



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:27 PM UTC

PDB ID : 3H6O / pdb_00003h6o
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtrriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

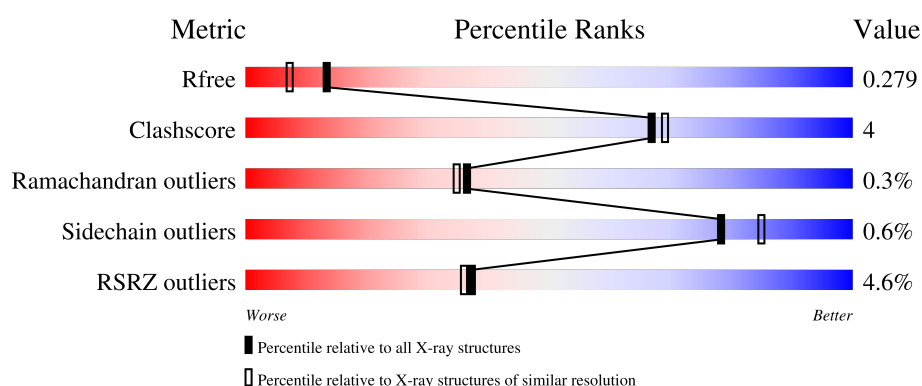
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	550	
1	C	550	
1	D	550	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	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	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	536	-	-	-	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	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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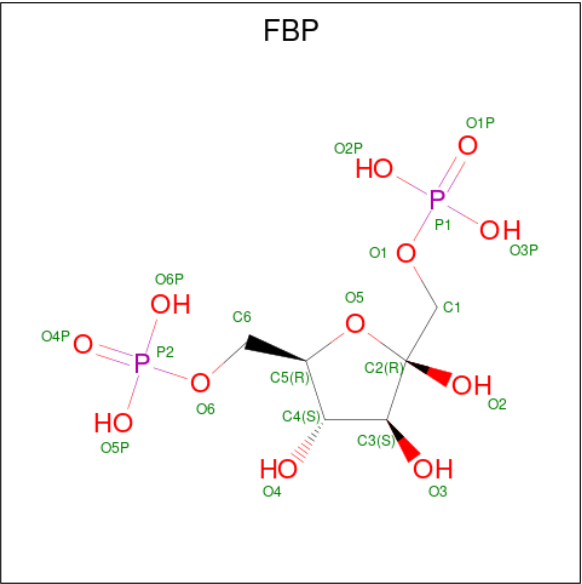
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP P14618
B	-15	SER	-	expression tag	UNP P14618
B	-14	HIS	-	expression tag	UNP P14618
B	-13	HIS	-	expression tag	UNP P14618
B	-12	HIS	-	expression tag	UNP P14618
B	-11	HIS	-	expression tag	UNP P14618
B	-10	HIS	-	expression tag	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 (CCD ID: FBP) (formula: $C_6H_{14}O_{12}P_2$).

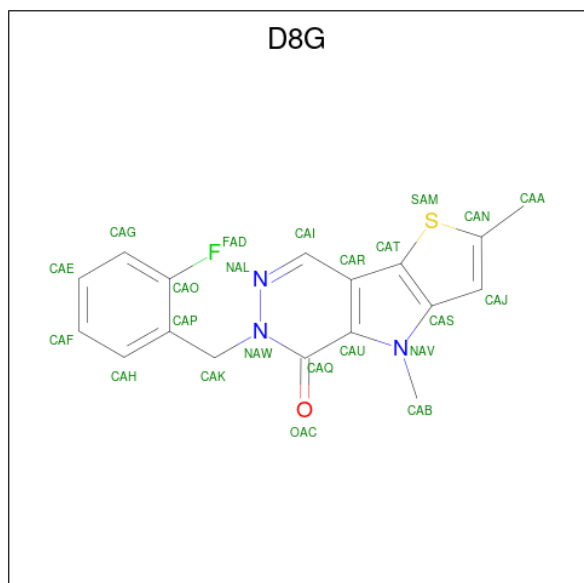


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total X 11 11	0	0
3	B	9	Total X 9 9	0	0
3	C	4	Total X 4 4	0	0
3	D	7	Total X 7 7	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 (CCD ID: 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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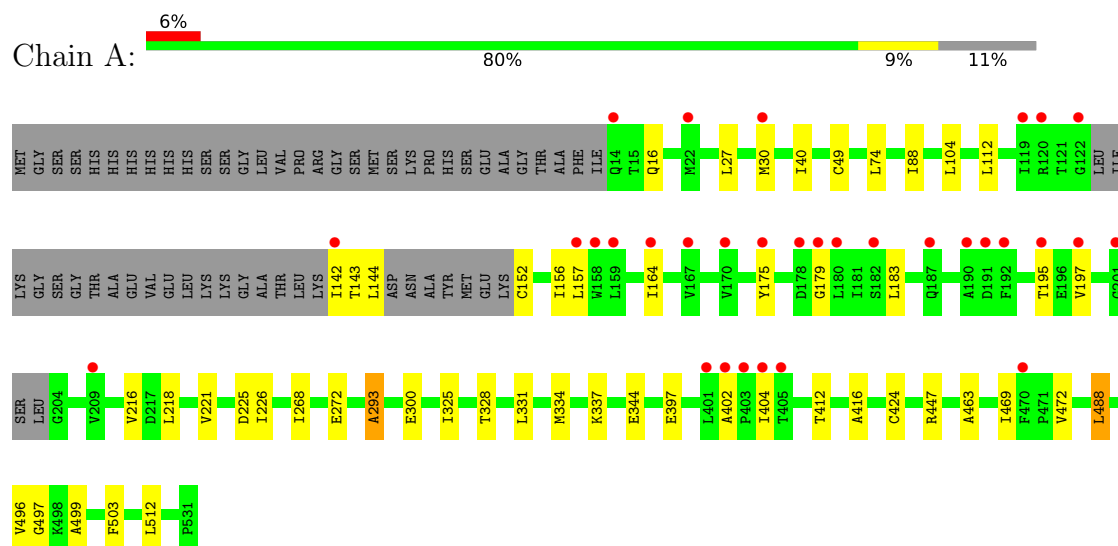
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	45	Total	O	0	0
			45	45		
5	D	55	Total	O	0	0
			55	55		

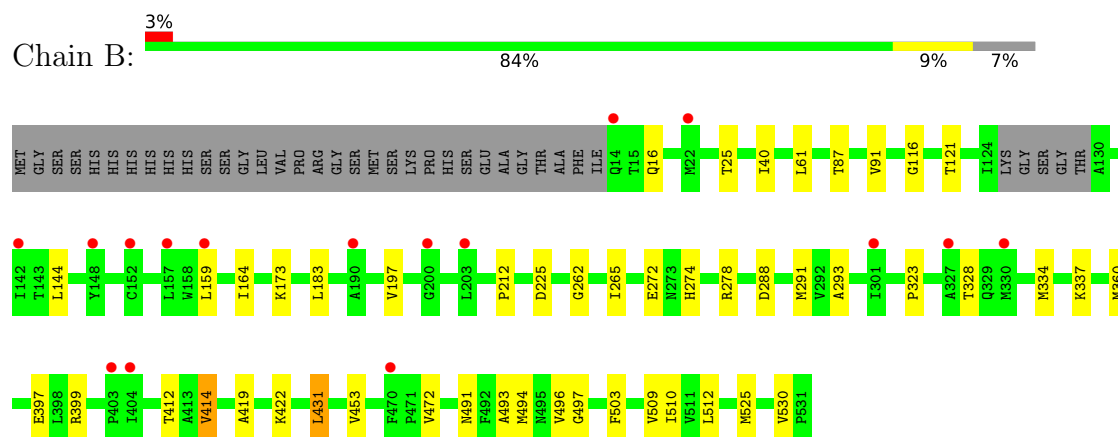
3 Residue-property plots [i](#)

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.

