



wwPDB X-ray Structure Validation Summary Report

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 4IP7 / pdb_00004ip7
Title : Structure of the S12D variant of human liver pyruvate kinase in complex with citrate and FBP.
Authors : Holyoak, T.; Fenton, A.W.
Deposited on : 2013-01-09
Resolution : 1.80 Å (reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  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](#) ) 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

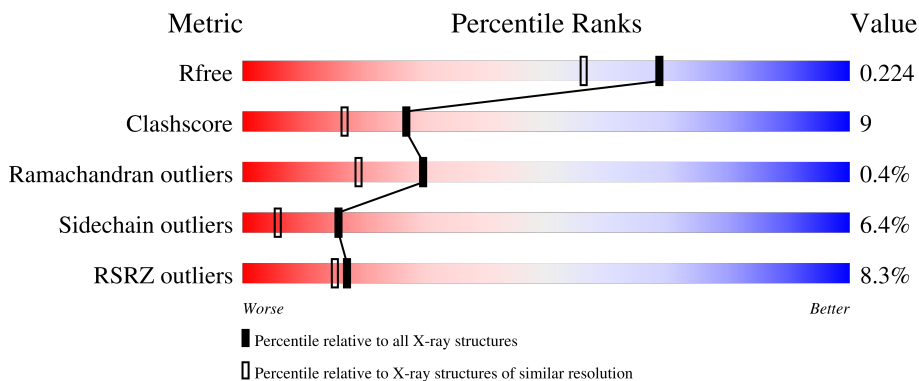
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

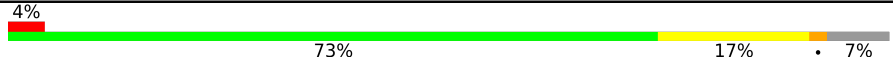



The reported resolution of this entry is 1.80 Å.

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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	543	
1	B	543	
1	C	543	
1	D	543	

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	FLC	B	602	-	-	X	-
6	PEG	A	606	-	-	X	-
8	1PE	C	605	-	X	-	-
8	1PE	C	606	-	X	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17146 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 L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	506	3944	2485	706	733	20	0	19	0
1	B	505	3882	2449	695	718	20	0	11	0
1	C	500	3831	2412	686	714	19	0	11	2
1	D	507	3920	2469	709	723	19	0	12	0

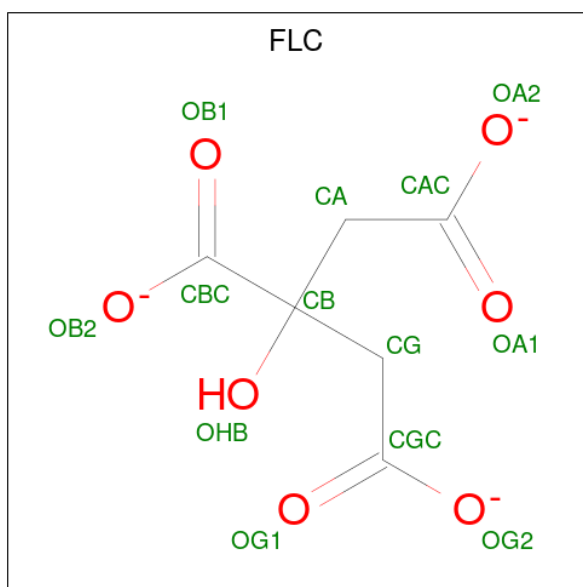
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	ASP	SER	engineered mutation	UNP P30613
B	12	ASP	SER	engineered mutation	UNP P30613
C	12	ASP	SER	engineered mutation	UNP P30613
D	12	ASP	SER	engineered mutation	UNP P30613

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

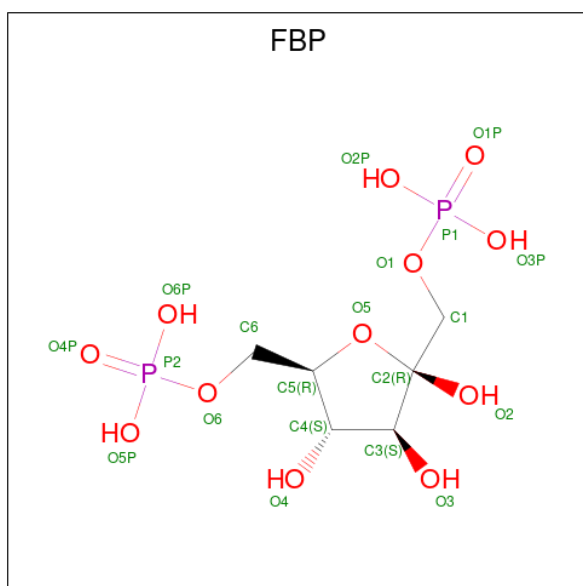
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mn 1	0	0
2	B	1	Total 1	Mn 1	0	0
2	C	1	Total 1	Mn 1	0	0
2	D	1	Total 1	Mn 1	0	0

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: C₆H₅O₇).



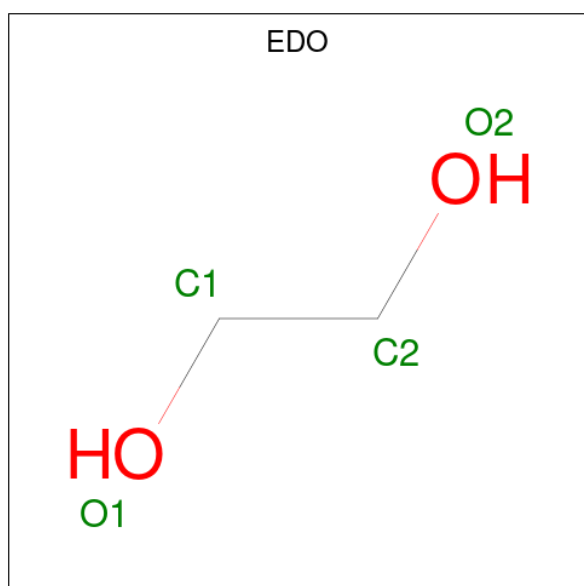
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	B	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0
3	D	1	Total C O 13 6 7	0	0

- Molecule 4 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
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		
4	C	1	Total	C	O	P	0	0
			20	6	12	2		
4	D	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



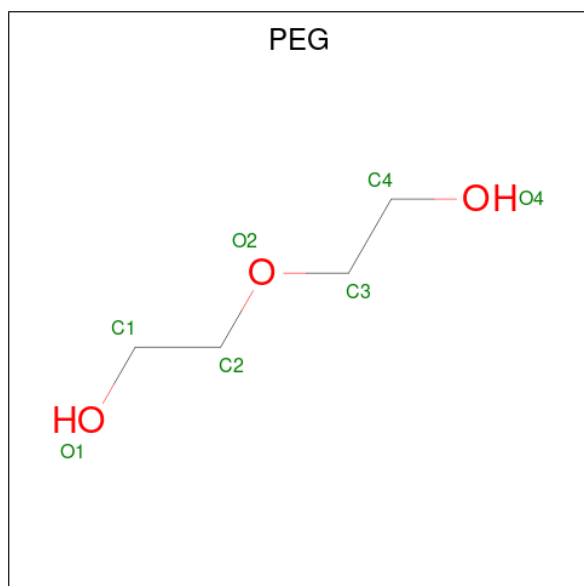
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).

