



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:10 AM BST

PDB ID : 3U2Z
Title : Activator-Bound Structure of Human Pyruvate Kinase M2
Authors : Hong, B.; Dimov, S.; Tempel, W.; Auld, D.; Thomas, C.; Boxer, M.; Jianq, J.-K.; Skoumbourdis, A.; Min, S.; Southall, N.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Weigelt, J.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2011-10-04
Resolution : 2.10 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 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	:	2.13.1
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)	:	2.13.1

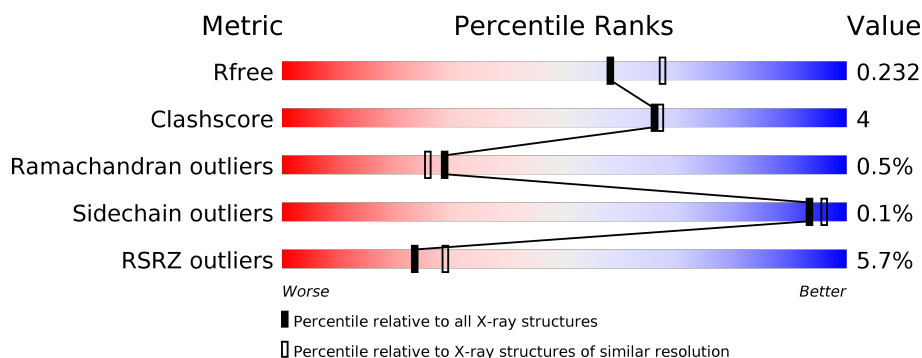
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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 $\leq 5\%$. 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	533	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div></div> </div> <div></div> </div>
1	B	533	<div> <div>8%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div></div> </div>
1	C	533	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div></div> </div> <div></div> </div>
1	D	533	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div></div> </div> <div></div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15896 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.

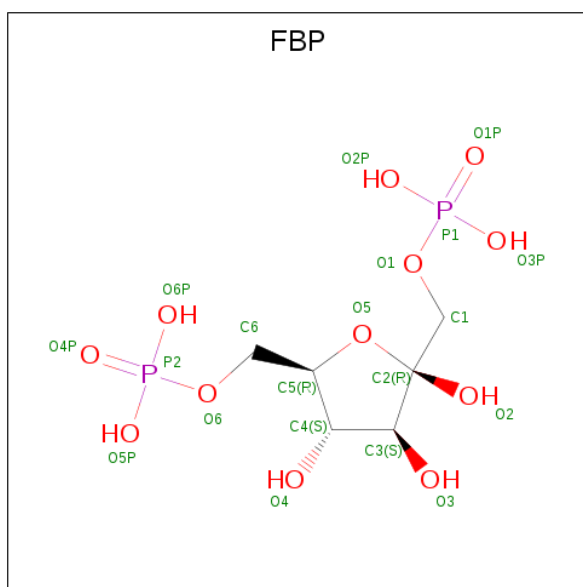
- Molecule 1 is a protein called Pyruvate kinase isozymes M1/M2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	5	1
			3826	2419	668	714	25			
1	B	514	Total	C	N	O	S	0	6	0
			3804	2407	671	699	27			
1	C	517	Total	C	N	O	S	0	6	0
			3835	2422	669	718	26			
1	D	513	Total	C	N	O	S	0	9	0
			3861	2441	681	713	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-1	GLY	-	expression tag	UNP P14618
D	0	SER	-	expression tag	UNP P14618

- Molecule 2 is 1,6-di-O-phosphono-beta-D-fructofuranose (three-letter code: FBP) (formula: $C_6H_{14}O_{12}P_2$).

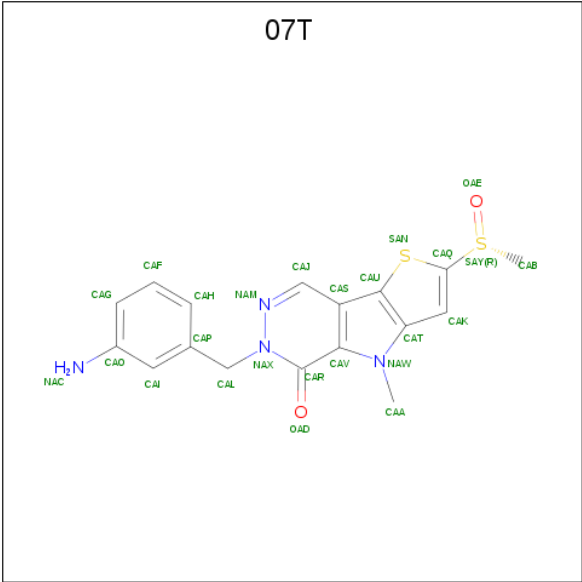


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	5	Total	X	0	0
			5	5		
3	A	6	Total	X	0	0
			6	6		
3	D	6	Total	X	0	0
			6	6		
3	C	4	Total	X	0	0
			4	4		

- Molecule 4 is 6-(3-aminobenzyl)-4-methyl-2-methylsulfinyl-4,6-dihydro-5H-thieno[2',3':4,5]pyrrolo[2,3-d]pyridazin-5-one (three-letter code: 07T) (formula: C₁₇H₁₆N₄O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	1
			50	34	8	4	4		
4	C	1	Total	C	N	O	S	0	1
			50	34	8	4	4		

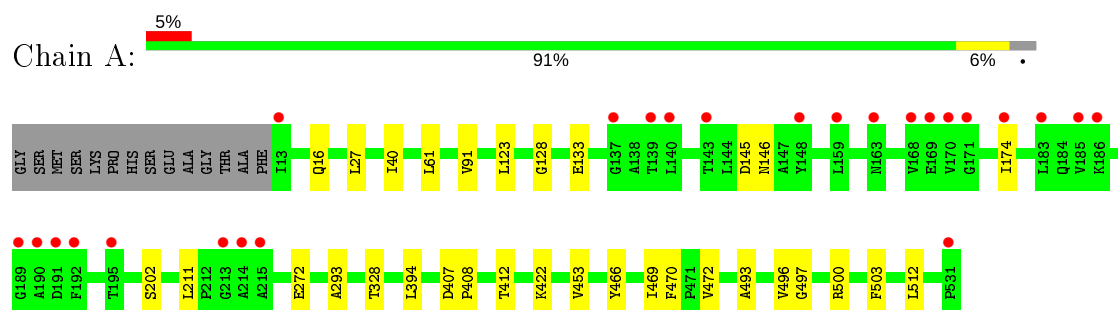
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		
5	B	90	Total	O	0	1
			91	91		
5	C	80	Total	O	0	1
			81	81		
5	D	99	Total	O	0	0
			99	99		

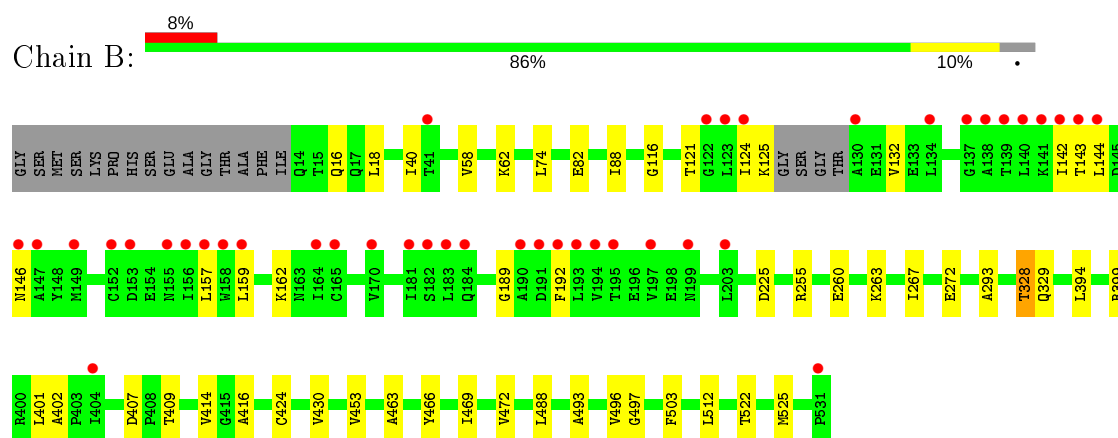
3 Residue-property plots [i](#)

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.

