



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 07:25 AM BST

PDB ID : 3H6O
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.; Bochkarev, A.; Inglese, J.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2009-04-23
Resolution : 2.00 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

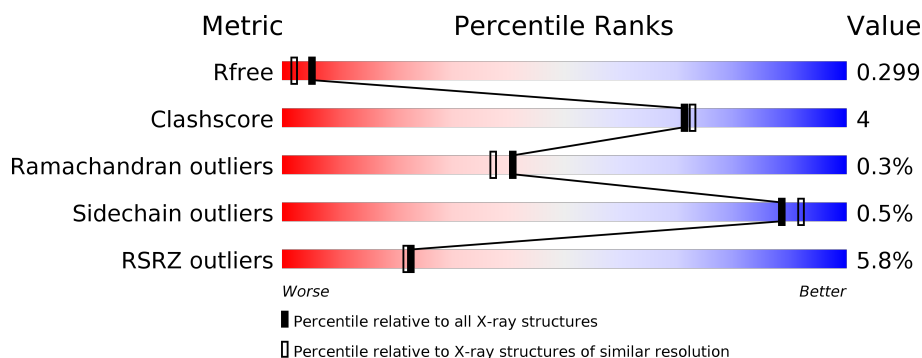
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	550	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>11%</div> </div> </div>
1	B	550	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>
1	C	550	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>5%</div> <div>15%</div> </div> </div>
1	D	550	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>8%</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
3	UNX	A	532	-	-	-	X
3	UNX	A	533	-	-	-	X
3	UNX	A	534	-	-	-	X
3	UNX	A	535	-	-	-	X
3	UNX	A	536	-	-	-	X
3	UNX	A	537	-	-	-	X
3	UNX	A	538	-	-	-	X
3	UNX	A	539	-	-	-	X
3	UNX	A	540	-	-	-	X
3	UNX	A	542	-	-	-	X
3	UNX	A	543	-	-	-	X
3	UNX	B	532	-	-	-	X
3	UNX	B	533	-	-	-	X
3	UNX	B	534	-	-	-	X
3	UNX	B	535	-	-	-	X
3	UNX	B	537	-	-	-	X
3	UNX	B	538	-	-	-	X
3	UNX	B	539	-	-	-	X
3	UNX	B	540	-	-	-	X
3	UNX	C	532	-	-	-	X
3	UNX	C	533	-	-	-	X
3	UNX	C	534	-	-	-	X
3	UNX	C	535	-	-	-	X
3	UNX	D	532	-	-	-	X
3	UNX	D	533	-	-	-	X
3	UNX	D	534	-	-	-	X
3	UNX	D	535	-	-	-	X
3	UNX	D	537	-	-	-	X
3	UNX	D	538	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15269 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	490	Total	C	N	O	S	0	1	0
			3676	2309	658	685	24			
1	B	513	Total	C	N	O	S	0	0	0
			3812	2391	672	725	24			
1	C	468	Total	C	N	O	S	0	0	0
			3497	2202	620	652	23			
1	D	507	Total	C	N	O	S	0	4	0
			3776	2376	673	703	24			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P14618
A	-17	GLY	-	expression tag	UNP P14618
A	-16	SER	-	expression tag	UNP P14618
A	-15	SER	-	expression tag	UNP P14618
A	-14	HIS	-	expression tag	UNP P14618
A	-13	HIS	-	expression tag	UNP P14618
A	-12	HIS	-	expression tag	UNP P14618
A	-11	HIS	-	expression tag	UNP P14618
A	-10	HIS	-	expression tag	UNP P14618
A	-9	HIS	-	expression tag	UNP P14618
A	-8	SER	-	expression tag	UNP P14618
A	-7	SER	-	expression tag	UNP P14618
A	-6	GLY	-	expression tag	UNP P14618
A	-5	LEU	-	expression tag	UNP P14618
A	-4	VAL	-	expression tag	UNP P14618
A	-3	PRO	-	expression tag	UNP P14618
A	-2	ARG	-	expression tag	UNP P14618
A	-1	GLY	-	expression tag	UNP P14618
A	0	SER	-	expression tag	UNP P14618
B	-18	MET	-	expression tag	UNP P14618
B	-17	GLY	-	expression tag	UNP P14618

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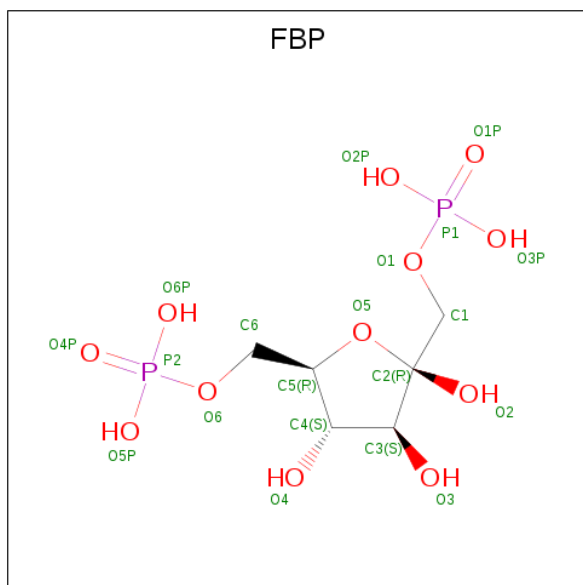
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	UNP P14618
B	-9	HIS	-	expression tag	UNP P14618
B	-8	SER	-	expression tag	UNP P14618
B	-7	SER	-	expression tag	UNP P14618
B	-6	GLY	-	expression tag	UNP P14618
B	-5	LEU	-	expression tag	UNP P14618
B	-4	VAL	-	expression tag	UNP P14618
B	-3	PRO	-	expression tag	UNP P14618
B	-2	ARG	-	expression tag	UNP P14618
B	-1	GLY	-	expression tag	UNP P14618
B	0	SER	-	expression tag	UNP P14618
C	-18	MET	-	expression tag	UNP P14618
C	-17	GLY	-	expression tag	UNP P14618
C	-16	SER	-	expression tag	UNP P14618
C	-15	SER	-	expression tag	UNP P14618
C	-14	HIS	-	expression tag	UNP P14618
C	-13	HIS	-	expression tag	UNP P14618
C	-12	HIS	-	expression tag	UNP P14618
C	-11	HIS	-	expression tag	UNP P14618
C	-10	HIS	-	expression tag	UNP P14618
C	-9	HIS	-	expression tag	UNP P14618
C	-8	SER	-	expression tag	UNP P14618
C	-7	SER	-	expression tag	UNP P14618
C	-6	GLY	-	expression tag	UNP P14618
C	-5	LEU	-	expression tag	UNP P14618
C	-4	VAL	-	expression tag	UNP P14618
C	-3	PRO	-	expression tag	UNP P14618
C	-2	ARG	-	expression tag	UNP P14618
C	-1	GLY	-	expression tag	UNP P14618
C	0	SER	-	expression tag	UNP P14618
D	-18	MET	-	expression tag	UNP P14618
D	-17	GLY	-	expression tag	UNP P14618
D	-16	SER	-	expression tag	UNP P14618
D	-15	SER	-	expression tag	UNP P14618
D	-14	HIS	-	expression tag	UNP P14618
D	-13	HIS	-	expression tag	UNP P14618

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP P14618
D	-11	HIS	-	expression tag	UNP P14618
D	-10	HIS	-	expression tag	UNP P14618
D	-9	HIS	-	expression tag	UNP P14618
D	-8	SER	-	expression tag	UNP P14618
D	-7	SER	-	expression tag	UNP P14618
D	-6	GLY	-	expression tag	UNP P14618
D	-5	LEU	-	expression tag	UNP P14618
D	-4	VAL	-	expression tag	UNP P14618
D	-3	PRO	-	expression tag	UNP P14618
D	-2	ARG	-	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: $C_6H_{14}O_{12}P_2$).

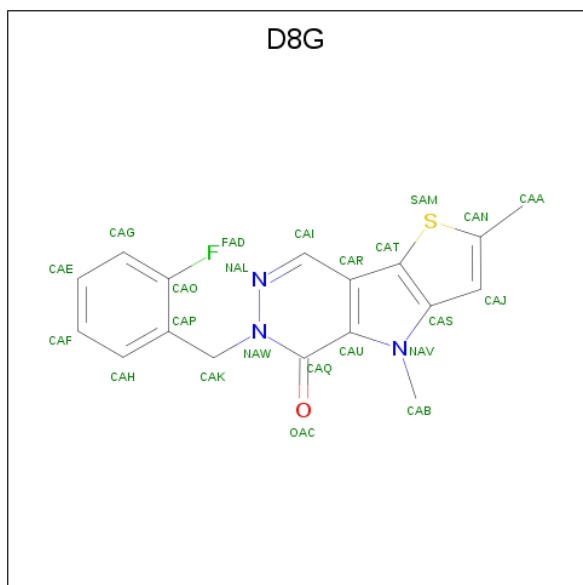


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	9	Total X 9 9	0	0
3	A	11	Total X 11 11	0	0
3	D	7	Total X 7 7	0	0
3	C	4	Total X 4 4	0	0

- Molecule 4 is 6-(2-fluorobenzyl)-2,4-dimethyl-4,6-dihydro-5H-thieno[2',3':4,5]pyrrolo[2,3-d]pyridazin-5-one (three-letter code: D8G) (formula: C₁₇H₁₄FN₃OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C F N O S 46 34 2 6 2 2	0	1
4	C	1	Total C F N O S 46 34 2 6 2 2	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	98	Total O 98 98	0	0
5	B	107	Total O 107 107	0	0