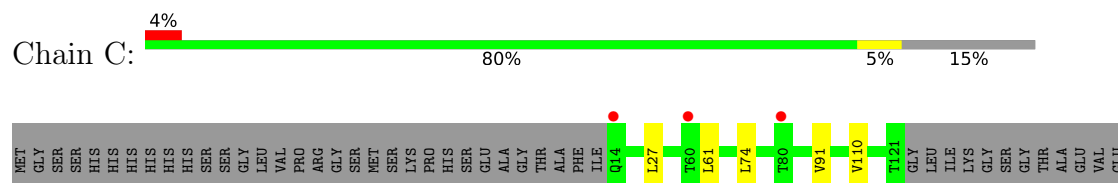
• Molecule 1: Pyruvate kinase isozymes M1/M2

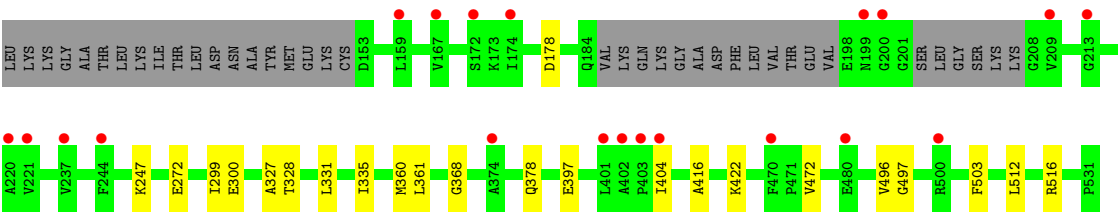


• Molecule 1: Pyruvate kinase isozymes M1/M2

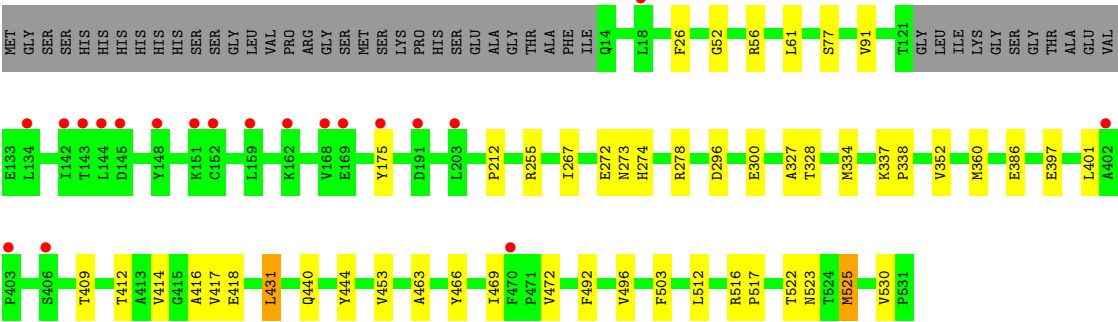
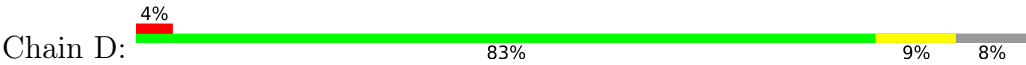


• Molecule 1: Pyruvate kinase isozymes M1/M2





● 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) 87.5 (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 (Not available) , 0.279	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)	0.30 , 54.8	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	0.94	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: D8G, FBP, UNX

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	0.83	2/3738 (0.1%)	0.83	0/5061
1	B	0.83	0/3874	0.84	0/5252
1	C	0.67	0/3555	0.78	0/4816
1	D	0.71	0/3851	0.80	0/5223
All	All	0.77	2/15018 (0.0%)	0.81	0/20352

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	ALA	CA-CB	-5.69	1.45	1.52
1	A	49	CYS	C-O	5.43	1.30	1.24

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	35	0
1	B	3812	0	3720	32	0
1	C	3497	0	3442	17	0
1	D	3776	0	3696	35	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	11	0	0	0	0
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	3	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	110	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 (110) 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:525:MET:HE3	1:D:525:MET:HE2	1.63	0.80
1:D:327:ALA:HB1	1:D:360:MET:HE2	1.70	0.72
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:A:488:LEU:C	1:A:488:LEU:HD23	2.23	0.63
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
1:C:327:ALA:HB1	1:C:360:MET:HE2	1.84	0.58
4:C:550[B]:D8G:HAF	1:D:397:GLU:OE1	2.03	0.58
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:61:LEU:HD13	1:B:91:VAL:HA	1.88	0.56
1:B:414:VAL:HG13	1:D:418:GLU:HG3	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:D:416:ALA:CB	1:D:512:LEU:HD21	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:52:GLY:O	1:D:56:ARG:HG3	2.09	0.52
1:D:412:THR:HG22	1:D:512:LEU:CD1	2.39	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:112:LEU:C	1:A:112:LEU:HD23	2.36	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:MET:HE2	1:B:360:MET:SD	2.57	0.45
1:B:472:VAL:HG11	1:B:496:VAL:HG11	1.98	0.45
1:A:404:ILE:HG22	1:A:404:ILE:O	2.16	0.45
1:B:453:VAL:CG2	1:B:493:ALA:HB2	2.47	0.45
1:B:494:MET:HE1	1:B:509:VAL:CG2	2.46	0.45
1:A:30:MET:HA	1:A:30:MET:HE2	1.99	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
1:C:74:LEU:HD11	1:C:110:VAL:HG13	1.99	0.45
1:D:334:MET:HE3	1:D:338:PRO:O	2.17	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: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
4:C:550[B]:D8G:HABA	1:D:26:PHE:CZ	2.54	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:B:494:MET:HE1	1:B:509:VAL:HG21	2.02	0.42
1:A:272:GLU:O	1:A:300:GLU:HG3	2.20	0.42
1:B:431:LEU:HD23	1:B:431:LEU:N	2.34	0.41
1:B:16:GLN:CD	1:B:40:ILE:HG23	2.46	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:C:472:VAL:HG11	1:C:496:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:397:GLU:CD	1:B:25:THR:HB	2.47	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 [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	483/550 (88%)	468 (97%)	14 (3%)	1 (0%)	43	42
1	B	509/550 (92%)	499 (98%)	9 (2%)	1 (0%)	43	42
1	C	460/550 (84%)	447 (97%)	12 (3%)	1 (0%)	43	42
1	D	507/550 (92%)	494 (97%)	11 (2%)	2 (0%)	30	27
All	All	1959/2200 (89%)	1908 (97%)	46 (2%)	5 (0%)	36	35

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	344/452 (76%)	343 (100%)	1 (0%)	86	91
1	B	385/452 (85%)	382 (99%)	3 (1%)	73	80
1	C	353/452 (78%)	351 (99%)	2 (1%)	78	85
1	D	377/452 (83%)	374 (99%)	3 (1%)	73	80
All	All	1459/1808 (81%)	1450 (99%)	9 (1%)	78	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	488	LEU
1	B	414	VAL
1	B	431	LEU
1	B	491	ASN
1	C	247	LYS
1	C	516	ARG
1	D	77	SER
1	D	431	LEU
1	D	525	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	A	479	GLN
1	B	44	ASN
1	B	78	HIS
1	B	199	ASN
1	C	391	HIS
1	D	16	GLN
1	D	90	ASN
1	D	146	ASN
1	D	458	GLN

