



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:38 PM UTC

PDB ID : 6ECH / pdb_00006ech
Title : Pyruvate Kinase Isoform L-type with phosphorylated Ser12 (pS12) in complex with FBP
Authors : Padyana, A.; Tong, S.
Deposited on : 2018-08-07
Resolution : 2.19 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 ⓘ](#)) 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

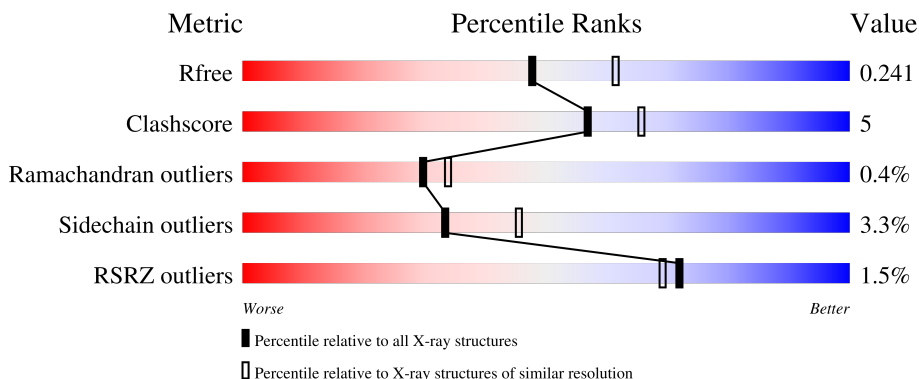
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


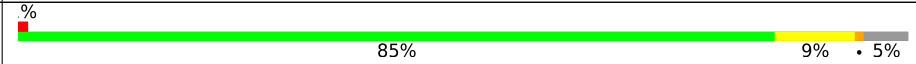
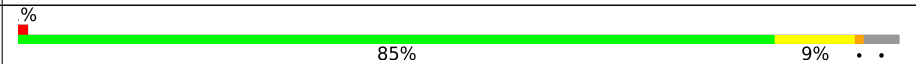

The reported resolution of this entry is 2.19 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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
5	OXL	A	607	-	X	-	-
5	OXL	B	607	-	X	-	-
5	OXL	C	604	-	X	-	-
5	OXL	D	606	-	X	-	-
6	EDO	C	611	-	-	X	-

2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 17686 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 PKLR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	528	4038	2537	722	761	18	0	2	0
1	B	525	4001	2516	715	752	18	0	1	0
1	C	528	4054	2546	734	756	18	0	2	0
1	D	527	4012	2522	717	755	18	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

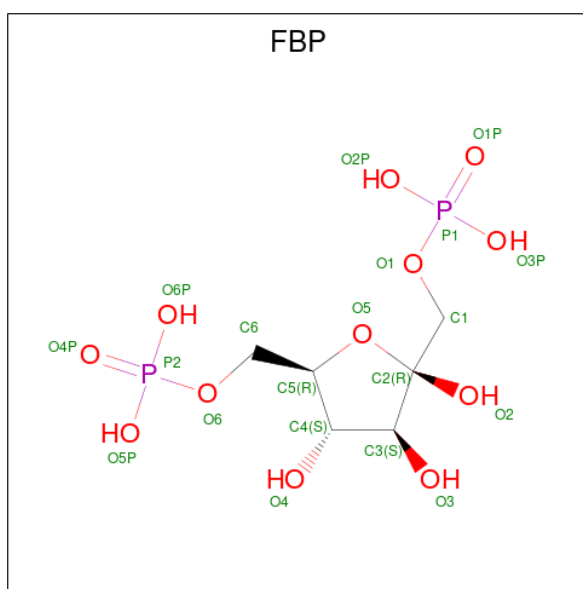
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P12928
A	544	HIS	-	expression tag	UNP P12928
A	545	HIS	-	expression tag	UNP P12928
A	546	HIS	-	expression tag	UNP P12928
A	547	HIS	-	expression tag	UNP P12928
A	548	HIS	-	expression tag	UNP P12928
A	549	HIS	-	expression tag	UNP P12928
B	0	HIS	-	expression tag	UNP P12928
B	544	HIS	-	expression tag	UNP P12928
B	545	HIS	-	expression tag	UNP P12928
B	546	HIS	-	expression tag	UNP P12928
B	547	HIS	-	expression tag	UNP P12928
B	548	HIS	-	expression tag	UNP P12928
B	549	HIS	-	expression tag	UNP P12928
C	0	HIS	-	expression tag	UNP P12928
C	544	HIS	-	expression tag	UNP P12928
C	545	HIS	-	expression tag	UNP P12928
C	546	HIS	-	expression tag	UNP P12928
C	547	HIS	-	expression tag	UNP P12928
C	548	HIS	-	expression tag	UNP P12928
C	549	HIS	-	expression tag	UNP P12928

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP P12928
D	544	HIS	-	expression tag	UNP P12928
D	545	HIS	-	expression tag	UNP P12928
D	546	HIS	-	expression tag	UNP P12928
D	547	HIS	-	expression tag	UNP P12928
D	548	HIS	-	expression tag	UNP P12928
D	549	HIS	-	expression tag	UNP P12928

- 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 MAGNESIUM ION (CCD ID: MG) (formula: Mg).