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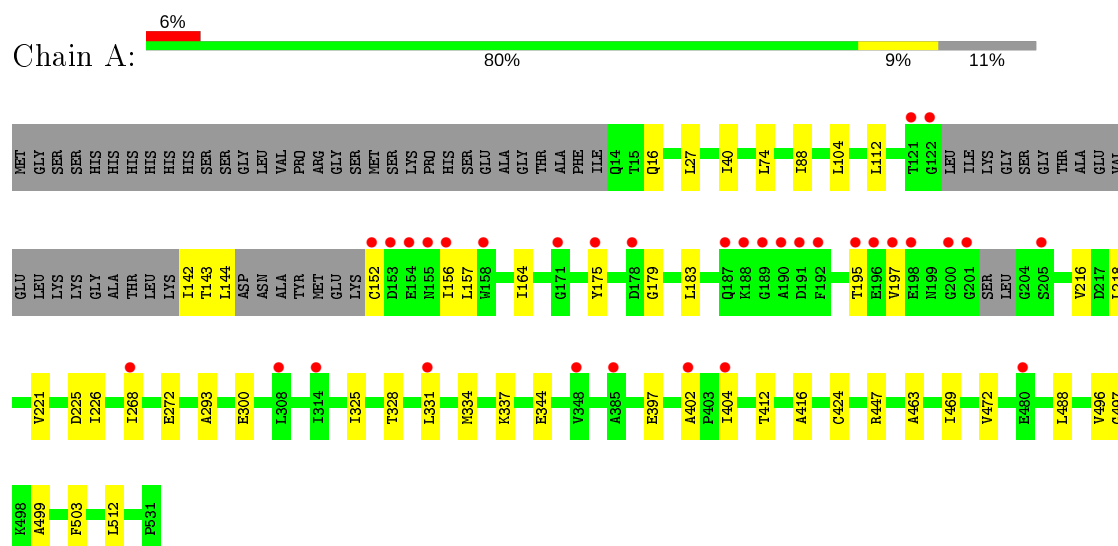
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	45	Total	O	0	0
			45	45		
5	D	55	Total	O	0	0
			55	55		

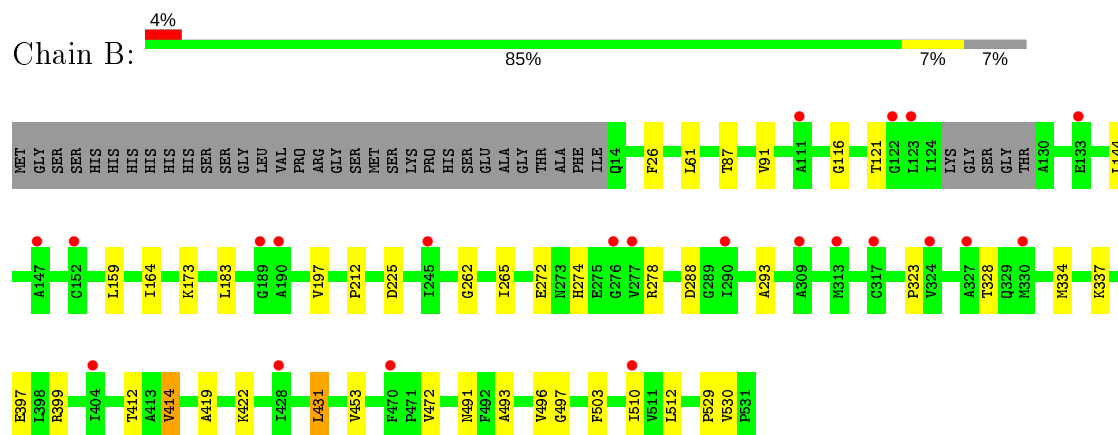
3 Residue-property plots [i](#)

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.

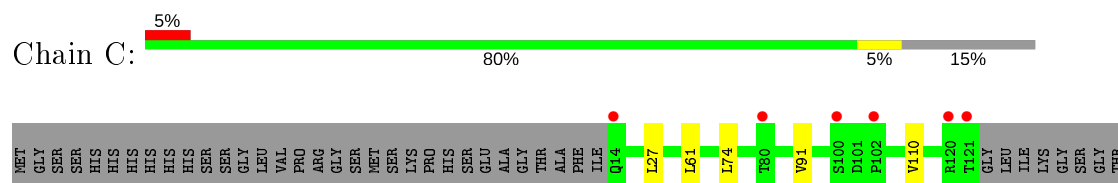
• Molecule 1: Pyruvate kinase isozymes M1/M2

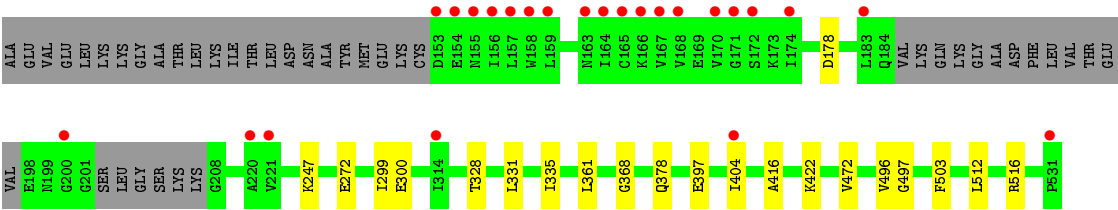


• Molecule 1: Pyruvate kinase isozymes M1/M2

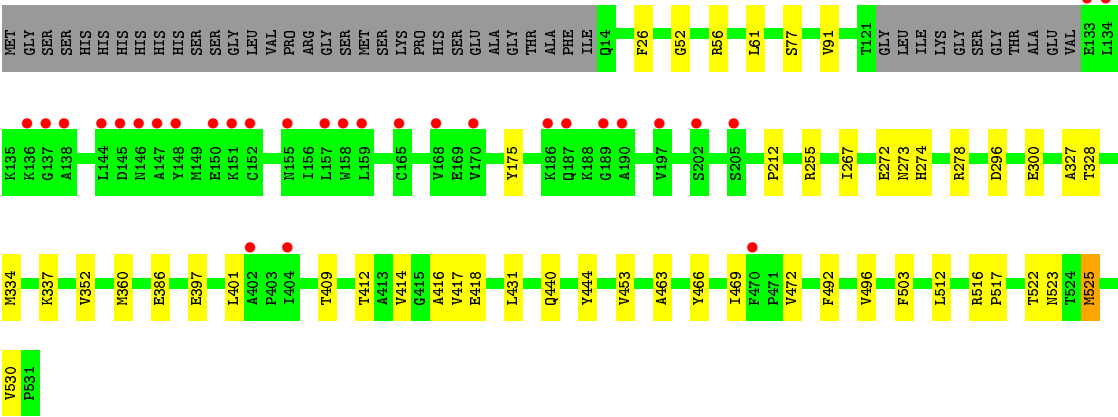
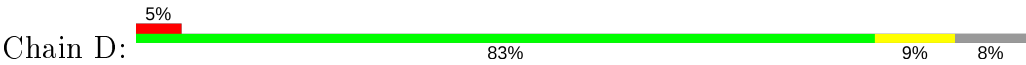


• Molecule 1: Pyruvate kinase isozymes M1/M2





● 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	81.34Å 155.69Å 101.79Å 90.00° 108.04° 90.00°	Depositor
Resolution (Å)	19.96 – 2.00 19.96 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.96-2.00) 94.2 (19.96-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.247 , 0.287 0.271 , 0.299	Depositor DCC
R_{free} test set	1859 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15269	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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, D8G, 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	0.62	0/3738	0.60	0/5061
1	B	0.61	0/3874	0.61	0/5252
1	C	0.49	0/3555	0.54	0/4816
1	D	0.52	0/3851	0.55	0/5223
All	All	0.56	0/15018	0.58	0/20352