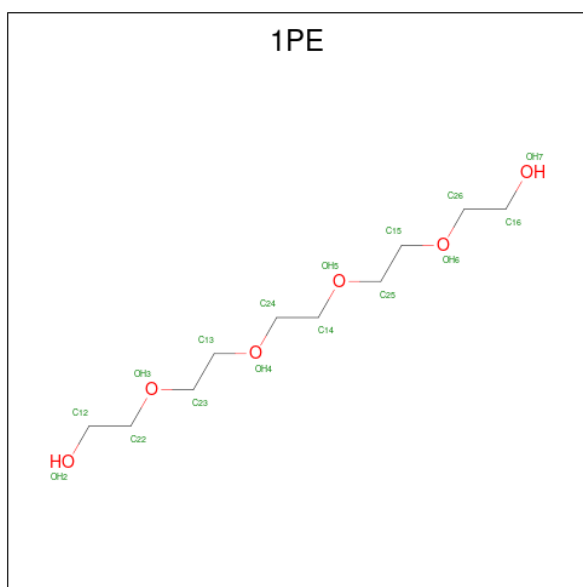


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	7	4	3	0	0
6	B	1	7	4	3	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

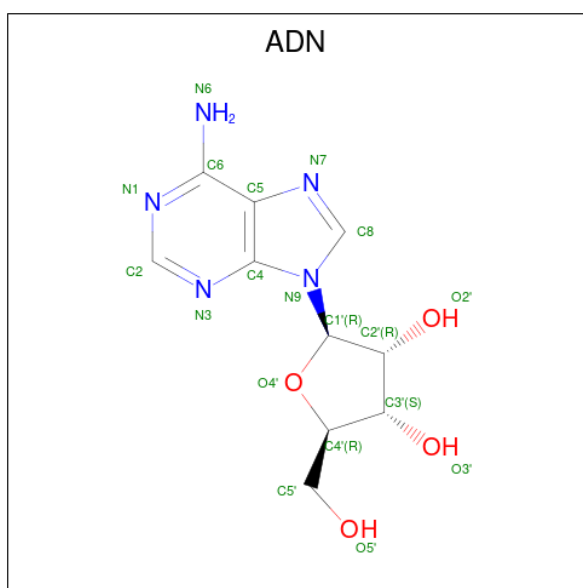
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	A	1	1	1	0	0
7	B	1	1	1	0	0
7	C	1	1	1	0	0
7	D	1	1	1	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			10	6	4		
8	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



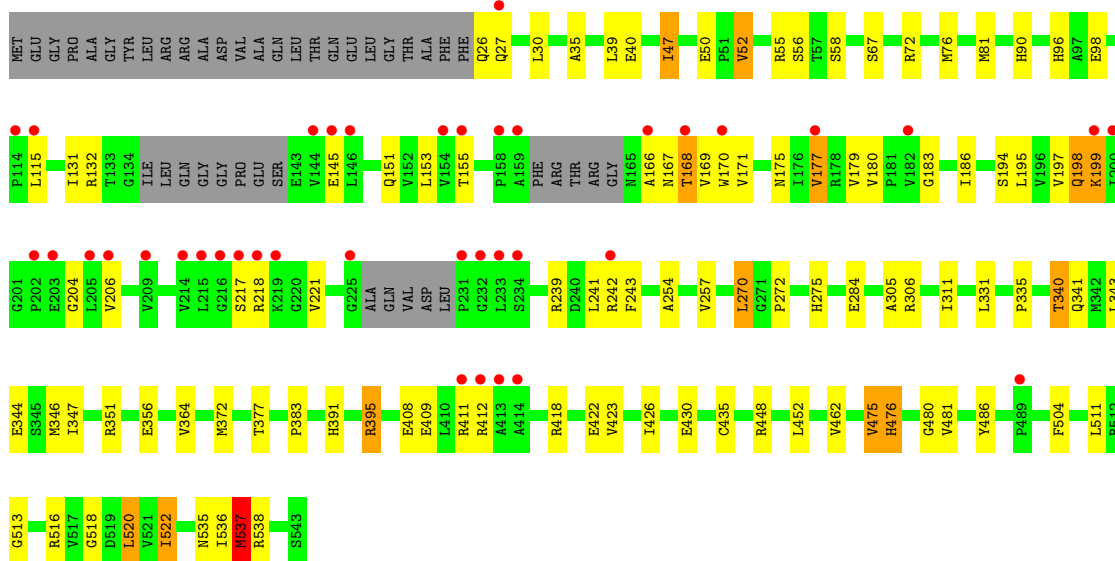
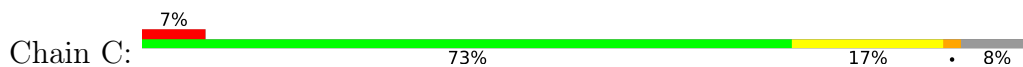
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	D	1	Total	C	N	O	0	1
			38	20	10	8		

- Molecule 10 is water.

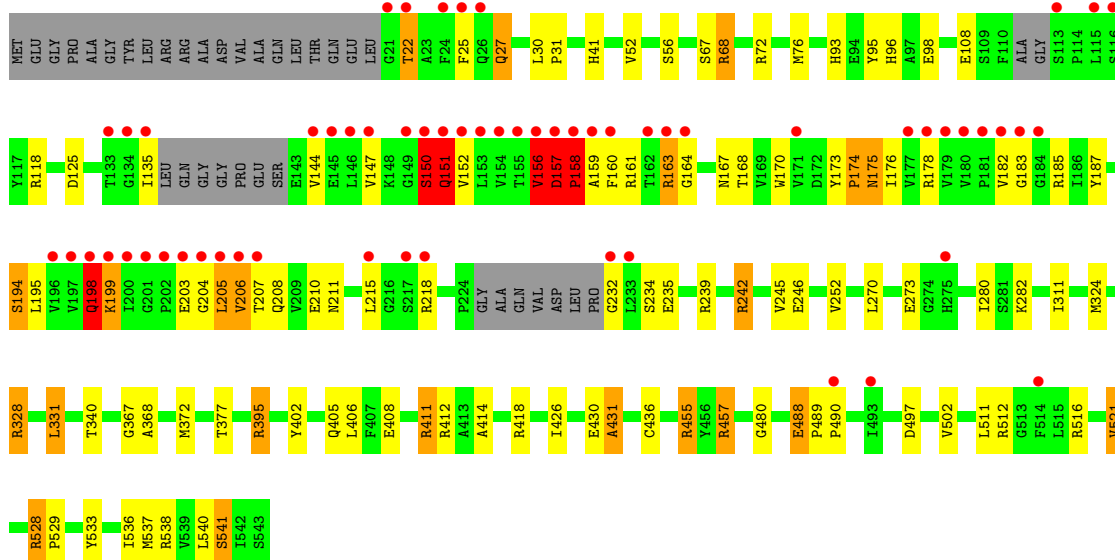
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	361	Total 361	O 361	0	0
10	B	324	Total 324	O 324	0	0
10	C	333	Total 333	O 333	0	0
10	D	306	Total 306	O 306	0	0

I542
S543

• Molecule 1: Pyruvate kinase isozymes L



• Molecule 1: Pyruvate kinase isozymes L



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.14Å 205.08Å 83.91Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	37.53 – 1.80 37.53 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (37.53-1.80) 97.5 (37.53-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.81Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.226 0.186 , 0.224	Depositor DCC
R_{free} test set	11896 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtrriage
Anisotropy	0.142	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17146	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: FLC, NA, PEG, EDO, ADN, MN, FBP, 1PE

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	1.50	25/4061 (0.6%)	1.37	23/5494 (0.4%)
1	B	1.37	11/3976 (0.3%)	1.29	17/5380 (0.3%)
1	C	1.42	17/3924 (0.4%)	1.25	14/5313 (0.3%)
1	D	1.58	41/4018 (1.0%)	1.38	45/5436 (0.8%)
All	All	1.47	94/15979 (0.6%)	1.32	99/21623 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	174	PRO	C-N	14.39	1.55	1.33
1	D	156	VAL	CA-C	14.20	1.70	1.52
1	D	204	GLY	C-N	13.11	1.52	1.33
1	D	203	GLU	CD-OE1	12.81	1.49	1.25
1	D	198	GLN	CD-NE2	12.32	1.59	1.33