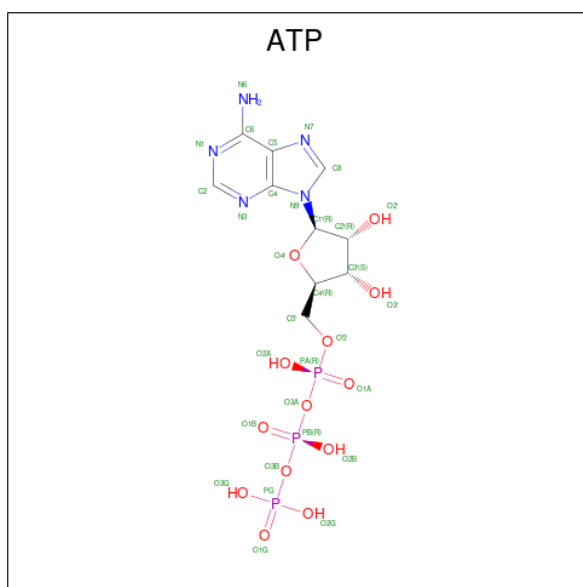
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

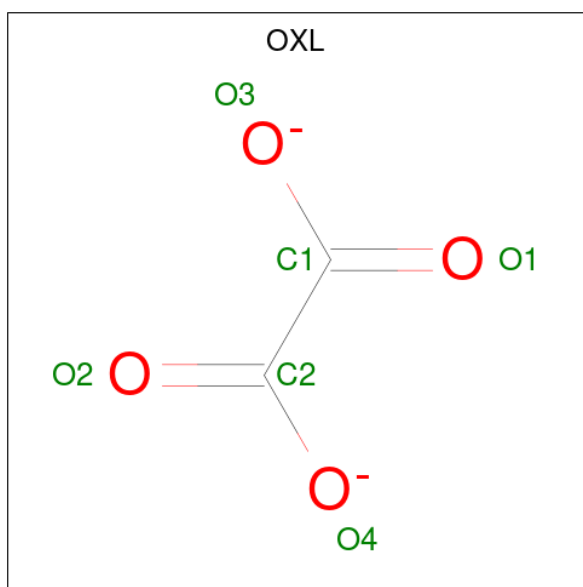
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Mg	0	0
			4	4		
3	C	2	Total	Mg	0	0
			2	2		
3	D	3	Total	Mg	0	0
			3	3		

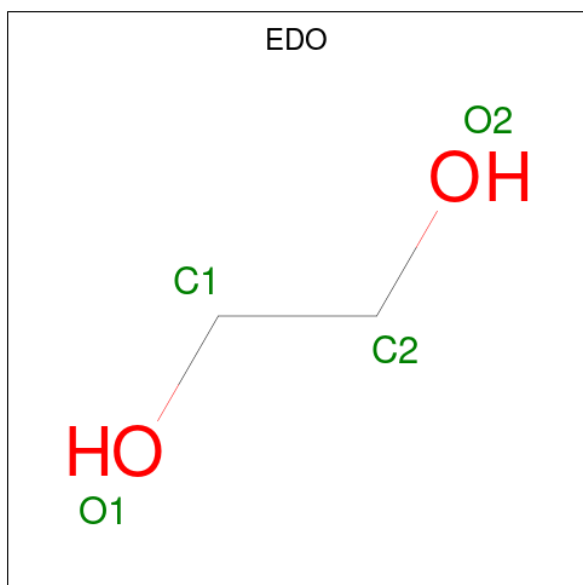
- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 2 4	0	0
5	B	1	Total C O 6 2 4	0	0
5	C	1	Total C O 6 2 4	0	0
5	D	1	Total C O 6 2 4	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