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	3676	0	3640	34	0
1	B	3812	0	3720	27	0
1	C	3497	0	3442	16	0
1	D	3776	0	3696	34	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	0	0	0
3	C	4	0	0	0	0
3	D	7	0	0	0	0
4	B	46	0	28	4	0
4	C	46	0	28	4	0
5	A	98	0	0	0	0
5	B	107	0	0	0	0
5	C	45	0	0	0	0
5	D	55	0	0	1	0
All	All	15269	0	14594	104	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 (104) 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:A:144:LEU:HD11	1:A:164:ILE:HG22	1.72	0.71
1:D:463:ALA:HB1	1:D:469:ILE:HG21	1.78	0.66
1:D:472:VAL:HG11	1:D:496:VAL:HG11	1.82	0.62
1:A:416:ALA:HB2	1:A:512:LEU:HD21	1.81	0.61
1:A:16:GLN:HG3	1:A:40:ILE:HG23	1.84	0.58
1:D:274[B]:HIS:CE1	1:D:278:ARG:CG	2.86	0.58
4:C:550[B]:D8G:HAF	1:D:397:GLU:OE1	2.03	0.58
1:A:488:LEU:C	1:A:488:LEU:HD23	2.23	0.57
1:A:221:VAL:HG11	1:A:226:ILE:HD13	1.86	0.57
1:A:402:ALA:HB1	1:C:422:LYS:HE2	1.85	0.57
1:B:414:VAL:HG13	1:D:418:GLU:HG3	1.88	0.56
1:B:61:LEU:HD13	1:B:91:VAL:HA	1.88	0.56
1:B:121:THR:HG22	1:B:159:LEU:CD2	2.35	0.56
1:A:152:CYS:SG	1:A:157:LEU:HD12	2.46	0.56
1:C:335:ILE:HG23	1:C:368:GLY:HA2	1.88	0.55
1:B:397:GLU:OE1	4:B:550[B]:D8G:HAF	2.07	0.54
1:B:26:PHE:CZ	4:B:550[B]:D8G:HABB	2.43	0.54
1:D:416:ALA:CB	1:D:512:LEU:HD21	2.37	0.54
1:A:143:THR:HB	1:A:156:ILE:HD11	1.89	0.54
1:B:497:GLY:HA3	1:B:503:PHE:CZ	2.43	0.53
1:D:492:PHE:O	1:D:496:VAL:HG23	2.08	0.53
1:A:183:LEU:HD22	1:A:195:THR:OG1	2.09	0.53
1:B:183:LEU:CD2	1:B:197:VAL:HG22	2.39	0.53
1:B:453:VAL:HG21	1:B:493:ALA:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:CYS:HB2	1:C:404:ILE:HG21	1.91	0.53
1:D:466:TYR:HB2	1:D:469:ILE:HD12	1.91	0.52
1:A:472:VAL:HG11	1:A:496:VAL:HG11	1.91	0.52
1:B:116:GLY:HA2	1:B:225:ASP:OD2	2.10	0.52
1:D:412:THR:HG22	1:D:512:LEU:CD1	2.39	0.52
1:D:52:GLY:O	1:D:56:ARG:HG3	2.09	0.52
1:C:27:LEU:HD23	1:D:401:LEU:HD12	1.92	0.51
1:A:27:LEU:HD13	4:B:550[B]:D8G:HAE	1.92	0.51
1:D:175:TYR:CE1	1:D:212:PRO:HG3	2.46	0.51
1:D:409:THR:HG23	1:D:522:THR:HB	1.92	0.51
1:A:175:TYR:HB3	1:A:179:GLY:HA2	1.93	0.51
1:B:87:THR:O	1:B:91:VAL:HG23	2.12	0.51
1:D:409:THR:HG22	1:D:440:GLN:OE1	2.11	0.50
1:B:288:ASP:O	1:B:323:PRO:HD2	2.11	0.50
1:D:334:MET:HA	1:D:337:LYS:O	2.11	0.50
1:D:417:VAL:HG21	1:D:444:TYR:HB2	1.94	0.50
1:A:142:ILE:HA	1:A:157:LEU:O	2.12	0.50
1:A:463:ALA:HB1	1:A:469:ILE:HG21	1.94	0.49
1:C:497:GLY:HA3	1:C:503:PHE:CZ	2.46	0.49
1:A:412:THR:HG22	1:A:512:LEU:HD22	1.94	0.49
1:A:497:GLY:HA3	1:A:503:PHE:CZ	2.48	0.49
1:C:397:GLU:OE1	4:C:550[A]:D8G:HAF	2.13	0.48
1:A:183:LEU:HD21	1:A:197:VAL:HG22	1.94	0.48
1:A:331:LEU:HD23	1:A:344:GLU:HB3	1.95	0.48
1:D:412:THR:HG22	1:D:512:LEU:HD11	1.96	0.47
1:B:503:PHE:CD1	1:B:530:VAL:HG21	2.50	0.47
1:B:412:THR:HG22	1:B:512:LEU:HD22	1.96	0.47
1:D:272:GLU:OE1	1:D:296:ASP:OD2	2.33	0.46
1:D:273:ASN:HB2	5:D:573:HOH:O	2.15	0.46
1:D:397:GLU:O	1:D:401:LEU:HG	2.15	0.46
1:C:272:GLU:O	1:C:300:GLU:HG3	2.15	0.46
1:B:272:GLU:HG2	1:B:293:ALA:HB3	1.97	0.46
4:C:550[A]:D8G:HABA	1:D:26:PHE:CZ	2.50	0.46
1:A:397:GLU:OE1	4:B:550[A]:D8G:HAF	2.16	0.46
1:B:144:LEU:HD11	1:B:164:ILE:HG22	1.98	0.45
1:A:112:LEU:HD23	1:A:112:LEU:C	2.36	0.45
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.98	0.45
1:A:404:ILE:O	1:A:404:ILE:HG22	2.16	0.45
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.47	0.45
1:C:61:LEU:HD13	1:C:91:VAL:HA	1.98	0.45
1:B:262:GLY:CA	1:B:265:ILE:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:HD11	1:C:110:VAL:HG13	1.99	0.45
1:D:352:VAL:HG11	1:D:386:GLU:HG3	1.98	0.45
1:C:416:ALA:HB2	1:C:512:LEU:HD21	1.99	0.44
1:A:16:GLN:HG2	1:A:447[A]:ARG:NH1	2.33	0.44
1:B:121:THR:HG22	1:B:159:LEU:HD21	1.98	0.44
1:A:74:LEU:HD21	1:A:88:ILE:HG13	1.99	0.44
1:D:416:ALA:HB2	1:D:512:LEU:HD21	1.98	0.44
1:C:331:LEU:HD12	1:C:361:LEU:HD21	2.00	0.43
1:D:525:MET:HE2	1:D:525:MET:HB3	1.72	0.43
1:D:255:ARG:CZ	1:D:267:ILE:HD12	2.48	0.43
1:C:331:LEU:HD11	1:C:378:GLN:HG3	2.00	0.43
1:A:424:CYS:HB2	1:C:404:ILE:CG2	2.49	0.43
1:D:61:LEU:HD13	1:D:91:VAL:HA	2.00	0.43
1:A:221:VAL:HG13	1:A:225:ASP:HB3	2.00	0.43
1:A:272:GLU:HG2	1:A:293:ALA:HB3	2.01	0.43
1:A:268:ILE:HG21	1:A:325:ILE:HD12	2.01	0.42
1:A:334:MET:HA	1:A:337:LYS:O	2.18	0.42
1:B:274:HIS:CE1	1:B:278:ARG:CG	3.02	0.42
1:D:327:ALA:HB1	1:D:360:MET:CE	2.50	0.42
1:A:272:GLU:O	1:A:300:GLU:HG3	2.20	0.42
1:B:431:LEU:N	1:B:431:LEU:HD23	2.34	0.41
1:B:121:THR:HG22	1:B:159:LEU:HD23	2.03	0.41
1:A:104:LEU:HD21	1:A:499:ALA:HB1	2.02	0.41
1:C:178:ASP:HA	1:C:299:ILE:HD13	2.03	0.41
1:A:183:LEU:HD23	1:A:197:VAL:HA	2.00	0.41
1:B:334:MET:HA	1:B:337:LYS:O	2.19	0.41
1:D:272:GLU:O	1:D:300:GLU:HG3	2.21	0.41
1:B:419:ALA:HB3	1:B:510:ILE:HD13	2.03	0.41
1:B:422:LYS:HB2	1:D:414:VAL:HG11	2.02	0.41
1:D:516:ARG:HB2	1:D:517:PRO:HD2	2.03	0.41
1:A:488:LEU:HD23	1:A:488:LEU:O	2.21	0.41
1:C:472:VAL:HG11	1:C:496:VAL:HG11	2.03	0.41
1:D:431:LEU:HD22	1:D:453:VAL:HB	2.03	0.41
1:B:399:ARG:HD2	1:D:418:GLU:OE2	2.21	0.40
1:A:216:VAL:HG12	1:A:218:LEU:H	1.86	0.40
1:D:503:PHE:CD1	1:D:530:VAL:HG21	2.56	0.40
1:B:173:LYS:O	1:B:212:PRO:HD2	2.21	0.40
1:C:27:LEU:HD13	4:C:550[B]:D8G:HAE	2.02	0.40
1:D:175:TYR:CE1	1:D:212:PRO:CG	3.05	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	483/550 (88%)	468 (97%)	14 (3%)	1 (0%)	47	44
1	B	509/550 (92%)	499 (98%)	9 (2%)	1 (0%)	47	44
1	C	460/550 (84%)	447 (97%)	12 (3%)	1 (0%)	47	44
1	D	507/550 (92%)	494 (97%)	11 (2%)	2 (0%)	34	30
All	All	1959/2200 (89%)	1908 (97%)	46 (2%)	5 (0%)	41	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	THR
1	C	328	THR
1	D	328	THR
1	D	523	ASN
1	B	328	THR

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	376/452 (83%)	376 (100%)	0	100	100
1	B	385/452 (85%)	381 (99%)	4 (1%)	76	81
1	C	353/452 (78%)	351 (99%)	2 (1%)	86	90
1	D	377/452 (83%)	375 (100%)	2 (0%)	88	92
All	All	1491/1808 (82%)	1483 (100%)	8 (0%)	88	92

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	414	VAL
1	B	431	LEU
1	B	491	ASN
1	B	529	PRO
1	C	247	LYS
1	C	516	ARG
1	D	77	SER
1	D	525	MET

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	90	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 31 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	D8G	C	550[B]	-	18,26,26	1.54	2 (11%)	18,39,39	2.10	5 (27%)
4	D8G	B	550[A]	-	18,26,26	1.57	2 (11%)	18,39,39	2.01	6 (33%)
4	D8G	C	550[A]	-	18,26,26	1.30	1 (5%)	18,39,39	1.96	5 (27%)
2	FBP	B	541	-	18,20,20	0.93	1 (5%)	23,32,32	0.83	0
2	FBP	D	541	-	18,20,20	0.95	1 (5%)	23,32,32	0.83	0
2	FBP	A	541	-	18,20,20	0.92	1 (5%)	23,32,32	0.78	0
2	FBP	C	541	-	18,20,20	0.98	1 (5%)	23,32,32	0.88	2 (8%)
4	D8G	B	550[B]	-	18,26,26	1.78	1 (5%)	18,39,39	1.85	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	D8G	C	550[B]	-	-	2/3/4/4	0/4/4/4
4	D8G	B	550[A]	-	-	2/3/4/4	0/4/4/4
4	D8G	C	550[A]	-	-	2/3/4/4	0/4/4/4
2	FBP	B	541	-	-	3/13/32/32	0/1/1/1
2	FBP	D	541	-	-	2/13/32/32	0/1/1/1
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	D8G	B	550[B]	-	-	2/3/4/4	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	550[B]	D8G	CAN-SAM	-6.45	1.64	1.73
4	B	550[A]	D8G	CAN-SAM	-4.83	1.67	1.73
4	C	550[B]	D8G	CAN-SAM	-4.29	1.67	1.73
4	C	550[A]	D8G	CAN-SAM	-3.40	1.69	1.73
2	C	541	FBP	O2-C2	3.06	1.46	1.40
2	D	541	FBP	O2-C2	2.86	1.45	1.40
2	B	541	FBP	O2-C2	2.73	1.45	1.40
2	A	541	FBP	O2-C2	2.59	1.45	1.40
4	C	550[B]	D8G	CAI-NAL	2.31	1.33	1.31
4	B	550[A]	D8G	CAI-NAL	2.30	1.33	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	550[A]	D8G	CAA-CAN-SAM	5.36	125.79	119.88
4	C	550[B]	D8G	CAA-CAN-SAM	5.34	125.77	119.88
4	B	550[A]	D8G	CAA-CAN-SAM	4.61	124.96	119.88
4	C	550[B]	D8G	CAR-CAI-NAL	-3.63	120.42	124.78
4	B	550[A]	D8G	CAP-CAK-NAW	-3.60	103.87	112.83
4	B	550[B]	D8G	CAR-CAI-NAL	-3.55	120.52	124.78
4	B	550[B]	D8G	CAA-CAN-SAM	3.48	123.72	119.88
4	C	550[B]	D8G	CAS-CAT-SAM	-3.43	107.40	111.84
4	C	550[A]	D8G	CAR-CAI-NAL	-3.23	120.90	124.78
4	B	550[B]	D8G	CAP-CAK-NAW	-3.18	104.93	112.83
4	B	550[B]	D8G	CAS-CAT-SAM	-3.16	107.76	111.84
4	C	550[A]	D8G	CAP-CAK-NAW	-3.11	105.09	112.83
4	B	550[A]	D8G	CAR-CAI-NAL	-3.09	121.07	124.78
4	B	550[A]	D8G	CAS-CAT-SAM	-2.98	107.99	111.84
4	C	550[B]	D8G	CAP-CAK-NAW	-2.85	105.73	112.83
4	C	550[A]	D8G	CAS-CAT-SAM	-2.69	108.37	111.84
4	C	550[B]	D8G	CAK-CAP-CAO	2.55	124.46	121.23
4	B	550[A]	D8G	CAK-NAW-CAQ	2.37	121.86	118.17
4	B	550[B]	D8G	CAK-NAW-CAQ	2.21	121.61	118.17
4	C	550[A]	D8G	CAK-NAW-CAQ	2.14	121.50	118.17
4	B	550[A]	D8G	CAK-CAP-CAO	2.11	123.91	121.23
2	C	541	FBP	O6P-P2-O6	2.03	112.15	106.73
2	C	541	FBP	P1-O1-C1	2.01	123.82	118.30