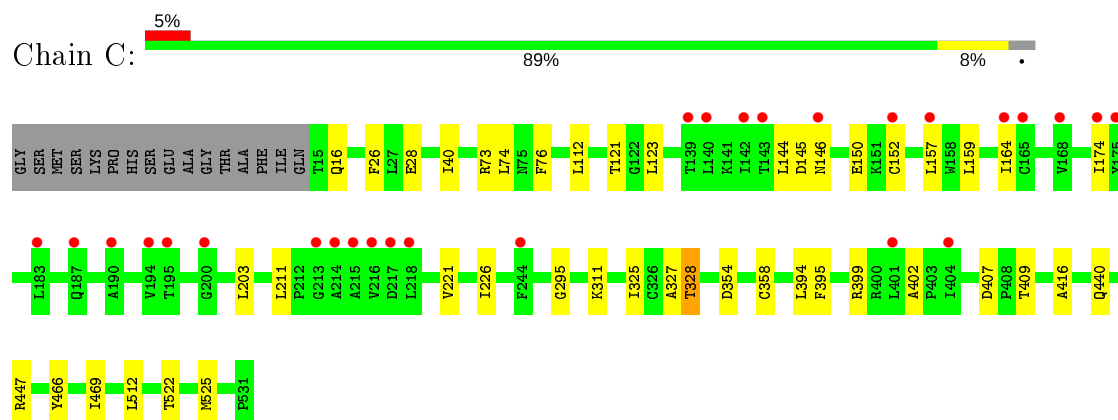
- Molecule 1: Pyruvate kinase isozymes M1/M2



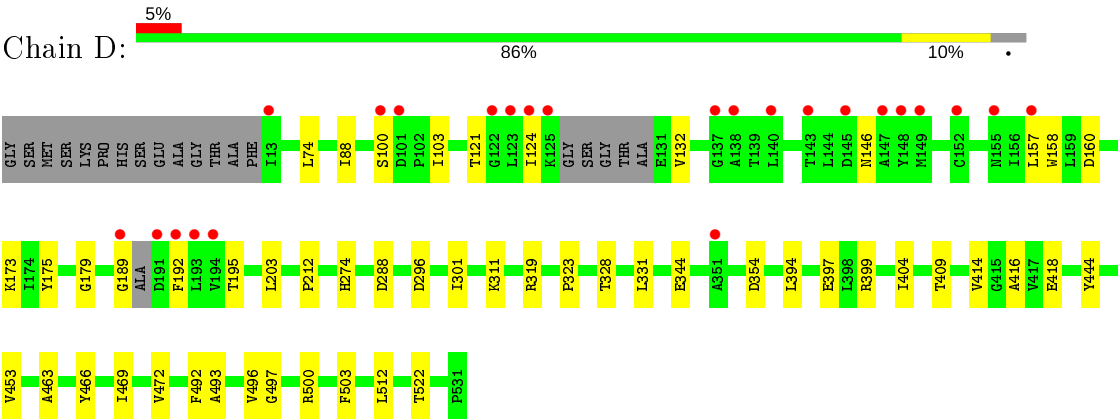
- Molecule 1: Pyruvate kinase isozymes M1/M2



- Molecule 1: Pyruvate kinase isozymes M1/M2



● Molecule 1: Pyruvate kinase isozymes M1/M2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.76 Å 151.16 Å 93.21 Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	44.45 – 2.10 43.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (44.45-2.10) 98.6 (43.50-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.190 , 0.231 0.197 , 0.232	Depositor DCC
R_{free} test set	1524 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15896	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: UNX, 07T, 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	0.67	0/3900	0.66	0/5288
1	B	0.65	0/3881	0.68	1/5264 (0.0%)
1	C	0.63	0/3911	0.67	1/5308 (0.0%)
1	D	0.67	0/3957	0.69	0/5361
All	All	0.66	0/15649	0.67	2/21221 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	525	MET	CG-SD-CE	6.39	110.42	100.20
1	B	407	ASP	CB-CG-OD1	6.00	123.70	118.30

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	3826	0	3730	22	0
1	B	3804	0	3754	42	0
1	C	3835	0	3770	33	0
1	D	3861	0	3809	37	0
2	A	20	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	6	0	0	0	0
3	B	5	0	0	0	0
3	C	4	0	0	0	0
3	D	6	0	0	1	0
4	B	50	0	32	3	0
4	C	50	0	32	5	0
5	A	98	0	0	0	0
5	B	91	0	0	0	0
5	C	81	0	0	0	0
5	D	99	0	0	0	0
All	All	15896	0	15167	122	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 4.

All (122) 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:399[A]:ARG:NH1	1:D:399[A]:ARG:CD	2.04	1.07
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:CD	1.62	1.00
1:B:399[A]:ARG:NH1	1:D:399[A]:ARG:HD3	1.87	0.86
1:C:157:LEU:HD13	1:C:203:LEU:HD21	1.63	0.81
1:B:424[B]:CYS:SG	1:D:404:ILE:HG21	2.22	0.79
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:HD3	1.47	0.74
1:C:407:ASP:OD1	1:C:409[B]:THR:HG22	1.88	0.72
1:C:395:PHE:CZ	1:C:399:ARG:HD2	2.26	0.70
1:A:422:LYS:NZ	1:C:402:ALA:HB1	2.07	0.69
1:D:296:ASP:OD2	3:D:534:UNX:UNK	1.74	0.68
1:B:399[A]:ARG:HH12	1:D:399[A]:ARG:HD2	1.57	0.65
1:C:409[B]:THR:HG23	1:C:440:GLN:OE1	1.96	0.65
1:C:157:LEU:CD1	1:C:203:LEU:HD21	2.30	0.62
1:B:466:TYR:HB2	1:B:469:ILE:HD12	1.82	0.61
1:A:272:GLU:HG2	1:A:293:ALA:HB3	1.83	0.61
1:D:311:LYS:NZ	1:D:354:ASP:OD1	2.33	0.60
1:D:414:VAL:HG12	1:D:444:TYR:CE2	2.38	0.59
1:B:124:ILE:HD12	1:B:132:VAL:HG22	1.85	0.58
1:A:412:THR:HG22	1:A:512:LEU:CD2	2.33	0.58
1:A:16:GLN:HG2	1:A:40:ILE:HG23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:LEU:HD23	1:B:488:LEU:C	2.24	0.58
1:B:394:LEU:HD13	4:B:551[B]:07T:H7	1.84	0.58
1:B:260:GLU:OE2	1:B:263:LYS:HE2	2.04	0.58
4:C:551[B]:07T:H7	1:D:394:LEU:HD13	1.84	0.57
1:B:142:ILE:HG21	1:B:159:LEU:HD12	1.85	0.57
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.86	0.57
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.86	0.56
1:A:422:LYS:HZ1	1:C:402:ALA:HB1	1.71	0.56
1:C:416:ALA:CB	1:C:512:LEU:HD21	2.35	0.56
1:C:394:LEU:HD13	4:C:551[A]:07T:H7	1.88	0.55
1:A:123:LEU:HD22	1:A:128:GLY:HA2	1.89	0.55
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.88	0.55
1:B:144:LEU:HD13	1:B:162:LYS:HA	1.89	0.54
1:D:274[B]:HIS:CD2	1:D:301:ILE:HG22	2.43	0.54
1:B:463:ALA:HB1	1:B:469:ILE:HG21	1.89	0.53
1:C:221:VAL:HG12	1:C:226:ILE:HG13	1.91	0.53
1:B:409[B]:THR:HG22	1:B:522:THR:O	2.08	0.53
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.91	0.52
1:B:121:THR:CG2	1:B:157:LEU:HD11	2.41	0.51
1:A:61:LEU:HD13	1:A:91:VAL:HA	1.91	0.51
1:C:26:PHE:CZ	4:C:551[B]:07T:H3	2.46	0.51
1:B:424[B]:CYS:SG	1:D:404:ILE:CG2	2.97	0.51
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.41	0.50
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.94	0.50
1:D:103:ILE:HD13	1:D:492:PHE:CE1	2.47	0.50
1:D:414:VAL:HG12	1:D:444:TYR:CZ	2.46	0.50
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.47	0.50
1:A:453:VAL:HG21	1:A:493:ALA:HB2	1.93	0.49
1:C:123:LEU:HD12	1:C:150:GLU:HG2	1.94	0.49
1:B:16:GLN:CD	1:B:40:ILE:HG23	2.32	0.49
1:C:144:LEU:HD21	1:C:164:ILE:HG22	1.93	0.49
1:C:16:GLN:HG2	1:C:40:ILE:HG23	1.95	0.49
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.48	0.48
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.94	0.48
1:A:27:LEU:HD23	1:B:401:LEU:HD12	1.94	0.48
1:D:189:GLY:HA3	1:D:192:PHE:CE1	2.48	0.48
1:A:412:THR:HG22	1:A:512:LEU:HD22	1.95	0.48
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.14	0.48
1:B:189:GLY:HA3	1:B:192:PHE:CE2	2.49	0.48
4:C:551[A]:07T:H14	1:D:397:GLU:OE1	2.14	0.47
1:D:175:TYR:HB3	1:D:179:GLY:HA2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.97	0.47
1:B:512:LEU:HD23	1:B:525:MET:HA	1.97	0.47
1:C:174:ILE:HG12	1:C:211:LEU:CD2	2.45	0.47
1:D:331:LEU:HD23	1:D:344:GLU:HB3	1.98	0.46
1:B:416:ALA:HB2	1:B:512:LEU:HD21	1.97	0.46
1:D:496:VAL:HG13	1:D:500[B]:ARG:NE	2.31	0.46
1:C:73:ARG:C	1:C:74:LEU:HD23	2.35	0.46
1:B:16:GLN:CG	1:B:40:ILE:HG23	2.46	0.45
1:C:74:LEU:HD23	1:C:74:LEU:N	2.32	0.45
1:D:414:VAL:CG1	1:D:444:TYR:CZ	3.00	0.45
1:A:412:THR:HG22	1:A:512:LEU:HD21	1.98	0.45
1:A:174:ILE:HG12	1:A:211:LEU:HD21	1.99	0.45
1:B:82:GLU:H	1:B:82:GLU:CD	2.20	0.45
1:C:28:GLU:OE2	1:D:319:ARG:NH1	2.50	0.44
1:B:74:LEU:HD11	1:B:88:ILE:HG13	1.99	0.44
1:C:409[A]:THR:HG22	1:C:522:THR:O	2.17	0.44
1:C:123:LEU:HD12	1:C:150:GLU:CG	2.47	0.44
1:C:16:GLN:O	1:C:447[A]:ARG:NH2	2.50	0.44
1:C:311:LYS:NZ	1:C:354:ASP:OD1	2.41	0.44
1:D:124:ILE:HD11	1:D:203:LEU:HG	2.00	0.44
1:A:466:TYR:HB2	1:A:469:ILE:HD12	1.99	0.43
1:A:453:VAL:CG2	1:A:493:ALA:HB2	2.48	0.43
1:C:144:LEU:HD21	1:C:164:ILE:CG2	2.48	0.43
1:C:395:PHE:CE1	1:C:399:ARG:HD2	2.53	0.43
1:D:414:VAL:CG1	1:D:444:TYR:CE2	3.00	0.43
1:B:272:GLU:HG2	1:B:293:ALA:HB3	2.01	0.43
1:B:58:VAL:HG12	1:B:62:LYS:HE3	2.01	0.43
1:C:152:CYS:HB3	1:C:157:LEU:HD12	2.01	0.43
1:D:472:VAL:HG11	1:D:496:VAL:HG11	2.00	0.43
1:D:409:THR:HG23	1:D:522:THR:HB	2.00	0.43
1:C:76:PHE:CE1	1:C:112:LEU:HG	2.55	0.42
1:D:497:GLY:HA3	1:D:503:PHE:CZ	2.54	0.42
1:B:255:ARG:CZ	1:B:267:ILE:HD12	2.48	0.42
1:D:288:ASP:O	1:D:323:PRO:HD2	2.19	0.42
1:D:453:VAL:CG2	1:D:493:ALA:HB2	2.49	0.42
1:D:74:LEU:HD11	1:D:88:ILE:HG13	2.00	0.42
1:A:133:GLU:HA	1:A:202:SER:HA	2.02	0.42
1:C:466:TYR:HB2	1:C:469:ILE:HD12	2.01	0.42
1:A:394:LEU:HA	4:B:551[A]:07T:H7	2.02	0.42
1:B:143:THR:C	1:B:144:LEU:HD23	2.39	0.42
1:D:132:VAL:HG23	1:D:203:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:LEU:HD23	1:B:18:LEU:HA	1.86	0.41
1:C:295:GLY:CA	1:C:328:THR:HG21	2.50	0.41
1:C:327:ALA:O	1:C:328:THR:HB	2.20	0.41
1:A:174:ILE:HG12	1:A:211:LEU:CD2	2.50	0.41
1:D:158:TRP:CH2	1:D:160:ASP:HB3	2.54	0.41
1:D:121:THR:HB	1:D:157:LEU:HD11	2.02	0.41
1:B:414:VAL:HG13	1:D:418:GLU:HG3	2.02	0.41
1:B:328:THR:HG22	1:B:329:GLN:HG3	2.03	0.41
1:C:121:THR:HG22	1:C:159:LEU:CD2	2.51	0.41
1:C:325:ILE:HG12	1:C:358:CYS:HB2	2.03	0.41
1:B:430:VAL:HG22	1:B:512:LEU:HD12	2.02	0.41
1:A:407:ASP:HA	1:A:408:PRO:HD3	1.97	0.41
1:A:470[B]:PHE:CZ	1:A:500:ARG:CD	3.04	0.41
1:B:74:LEU:HD11	1:B:88:ILE:CG1	2.50	0.41
1:B:394:LEU:CD1	4:B:551[B]:07T:H7	2.51	0.41
1:C:394:LEU:HA	4:C:551[A]:07T:H6	2.03	0.41
1:D:173:LYS:O	1:D:212:PRO:HD2	2.20	0.41
1:A:412:THR:CG2	1:A:512:LEU:HD22	2.50	0.40
1:B:124:ILE:O	1:B:125:LYS:O	2.39	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	520/533 (98%)	509 (98%)	8 (2%)	3 (1%)	25	21
1	B	515/533 (97%)	503 (98%)	10 (2%)	2 (0%)	34	32
1	C	521/533 (98%)	504 (97%)	14 (3%)	3 (1%)	25	21
1	D	515/533 (97%)	502 (98%)	11 (2%)	2 (0%)	34	32
All	All	2071/2132 (97%)	2018 (97%)	43 (2%)	10 (0%)	29	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	B	328	THR
1	C	146	ASN
1	C	328	THR
1	D	146	ASN
1	D	328	THR
1	A	146	ASN
1	B	146	ASN
1	A	145	ASP
1	C	145	ASP