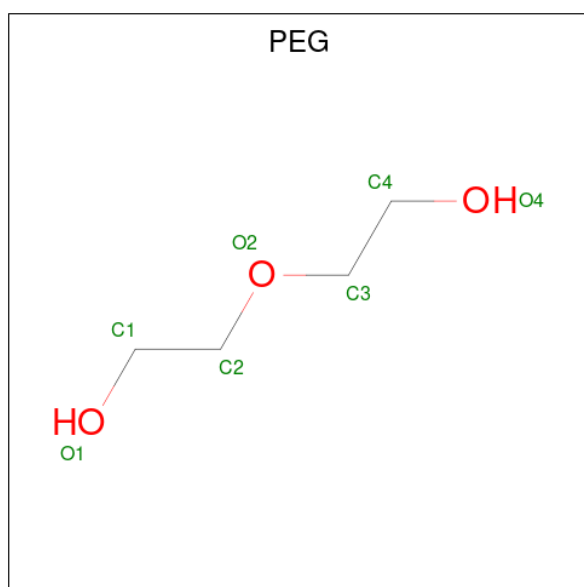
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0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

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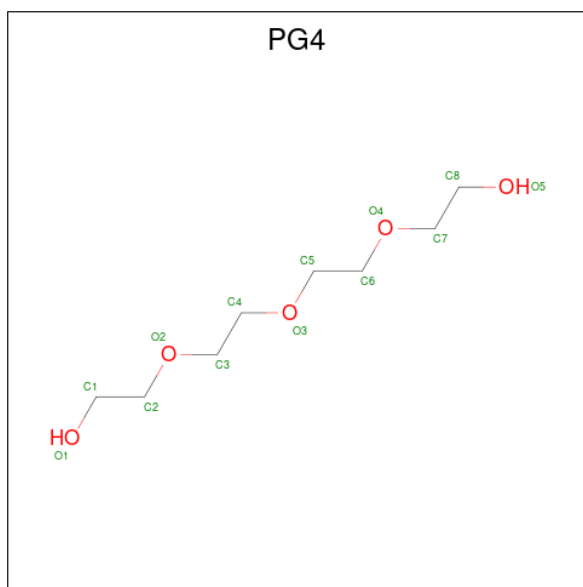
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



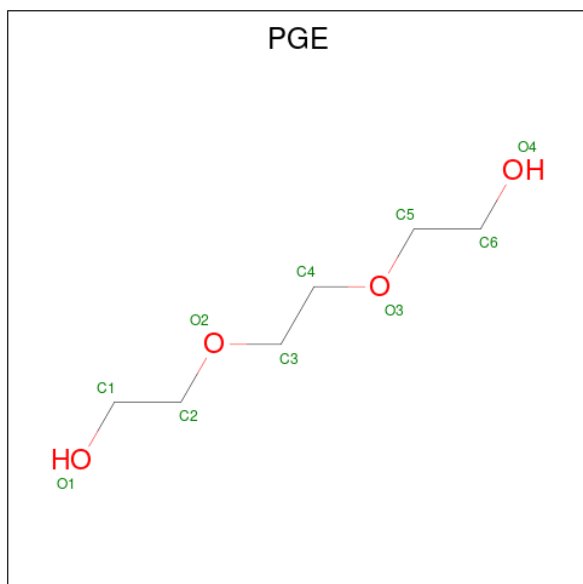
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Cl	0	0
			1	1		

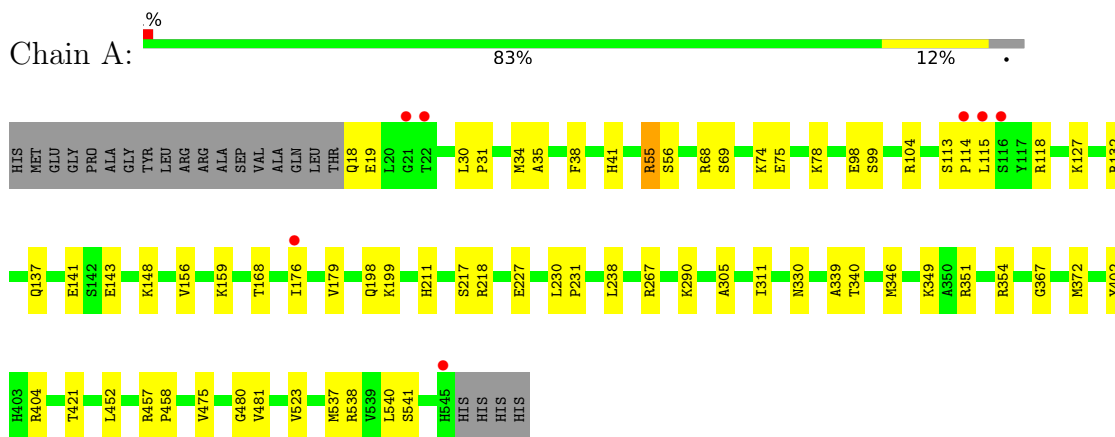
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	320	Total	O	0	0
			320	320		
11	B	281	Total	O	0	0
			281	281		
11	C	306	Total	O	0	0
			306	306		
11	D	294	Total	O	0	0
			294	294		