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Mol	Chain	Res	Type
1	D	523	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
2	FBP	A	541	-	18,20,20	0.92	1 (5%)	21,32,32	0.67	0
2	FBP	C	541	-	18,20,20	0.99	1 (5%)	21,32,32	0.80	1 (4%)
4	D8G	B	550[A]	-	26,26,26	2.15	9 (34%)	30,39,39	2.83	10 (33%)
4	D8G	B	550[B]	-	26,26,26	2.10	7 (26%)	30,39,39	2.67	10 (33%)
4	D8G	C	550[A]	-	26,26,26	2.15	7 (26%)	30,39,39	2.56	11 (36%)
4	D8G	C	550[B]	-	26,26,26	2.13	7 (26%)	30,39,39	2.59	9 (30%)
2	FBP	B	541	-	18,20,20	0.92	1 (5%)	21,32,32	0.84	0
2	FBP	D	541	-	18,20,20	0.95	1 (5%)	21,32,32	0.85	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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[A]	-	-	0/4/4/4	0/4/4/4
4	D8G	B	550[B]	-	-	0/4/4/4	0/4/4/4
4	D8G	C	550[A]	-	-	0/4/4/4	0/4/4/4
4	D8G	C	550[B]	-	-	0/4/4/4	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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	550[A]	D8G	NAW-NAL	-7.20	1.24	1.36
4	B	550[B]	D8G	NAW-NAL	-7.11	1.24	1.36
4	C	550[A]	D8G	NAW-NAL	-7.02	1.24	1.36
4	C	550[B]	D8G	NAW-NAL	-6.65	1.25	1.36
4	C	550[A]	D8G	CAT-SAM	-3.67	1.66	1.74
4	C	550[B]	D8G	CAU-NAV	-3.48	1.33	1.39
4	B	550[A]	D8G	CAT-SAM	-3.15	1.67	1.74
4	C	550[B]	D8G	CAI-NAL	3.08	1.33	1.29
4	B	550[A]	D8G	CAI-NAL	3.08	1.33	1.29
4	B	550[B]	D8G	CAN-SAM	-3.06	1.64	1.72
2	C	541	FBP	O2-C2	3.03	1.46	1.40
4	C	550[A]	D8G	CAU-NAV	-2.90	1.34	1.39
4	B	550[B]	D8G	CAT-SAM	-2.89	1.68	1.74
2	D	541	FBP	O2-C2	2.84	1.45	1.40
4	C	550[A]	D8G	CAJ-CAS	-2.82	1.35	1.42
2	B	541	FBP	O2-C2	2.71	1.45	1.40
4	C	550[B]	D8G	CAJ-CAS	-2.62	1.36	1.42
4	C	550[A]	D8G	CAI-NAL	2.60	1.32	1.29
4	B	550[B]	D8G	CAU-NAV	-2.60	1.35	1.39
2	A	541	FBP	O2-C2	2.57	1.45	1.40
4	C	550[B]	D8G	CAT-SAM	-2.48	1.68	1.74
4	B	550[B]	D8G	CAI-NAL	2.47	1.32	1.29
4	B	550[A]	D8G	CAJ-CAS	-2.36	1.37	1.42
4	C	550[B]	D8G	CAK-NAW	2.35	1.50	1.46
4	C	550[B]	D8G	CAS-NAV	-2.31	1.33	1.39
4	C	550[A]	D8G	CAR-CAT	-2.28	1.37	1.44
4	B	550[A]	D8G	CAU-NAV	-2.27	1.35	1.39
4	B	550[B]	D8G	CAJ-CAS	-2.26	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	550[A]	D8G	CAN-SAM	-2.22	1.67	1.72
4	B	550[B]	D8G	CAR-CAT	-2.21	1.38	1.44
4	C	550[A]	D8G	CAS-NAV	-2.18	1.34	1.39
4	B	550[A]	D8G	CAQ-NAW	2.15	1.44	1.39
4	B	550[A]	D8G	CAR-CAT	-2.13	1.38	1.44
4	B	550[A]	D8G	CAK-NAW	2.06	1.49	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	550[A]	D8G	CAP-CAK-NAW	-9.58	103.87	113.08
4	B	550[B]	D8G	CAP-CAK-NAW	-8.48	104.93	113.08
4	C	550[A]	D8G	CAP-CAK-NAW	-8.31	105.09	113.08
4	C	550[B]	D8G	CAP-CAK-NAW	-7.64	105.73	113.08
4	B	550[B]	D8G	CAT-CAS-NAV	-6.16	105.50	110.19
4	B	550[A]	D8G	CAT-CAS-NAV	-5.96	105.65	110.19
4	C	550[A]	D8G	CAT-CAS-NAV	-5.58	105.94	110.19
4	C	550[B]	D8G	CAT-CAS-NAV	-5.56	105.96	110.19
4	C	550[B]	D8G	CAS-CAT-SAM	-5.01	107.40	111.16
4	B	550[A]	D8G	CAQ-CAU-NAV	4.65	136.69	131.26
4	B	550[B]	D8G	CAS-CAT-SAM	-4.53	107.76	111.16
4	B	550[A]	D8G	CAS-CAT-SAM	-4.22	107.99	111.16
4	C	550[A]	D8G	CAQ-CAU-NAV	4.15	136.11	131.26
4	C	550[B]	D8G	CAK-NAW-NAL	4.05	119.21	114.38
4	B	550[B]	D8G	CAN-SAM-CAT	3.98	95.67	92.32
4	C	550[B]	D8G	CAU-NAV-CAS	3.97	111.90	108.61
4	C	550[A]	D8G	CAU-NAV-CAS	3.87	111.82	108.61
4	C	550[A]	D8G	CAS-CAT-SAM	-3.72	108.37	111.16
4	B	550[B]	D8G	CAQ-CAU-NAV	3.72	135.61	131.26
4	B	550[A]	D8G	CAN-SAM-CAT	3.62	95.37	92.32
4	B	550[A]	D8G	CAU-NAV-CAS	3.53	111.54	108.61
4	B	550[B]	D8G	CAU-NAV-CAS	3.49	111.50	108.61
4	C	550[B]	D8G	CAN-SAM-CAT	3.24	95.05	92.32
4	B	550[A]	D8G	OAC-CAQ-CAU	-3.15	119.92	126.38
4	C	550[B]	D8G	CAQ-CAU-NAV	3.14	134.93	131.26
4	B	550[B]	D8G	OAC-CAQ-CAU	-3.02	120.19	126.38
4	C	550[B]	D8G	OAC-CAQ-CAU	-3.02	120.20	126.38
4	C	550[A]	D8G	OAC-CAQ-CAU	-2.82	120.59	126.38
4	B	550[A]	D8G	CAK-NAW-CAQ	2.82	121.86	119.22
4	C	550[A]	D8G	CAN-SAM-CAT	2.74	94.63	92.32
4	B	550[B]	D8G	CAK-NAW-CAQ	2.55	121.61	119.22
4	B	550[A]	D8G	CAK-NAW-NAL	2.54	117.40	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	550[A]	D8G	CAR-CAU-NAV	-2.46	107.00	109.41
4	C	550[A]	D8G	CAK-NAW-CAQ	2.43	121.50	119.22
4	B	550[A]	D8G	CAR-CAU-NAV	-2.43	107.02	109.41
4	B	550[B]	D8G	CAK-NAW-NAL	2.36	117.19	114.38
4	C	550[A]	D8G	CAK-NAW-NAL	2.36	117.19	114.38
4	C	550[A]	D8G	CAA-CAN-SAM	2.31	125.79	121.03
4	C	550[B]	D8G	CAA-CAN-SAM	2.30	125.77	121.03
2	C	541	FBP	O6P-P2-O6	2.10	112.15	106.67
4	B	550[B]	D8G	CAR-CAU-NAV	-2.02	107.42	109.41

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

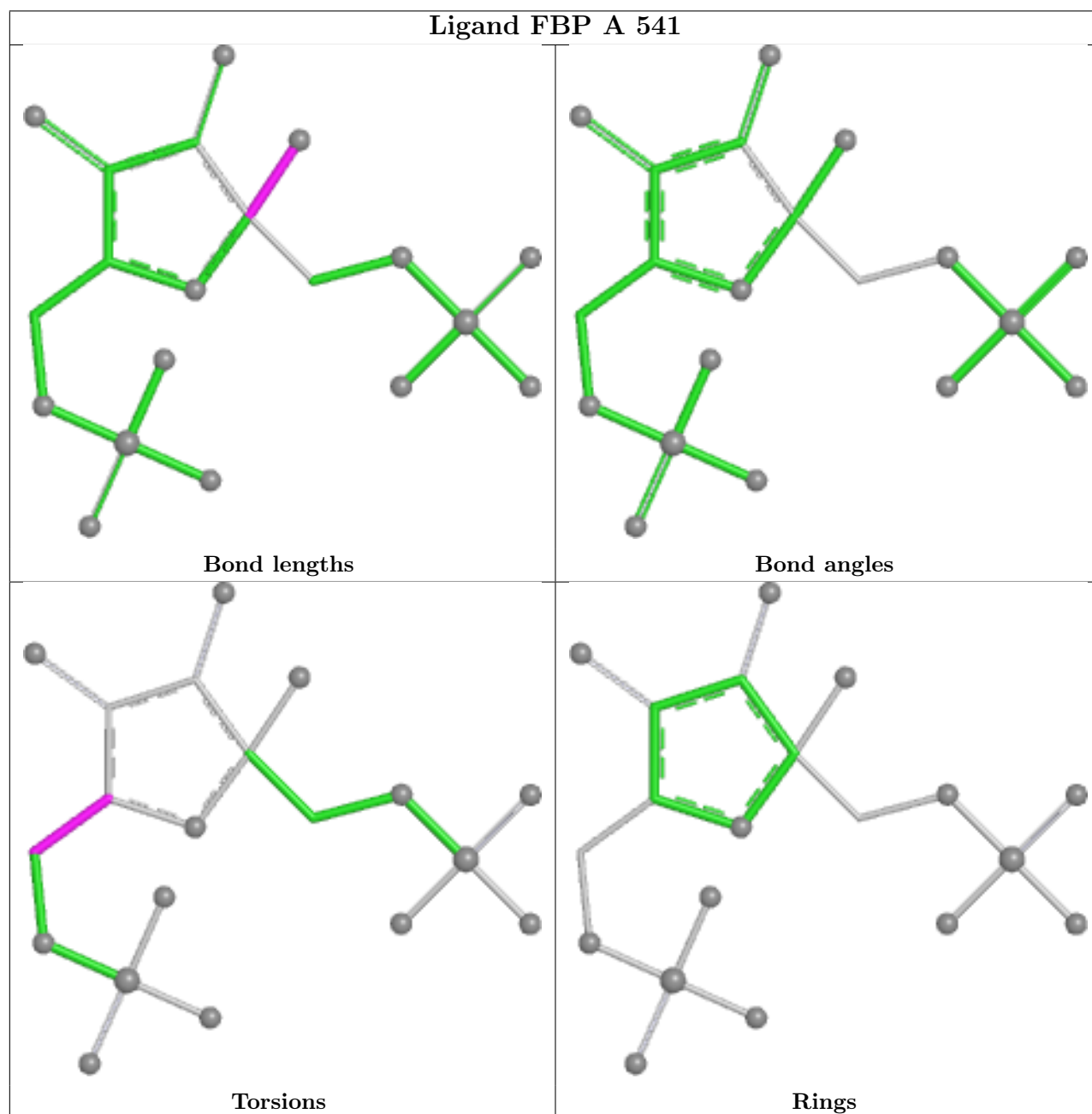
There are no ring outliers.