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	376/437 (86%)	376 (100%)	0	100	100
1	B	379/437 (87%)	379 (100%)	0	100	100
1	C	385/437 (88%)	385 (100%)	0	100	100
1	D	391/437 (90%)	389 (100%)	2 (0%)	88	92
All	All	1531/1748 (88%)	1529 (100%)	2 (0%)	93	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	100	SER
1	D	195	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	491	ASN

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 ⓘ

Of 29 ligands modelled in this entry, 21 are unknown - leaving 8 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	$\# Z > 2$
4	07T	C	551[B]	-	19,28,28	1.76	3 (15%)	18,42,42	2.25	5 (27%)
2	FBP	A	541	-	18,20,20	1.03	1 (5%)	23,32,32	0.85	2 (8%)
2	FBP	C	541	-	18,20,20	1.00	1 (5%)	23,32,32	0.82	0
4	07T	B	551[B]	-	19,28,28	1.66	3 (15%)	18,42,42	2.08	4 (22%)
4	07T	B	551[A]	-	19,28,28	1.74	2 (10%)	18,42,42	2.27	4 (22%)
2	FBP	B	541	-	18,20,20	1.14	1 (5%)	23,32,32	0.82	0
2	FBP	D	541	-	18,20,20	0.91	1 (5%)	23,32,32	1.10	2 (8%)
4	07T	C	551[A]	-	19,28,28	1.63	2 (10%)	18,42,42	2.86	5 (27%)

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
4	07T	C	551[B]	-	-	0/3/8/8	0/4/4/4
2	FBP	A	541	-	-	2/13/32/32	0/1/1/1
2	FBP	C	541	-	-	2/13/32/32	0/1/1/1
4	07T	B	551[B]	-	-	0/3/8/8	0/4/4/4
4	07T	B	551[A]	-	-	0/3/8/8	0/4/4/4
2	FBP	B	541	-	-	2/13/32/32	0/1/1/1
2	FBP	D	541	-	-	2/13/32/32	0/1/1/1
4	07T	C	551[A]	-	-	0/3/8/8	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	551[B]	07T	CAQ-SAY	-4.98	1.71	1.79
4	B	551[B]	07T	CAQ-SAY	-4.62	1.72	1.79
4	B	551[A]	07T	CAQ-SAY	-4.53	1.72	1.79
4	C	551[A]	07T	CAQ-SAY	-4.29	1.72	1.79
4	C	551[A]	07T	CAQ-SAN	-4.02	1.65	1.72
4	B	551[A]	07T	CAQ-SAN	-3.96	1.65	1.72
2	B	541	FBP	O2-C2	3.61	1.46	1.40
4	C	551[B]	07T	CAQ-SAN	-3.60	1.66	1.72
2	D	541	FBP	O2-C2	3.03	1.45	1.40
2	A	541	FBP	O2-C2	3.01	1.45	1.40
4	B	551[B]	07T	CAQ-SAN	-2.88	1.67	1.72
2	C	541	FBP	O2-C2	2.63	1.45	1.40
4	B	551[B]	07T	CAA-NAW	2.47	1.52	1.48
4	C	551[B]	07T	CAJ-NAM	2.35	1.33	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	551[A]	07T	CAB-SAY-CAQ	7.67	106.24	97.61
4	B	551[A]	07T	CAP-CAL-NAX	-7.52	101.47	112.48
4	C	551[B]	07T	CAP-CAL-NAX	-6.47	103.01	112.48
4	C	551[A]	07T	CAP-CAL-NAX	-6.44	103.06	112.48
4	B	551[B]	07T	CAP-CAL-NAX	-5.69	104.15	112.48
4	B	551[B]	07T	CAS-CAJ-NAM	-4.75	119.08	124.78
4	C	551[B]	07T	CAB-SAY-CAQ	4.38	102.54	97.61
4	C	551[A]	07T	OAE-SAY-CAQ	4.01	109.69	105.59
4	B	551[B]	07T	CAB-SAY-CAQ	3.43	101.47	97.61
4	C	551[B]	07T	CAS-CAJ-NAM	-3.40	120.70	124.78
4	C	551[A]	07T	CAT-CAU-SAN	-3.24	107.65	111.84
4	B	551[A]	07T	CAB-SAY-CAQ	3.19	101.20	97.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	551[A]	07T	CAT-CAU-SAN	-3.12	107.80	111.84
4	C	551[B]	07T	CAT-CAU-SAN	-3.07	107.87	111.84
4	C	551[A]	07T	CAS-CAJ-NAM	-2.91	121.28	124.78
4	B	551[A]	07T	CAS-CAJ-NAM	-2.71	121.52	124.78
2	D	541	FBP	P1-O1-C1	2.49	125.17	118.30
2	A	541	FBP	P1-O1-C1	2.45	125.03	118.30
4	B	551[B]	07T	CAT-CAU-SAN	-2.29	108.89	111.84
4	C	551[B]	07T	OAE-SAY-CAB	2.03	109.14	105.45
2	A	541	FBP	O6P-P2-O5P	2.02	115.36	107.64
2	D	541	FBP	O6P-P2-O5P	2.00	115.30	107.64

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	541	FBP	C4-C5-C6-O6
2	A	541	FBP	C4-C5-C6-O6
2	C	541	FBP	C4-C5-C6-O6
2	D	541	FBP	C4-C5-C6-O6
2	B	541	FBP	O5-C5-C6-O6
2	A	541	FBP	O5-C5-C6-O6
2	C	541	FBP	O5-C5-C6-O6
2	D	541	FBP	O5-C5-C6-O6