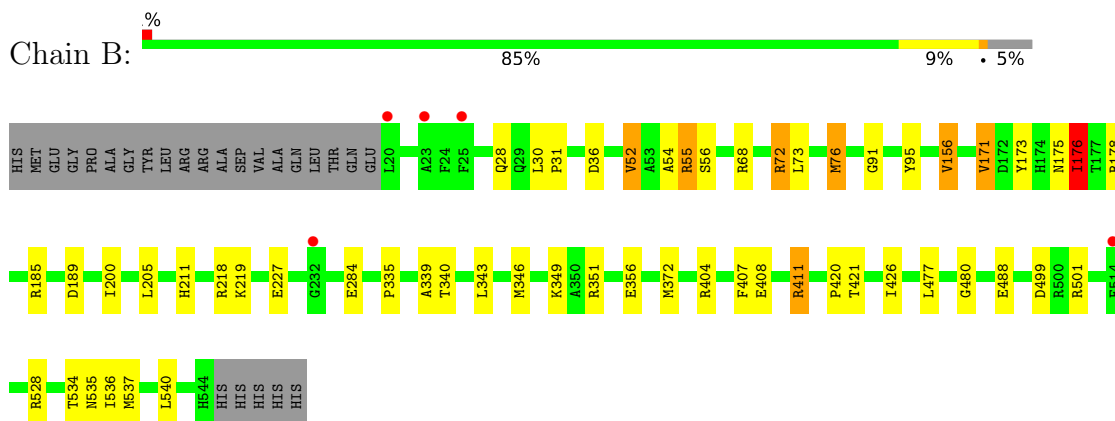
3 Residue-property plots [i](#)

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.

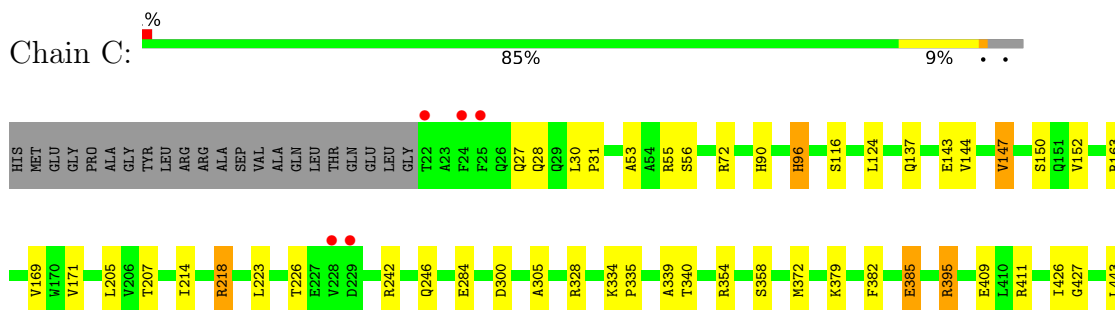
- Molecule 1: Pyruvate kinase PKLR

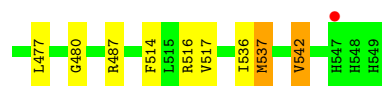


- Molecule 1: Pyruvate kinase PKLR

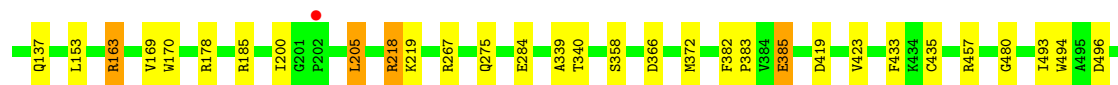
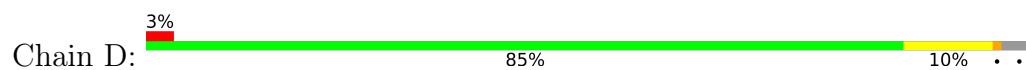


- Molecule 1: Pyruvate kinase PKLR





- Molecule 1: Pyruvate kinase PKLR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.55Å 108.90Å 296.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.19 49.52 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.52-2.19) 99.9 (49.52-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.18Å)	Xtrriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.181 , 0.238 0.189 , 0.241	Depositor DCC
R_{free} test set	7124 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17686	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: PEG, ATP, EDO, FBP, PG4, PGE, CL, MG, OXL

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	0.90	0/4104	1.02	2/5560 (0.0%)
1	B	0.89	1/4066 (0.0%)	1.04	3/5509 (0.1%)
1	C	0.87	0/4125	1.04	2/5587 (0.0%)
1	D	0.87	0/4077	1.02	4/5523 (0.1%)
All	All	0.88	1/16372 (0.0%)	1.03	11/22179 (0.0%)