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	550[B]	D8G	NAW-CAK-CAP-CAO
4	C	550[A]	D8G	NAW-CAK-CAP-CAH
4	C	550[A]	D8G	NAW-CAK-CAP-CAO
2	B	541	FBP	C4-C5-C6-O6
2	C	541	FBP	C4-C5-C6-O6
4	B	550[B]	D8G	NAW-CAK-CAP-CAH
4	B	550[B]	D8G	NAW-CAK-CAP-CAO
4	B	550[A]	D8G	NAW-CAK-CAP-CAO
2	D	541	FBP	C4-C5-C6-O6
2	A	541	FBP	C4-C5-C6-O6
2	C	541	FBP	O5-C5-C6-O6
2	A	541	FBP	O5-C5-C6-O6
2	B	541	FBP	O5-C5-C6-O6
2	D	541	FBP	O5-C5-C6-O6
4	C	550[B]	D8G	NAW-CAK-CAP-CAH

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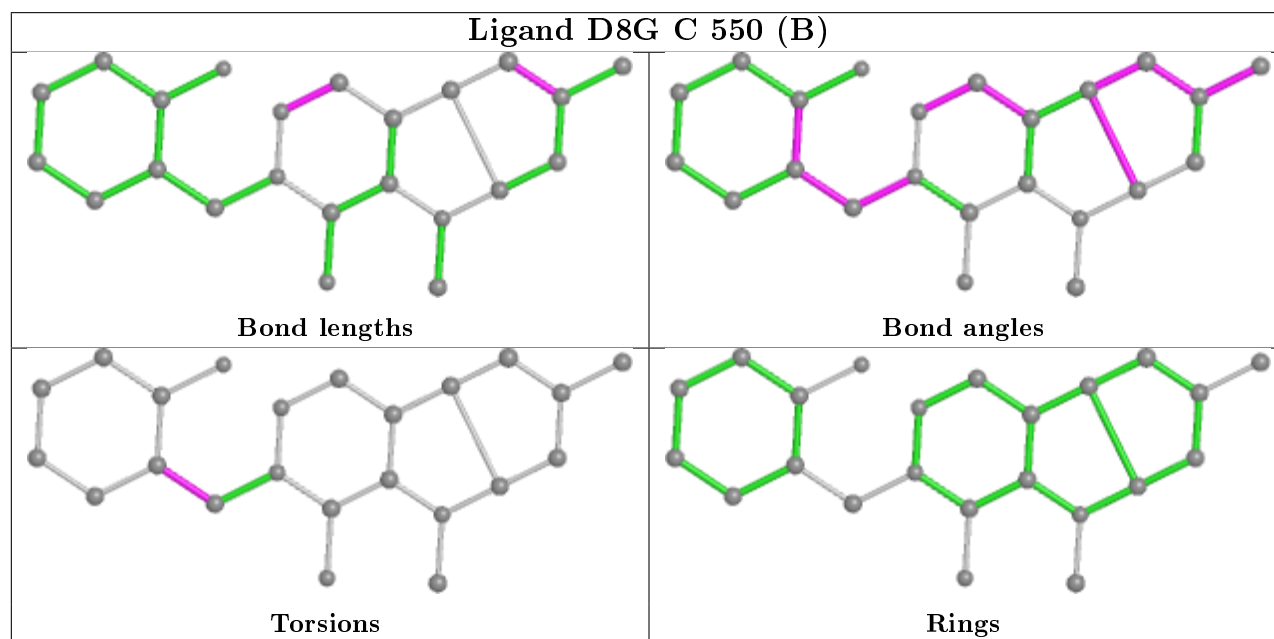
Mol	Chain	Res	Type	Atoms
4	B	550[A]	D8G	NAW-CAK-CAP-CAH
2	B	541	FBP	O1-C1-C2-O5

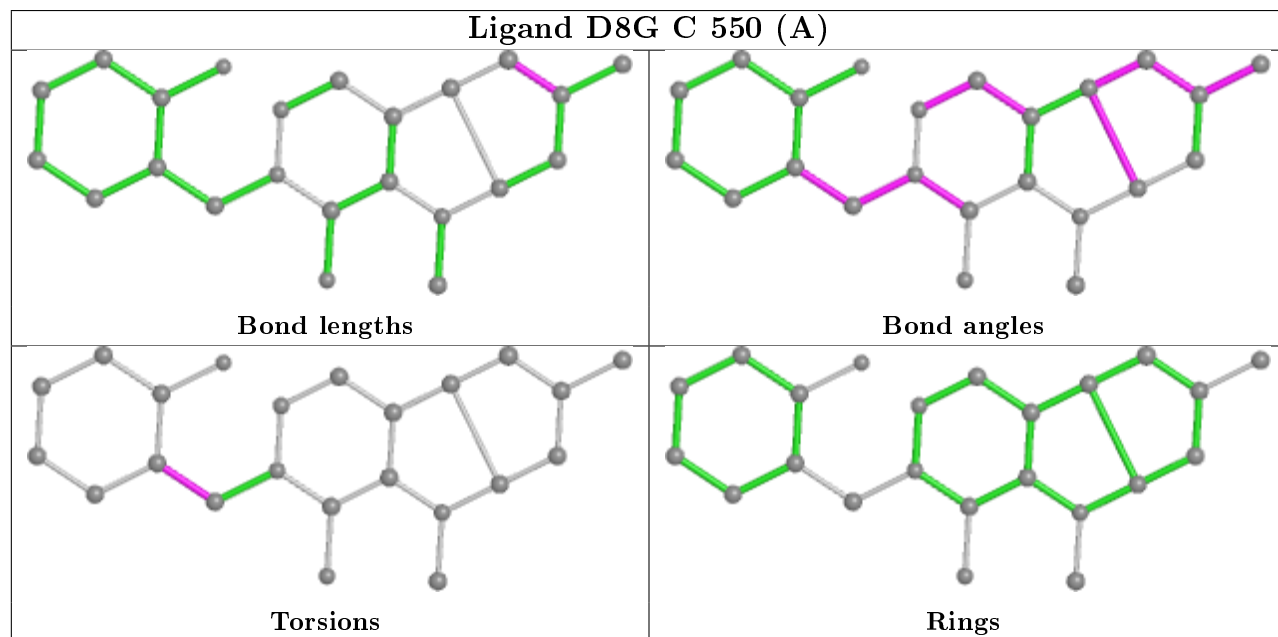
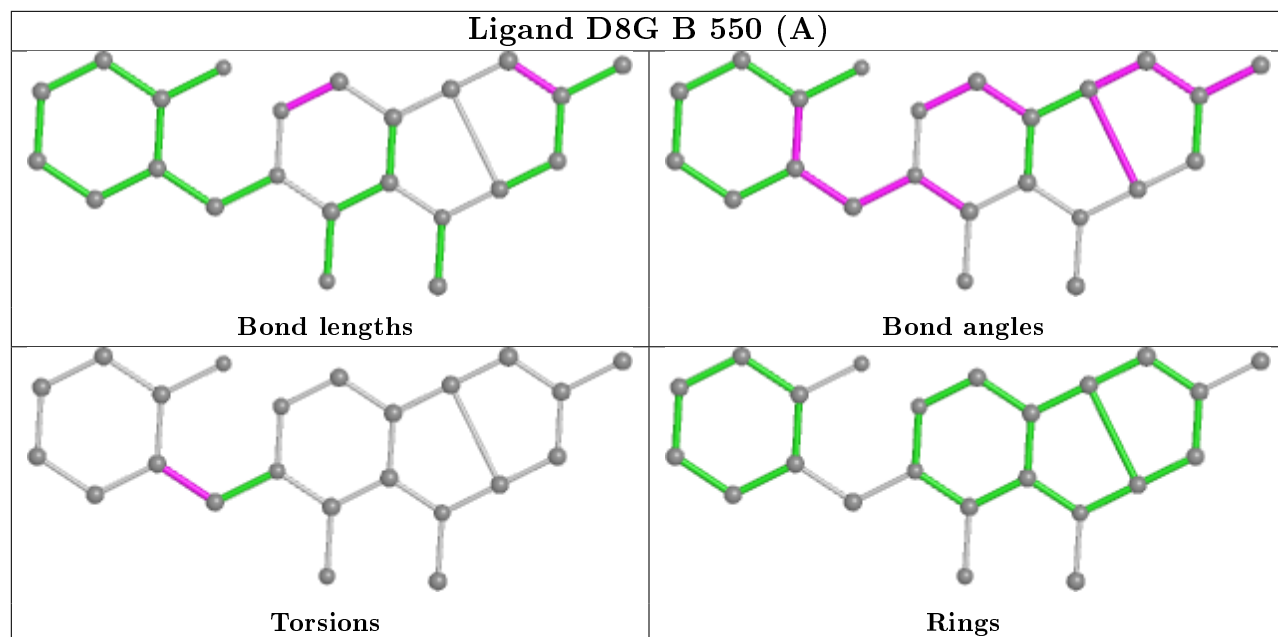
There are no ring outliers.