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ALA	CA-C-N	-12.76	103.89	119.84
1	A	414	ALA	C-N-CA	-12.76	103.89	119.84
1	D	151	GLN	CA-C-N	-11.51	107.53	122.37
1	D	151	GLN	C-N-CA	-11.51	107.53	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	158	PRO	N-CA-CB	-9.01	93.79	103.25

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	151	GLN	Mainchain
1	D	157	ASP	Mainchain

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	3944	0	4061	69	1
1	B	3882	0	3990	78	0
1	C	3831	0	3928	79	0
1	D	3920	0	4026	79	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	4	1	0
3	B	13	0	4	4	0
3	C	13	0	4	1	0
3	D	13	0	4	2	0
4	A	20	0	10	0	0
4	B	20	0	10	0	0
4	C	20	0	10	0	0
4	D	20	0	10	0	0
5	A	8	0	12	0	0
5	B	8	0	12	1	0
5	C	8	0	12	1	0
5	D	12	0	18	0	0
6	A	7	0	10	9	0
6	B	7	0	10	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	C	17	0	22	22	0
9	D	38	0	26	3	0
10	A	361	0	0	13	1
10	B	324	0	0	6	0
10	C	333	0	0	12	0
10	D	306	0	0	11	0
All	All	17146	0	16183	294	2

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 9.

The worst 5 of 294 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)
8:C:606:1PE:H232	10:C:734:HOH:O	1.45	1.17
1:C:58:SER:N	8:C:606:1PE:H131	1.66	1.09
1:D:455:ARG:HG3	1:D:455:ARG:HH11	1.10	1.09
1:B:156:VAL:HG21	1:B:174:PRO:HA	1.34	1.08
1:C:476:HIS:ND1	8:C:606:1PE:H122	1.70	1.06

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:994:HOH:O	10:A:1017:HOH:O[1_455]	1.83	0.37
1:A:74:LYS:NZ	1:D:246:GLU:OE1[2_645]	2.13	0.07

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	517/543 (95%)	504 (98%)	11 (2%)	2 (0%)	30 19
1	B	508/543 (94%)	491 (97%)	15 (3%)	2 (0%)	30 19
1	C	503/543 (93%)	492 (98%)	9 (2%)	2 (0%)	30 19
1	D	511/543 (94%)	494 (97%)	16 (3%)	1 (0%)	43 31
All	All	2039/2172 (94%)	1981 (97%)	51 (2%)	7 (0%)	30 25

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	GLY
1	D	340	THR
1	B	340	THR
1	C	340	THR
1	A	535	ASN

5.3.2 Protein sidechains [i](#)

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	426/433 (98%)	400 (94%)	26 (6%)	17 6
1	B	415/433 (96%)	378 (91%)	37 (9%)	9 2
1	C	412/433 (95%)	393 (95%)	19 (5%)	24 12
1	D	420/433 (97%)	394 (94%)	26 (6%)	16 6
All	All	1673/1732 (97%)	1565 (94%)	108 (6%)	16 5

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	511	LEU
1	C	198	GLN
1	D	331	LEU
1	B	521	VAL
1	C	168	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	27	GLN
1	C	151	GLN
1	D	211	ASN
1	C	167	ASN
1	B	211	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 8 are monoatomic - leaving 23 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
8	1PE	C	605	-	9,9,15	2.11	5 (55%)	8,8,14	1.72	2 (25%)
4	FBP	A	603	-	18,20,20	1.13	2 (11%)	21,32,32	1.64	5 (23%)
5	EDO	A	605	-	3,3,3	0.70	0	2,2,2	0.55	0
9	ADN	D	604[B]	-	21,21,21	1.58	3 (14%)	31,31,31	2.39	13 (41%)
3	FLC	B	602	2	12,12,12	1.28	1 (8%)	17,17,17	1.60	2 (11%)
5	EDO	D	607	-	3,3,3	1.10	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	PEG	B	605	-	6,6,6	0.93	0	5,5,5	0.56	0
3	FLC	D	602	2	12,12,12	1.74	4 (33%)	17,17,17	1.63	4 (23%)
9	ADN	D	604[A]	-	21,21,21	1.60	3 (14%)	31,31,31	2.22	12 (38%)
5	EDO	D	605	-	3,3,3	0.95	0	2,2,2	0.69	0
5	EDO	D	606	-	3,3,3	0.77	0	2,2,2	1.11	0
5	EDO	B	606	-	3,3,3	1.55	1 (33%)	2,2,2	0.62	0
4	FBP	B	603	-	18,20,20	1.15	3 (16%)	21,32,32	1.64	3 (14%)
4	FBP	C	604	-	18,20,20	0.94	1 (5%)	21,32,32	1.29	3 (14%)
5	EDO	C	601	-	3,3,3	0.85	0	2,2,2	1.04	0
5	EDO	A	604	-	3,3,3	0.68	0	2,2,2	0.87	0
4	FBP	D	603	-	18,20,20	1.54	4 (22%)	21,32,32	1.69	7 (33%)
5	EDO	C	607	-	3,3,3	0.80	0	2,2,2	0.29	0
3	FLC	A	602	2	12,12,12	1.76	2 (16%)	17,17,17	2.09	5 (29%)
5	EDO	B	604	-	3,3,3	0.73	0	2,2,2	0.77	0
3	FLC	C	603	2	12,12,12	1.85	3 (25%)	17,17,17	1.84	4 (23%)
8	1PE	C	606	-	6,6,15	2.66	2 (33%)	5,5,14	4.14	3 (60%)
6	PEG	A	606	-	6,6,6	0.68	0	5,5,5	1.53	2 (40%)

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
8	1PE	C	605	-	-	5/7/7/13	-
4	FBP	A	603	-	-	3/13/32/32	0/1/1/1
5	EDO	A	605	-	-	0/1/1/1	-
9	ADN	D	604[B]	-	-	3/6/22/22	0/3/3/3
3	FLC	B	602	2	-	8/16/16/16	-
5	EDO	D	607	-	-	0/1/1/1	-
6	PEG	B	605	-	-	3/4/4/4	-
3	FLC	D	602	2	-	2/16/16/16	-
9	ADN	D	604[A]	-	-	5/6/22/22	0/3/3/3
5	EDO	D	605	-	-	1/1/1/1	-
5	EDO	D	606	-	-	1/1/1/1	-
5	EDO	B	606	-	-	0/1/1/1	-
4	FBP	B	603	-	-	2/13/32/32	0/1/1/1
4	FBP	C	604	-	-	2/13/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	601	-	-	0/1/1/1	-
5	EDO	A	604	-	-	0/1/1/1	-
4	FBP	D	603	-	-	2/13/32/32	0/1/1/1
5	EDO	C	607	-	-	1/1/1/1	-
3	FLC	A	602	2	-	3/16/16/16	-
5	EDO	B	604	-	-	0/1/1/1	-
3	FLC	C	603	2	-	2/16/16/16	-
8	1PE	C	606	-	-	2/4/4/13	-
6	PEG	A	606	-	-	3/4/4/4	-

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	606	1PE	OH3-C23	4.88	1.63	1.42
9	D	604[A]	ADN	C5-C4	4.83	1.47	1.39
9	D	604[B]	ADN	C5-C4	4.82	1.47	1.39
3	A	602	FLC	CG-CB	4.25	1.59	1.54
3	C	603	FLC	CG-CB	3.95	1.58	1.54

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	606	1PE	OH3-C23-C13	6.59	139.17	110.11
9	D	604[B]	ADN	C5-C4-N3	-5.78	118.75	126.72
8	C	606	1PE	OH4-C13-C23	5.28	142.93	111.82
9	D	604[A]	ADN	C5-C4-N3	-5.12	119.67	126.72
3	B	602	FLC	OB2-CBC-CB	4.85	122.45	113.14