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	A	0	6
1	B	0	4
1	C	0	4
1	D	0	5
All	All	0	19

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	ILE	N-CA	7.96	1.55	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	THR	CB-CA-C	6.54	121.54	109.70
1	B	52	VAL	N-CA-C	-6.02	107.02	111.90
1	B	176	ILE	N-CA-CB	5.89	117.83	110.47
1	C	96	HIS	CA-CB-CG	-5.80	108.00	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	514	PHE	CA-CB-CG	5.39	119.19	113.80
1	B	72	ARG	CG-CD-NE	-5.35	100.22	112.00
1	A	311	ILE	N-CA-C	-5.25	108.39	113.53
1	D	366	ASP	CA-CB-CG	5.01	117.61	112.60
1	D	275	GLN	CB-CA-C	-5.01	102.17	110.68
1	D	219	LYS	CA-C-N	5.00	124.72	119.92
1	D	219	LYS	C-N-CA	5.00	124.72	119.92

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	ARG	Sidechain
1	A	132	ARG	Sidechain
1	A	218	ARG	Sidechain
1	A	267	ARG	Sidechain
1	A	457	ARG	Sidechain
1	A	55	ARG	Sidechain
1	B	404	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	55	ARG	Sidechain
1	B	72	ARG	Sidechain
1	C	163	ARG	Sidechain
1	C	328	ARG	Sidechain
1	C	516	ARG	Sidechain
1	C	72	ARG	Sidechain
1	D	185	ARG	Sidechain
1	D	218	ARG	Sidechain
1	D	267	ARG	Sidechain
1	D	457	ARG	Sidechain
1	D	55	ARG	Sidechain

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	4038	0	4098	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4001	0	4072	39	0
1	C	4054	0	4105	40	0
1	D	4012	0	4080	29	0
2	A	20	0	10	0	0
2	B	20	0	10	2	0
2	C	20	0	10	0	0
2	D	20	0	10	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	31	0	12	0	0
4	B	31	0	12	0	0
4	D	31	0	12	0	0
5	A	6	0	0	1	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
6	A	28	0	42	9	0
6	B	36	0	54	5	0
6	C	36	0	54	7	0
6	D	32	0	48	3	0
7	A	7	0	10	3	0
7	D	7	0	10	0	0
8	A	13	0	18	2	0
9	B	10	0	14	5	0
10	D	1	0	0	0	0
11	A	320	0	0	10	0
11	B	281	0	0	8	0
11	C	306	0	0	8	0
11	D	294	0	0	7	0
All	All	17686	0	16681	152	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 5.