4 monomers are involved in 7 short contacts:

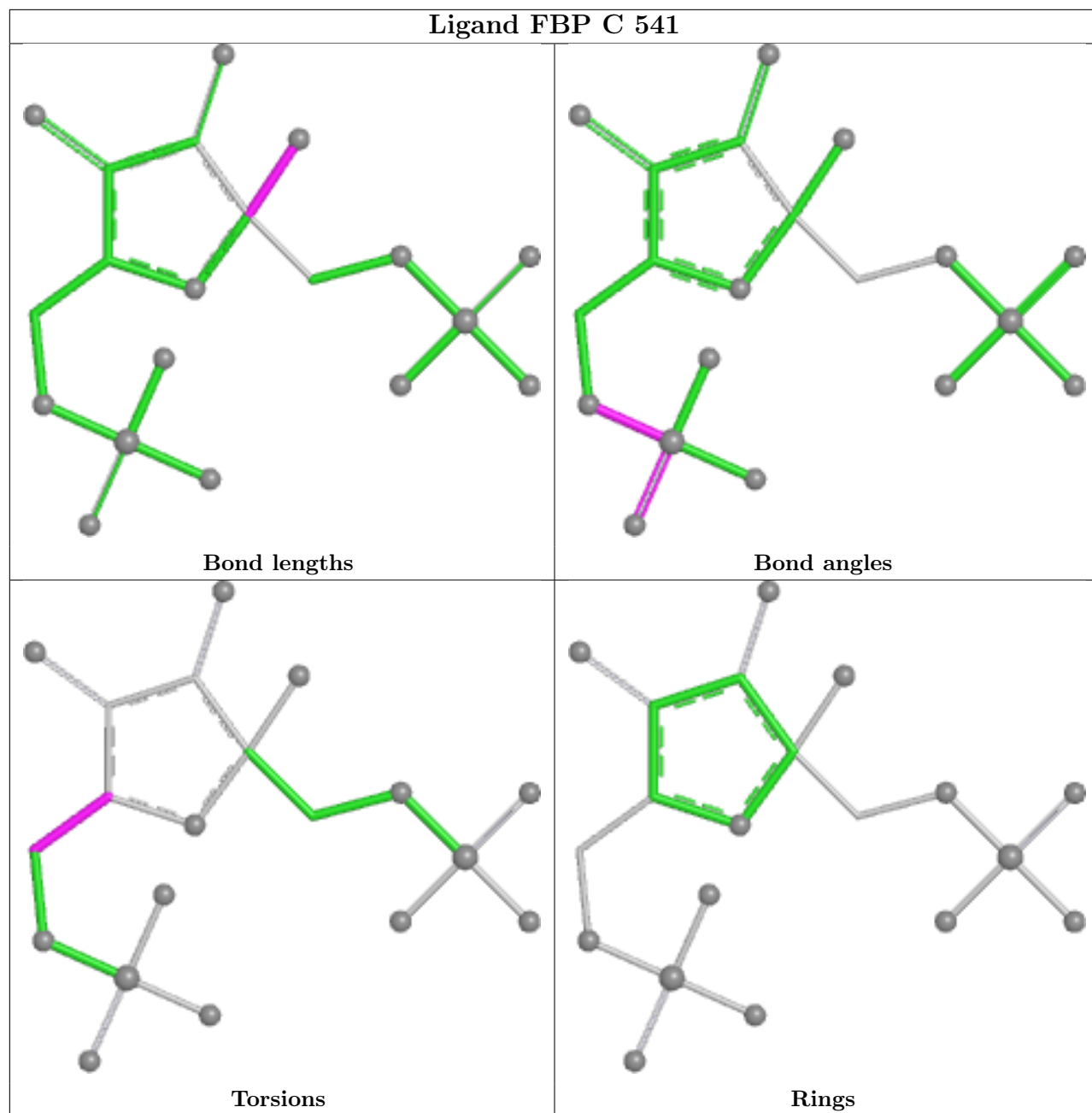
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	550[A]	D8G	1	0
4	B	550[B]	D8G	2	0
4	C	550[A]	D8G	1	0
4	C	550[B]	D8G	3	0

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.

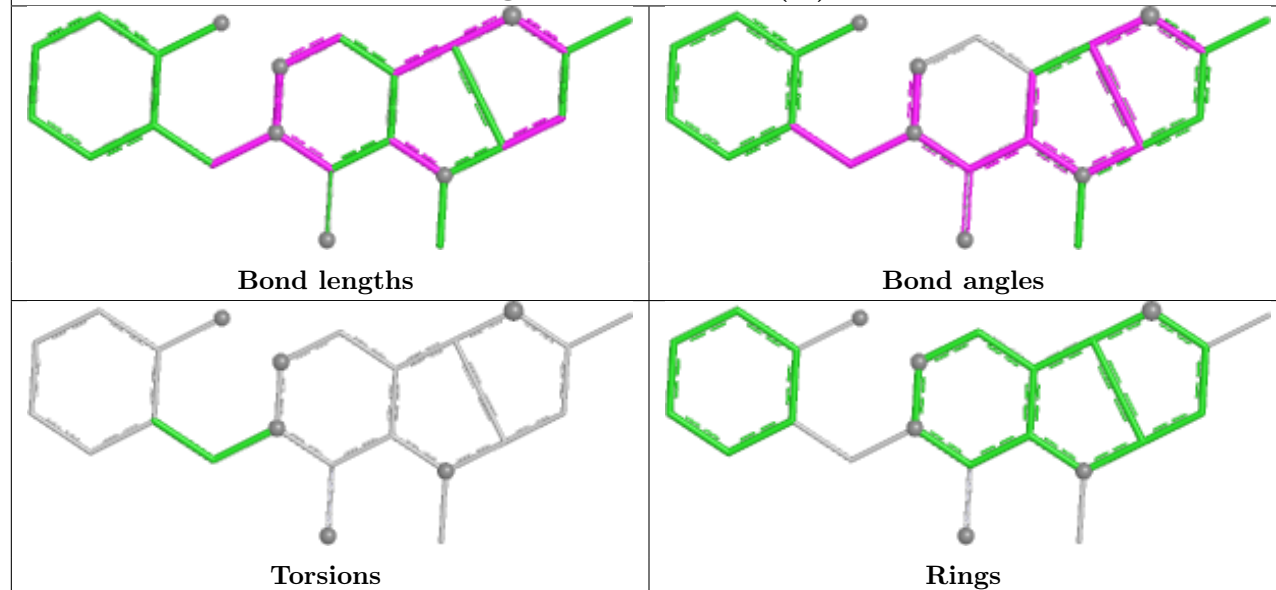
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