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

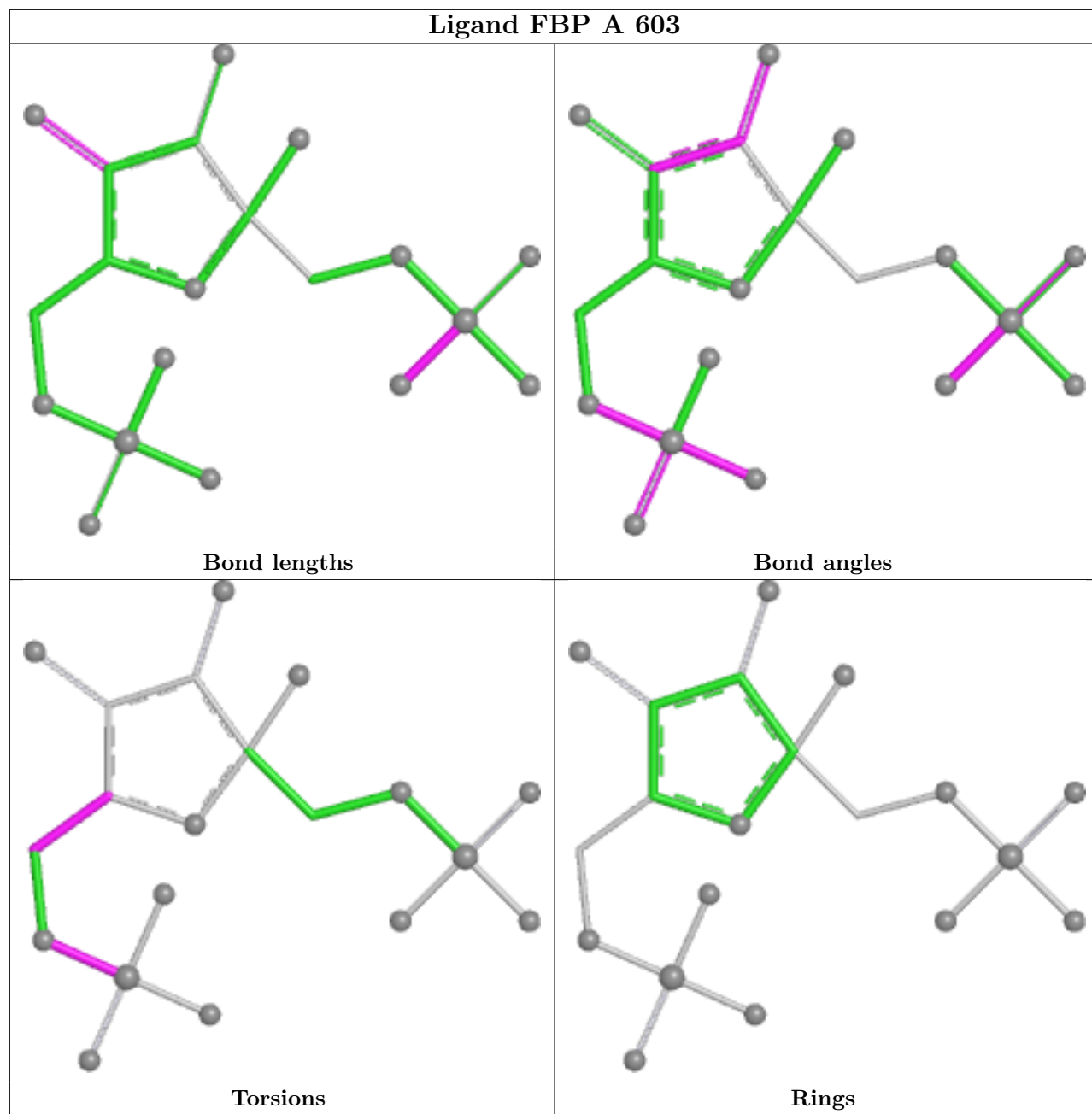
Mol	Chain	Res	Type	Atoms
9	D	604[A]	ADN	C2'-C1'-N9-C8
8	C	605	1PE	C23-C13-OH4-C24
9	D	604[A]	ADN	C3'-C4'-C5'-O5'
9	D	604[A]	ADN	O4'-C4'-C5'-O5'
4	B	603	FBP	C4-C5-C6-O6

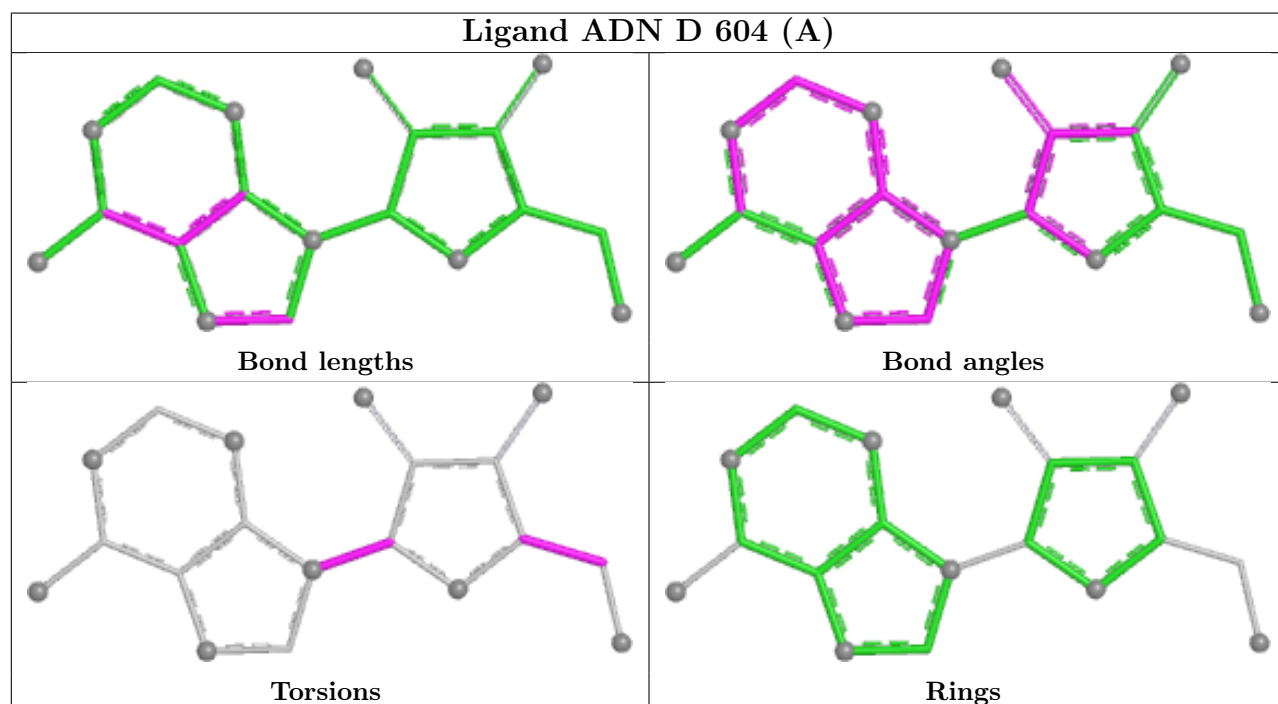
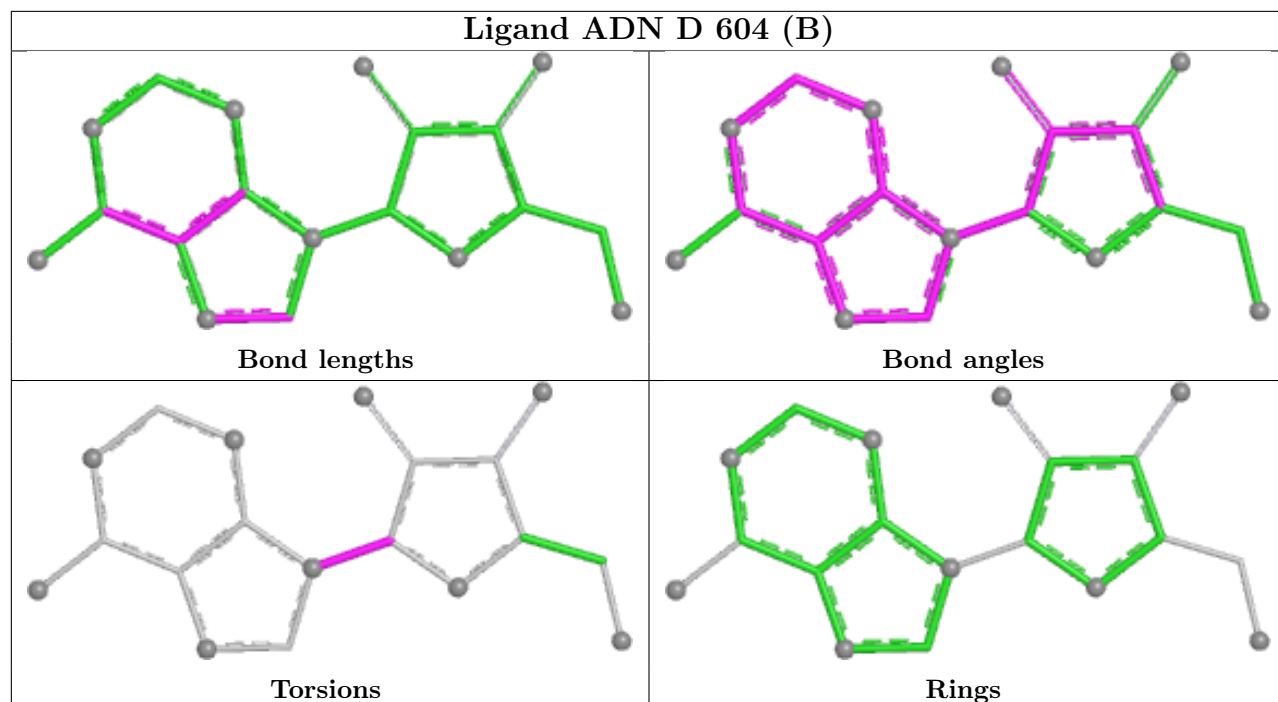
There are no ring outliers.