All (152) 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:537:MET:HE3	1:C:537:MET:HE3	1.52	0.92
1:C:382:PHE:HB3	1:C:385:GLU:HG2	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:MET:HE3	1:D:537:MET:HE3	1.65	0.77
1:D:435:CYS:HB2	1:D:520:LEU:HD12	1.68	0.76
1:C:354:ARG:HH12	6:C:608:EDO:H11	1.52	0.73
1:C:242:ARG:CZ	11:C:702:HOH:O	2.37	0.71
1:C:339:ALA:HB1	1:C:372:MET:HE2	1.76	0.68
1:C:242:ARG:NE	11:C:702:HOH:O	2.26	0.68
1:D:493:ILE:HB	1:D:496:ASP:OD2	1.94	0.67
1:D:382:PHE:HB3	1:D:385:GLU:HG2	1.75	0.67
1:A:351:ARG:NH2	1:B:211:HIS:ND1	2.43	0.67
1:C:143:GLU:CD	1:C:214:ILE:HD11	2.20	0.66
1:D:137:GLN:OE1	1:D:163:ARG:HG3	1.97	0.65
1:B:91:GLY:H	9:B:608:PGE:H32	1.61	0.65
1:C:56:SER:HB2	1:C:480:GLY:HA2	1.80	0.63
1:A:55:ARG:H	6:A:608:EDO:H12	1.64	0.62
1:A:211:HIS:ND1	1:B:351:ARG:NH1	2.47	0.62
1:C:218:ARG:HD2	11:C:965:HOH:O	1.99	0.62
1:C:354:ARG:HH12	6:C:608:EDO:C1	2.13	0.62
1:A:30:LEU:O	1:A:34:MET:HG2	2.01	0.61
1:A:458:PRO:HG2	7:A:615:PEG:H11	1.82	0.60
1:B:156:VAL:HG23	1:B:176:ILE:HD11	1.83	0.60
1:A:538:ARG:HG2	1:C:536:ILE:HG12	1.84	0.59
1:C:300:ASP:OD1	6:C:611:EDO:C2	2.50	0.59
1:A:113:SER:C	1:A:115:LEU:H	2.11	0.59
1:D:68:ARG:NH2	1:D:95:TYR:O	2.36	0.59
1:A:480:GLY:HA3	7:A:615:PEG:H12	1.83	0.59
1:A:18:GLN:N	11:A:705:HOH:O	2.35	0.58
1:A:354:ARG:HH22	6:A:612:EDO:H12	1.69	0.58
1:D:516:ARG:NH2	11:D:705:HOH:O	2.34	0.57
1:D:68:ARG:HH22	1:D:98:GLU:HB2	1.69	0.56
1:A:537:MET:CE	1:C:537:MET:HE3	2.32	0.56
1:A:118:ARG:NH2	11:A:707:HOH:O	2.38	0.56
1:B:501:ARG:NH2	2:B:601:FBP:O3P	2.39	0.56
1:B:501:ARG:HH22	2:B:601:FBP:P1	2.29	0.56
6:A:612:EDO:C1	11:B:842:HOH:O	2.54	0.55
1:A:421[B]:THR:HG23	11:A:760:HOH:O	2.07	0.55
1:D:96:HIS:HD2	11:D:887:HOH:O	1.90	0.55
1:A:68:ARG:NH2	11:A:708:HOH:O	2.39	0.55
1:A:421[B]:THR:HG21	11:A:881:HOH:O	2.06	0.55
6:A:612:EDO:H12	11:B:842:HOH:O	2.06	0.55
1:A:480:GLY:HA3	7:A:615:PEG:C1	2.38	0.54
1:A:523:VAL:HG21	1:A:540:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:O	1:A:115:LEU:N	2.40	0.54
1:C:147:VAL:HG22	1:C:150:SER:HB3	1.90	0.53
1:C:517:VAL:HA	1:C:542:VAL:HG22	1.89	0.53
1:A:305:ALA:HB1	5:A:607:OXL:C2	2.39	0.53
1:A:330:ASN:HD21	1:A:367:GLY:HA3	1.74	0.53
1:A:75[A]:GLU:OE1	1:A:78:LYS:NZ	2.36	0.52
1:B:55:ARG:H	6:B:610:EDO:C1	2.23	0.52
1:B:175:ASN:ND2	1:B:178:ARG:HH11	2.07	0.52
1:D:115:LEU:O	1:D:512:ARG:NE	2.41	0.51
1:A:56:SER:HB2	1:A:480:GLY:HA2	1.92	0.51
1:C:382:PHE:HB3	1:C:385:GLU:CG	2.38	0.51
1:B:68:ARG:NH1	1:B:95:TYR:O	2.36	0.51
1:D:38:PHE:O	1:D:41:HIS:HB3	2.12	0.50
1:B:91:GLY:N	9:B:608:PGE:H32	2.27	0.50
1:C:242:ARG:CZ	1:C:246:GLN:HE22	2.24	0.50
1:A:55:ARG:N	6:A:608:EDO:H12	2.26	0.50
1:B:91:GLY:H	9:B:608:PGE:C3	2.25	0.50
1:B:421[A]:THR:HG23	1:B:534:THR:HB	1.92	0.50
1:C:411:ARG:HG2	1:C:426:ILE:HD11	1.94	0.50
1:D:118:ARG:NH1	11:D:706:HOH:O	2.34	0.49
1:B:54:ALA:HA	6:B:610:EDO:H21	1.94	0.49
1:B:189:ASP:CG	1:B:219:LYS:HD2	2.38	0.49
1:D:68:ARG:NH2	1:D:98:GLU:HB2	2.27	0.49
1:A:230:LEU:O	1:A:231:PRO:C	2.56	0.49
1:C:300:ASP:OD1	6:C:611:EDO:H22	2.12	0.49
1:A:346:MET:HA	1:A:349:LYS:O	2.12	0.48
1:C:90:HIS:O	1:C:96:HIS:HE1	1.95	0.48
1:C:124:LEU:C	1:C:124:LEU:HD23	2.39	0.48
1:B:420:PRO:HB2	11:B:718:HOH:O	2.12	0.48
1:C:300:ASP:OD1	6:C:611:EDO:H21	2.14	0.48
1:D:200:ILE:HG12	1:D:205:LEU:HD23	1.94	0.48
1:B:540:LEU:HD22	6:B:611:EDO:C1	2.44	0.47
1:C:300:ASP:HA	6:C:611:EDO:H22	1.94	0.47
1:B:536:ILE:HG12	1:D:538:ARG:HG2	1.96	0.47
1:B:56:SER:HB2	1:B:480:GLY:HA2	1.96	0.47
1:C:284:GLU:HG2	1:C:305:ALA:HB3	1.96	0.47
1:C:335:PRO:HB3	1:C:477:LEU:O	2.14	0.47
1:D:544:HIS:C	1:D:544:HIS:CD2	2.92	0.47