4 monomers are involved in 8 short contacts:

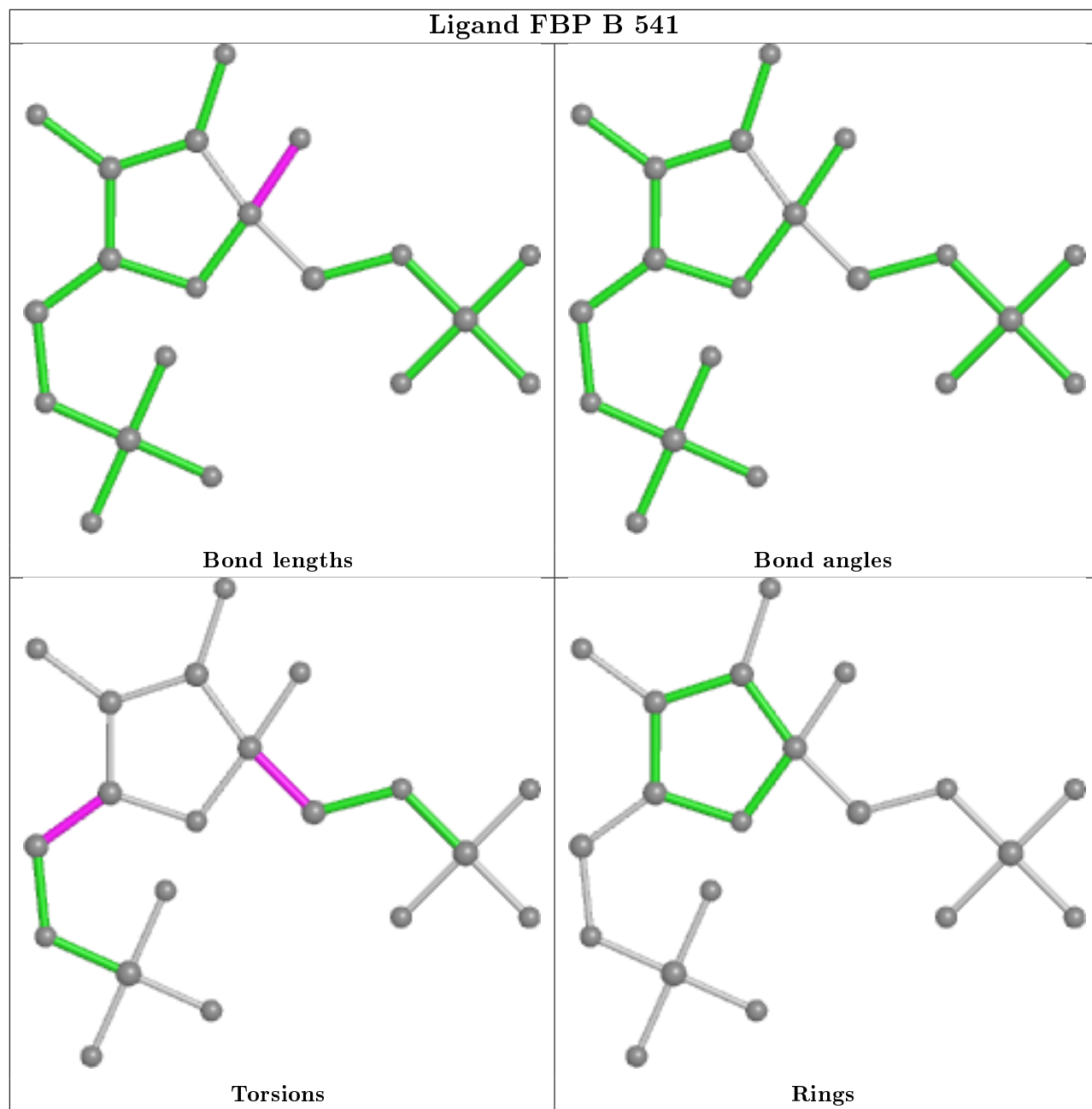
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	550[B]	D8G	2	0
4	B	550[A]	D8G	1	0
4	C	550[A]	D8G	2	0
4	B	550[B]	D8G	3	0

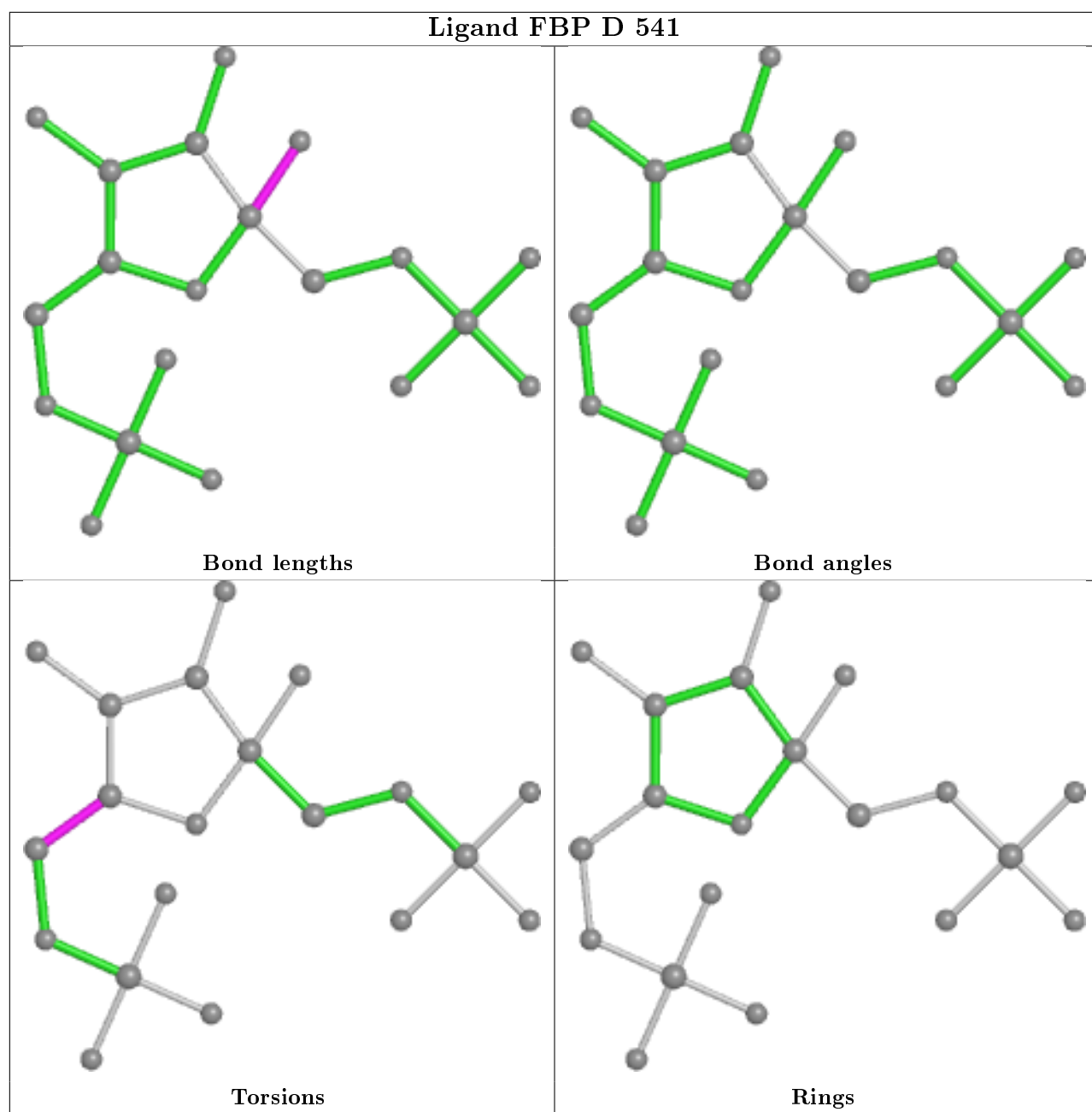
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