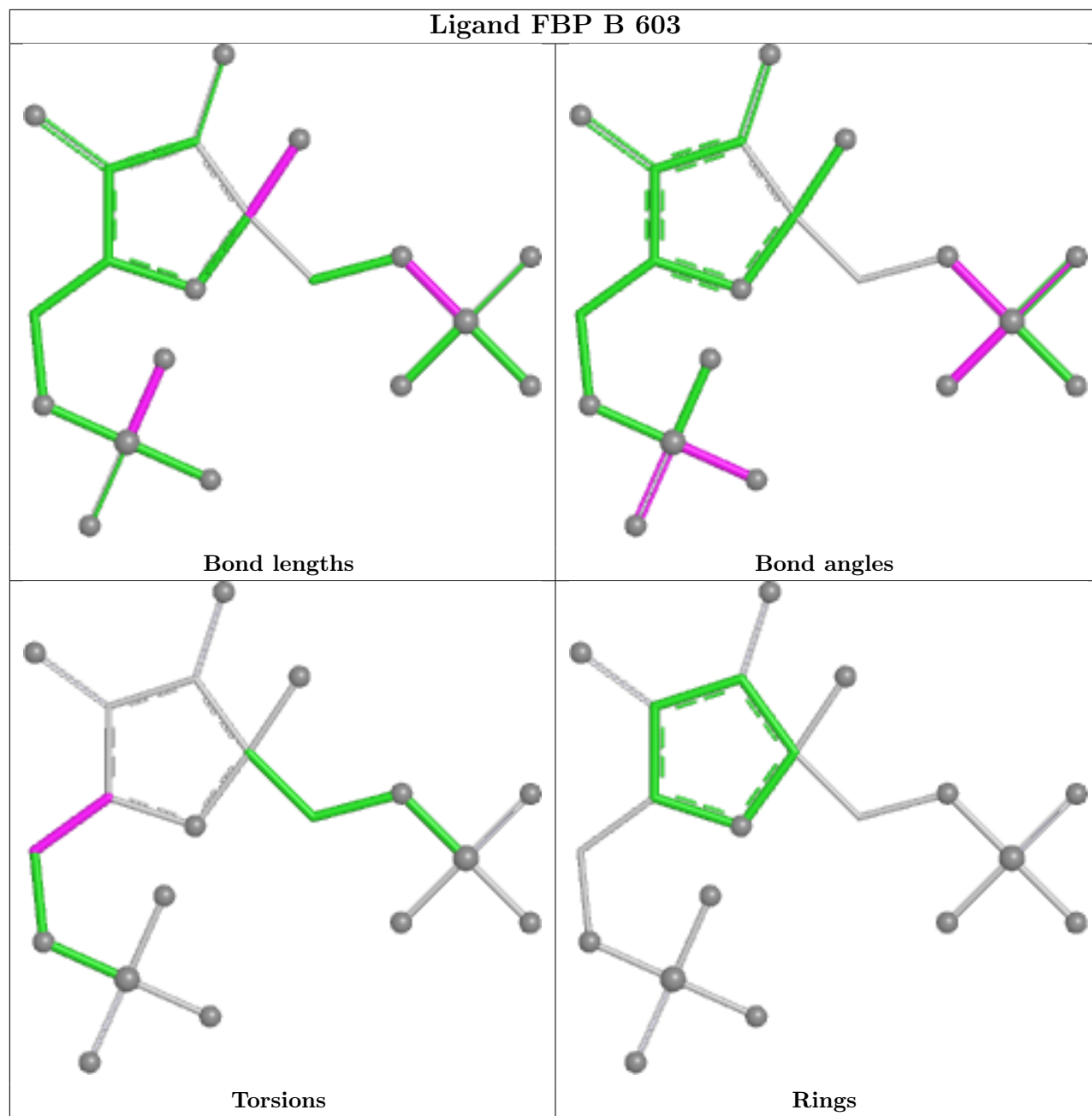
11 monomers are involved in 45 short contacts:

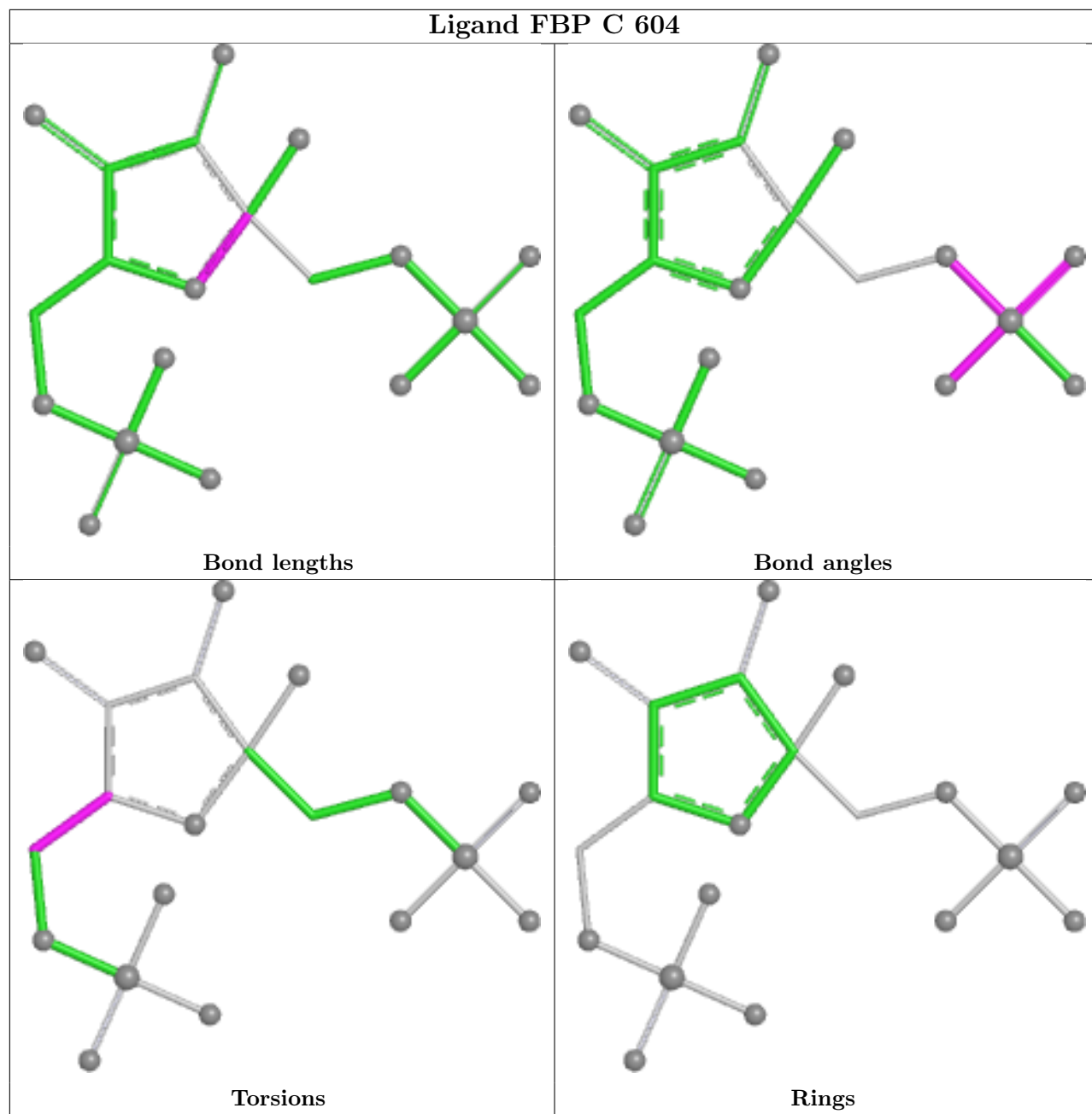
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	605	1PE	3	0
9	D	604[B]	ADN	3	0
3	B	602	FLC	4	0
6	B	605	PEG	1	0
3	D	602	FLC	2	0
5	B	606	EDO	1	0
5	C	601	EDO	1	0
3	A	602	FLC	1	0
3	C	603	FLC	1	0
8	C	606	1PE	19	0
6	A	606	PEG	9	0

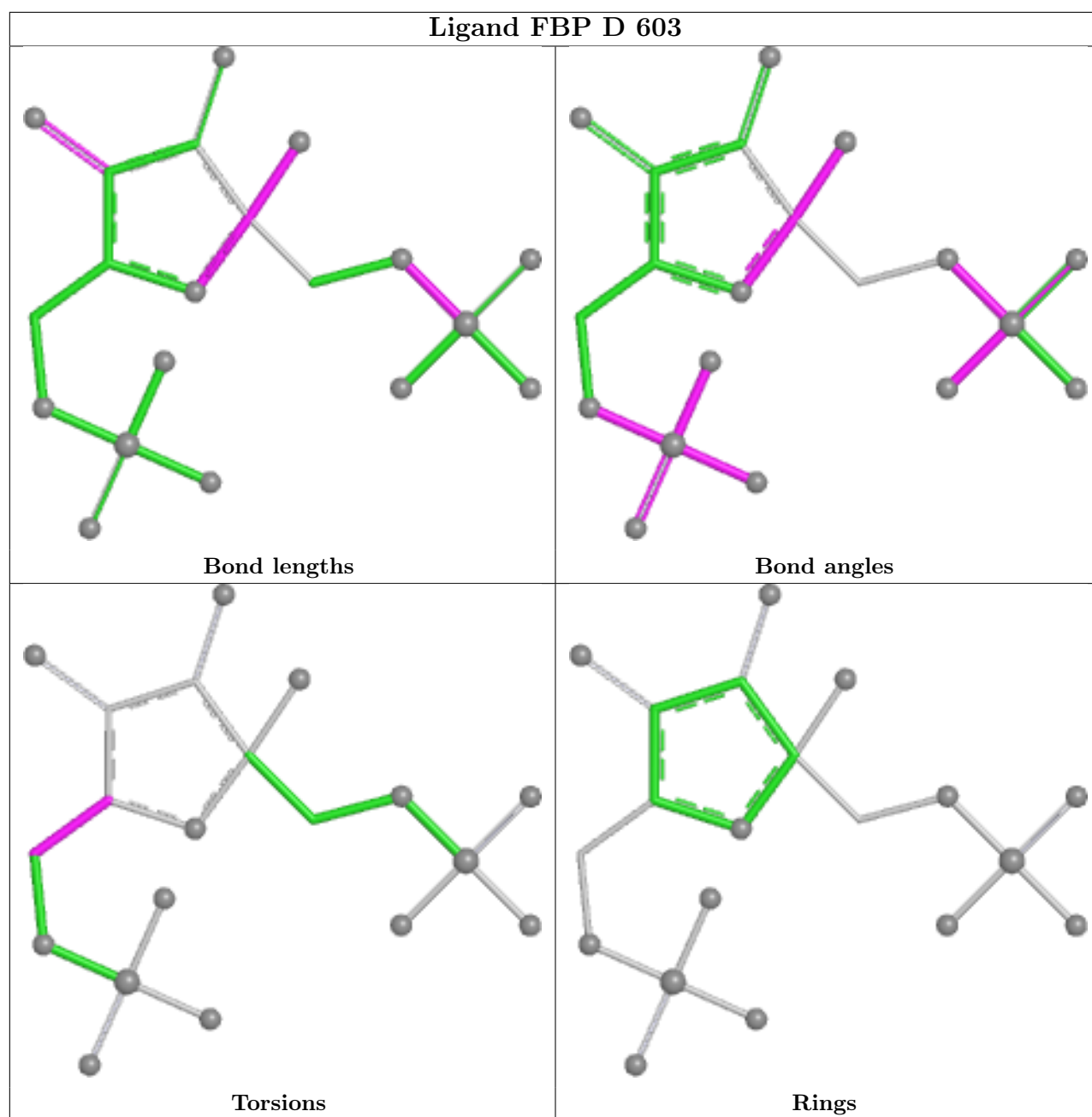
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	506/543 (93%)	0.01	24 (4%) 36 35	15, 31, 73, 103	19 (3%)
1	B	505/543 (93%)	0.22	45 (8%) 15 13	16, 33, 96, 125	11 (2%)
1	C	500/543 (92%)	0.22	39 (7%) 19 17	16, 34, 95, 120	12 (2%)
1	D	507/543 (93%)	0.27	60 (11%) 9 7	16, 34, 115, 197	12 (2%)
All	All	2018/2172 (92%)	0.18	168 (8%) 17 15	15, 33, 96, 197	54 (2%)

The worst 5 of 168 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	228	VAL	8.8
1	B	135	ILE	6.3
1	C	233	LEU	6.3
1	D	160	PHE	6.0
1	D	21	GLY	5.6

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](#)