1:C:27:GLN:HG2	11:C:958:HOH:O	2.14	0.47
1:C:55:ARG:HB2	1:C:395:ARG:HG3	1.97	0.47
1:C:28:GLN:HG2	11:C:804:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:O	1:C:207:THR:HG23	2.16	0.46
1:B:421[B]:THR:HG23	11:B:762:HOH:O	2.15	0.46
1:C:218:ARG:NH1	11:C:709:HOH:O	2.42	0.46
1:C:53:ALA:O	1:C:395:ARG:NH1	2.44	0.46
1:C:427:GLY:C	1:C:537:MET:HE2	2.40	0.46
1:B:408:GLU:HG2	11:D:884:HOH:O	2.16	0.45
1:D:494:TRP:NE1	1:D:529:PRO:HG3	2.31	0.45
1:D:494:TRP:CD1	1:D:529:PRO:HG3	2.51	0.45
1:B:339:ALA:HB1	1:B:372:MET:HE2	1.98	0.45
6:B:610:EDO:O2	11:B:701:HOH:O	2.21	0.45
1:A:421[B]:THR:OG1	1:A:452:LEU:HD12	2.16	0.45
1:D:61:ALA:HB3	1:D:81:MET:SD	2.57	0.45
1:A:38:PHE:O	1:A:41:HIS:HB3	2.17	0.44
1:B:411:ARG:HG3	1:B:426:ILE:HD11	1.99	0.44
1:C:30:LEU:N	1:C:31:PRO:CD	2.80	0.44
1:B:421[B]:THR:CG2	11:B:762:HOH:O	2.64	0.44
1:B:156:VAL:CG2	1:B:176:ILE:HD11	2.48	0.44
1:B:200:ILE:HG12	1:B:205:LEU:HD23	2.00	0.44
1:A:475:VAL:HB	1:A:481:VAL:HG11	2.00	0.44
1:B:218:ARG:HH11	9:B:608:PGE:H32	1.83	0.44
1:D:435:CYS:CB	1:D:520:LEU:HD12	2.44	0.44
1:A:351:ARG:HD2	11:A:997:HOH:O	2.17	0.43
1:B:73:LEU:HA	1:B:76:MET:HG3	2.00	0.43
1:B:218:ARG:HE	9:B:608:PGE:H4	1.83	0.43
1:C:409:GLU:OE2	1:D:37:THR:HB	2.18	0.43
1:A:35:ALA:O	1:A:402:TYR:OH	2.35	0.43
1:B:421[B]:THR:HG22	1:B:534:THR:HB	2.01	0.43
1:D:339:ALA:HB1	1:D:372:MET:HE2	2.01	0.43
1:B:171:VAL:HG11	1:B:176:ILE:HG12	2.01	0.42
1:D:382:PHE:N	1:D:383:PRO:CD	2.82	0.42
1:A:217:SER:HB2	6:A:610:EDO:H12	2.01	0.42
1:C:487:ARG:NH1	11:C:705:HOH:O	2.35	0.42
1:D:528:ARG:HB2	1:D:529:PRO:CD	2.49	0.42
6:B:611:EDO:H22	11:B:896:HOH:O	2.18	0.42
1:D:133:THR:HA	1:D:170:TRP:O	2.20	0.42
1:A:118:ARG:HH12	6:A:611:EDO:H11	1.84	0.42
1:C:143:GLU:OE1	1:C:214:ILE:HD11	2.20	0.42
6:A:608:EDO:H22	6:A:611:EDO:C2	2.49	0.42
1:A:339:ALA:HB1	1:A:372:MET:HE2	2.02	0.42
1:B:343:LEU:HD23	1:B:356:GLU:HB3	2.02	0.42
1:A:30:LEU:N	1:A:31:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:HD2	1:A:99:SER:OG	2.19	0.42
1:A:68:ARG:HH12	1:A:98:GLU:HB3	1.84	0.42
1:B:335:PRO:HB3	1:B:477:LEU:O	2.19	0.42
1:C:334:LYS:HE2	6:C:611:EDO:H11	2.02	0.41
1:D:433:PHE:CD2	6:D:607:EDO:H22	2.55	0.41
1:A:541:SER:H	8:A:616:PG4:C3	2.33	0.41
1:B:28:GLN:HG2	11:B:878:HOH:O	2.20	0.41
1:A:137:GLN:NE2	11:A:735:HOH:O	2.54	0.41
1:B:346:MET:HA	1:B:349:LYS:O	2.20	0.41
1:C:443:LEU:N	1:C:443:LEU:HD23	2.36	0.41
6:D:613:EDO:H21	11:D:921:HOH:O	2.20	0.41
1:A:69:SER:HB2	6:A:613:EDO:H12	2.03	0.41
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.93	0.41
1:B:30:LEU:N	1:B:31:PRO:CD	2.83	0.41
1:D:56:SER:HB2	1:D:480:GLY:HA2	2.01	0.41
1:A:127:LYS:NZ	11:A:716:HOH:O	2.53	0.41
11:A:753:HOH:O	1:B:36:ASP:HB3	2.21	0.41
6:D:613:EDO:C1	11:D:875:HOH:O	2.69	0.41
1:B:173:TYR:O	1:B:176:ILE:HG13	2.20	0.41
1:B:407:PHE:CE2	1:B:411:ARG:HD3	2.56	0.41
1:A:74:LYS:HE3	11:A:846:HOH:O	2.20	0.41
1:A:113:SER:C	1:A:115:LEU:N	2.78	0.41
1:C:90:HIS:O	1:C:96:HIS:CE1	2.72	0.41
1:C:242:ARG:HD2	11:C:888:HOH:O	2.21	0.41
1:D:419:ASP:O	1:D:423:VAL:HG23	2.20	0.40
1:D:218:ARG:NH2	11:D:735:HOH:O	2.53	0.40
1:A:541:SER:H	8:A:616:PG4:H31	1.86	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	528/550 (96%)	512 (97%)	14 (3%)	2 (0%)	30	34
1	B	524/550 (95%)	513 (98%)	9 (2%)	2 (0%)	30	34
1	C	528/550 (96%)	517 (98%)	10 (2%)	1 (0%)	43	51
1	D	525/550 (96%)	508 (97%)	14 (3%)	3 (1%)	21	23
All	All	2105/2200 (96%)	2050 (97%)	47 (2%)	8 (0%)	30	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	PRO
1	A	340	THR
1	B	340	THR
1	B	535	ASN
1	C	340	THR
1	D	535	ASN
1	D	112	THR
1	D	340	THR