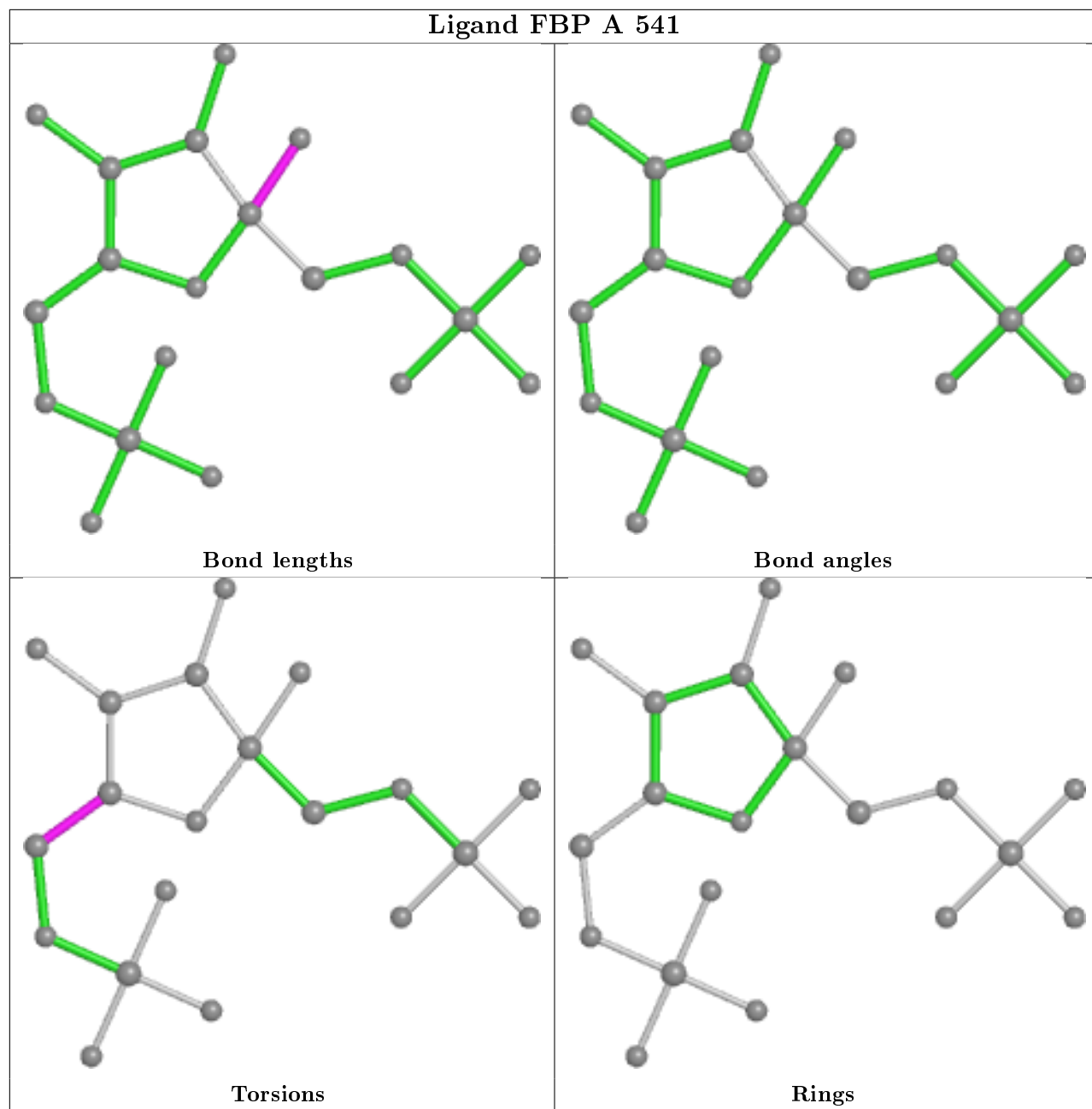




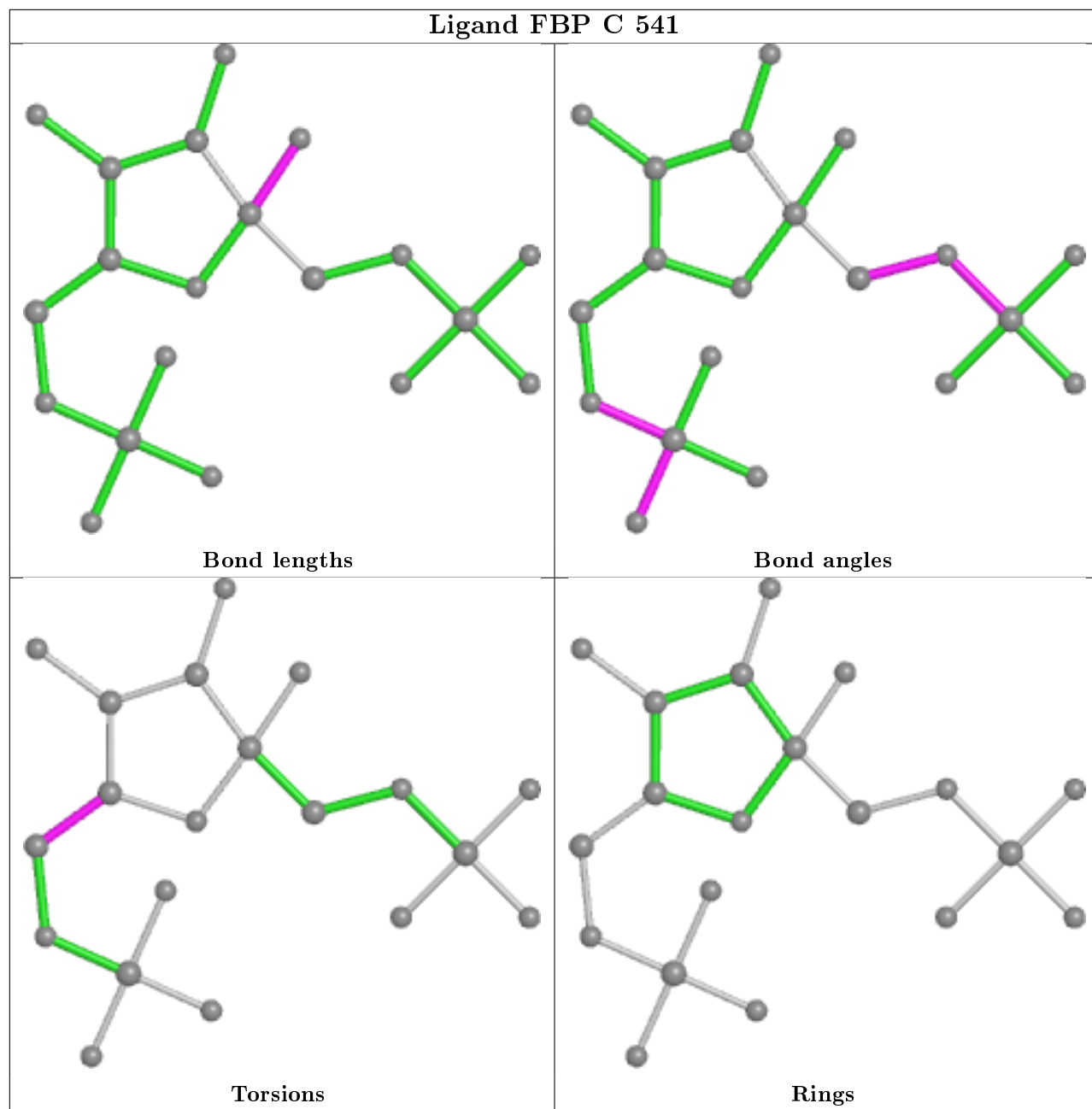
Ligand FBP B 541

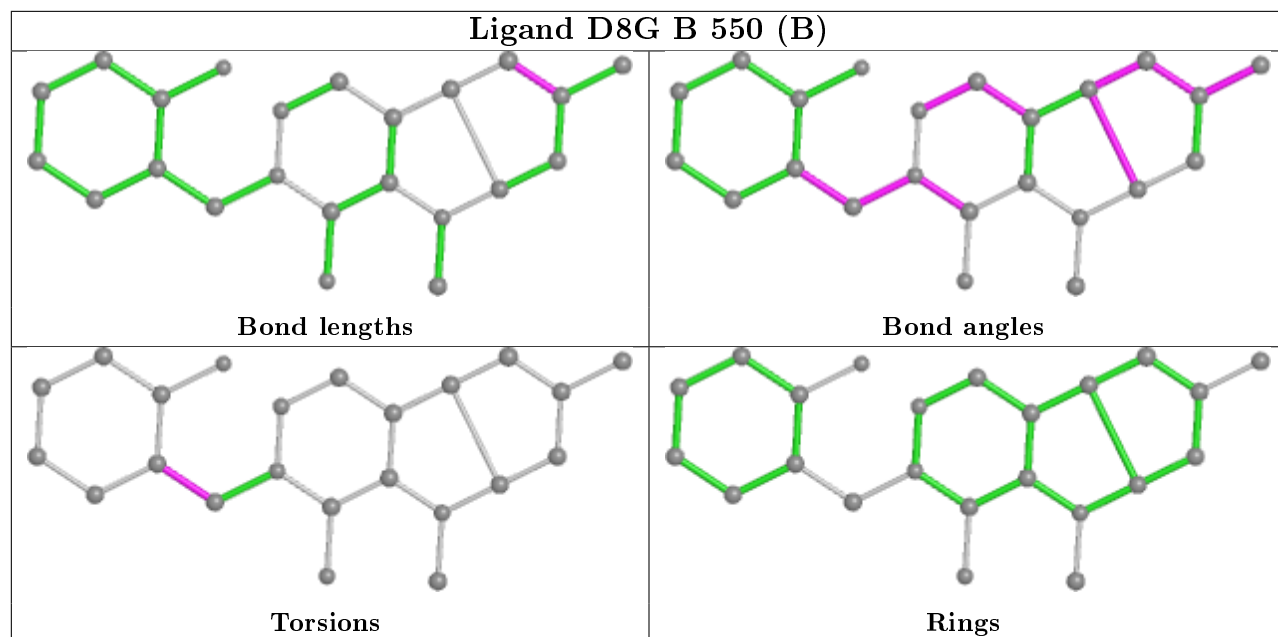






Ligand FBP C 541





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	490/550 (89%)	0.44	33 (6%)	17 17	31, 40, 58, 63	1 (0%)
1	B	513/550 (93%)	0.26	22 (4%)	35 34	32, 40, 48, 59	4 (0%)
1	C	468/550 (85%)	0.36	30 (6%)	19 18	33, 41, 51, 61	0
1	D	507/550 (92%)	0.34	30 (5%)	22 21	33, 40, 54, 63	1 (0%)
All	All	1978/2200 (89%)	0.35	115 (5%)	23 22	31, 40, 53, 63	6 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	190	ALA	6.9
1	D	147	ALA	6.5
1	D	152	CYS	5.8
1	A	197	VAL	5.3
1	D	134	LEU	5.3
1	C	157	LEU	5.3
1	C	156	ILE	5.1
1	A	152	CYS	4.8
1	B	330	MET	4.7
1	D	190	ALA	4.5
1	A	191	ASP	4.5
1	C	170	VAL	4.3
1	A	192	PHE	4.2
1	C	404	ILE	4.2
1	D	155	ASN	4.1
1	B	190	ALA	4.1
1	C	158	TRP	4.1
1	D	159	LEU	4.1
1	A	153	ASP	4.0
1	D	150	GLU	4.0
1	A	404	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	147	ALA	3.9
1	D	170	VAL	3.9
1	C	167	VAL	3.6
1	C	80	THR	3.6
1	D	136	LYS	3.6
1	D	151	LYS	3.6
1	D	148	TYR	3.6
1	A	205	SER	3.5
1	A	196	GLU	3.5
1	C	165	CYS	3.4
1	D	146	ASN	3.3
1	A	122	GLY	3.3
1	A	158	TRP	3.3
1	C	171	GLY	3.3
1	C	153	ASP	3.3
1	C	159	LEU	3.2
1	D	133	GLU	3.2
1	C	163	ASN	3.1
1	A	480	GLU	3.1
1	D	144	LEU	3.1
1	B	404	ILE	3.1
1	C	121	THR	3.1
1	D	168	VAL	3.1
1	C	155	ASN	3.0
1	D	186	LYS	3.0
1	D	187	GLN	3.0
1	C	200	GLY	3.0
1	A	155	ASN	2.9
1	B	123	LEU	2.9
1	A	156	ILE	2.9
1	D	189	GLY	2.9
1	D	158	TRP	2.9
1	C	100	SER	2.9
1	B	327	ALA	2.8
1	A	171	GLY	2.8
1	C	220	ALA	2.7
1	A	154	GLU	2.7
1	B	309	ALA	2.7
1	A	187	GLN	2.7
1	B	510	ILE	2.7
1	D	197	VAL	2.7
1	B	245	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	164	ILE	2.6
1	D	165	CYS	2.6
1	C	183	LEU	2.6
1	A	178	ASP	2.6
1	D	205	SER	2.6
1	A	201	GLY	2.5
1	B	317	CYS	2.5
1	C	120	ARG	2.5
1	D	404	ILE	2.5
1	B	470	PHE	2.5
1	C	531	PRO	2.4
1	C	166	LYS	2.4
1	D	145	ASP	2.4
1	A	200	GLY	2.4
1	A	195	THR	2.4
1	B	313	MET	2.4
1	D	137	GLY	2.4
1	A	308	LEU	2.3
1	B	276	GLY	2.3
1	D	470[A]	PHE	2.3
1	C	102	PRO	2.3
1	B	324	VAL	2.3
1	A	198	GLU	2.3
1	A	268	ILE	2.3
1	C	174	ILE	2.3
1	A	121	THR	2.3
1	A	314	ILE	2.3
1	A	402	ALA	2.2
1	C	14	GLN	2.2
1	A	348	VAL	2.2
1	D	202	SER	2.2
1	D	138	ALA	2.2
1	D	402	ALA	2.2
1	A	331	LEU	2.2
1	B	189	GLY	2.2
1	C	168	VAL	2.1
1	A	188	LYS	2.1
1	B	277	VAL	2.1
1	A	189	GLY	2.1
1	B	122	GLY	2.1
1	C	154	GLU	2.1
1	A	385	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	111	ALA	2.1