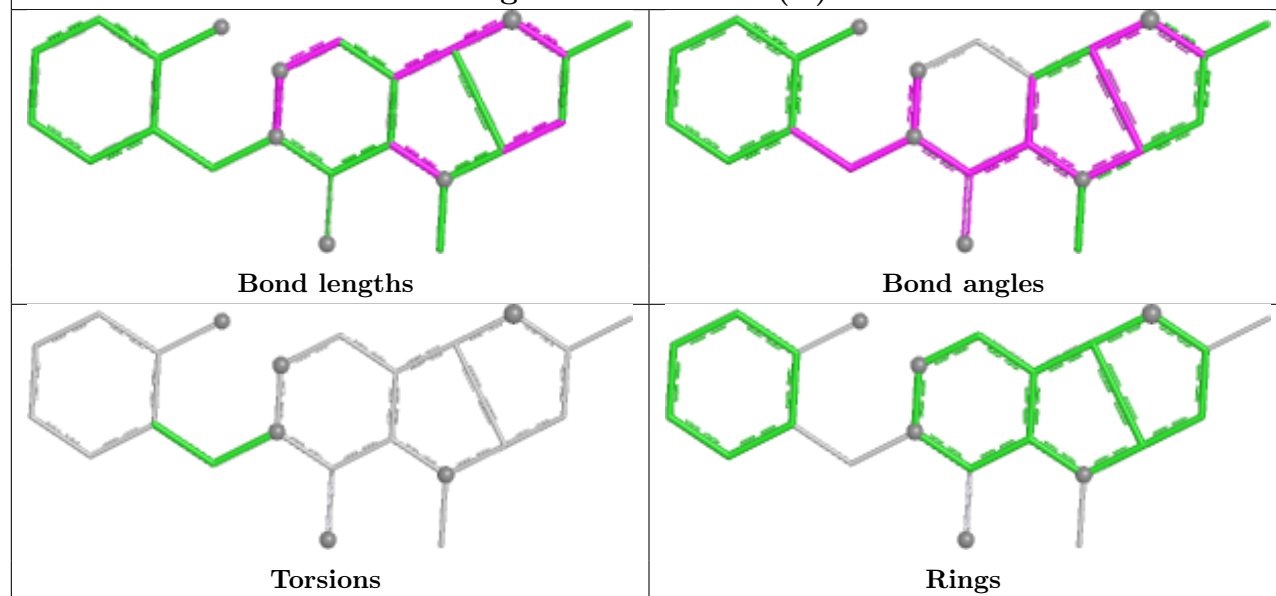
Ligand FBP C 541

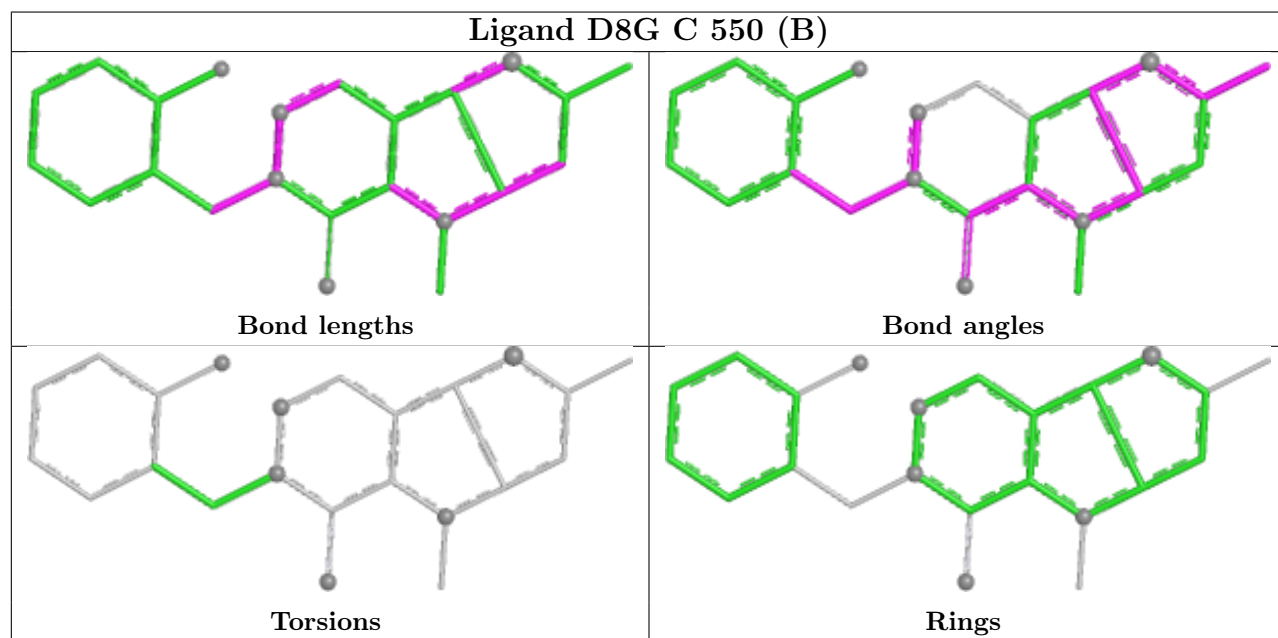
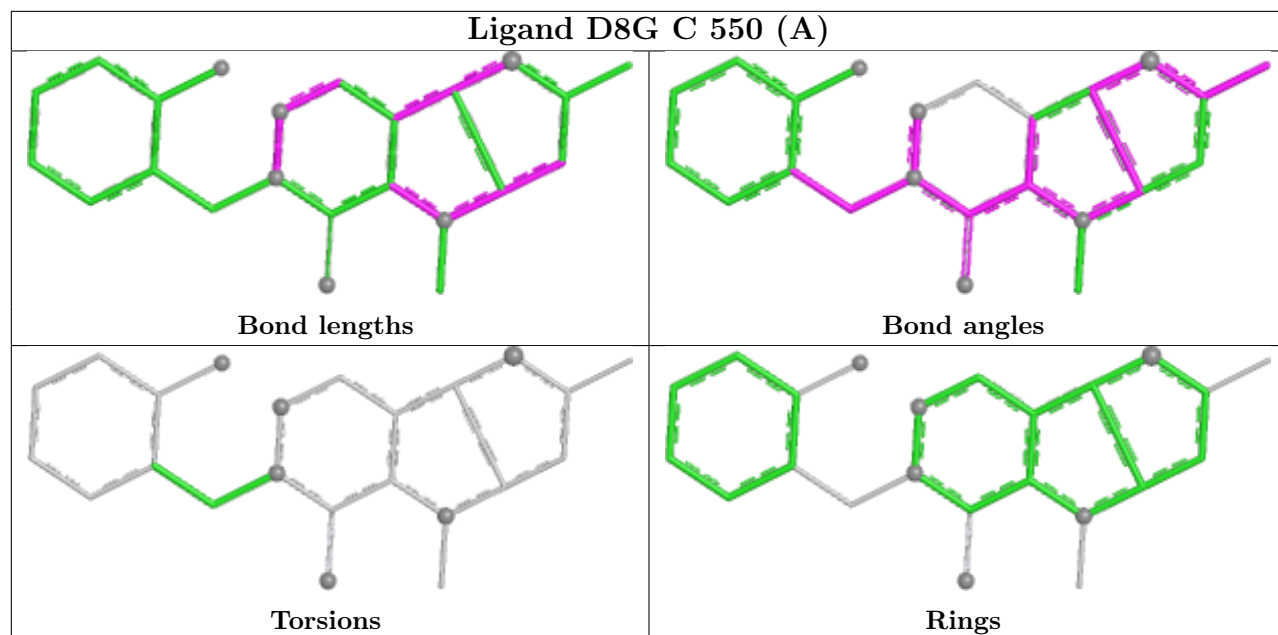


Ligand D8G B 550 (A)