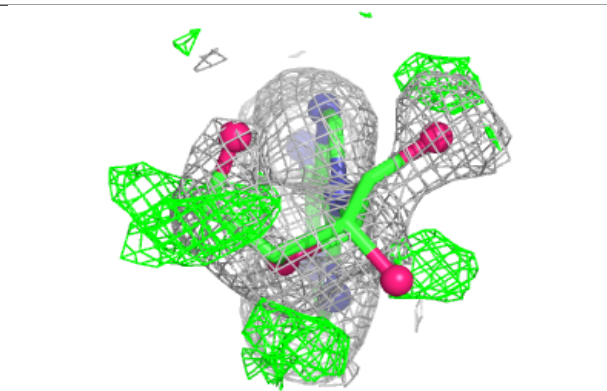
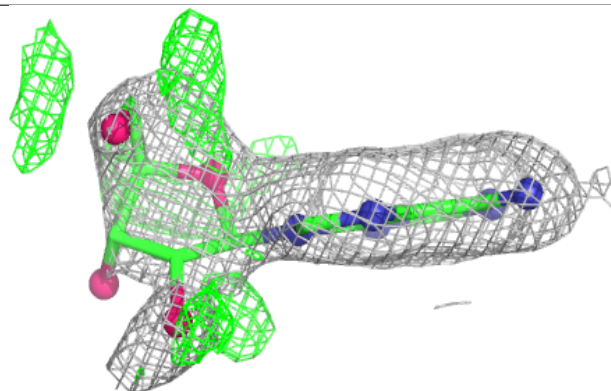
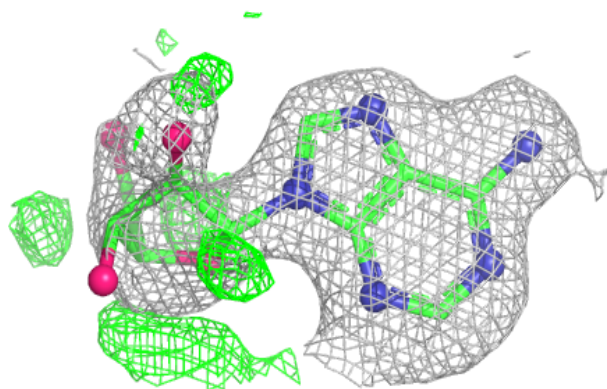
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PEG	B	605	7/7	0.77	0.16	42,50,59,60	0
8	1PE	C	605	10/16	0.81	0.14	41,46,48,49	0
5	EDO	C	607	4/4	0.82	0.13	44,52,55,56	0
9	ADN	D	604[A]	19/19	0.82	0.14	26,30,41,43	19
9	ADN	D	604[B]	19/19	0.82	0.14	26,30,47,49	19
6	PEG	A	606	7/7	0.84	0.14	37,42,47,48	0
5	EDO	B	606	4/4	0.87	0.19	32,36,36,44	0
5	EDO	D	606	4/4	0.89	0.13	42,43,52,55	0
8	1PE	C	606	7/16	0.91	0.11	29,32,41,42	0
7	NA	C	608	1/1	0.92	0.10	41,41,41,41	0
7	NA	B	607	1/1	0.93	0.10	37,37,37,37	0
3	FLC	B	602	13/13	0.94	0.07	26,30,42,44	0
5	EDO	A	605	4/4	0.94	0.08	30,35,36,38	0
5	EDO	D	605	4/4	0.94	0.11	27,29,32,38	0
3	FLC	D	602	13/13	0.95	0.08	25,32,42,42	0
7	NA	A	607	1/1	0.95	0.11	40,40,40,40	0
5	EDO	C	601	4/4	0.95	0.09	35,35,37,38	0
3	FLC	C	603	13/13	0.95	0.07	24,31,41,47	0
5	EDO	A	604	4/4	0.96	0.07	25,27,28,34	0
3	FLC	A	602	13/13	0.96	0.06	21,27,36,39	0
5	EDO	D	607	4/4	0.96	0.07	31,35,36,38	0
5	EDO	B	604	4/4	0.96	0.07	27,32,34,37	0
7	NA	D	608	1/1	0.97	0.10	38,38,38,38	0
4	FBP	D	603	20/20	0.98	0.05	26,28,32,32	0
4	FBP	C	604	20/20	0.98	0.05	23,27,29,30	0
2	MN	C	602	1/1	0.99	0.05	28,28,28,28	0
4	FBP	A	603	20/20	0.99	0.04	22,25,28,28	0
4	FBP	B	603	20/20	0.99	0.04	23,26,29,30	0
2	MN	A	601	1/1	0.99	0.02	26,26,26,26	0
2	MN	D	601	1/1	1.00	0.02	28,28,28,28	0
2	MN	B	601	1/1	1.00	0.04	27,27,27,27	0

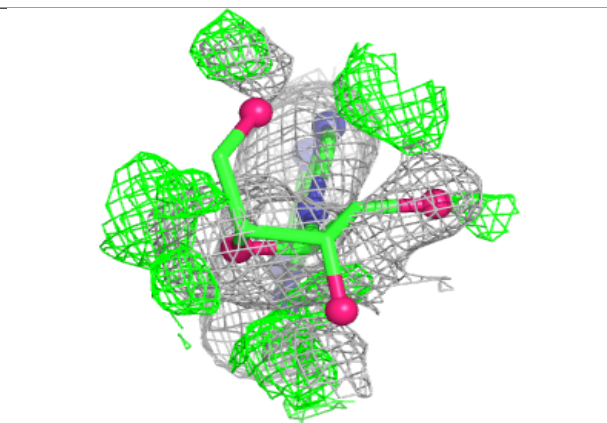
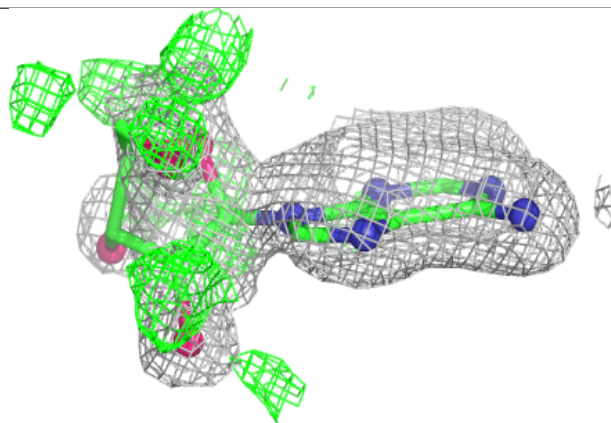
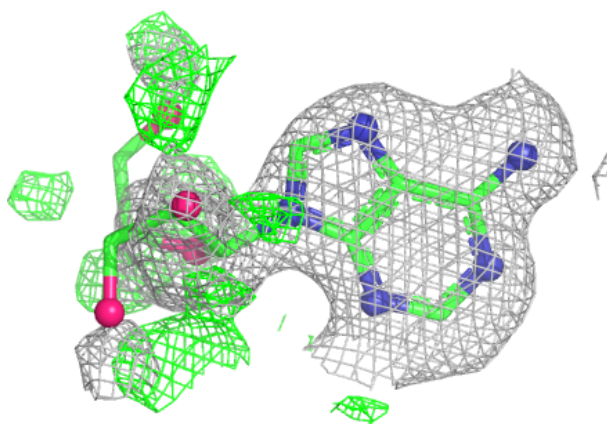
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADN D 604 (A):