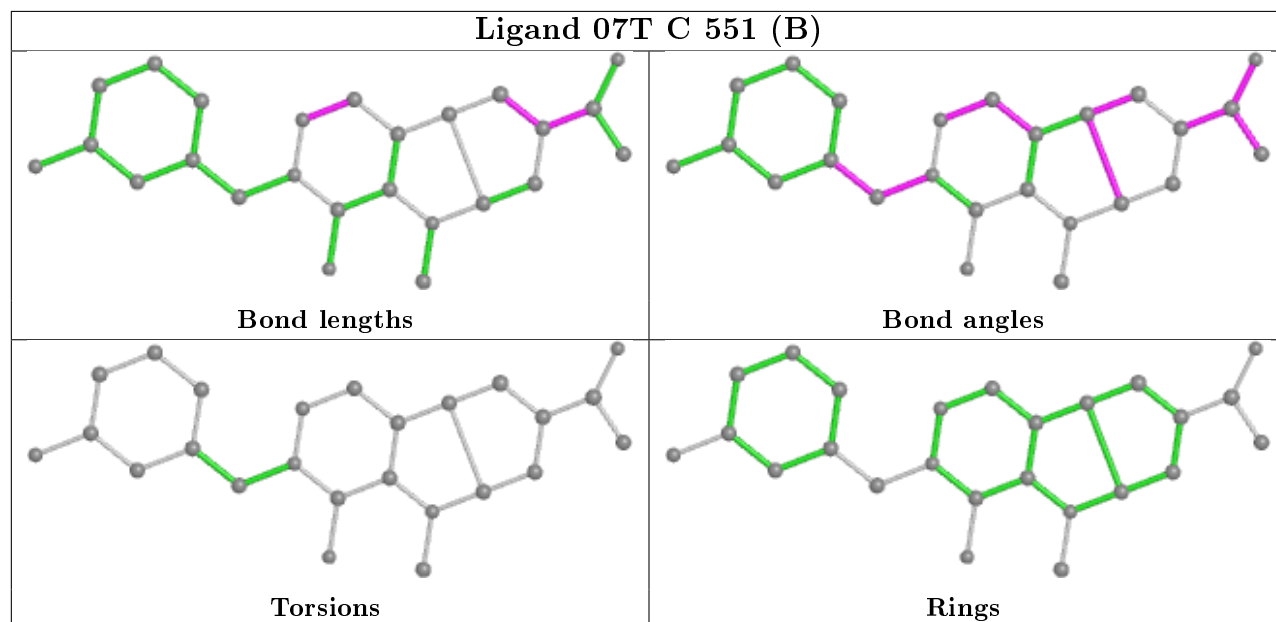
There are no ring outliers.

4 monomers are involved in 8 short contacts:

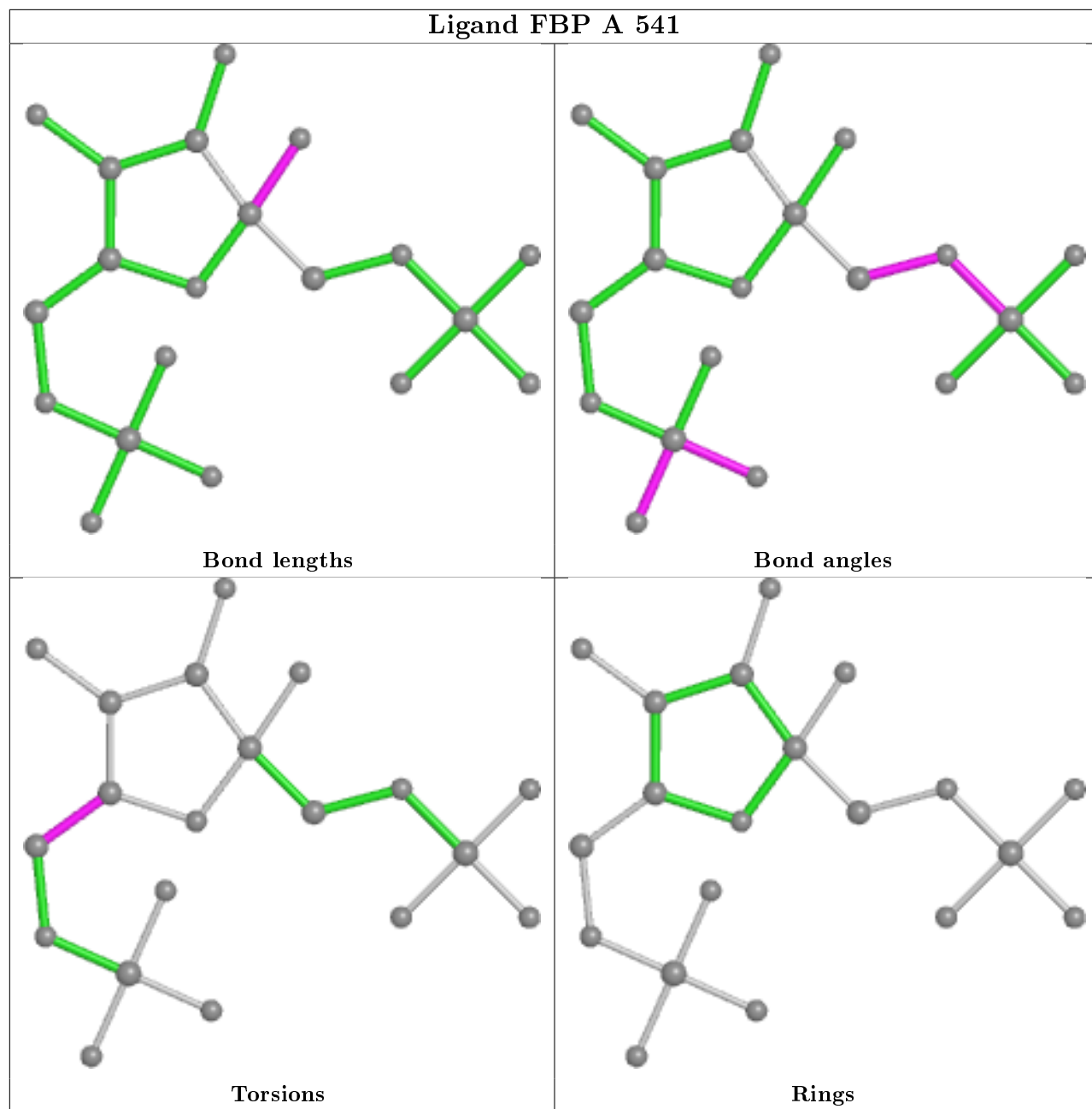
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	551[B]	07T	2	0
4	B	551[B]	07T	2	0
4	B	551[A]	07T	1	0
4	C	551[A]	07T	3	0

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

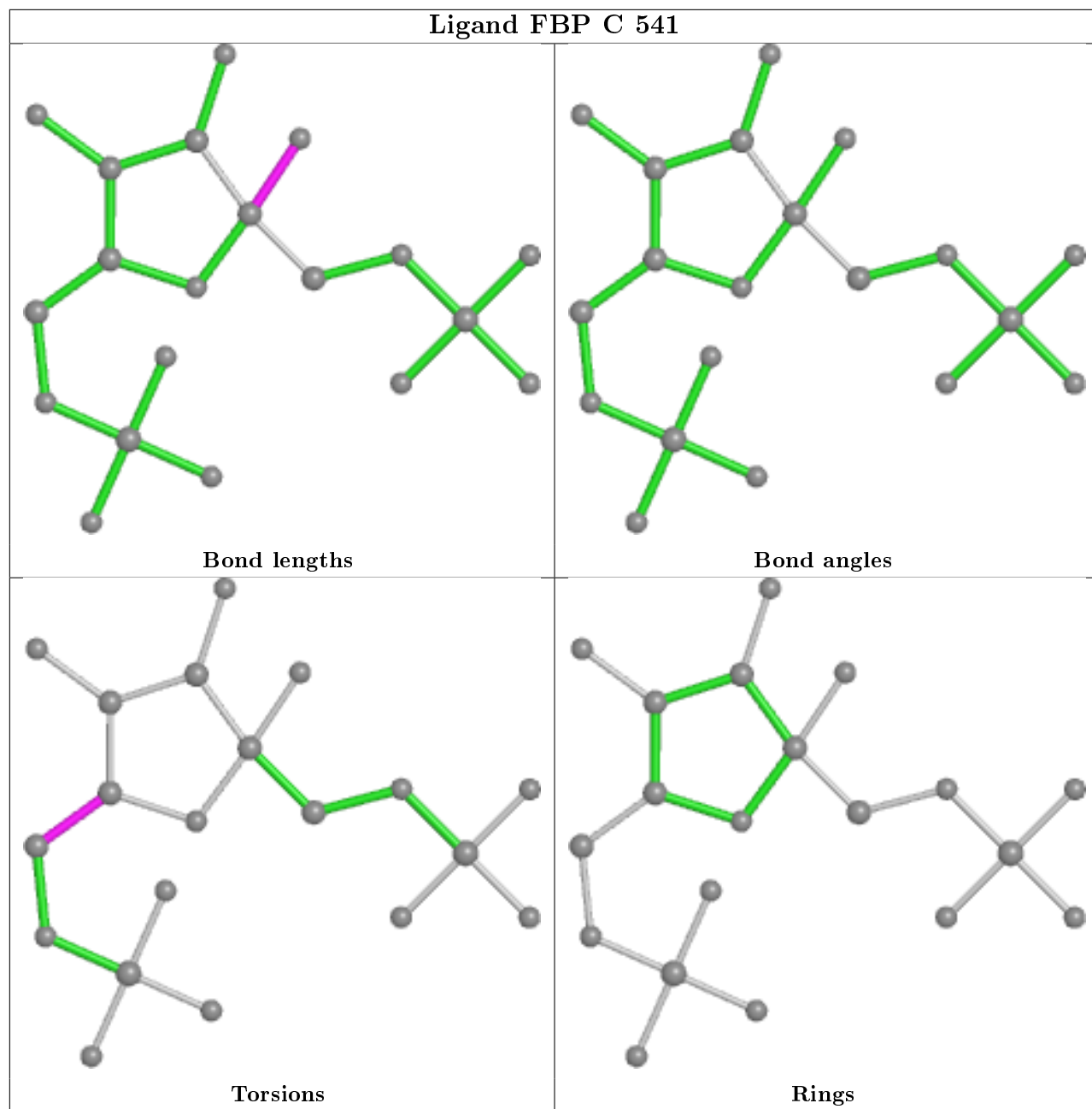
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