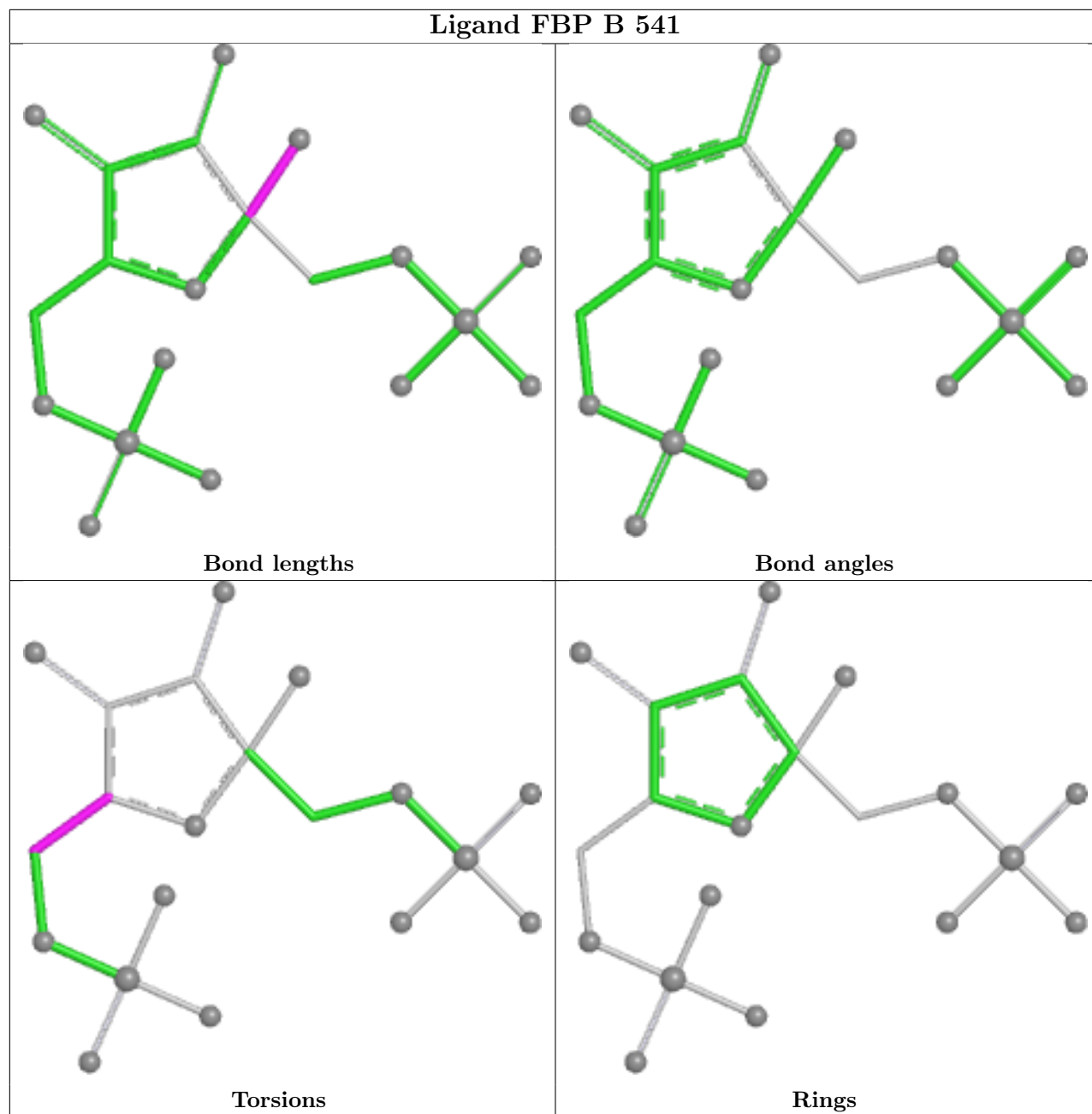


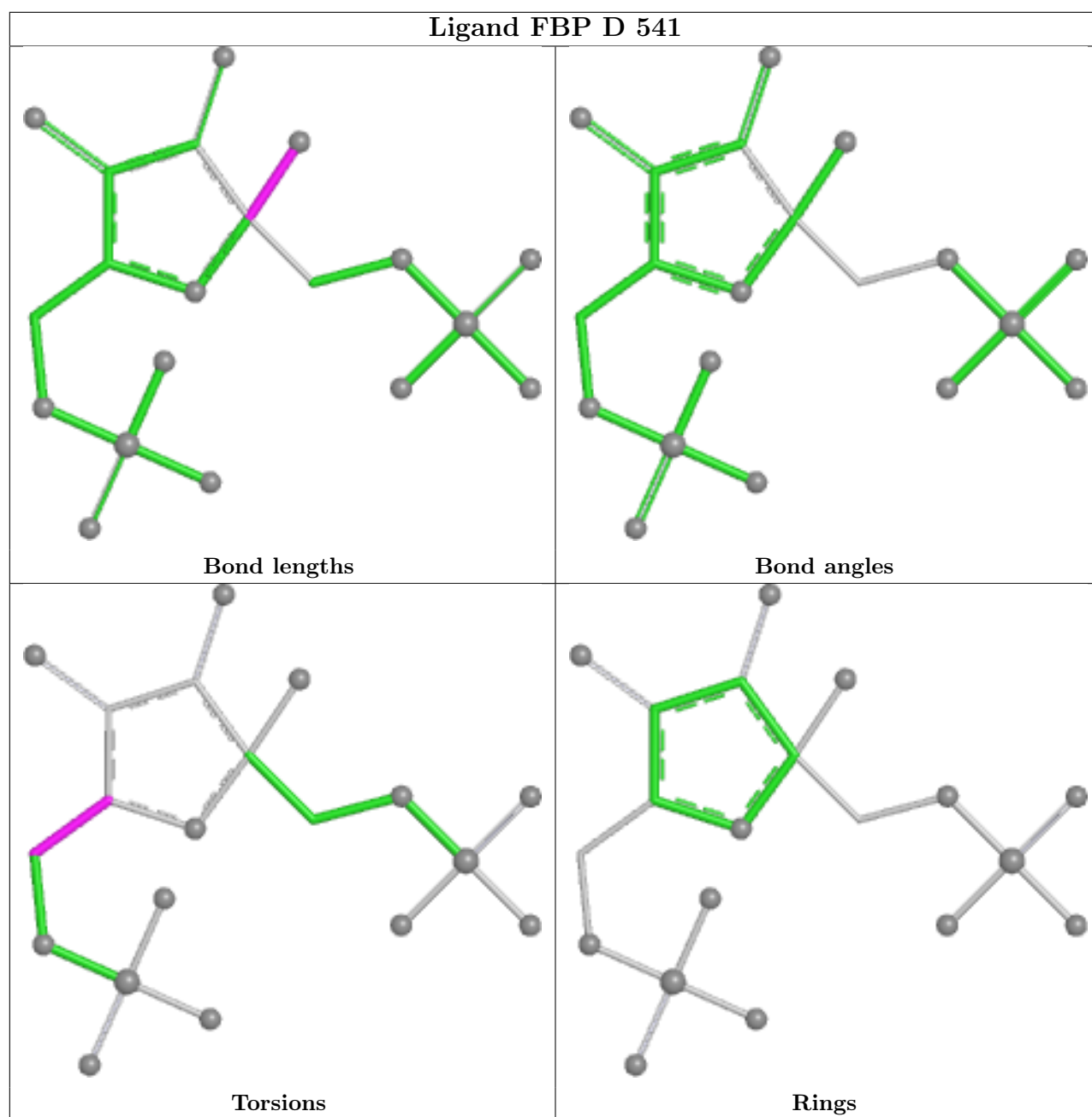
Ligand D8G B 550 (B)





Ligand FBP B 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%)	0.54	32 (6%)	25 23	23, 40, 58, 63	2 (0%)
1	B	513/550 (93%)	0.50	16 (3%)	51 50	31, 40, 48, 59	4 (0%)
1	C	468/550 (85%)	0.64	23 (4%)	35 34	33, 41, 51, 61	0
1	D	507/550 (92%)	0.60	20 (3%)	43 42	21, 40, 54, 63	5 (0%)
All	All	1978/2200 (89%)	0.57	91 (4%)	37 36	21, 40, 53, 63	11 (0%)

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	MET	4.7
1	C	220	ALA	4.6
1	A	190	ALA	4.1
1	A	192	PHE	4.1
1	D	403	PRO	4.1
1	D	134	LEU	3.9
1	D	159	LEU	3.7
1	C	167	VAL	3.7
1	C	14	GLN	3.5
1	A	14	GLN	3.4
1	A	209	VAL	3.3
1	B	470	PHE	3.2
1	D	152	CYS	3.2
1	A	159	LEU	3.1
1	A	197	VAL	3.0
1	B	403	PRO	3.0
1	B	14	GLN	3.0
1	B	327	ALA	3.0
1	A	22	MET	2.9
1	A	175	TYR	2.9
1	C	237	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	148	TYR	2.8
1	A	157	LEU	2.8
1	B	404	ILE	2.8
1	D	406	SER	2.7
1	C	404	ILE	2.7
1	B	159	LEU	2.7
1	C	159	LEU	2.7
1	A	167	VAL	2.7
1	C	200	GLY	2.7
1	A	180	LEU	2.7
1	A	403	PRO	2.7
1	C	500	ARG	2.7
1	C	402	ALA	2.6
1	D	142	ILE	2.6
1	D	168	VAL	2.6
1	B	190	ALA	2.6
1	C	403	PRO	2.6
1	B	142	ILE	2.5
1	A	402	ALA	2.5
1	D	402	ALA	2.5
1	A	470	PHE	2.5
1	D	203	LEU	2.5
1	C	470	PHE	2.5
1	A	179	GLY	2.4
1	A	201	GLY	2.4
1	D	145	ASP	2.4
1	A	404	ILE	2.4
1	B	22	MET	2.4
1	A	195	THR	2.4
1	A	401	LEU	2.4
1	C	209	VAL	2.4
1	A	405	THR	2.4
1	B	157	LEU	2.3
1	C	213	GLY	2.3
1	A	30	MET	2.3
1	C	480	GLU	2.3
1	A	164	ILE	2.3
1	C	221	VAL	2.3
1	C	80	THR	2.3
1	C	374	ALA	2.3
1	B	200	GLY	2.3
1	C	174	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLN	2.2
1	C	172	SER	2.2
1	A	142	ILE	2.2
1	D	143	THR	2.2
1	A	122	GLY	2.2
1	A	120	ARG	2.2
1	D	148	TYR	2.2
1	A	191	ASP	2.2
1	D	18	LEU	2.1
1	C	199	ASN	2.1
1	A	178	ASP	2.1
1	A	119	ILE	2.1
1	D	144	LEU	2.1
1	D	162	LYS	2.1
1	A	182	SER	2.1
1	B	152	CYS	2.1
1	B	301	ILE	2.1
1	C	401	LEU	2.1
1	D	151	LYS	2.1
1	A	170	VAL	2.1
1	D	470[A]	PHE	2.1
1	D	191	ASP	2.0
1	D	175	TYR	2.0
1	C	244	PHE	2.0
1	D	169	GLU	2.0
1	A	158	TRP	2.0
1	B	203	LEU	2.0
1	C	60	THR	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 oligosaccharides 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,