1	B	152	CYS	2.1
1	D	157	LEU	2.0
1	A	175	TYR	2.0
1	B	133	GLU	2.0
1	C	314	ILE	2.0
1	C	172	SER	2.0
1	B	290	ILE	2.0
1	B	428	ILE	2.0
1	C	221	VAL	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(Å ²)	Q<0.9
3	UNX	A	543	1/1	-0.61	0.84	2,2,2,2	1
3	UNX	D	537	1/1	-0.54	2.29	2,2,2,2	1
3	UNX	C	533	1/1	-0.45	5.73	2,2,2,2	1
3	UNX	A	540	1/1	-0.40	1.41	2,2,2,2	1
3	UNX	D	532	1/1	-0.35	3.20	2,2,2,2	1
3	UNX	B	538	1/1	-0.30	0.85	2,2,2,2	1
3	UNX	A	535	1/1	-0.30	2.30	2,2,2,2	1
3	UNX	A	542	1/1	-0.28	2.47	2,2,2,2	1
3	UNX	A	532	1/1	-0.28	2.82	2,2,2,2	1
3	UNX	C	535	1/1	-0.21	1.34	2,2,2,2	1
3	UNX	B	532	1/1	-0.20	1.97	2,2,2,2	1
3	UNX	A	533	1/1	-0.20	1.76	2,2,2,2	1
3	UNX	B	539	1/1	-0.18	2.15	2,2,2,2	1

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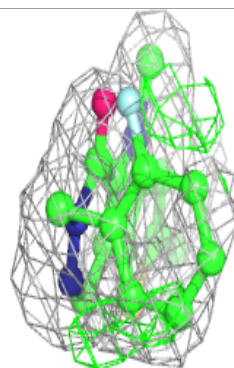
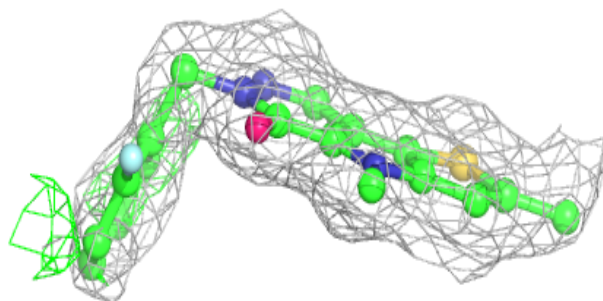
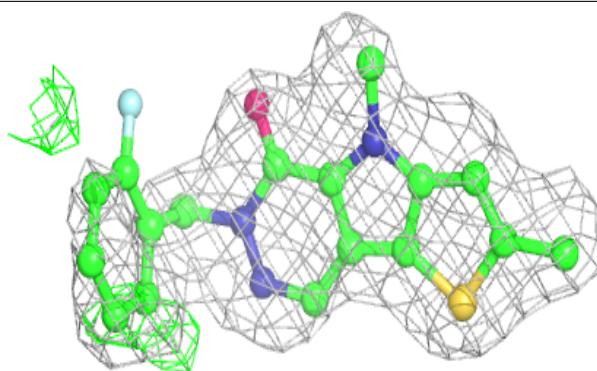
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	UNX	C	534	1/1	-0.15	1.95	22,22,22,22	1
3	UNX	A	539	1/1	-0.14	2.20	2,2,2,2	1
3	UNX	B	537	1/1	-0.12	1.31	2,2,2,2	1
3	UNX	A	537	1/1	-0.07	3.35	2,2,2,2	1
3	UNX	B	540	1/1	-0.06	1.89	2,2,2,2	1
3	UNX	B	535	1/1	0.01	3.78	2,2,2,2	1
3	UNX	B	533	1/1	0.10	2.50	2,2,2,2	1
3	UNX	D	535	1/1	0.22	1.59	2,2,2,2	1
3	UNX	A	538	1/1	0.22	1.73	2,2,2,2	1
3	UNX	A	536	1/1	0.35	3.83	2,2,2,2	1
3	UNX	B	534	1/1	0.38	3.01	2,2,2,2	1
3	UNX	C	532	1/1	0.38	2.37	2,2,2,2	1
3	UNX	D	533	1/1	0.42	2.60	2,2,2,2	1
3	UNX	D	538	1/1	0.42	2.87	2,2,2,2	1
3	UNX	D	534	1/1	0.42	2.78	2,2,2,2	1
3	UNX	A	534	1/1	0.42	2.45	2,2,2,2	1
3	UNX	D	536	1/1	0.80	3.39	2,2,2,2	1
3	UNX	B	536	1/1	0.90	2.09	2,2,2,2	1
4	D8G	B	550[B]	23/23	0.93	0.16	33,34,34,35	23
4	D8G	B	550[A]	23/23	0.93	0.16	30,31,31,31	23
4	D8G	C	550[A]	23/23	0.94	0.14	32,34,34,34	23
4	D8G	C	550[B]	23/23	0.94	0.14	32,35,35,35	23
2	FBP	C	541	20/20	0.95	0.09	41,44,46,46	0
2	FBP	B	541	20/20	0.97	0.10	30,34,37,37	0
2	FBP	D	541	20/20	0.97	0.08	38,41,43,44	0
2	FBP	A	541	20/20	0.97	0.09	38,41,46,46	0

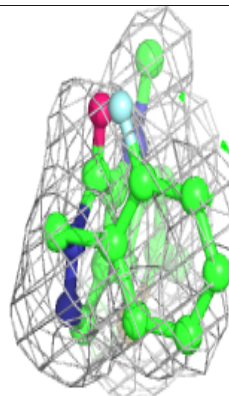
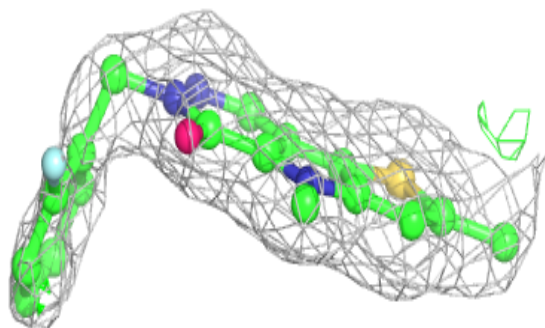
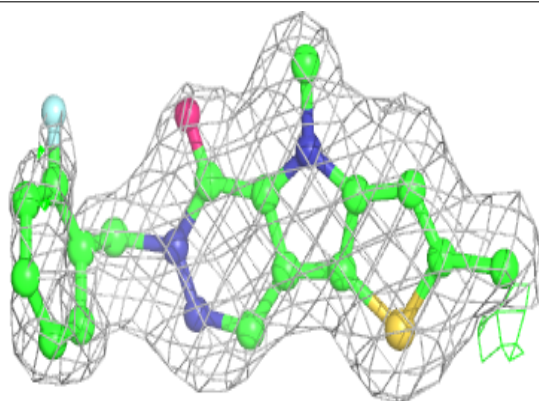
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around D8G B 550 (B):

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

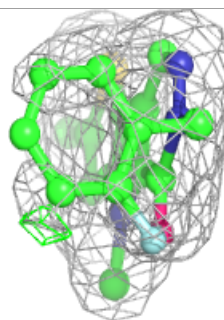
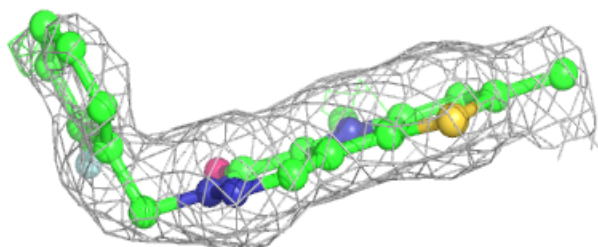
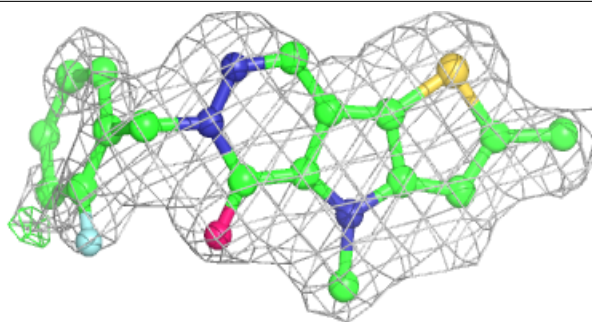
**Electron density around D8G B 550 (A):**