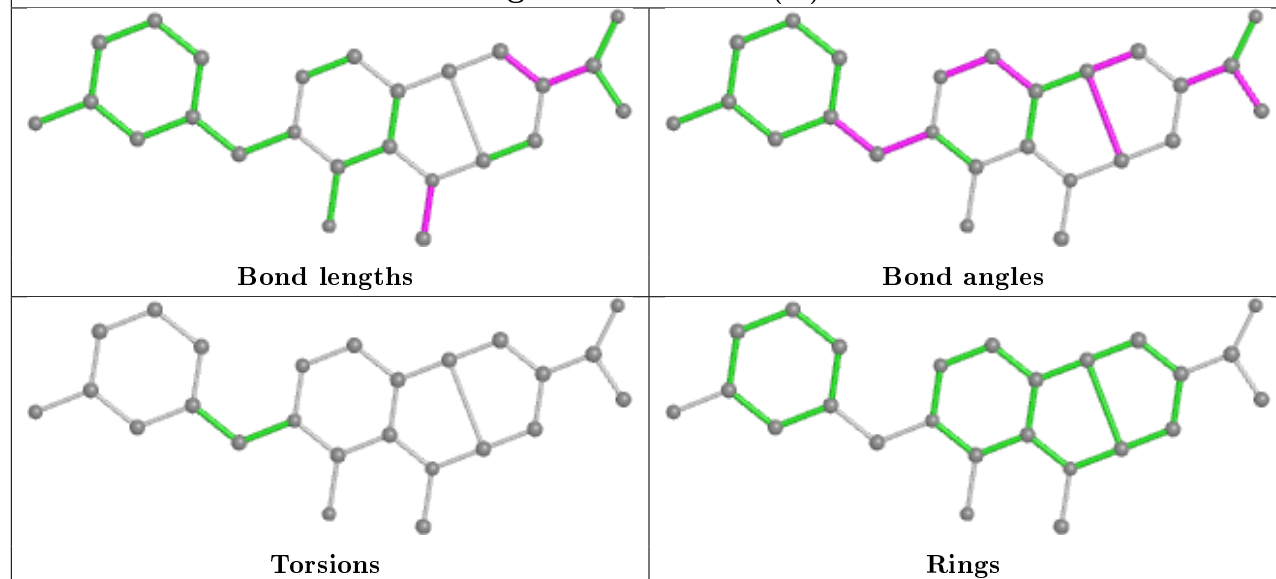
Ligand FBP A 541



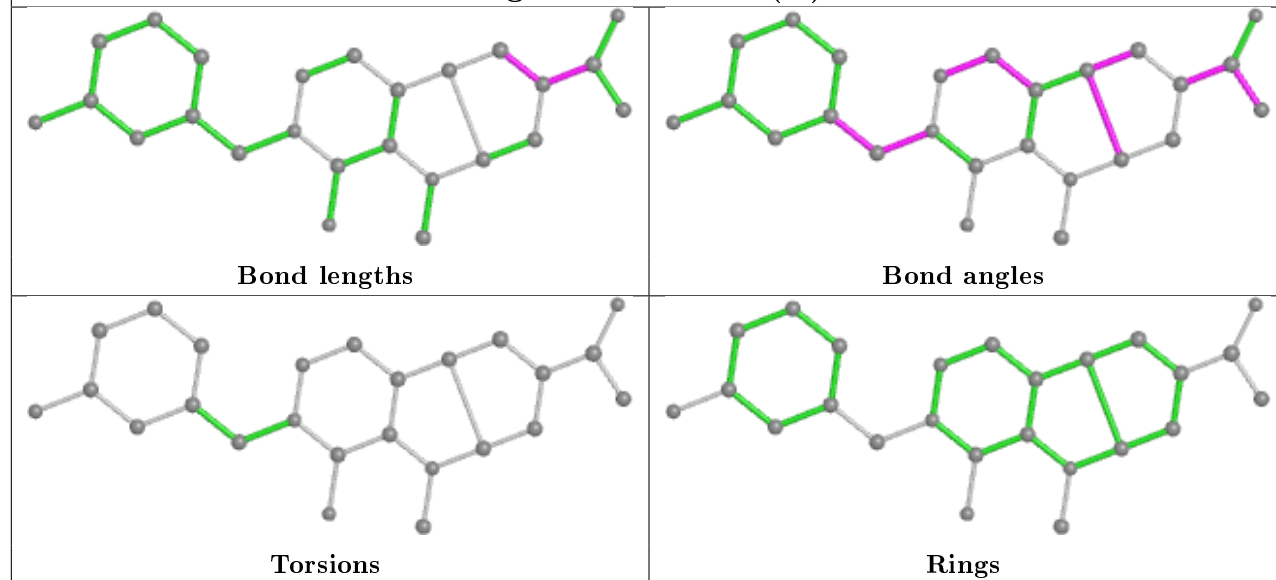
Ligand FBP C 541



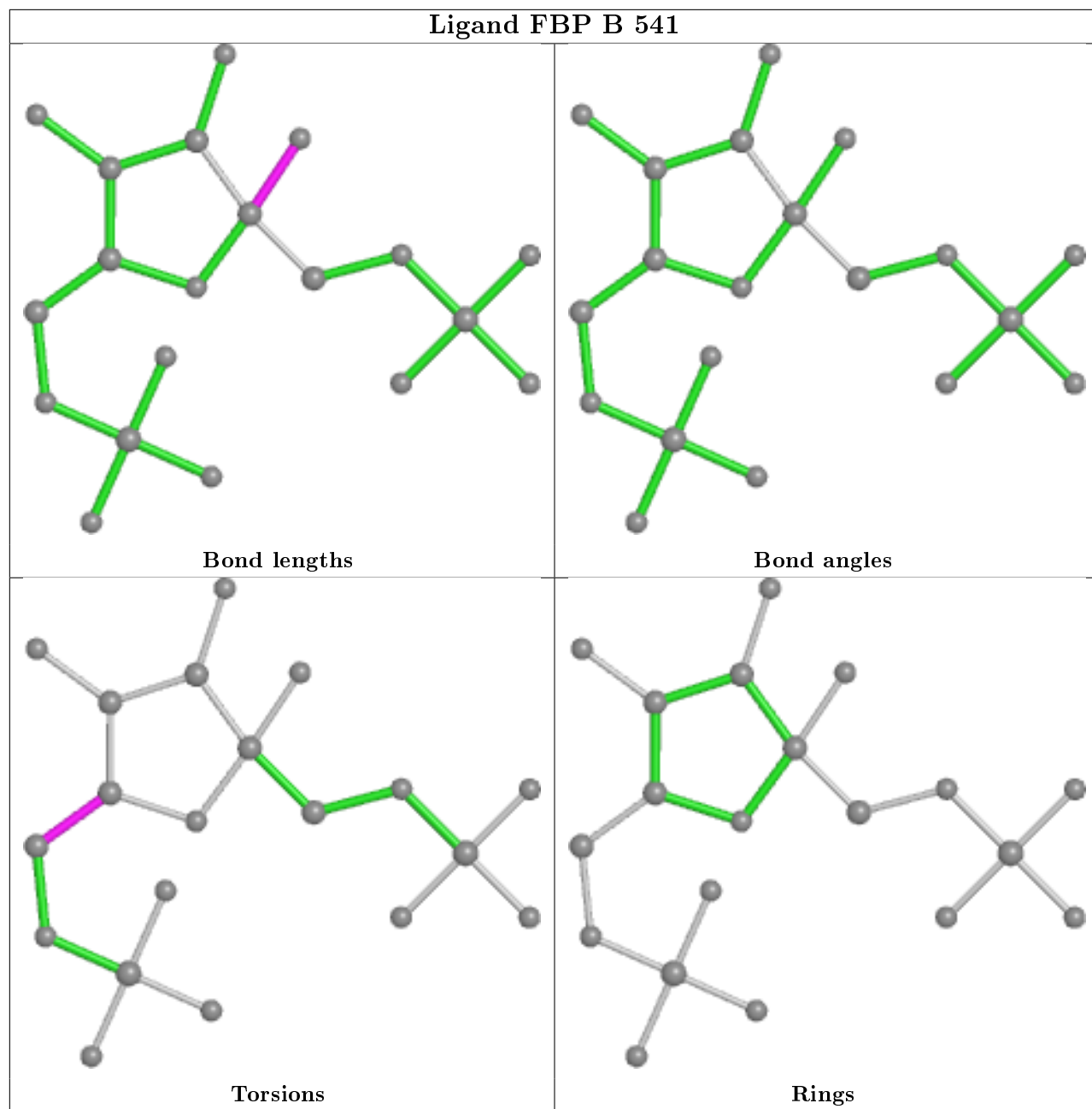
Ligand 07T B 551 (B)