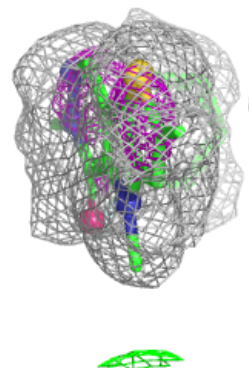
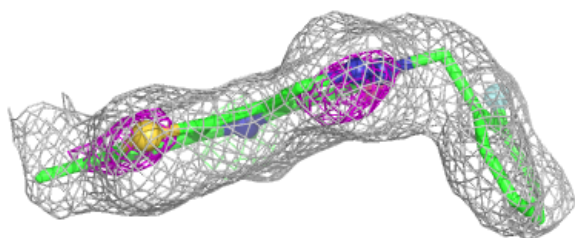
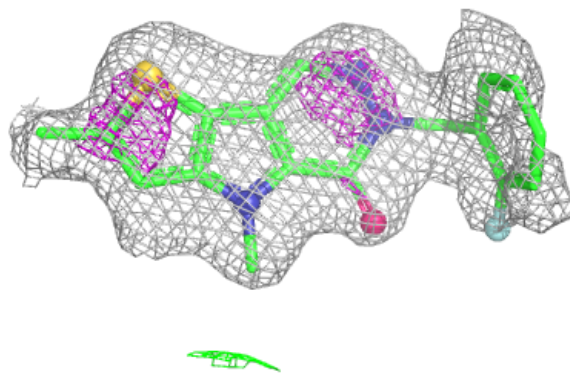
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	UNX	B	538	1/1	-0.52	1.63	2,2,2,2	1
3	UNX	D	537	1/1	-0.48	1.27	2,2,2,2	1
3	UNX	C	535	1/1	-0.40	2.49	2,2,2,2	1
3	UNX	A	532	1/1	-0.28	1.56	2,2,2,2	1
3	UNX	B	532	1/1	-0.22	1.65	2,2,2,2	1
3	UNX	C	534	1/1	-0.16	1.30	22,22,22,22	1
3	UNX	A	535	1/1	0.16	1.63	2,2,2,2	1
3	UNX	D	532	1/1	0.18	4.71	2,2,2,2	1
3	UNX	B	536	1/1	0.20	1.19	2,2,2,2	1
3	UNX	C	532	1/1	0.20	1.74	2,2,2,2	1
3	UNX	D	535	1/1	0.25	2.17	2,2,2,2	1
3	UNX	A	533	1/1	0.25	1.17	2,2,2,2	1
3	UNX	A	543	1/1	0.37	1.28	2,2,2,2	1
3	UNX	B	533	1/1	0.42	2.70	2,2,2,2	1
3	UNX	A	537	1/1	0.43	2.24	2,2,2,2	1
3	UNX	B	539	1/1	0.43	1.83	2,2,2,2	1
3	UNX	B	534	1/1	0.46	2.12	2,2,2,2	1
3	UNX	A	538	1/1	0.55	2.44	2,2,2,2	1
3	UNX	A	536	1/1	0.55	1.55	2,2,2,2	1
3	UNX	D	533	1/1	0.56	0.93	2,2,2,2	1
3	UNX	B	540	1/1	0.58	1.05	2,2,2,2	1
3	UNX	B	537	1/1	0.58	2.70	2,2,2,2	1
3	UNX	A	539	1/1	0.70	1.28	2,2,2,2	1
3	UNX	A	534	1/1	0.71	1.41	2,2,2,2	1
3	UNX	A	542	1/1	0.71	1.17	2,2,2,2	1
3	UNX	B	535	1/1	0.73	1.77	2,2,2,2	1
3	UNX	D	534	1/1	0.73	1.89	2,2,2,2	1
3	UNX	D	538	1/1	0.78	1.29	2,2,2,2	1
3	UNX	D	536	1/1	0.80	1.53	2,2,2,2	1
3	UNX	C	533	1/1	0.82	1.19	2,2,2,2	1
4	D8G	C	550[A]	23/23	0.82	0.14	32,34,34,34	23
4	D8G	C	550[B]	23/23	0.82	0.14	32,35,35,35	23
4	D8G	B	550[A]	23/23	0.83	0.15	30,31,31,31	23
4	D8G	B	550[B]	23/23	0.83	0.15	33,34,34,35	23
3	UNX	A	540	1/1	0.84	1.05	2,2,2,2	1
2	FBP	C	541	20/20	0.91	0.11	41,44,46,46	0
2	FBP	A	541	20/20	0.93	0.10	38,41,46,46	0
2	FBP	D	541	20/20	0.94	0.10	38,41,43,44	0
2	FBP	B	541	20/20	0.95	0.09	30,34,37,37	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.

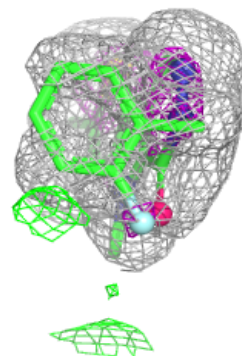
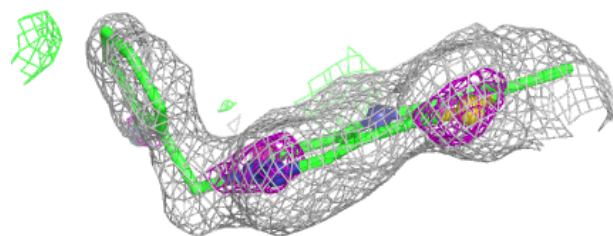
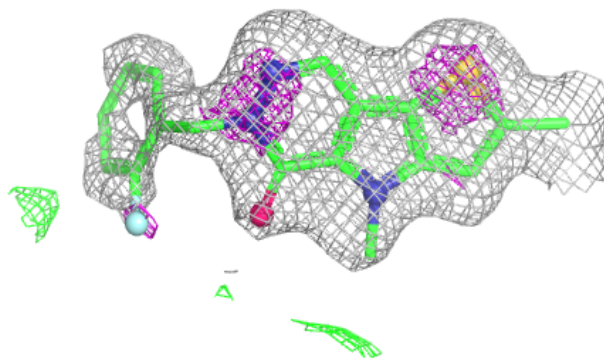
Electron density around D8G C 550 (A):

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

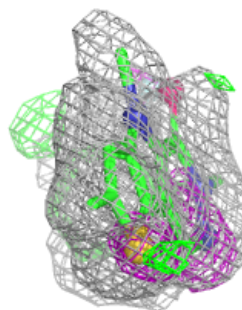
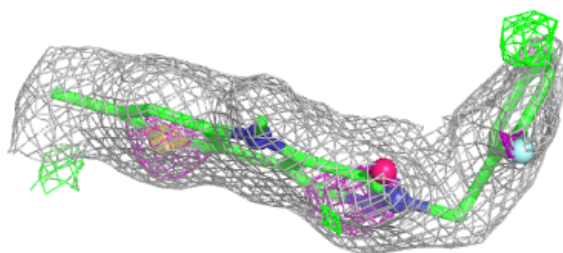
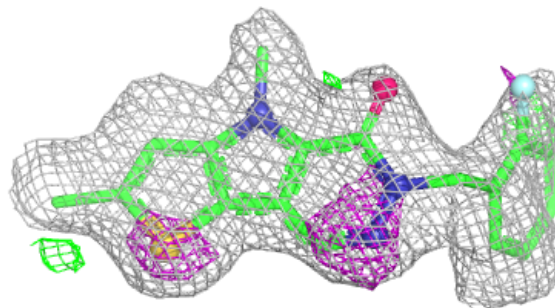


Electron density around D8G C 550 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

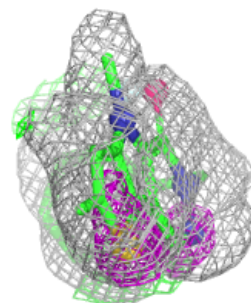
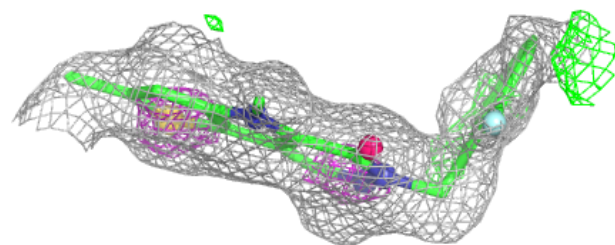
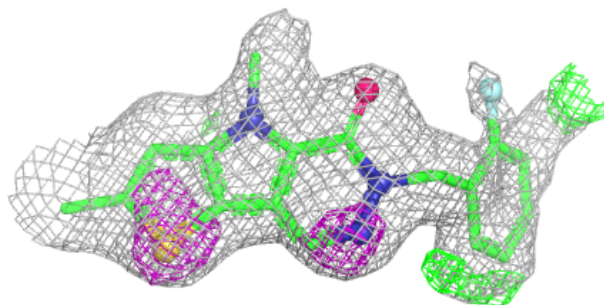
**Electron density around D8G B 550 (A):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

