

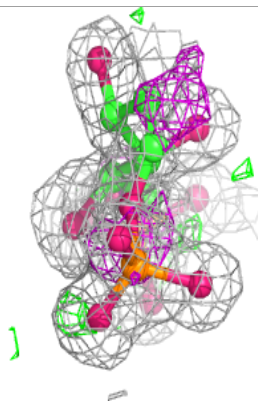
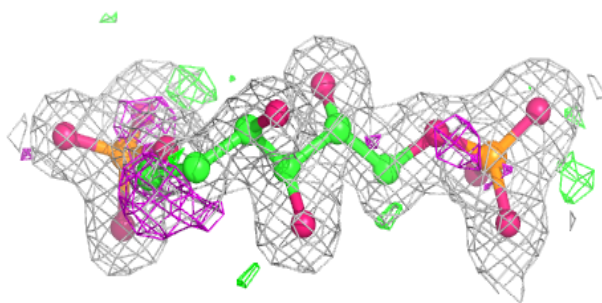
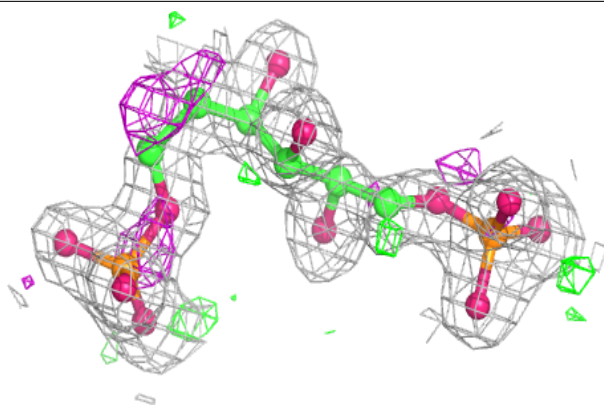
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



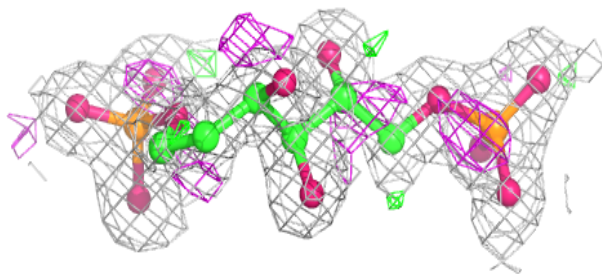
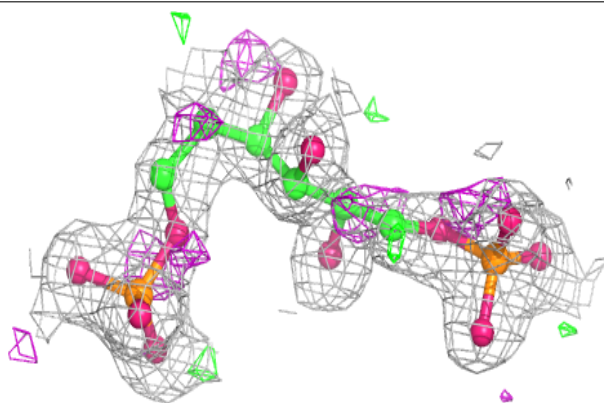


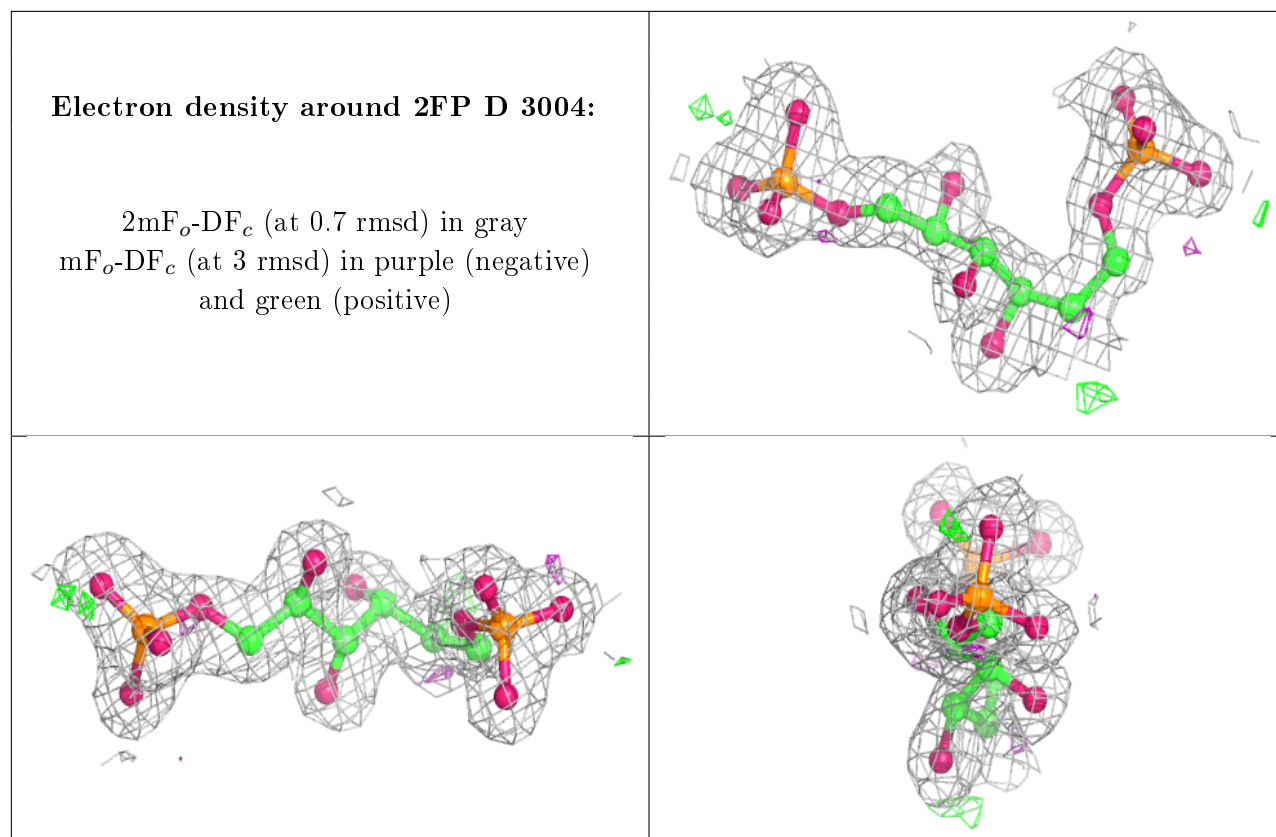
**Electron density around 2FP C 3003:**

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

**Electron density around 2FP A 3001:**

$2mF_o-DF_c$  (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.