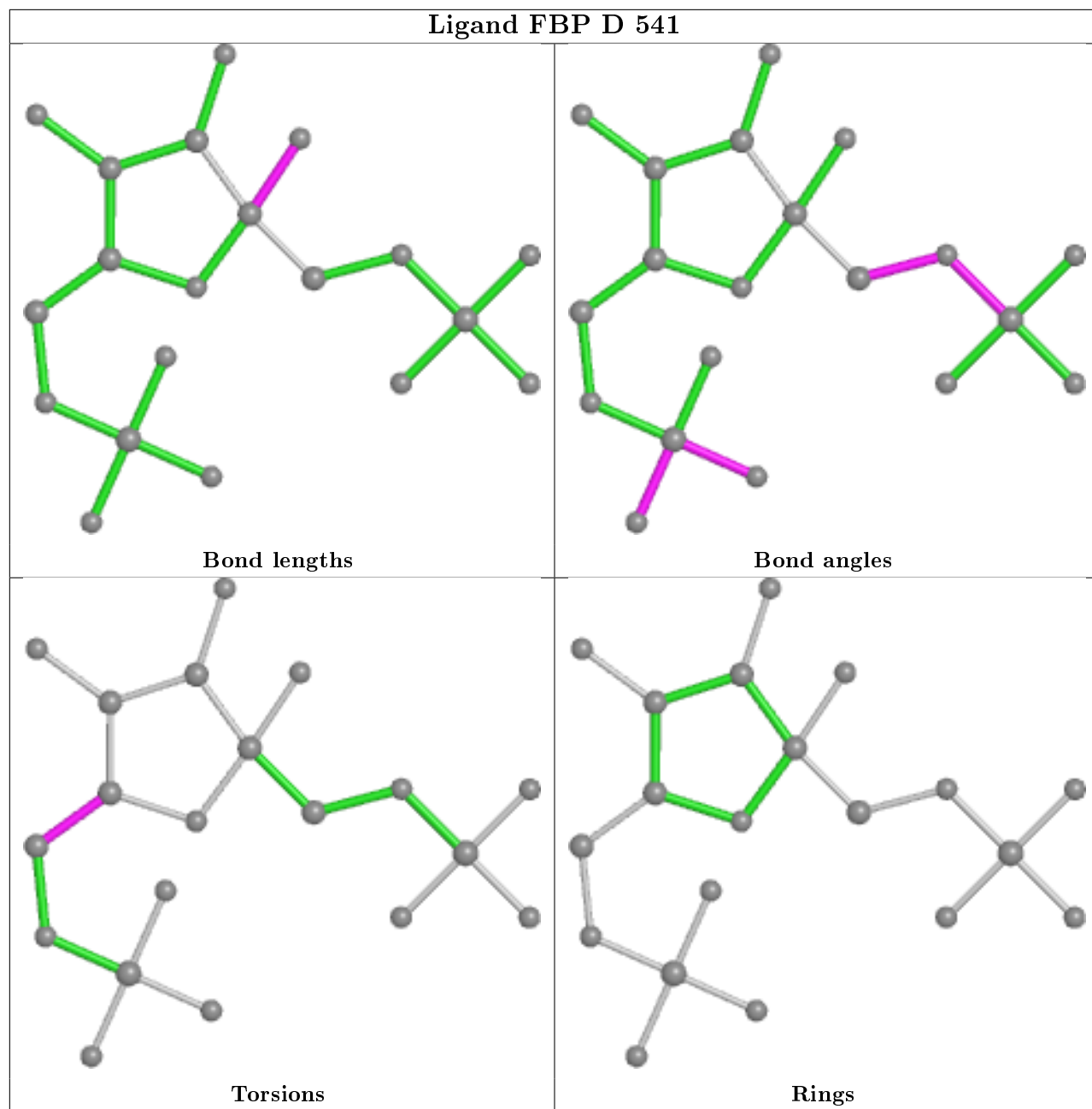
Ligand 07T B 551 (A)