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

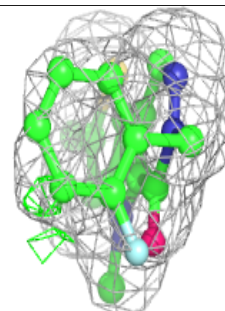
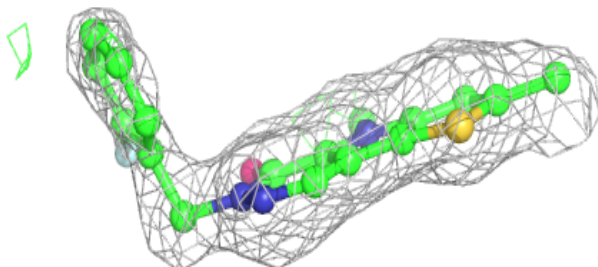
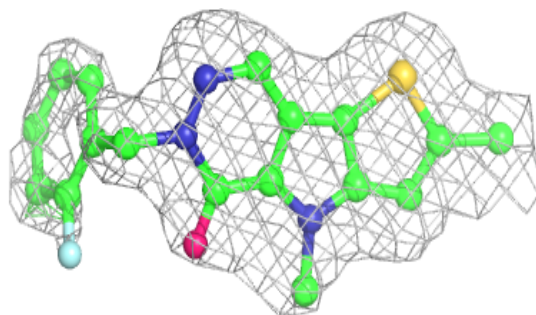


Electron density around D8G C 550 (A):

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

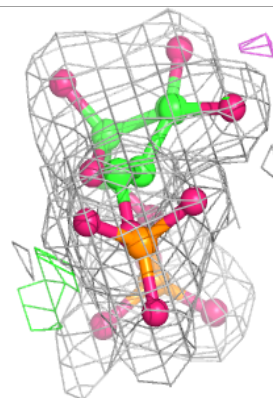
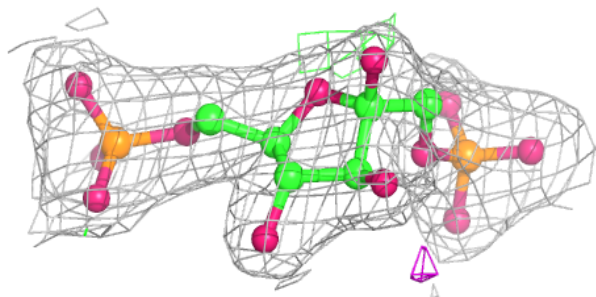
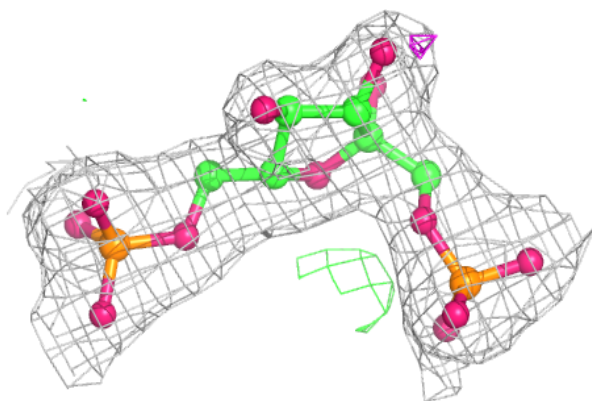
**Electron density around D8G C 550 (B):**

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

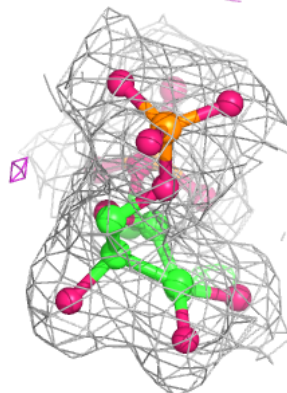
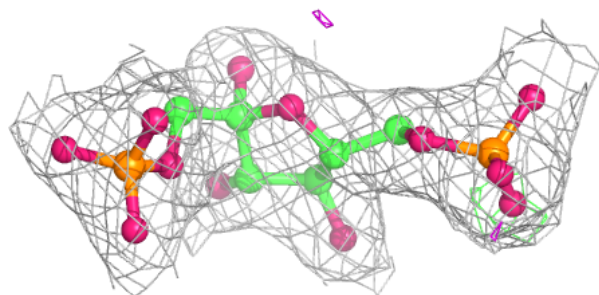
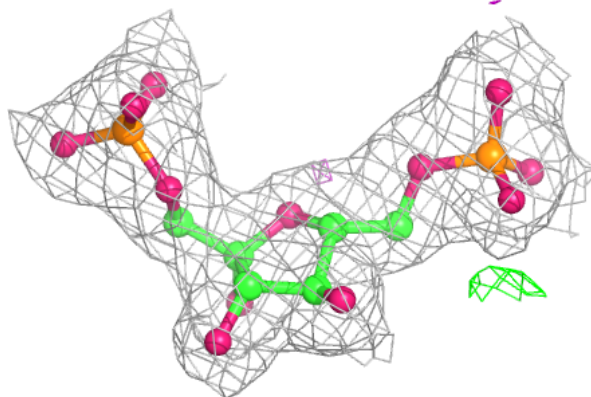


Electron density around FBP C 541:

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

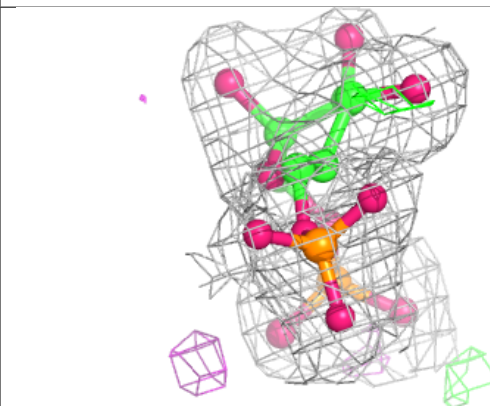
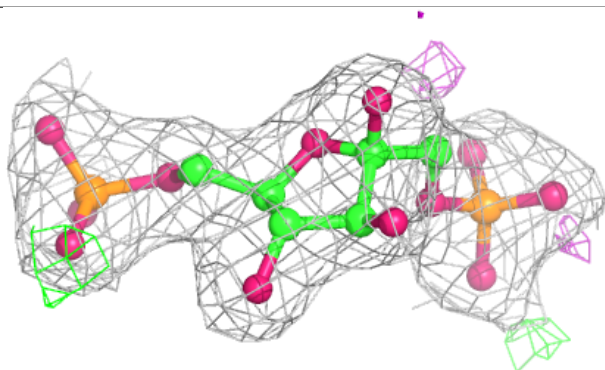
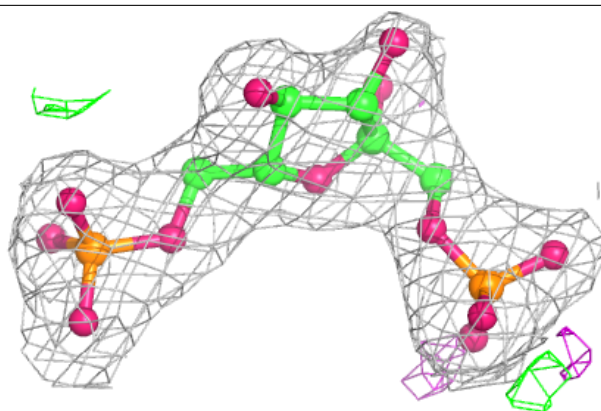
**Electron density around FBP B 541:**

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

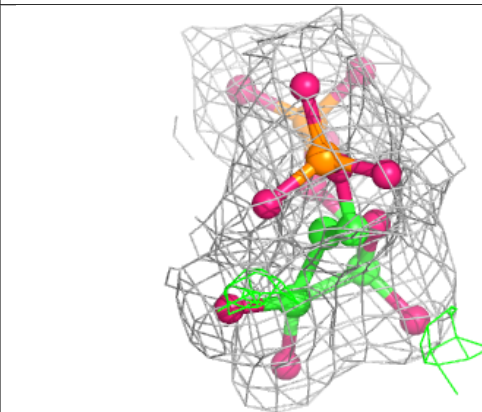
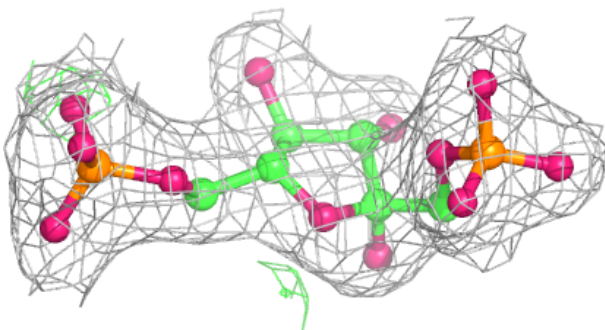
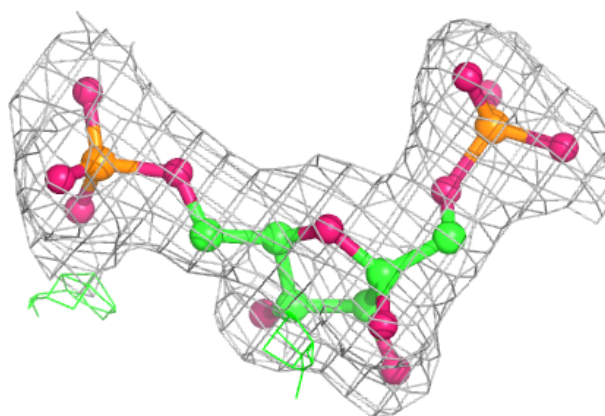


Electron density around FBP D 541:

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

**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)



6.5 Other polymers

There are no such residues in this entry.