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

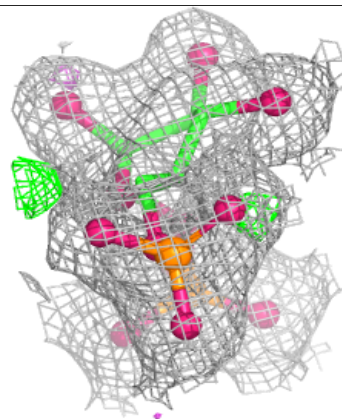
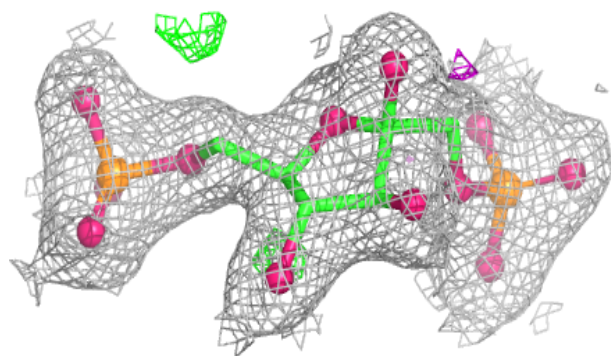
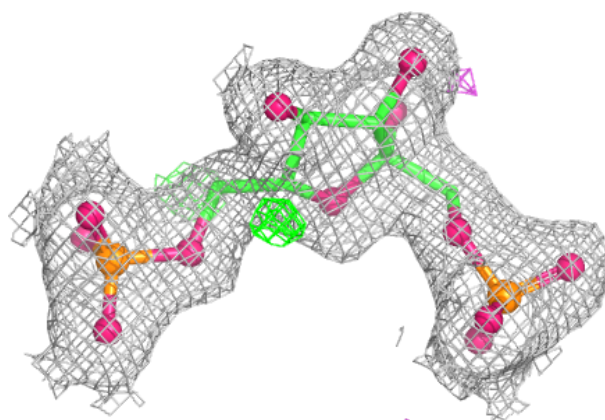
**Electron density around ADN D 604 (B):**

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



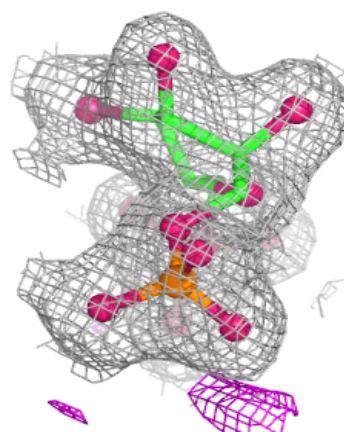
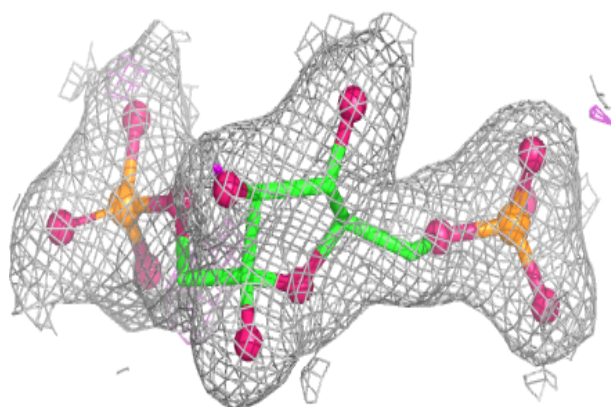
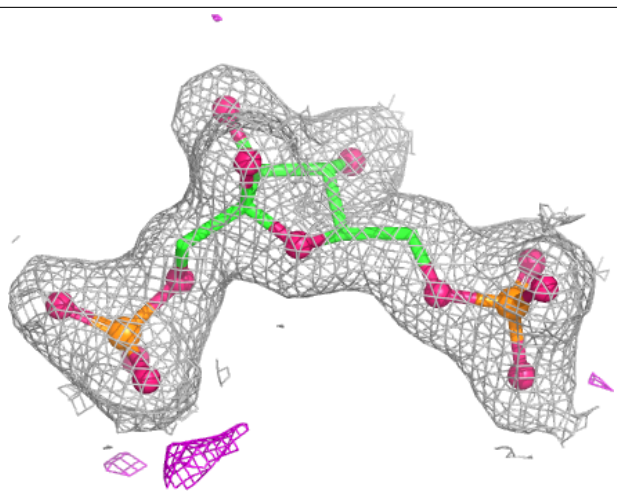
Electron density around FBP D 603:

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



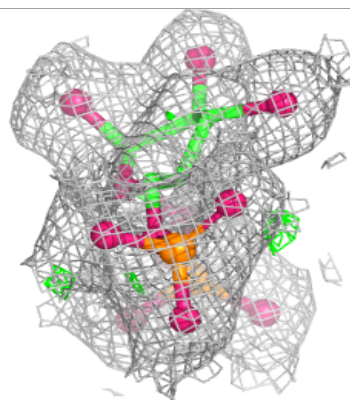
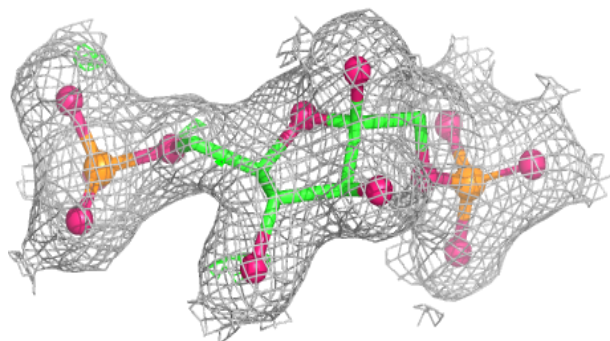
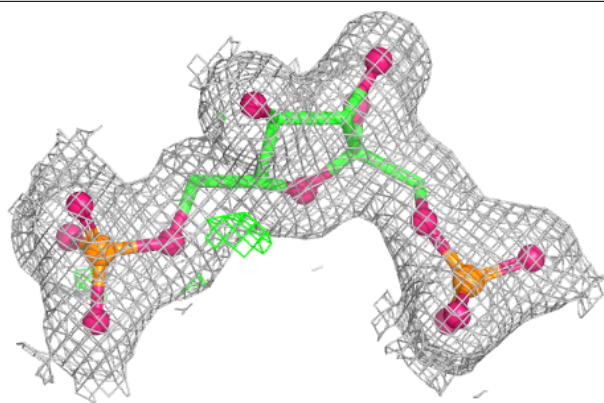
Electron density around FBP C 604:

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

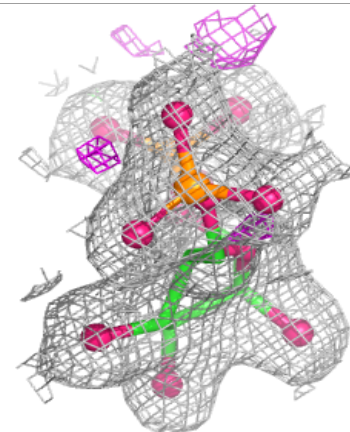
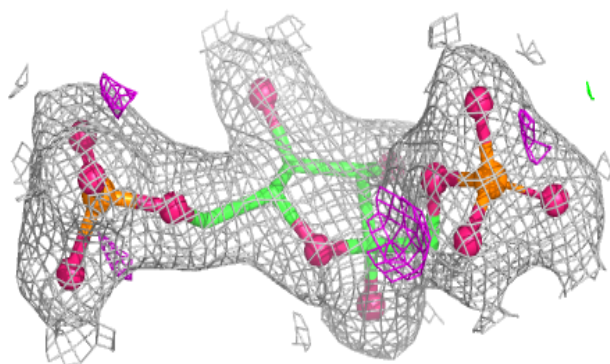
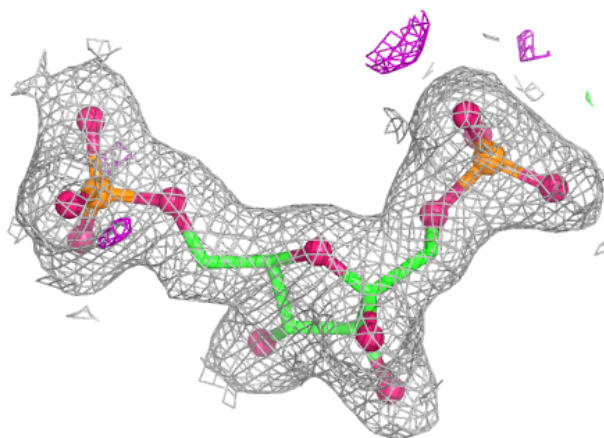


Electron density around FBP A 603:

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

**Electron density around FBP B 603:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.