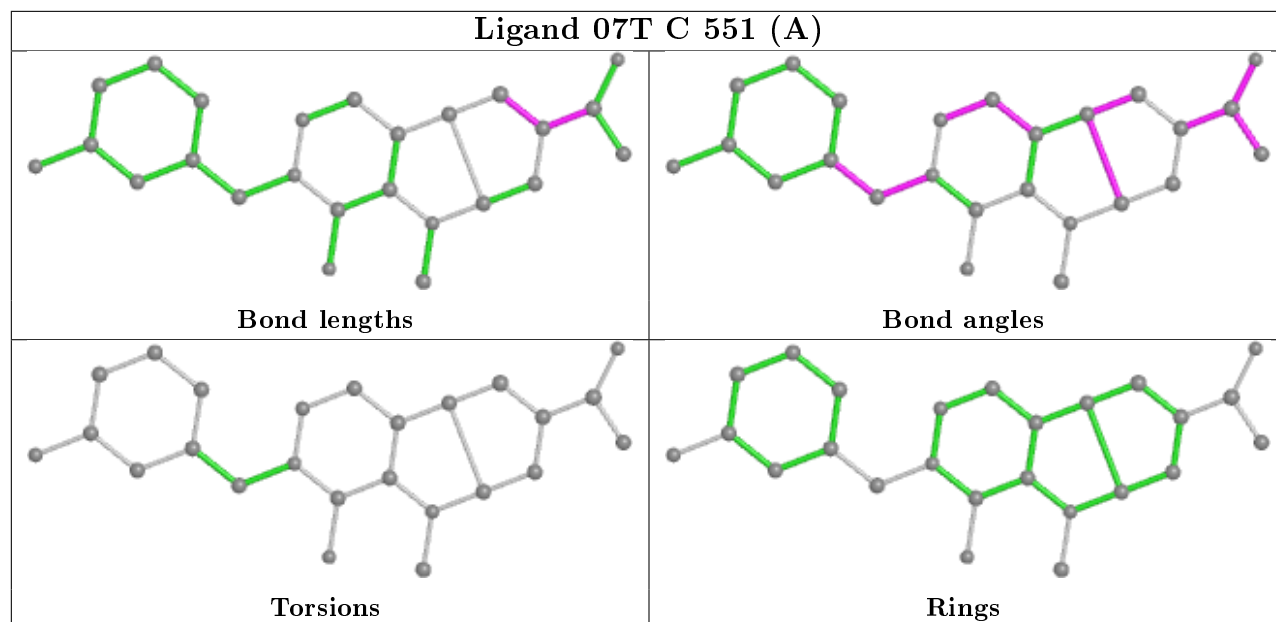


Ligand FBP B 541



Ligand FBP D 541





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, 95th 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 ²)	Q<0.9
1	A	519/533 (97%)	-0.02	25 (4%)	30	36	18, 30, 68, 83	0
1	B	514/533 (96%)	0.15	42 (8%)	11	15	17, 33, 75, 93	1 (0%)
1	C	517/533 (96%)	0.14	27 (5%)	27	32	19, 34, 59, 72	0
1	D	513/533 (96%)	0.08	24 (4%)	31	37	17, 30, 63, 81	3 (0%)
All	All	2063/2132 (96%)	0.09	118 (5%)	23	29	17, 32, 67, 93	4 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	13	ILE	6.0
1	B	190	ALA	5.9
1	C	215	ALA	5.9
1	C	140	LEU	5.9
1	B	138	ALA	5.7
1	C	165	CYS	5.7
1	B	144	LEU	5.3
1	B	142	ILE	5.1
1	A	192	PHE	5.1
1	B	123	LEU	4.8
1	B	203	LEU	4.7
1	D	152	CYS	4.7
1	D	148	TYR	4.7
1	C	195	THR	4.7
1	B	156	ILE	4.7
1	D	192	PHE	4.7
1	C	214	ALA	4.3
1	B	197	VAL	4.3
1	B	170	VAL	4.2
1	C	216	VAL	4.2
1	A	183	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	134	LEU	4.1
1	B	194	VAL	4.1
1	B	137	GLY	4.1
1	B	152	CYS	4.1
1	C	164	ILE	4.1
1	B	193	LEU	4.0
1	C	139	THR	3.9
1	B	192	PHE	3.9
1	A	185	VAL	3.9
1	B	158	TRP	3.9
1	A	190	ALA	3.9
1	B	140	LEU	3.9
1	C	190	ALA	3.9
1	D	123	LEU	3.9
1	D	191	ASP	3.9
1	A	170	VAL	3.8
1	A	163	ASN	3.7
1	C	404	ILE	3.7
1	A	213[A]	GLY	3.7
1	A	214	ALA	3.7
1	B	147	ALA	3.6
1	C	142	ILE	3.5
1	D	193	LEU	3.5
1	B	143	THR	3.5
1	B	165	CYS	3.3
1	B	139	THR	3.3
1	B	181	ILE	3.3
1	B	183	LEU	3.3
1	D	189	GLY	3.2
1	B	41	THR	3.2
1	D	147	ALA	3.2
1	B	195	THR	3.2
1	D	140	LEU	3.1
1	A	159	LEU	3.1
1	D	124	ILE	3.1
1	D	125	LYS	3.1
1	B	122	GLY	3.1
1	A	148	TYR	3.0
1	A	13	ILE	2.9
1	B	153	ASP	2.9
1	A	168	VAL	2.9
1	B	149	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	140	LEU	2.9
1	C	213[A]	GLY	2.9
1	A	143	THR	2.9
1	A	531	PRO	2.9
1	C	244	PHE	2.8
1	B	141	LYS	2.8
1	D	138	ALA	2.8
1	C	157	LEU	2.8
1	A	186	LYS	2.8
1	B	191	ASP	2.8
1	B	184	GLN	2.8
1	A	191	ASP	2.7
1	B	531	PRO	2.7
1	C	143	THR	2.7
1	B	159	LEU	2.7
1	D	155	ASN	2.7
1	C	174	ILE	2.7
1	A	139	THR	2.7
1	B	199	ASN	2.6
1	B	164	ILE	2.5
1	D	157	LEU	2.5
1	C	200	GLY	2.5
1	A	171	GLY	2.5
1	C	152	CYS	2.5
1	D	100	SER	2.4
1	D	137	GLY	2.4
1	B	157	LEU	2.4
1	A	174	ILE	2.4
1	B	182	SER	2.4
1	C	168	VAL	2.3
1	C	194	VAL	2.3
1	B	146	ASN	2.3
1	B	155	ASN	2.3
1	A	169	GLU	2.3
1	B	130	ALA	2.2
1	C	187	GLN	2.2
1	B	404	ILE	2.2
1	A	189	GLY	2.2
1	C	401	LEU	2.1
1	C	175	TYR	2.1
1	D	149	MET	2.1
1	C	183	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	122	GLY	2.1
1	B	124	ILE	2.1
1	C	218	LEU	2.1
1	C	217	ASP	2.1
1	D	194	VAL	2.1
1	D	143	THR	2.1
1	D	351	ALA	2.1
1	A	137	GLY	2.0
1	A	195	THR	2.0
1	C	146	ASN	2.0
1	A	215	ALA	2.0
1	D	101	ASP	2.0
1	D	145	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 95th 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(\AA^2)	Q<0.9
3	UNX	A	537	1/1	0.69	0.15	30,30,30,30	0
3	UNX	B	532	1/1	0.70	0.16	30,30,30,30	0
3	UNX	C	534	1/1	0.78	0.26	30,30,30,30	0
3	UNX	C	535	1/1	0.80	0.42	30,30,30,30	0
3	UNX	D	533	1/1	0.82	0.61	30,30,30,30	0
3	UNX	B	533	1/1	0.83	0.40	30,30,30,30	0
3	UNX	A	534	1/1	0.83	0.23	30,30,30,30	0
3	UNX	A	533	1/1	0.86	0.10	30,30,30,30	0
3	UNX	D	534	1/1	0.86	0.10	30,30,30,30	0
3	UNX	B	536	1/1	0.86	0.20	30,30,30,30	0

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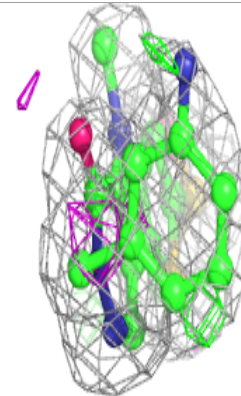
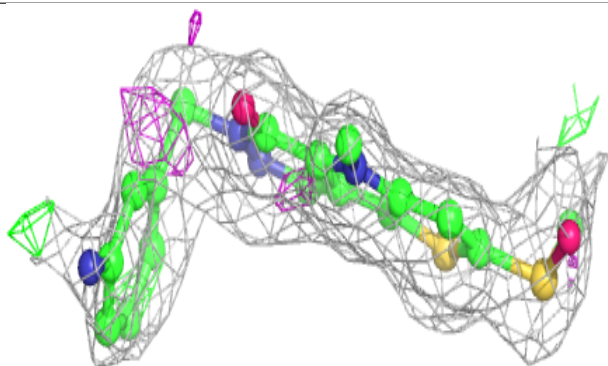
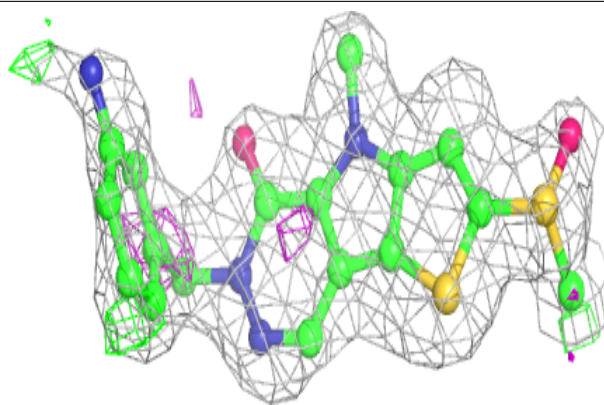
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	A	535	1/1	0.86	0.43	30,30,30,30	0
3	UNX	A	536	1/1	0.86	0.17	30,30,30,30	0
3	UNX	D	537	1/1	0.88	0.22	30,30,30,30	0
3	UNX	D	532	1/1	0.91	0.30	30,30,30,30	0
3	UNX	B	534	1/1	0.92	0.27	30,30,30,30	0
3	UNX	C	532	1/1	0.92	0.17	30,30,30,30	0
3	UNX	C	533	1/1	0.93	0.32	30,30,30,30	0
4	07T	B	551[A]	25/25	0.94	0.15	14,22,28,31	25
4	07T	B	551[B]	25/25	0.94	0.15	17,21,33,36	25
3	UNX	B	535	1/1	0.94	0.28	30,30,30,30	0
4	07T	C	551[A]	25/25	0.95	0.13	14,23,29,32	25
4	07T	C	551[B]	25/25	0.95	0.13	14,22,33,36	25
2	FBP	C	541	20/20	0.98	0.09	27,38,43,45	0
2	FBP	B	541	20/20	0.98	0.09	21,26,30,32	0
3	UNX	A	532	1/1	0.98	0.49	30,30,30,30	0
2	FBP	A	541	20/20	0.98	0.07	21,31,33,34	0
2	FBP	D	541	20/20	0.98	0.09	19,24,27,28	0
3	UNX	D	535	1/1	0.99	0.35	30,30,30,30	0
3	UNX	D	536	1/1	0.99	0.23	30,30,30,30	0

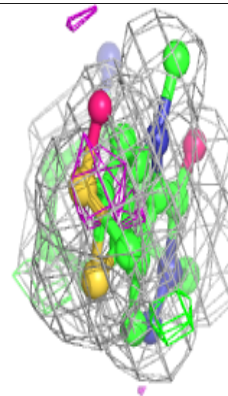
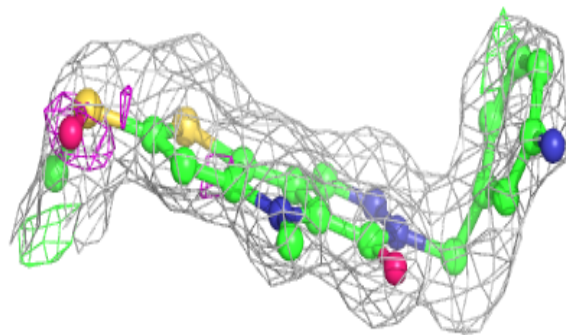
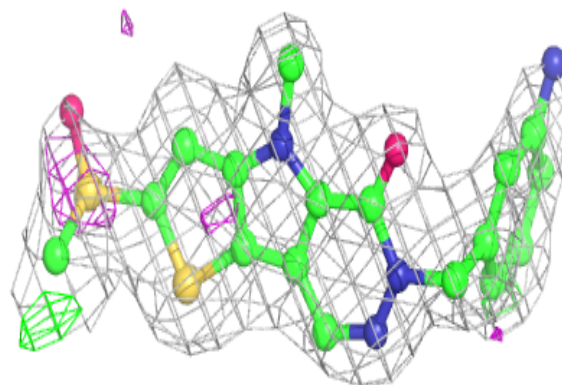
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 07T B 551 (A):

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

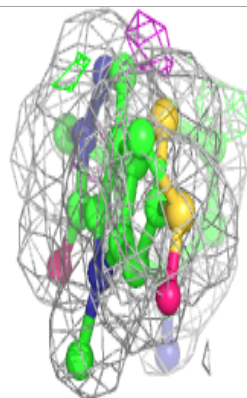
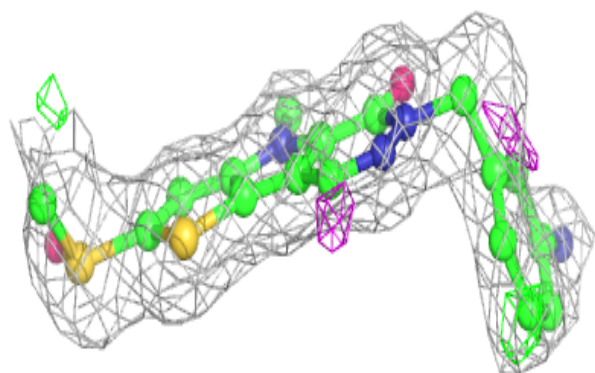
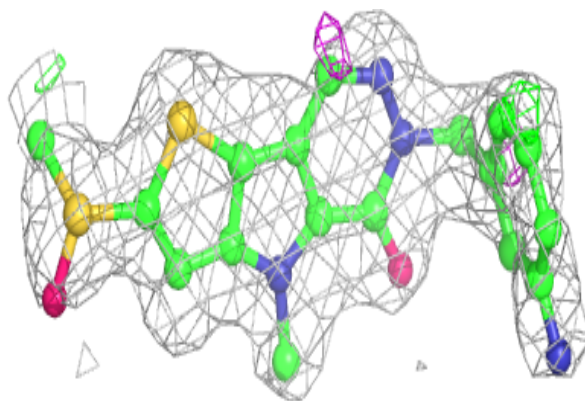
**Electron density around 07T B 551 (B):**