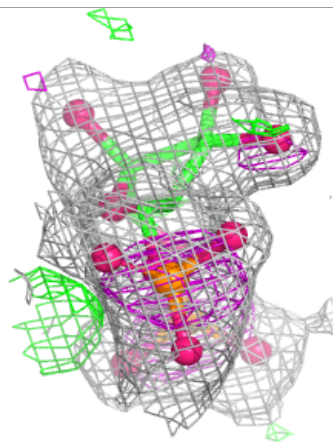
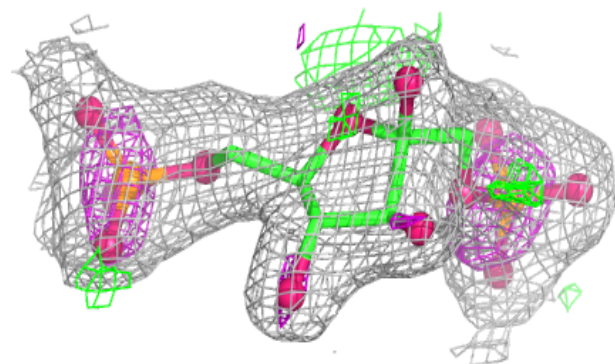
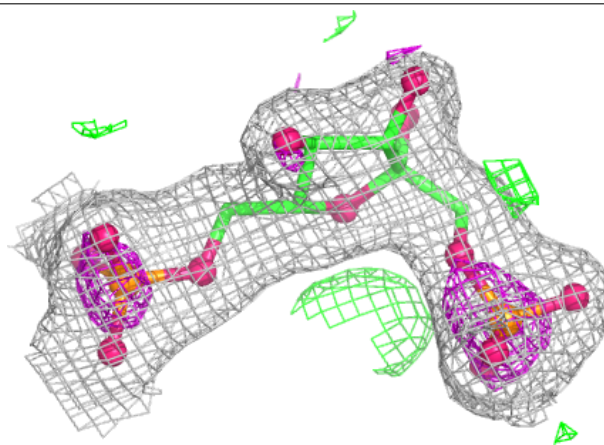


Electron density around D8G B 550 (B):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

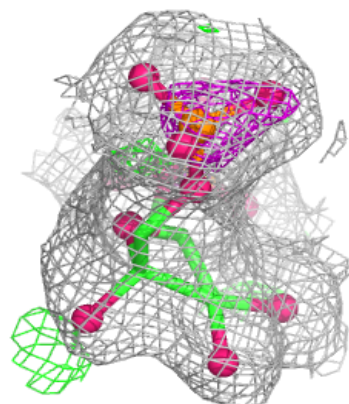
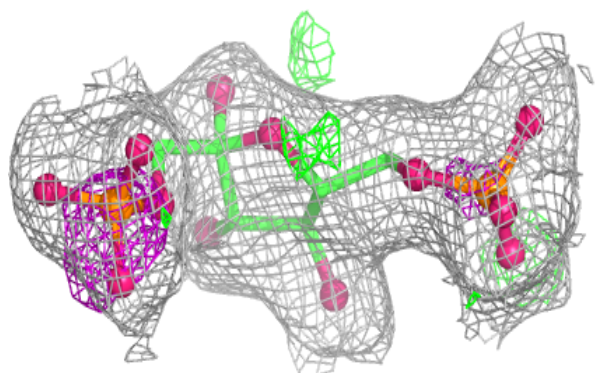
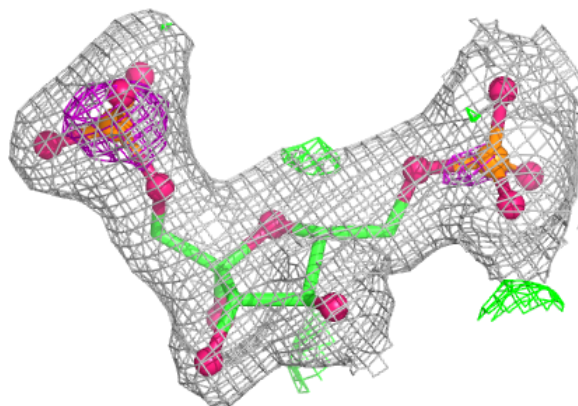
**Electron density around FBP C 541:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

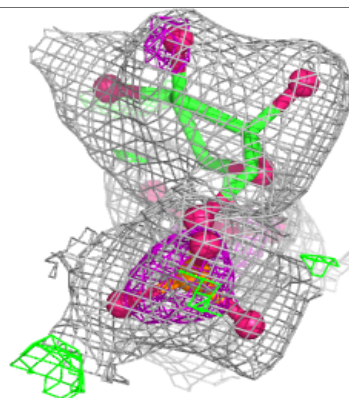
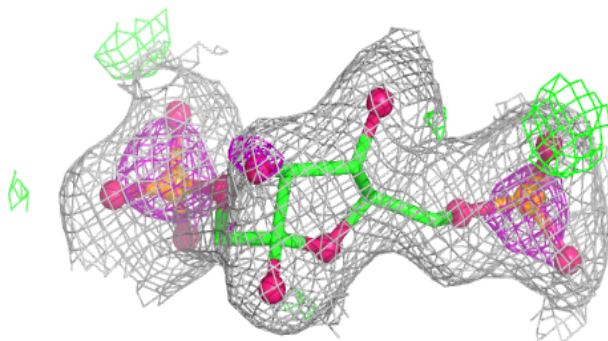
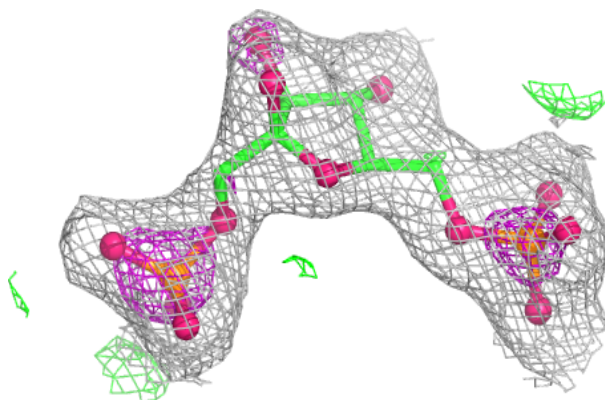


Electron density around FBP A 541:

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and green (positive)

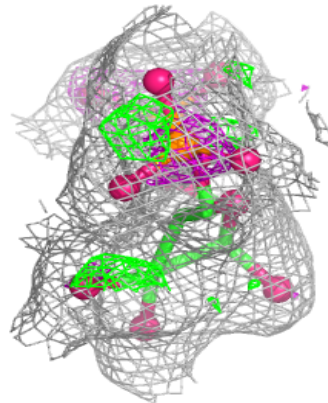
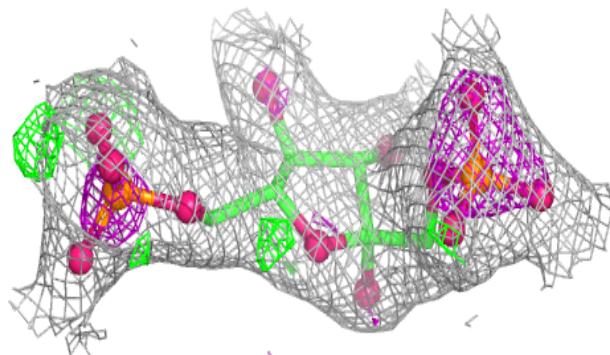
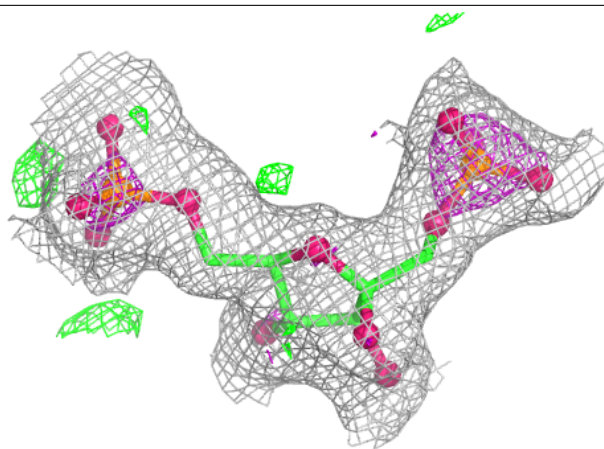
**Electron density around FBP D 541:**

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



Electron density around FBP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.