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

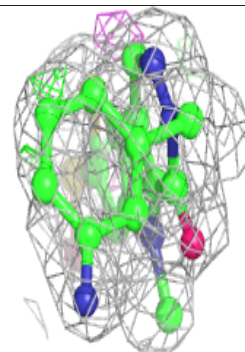
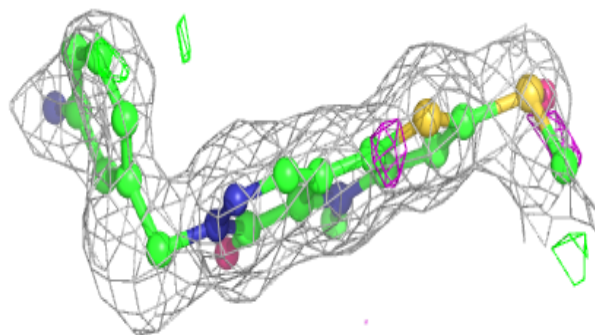
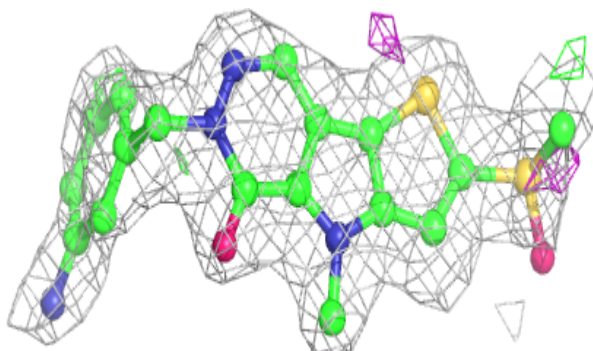


Electron density around 07T C 551 (A):

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

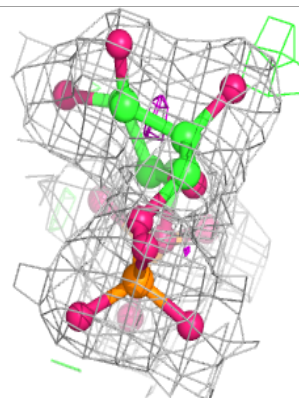
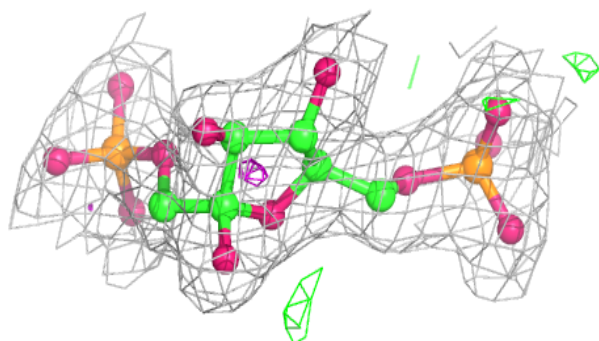
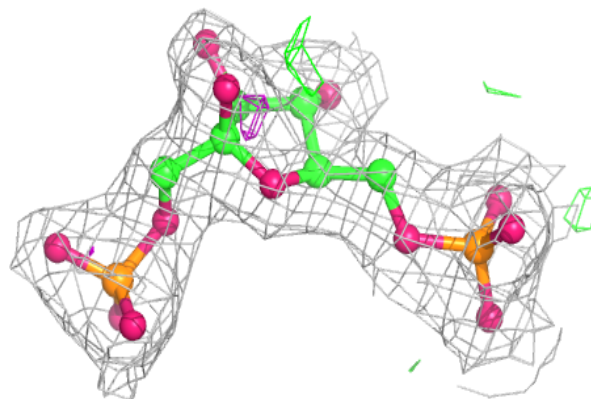
**Electron density around 07T C 551 (B):**

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

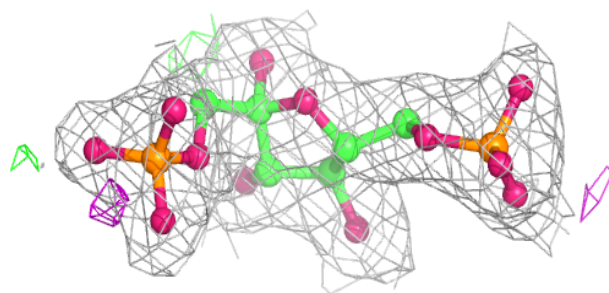
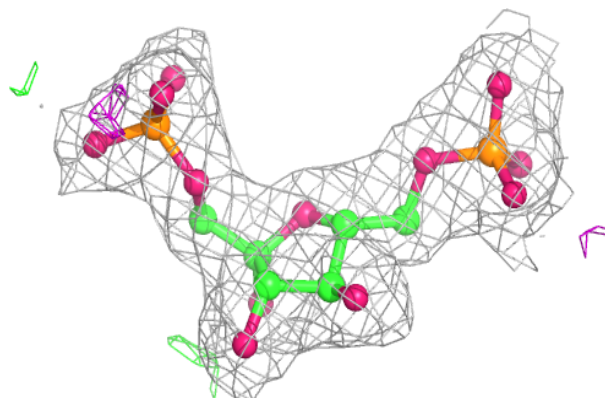


Electron density around FBP C 541:

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

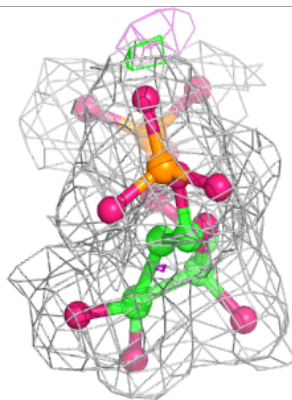
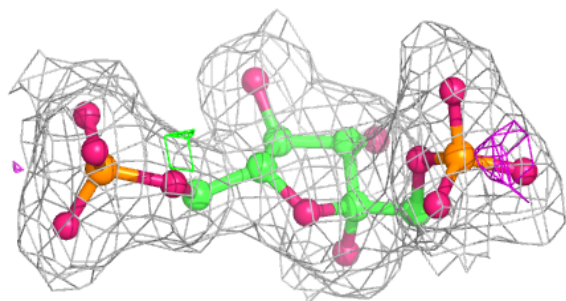
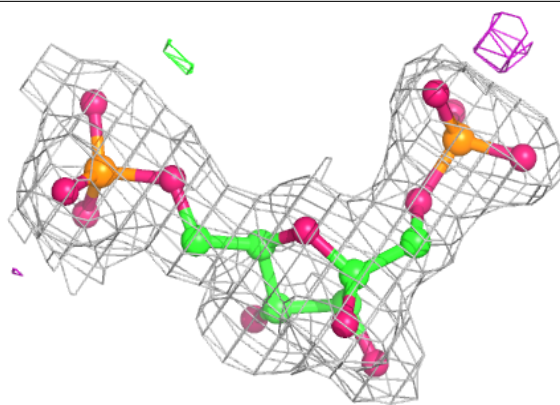
**Electron density around FBP B 541:**

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

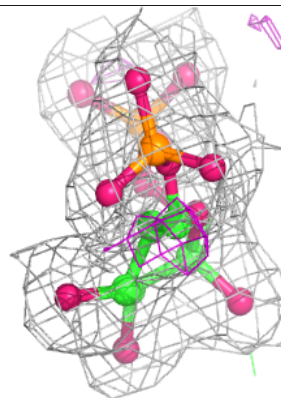
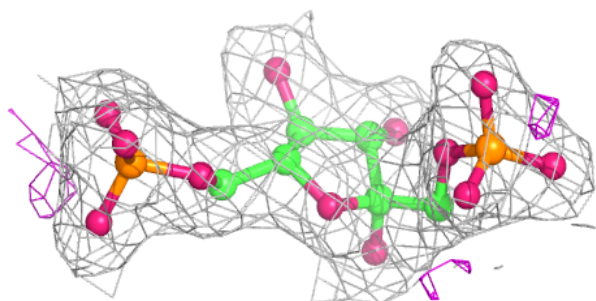
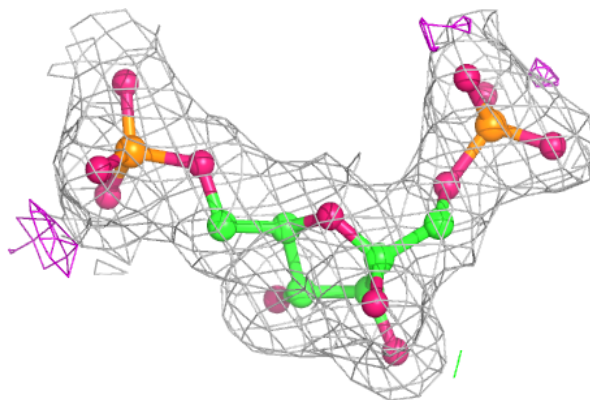


Electron density around FBP A 541:

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

**Electron density around FBP D 541:**

$2mF_o-DF_c$ (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.