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	432/446 (97%)	418 (97%)	14 (3%)	34	47
1	B	428/446 (96%)	417 (97%)	11 (3%)	40	55
1	C	433/446 (97%)	417 (96%)	16 (4%)	30	41
1	D	429/446 (96%)	413 (96%)	16 (4%)	30	41
All	All	1722/1784 (96%)	1665 (97%)	57 (3%)	33	45

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLU
1	A	141	GLU
1	A	143	GLU

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	156	VAL
1	A	159	LYS
1	A	176	ILE
1	A	179	VAL
1	A	198	GLN
1	A	199	LYS
1	A	227	GLU
1	A	238	LEU
1	A	290	LYS
1	A	404	ARG
1	B	52	VAL
1	B	76	MET
1	B	156	VAL
1	B	171	VAL
1	B	176	ILE
1	B	185	ARG
1	B	227	GLU
1	B	284	GLU
1	B	411	ARG
1	B	488	GLU
1	B	499	ASP
1	C	116	SER
1	C	137	GLN
1	C	144	VAL
1	C	147	VAL
1	C	152	VAL
1	C	169	VAL
1	C	171	VAL
1	C	218	ARG
1	C	223	LEU
1	C	226	THR
1	C	358	SER
1	C	379	LYS
1	C	385	GLU
1	C	395	ARG
1	C	537	MET
1	C	542	VAL
1	D	20	LEU
1	D	52	VAL
1	D	68	ARG
1	D	78	LYS

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Mol	Chain	Res	Type
1	D	127	LYS
1	D	153	LEU
1	D	163	ARG
1	D	169	VAL
1	D	178	ARG
1	D	205	LEU
1	D	284	GLU
1	D	358	SER
1	D	385	GLU
1	D	499	ASP
1	D	543	SER
1	D	544	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	161	GLN
1	A	174	HIS
1	A	175	ASN
1	A	246	GLN
1	A	275	GLN
1	A	330	ASN
1	A	470	GLN
1	B	27	GLN
1	B	161	GLN
1	B	175	ASN
1	B	236	GLN
1	B	470	GLN
1	B	544	HIS
1	C	28	GLN
1	C	96	HIS
1	C	161	GLN
1	C	236	GLN
1	C	246	GLN
1	C	405	GLN
1	C	470	GLN
1	C	545	HIS
1	C	546	HIS
1	D	28	GLN
1	D	96	HIS
1	D	102	ASN

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Mol	Chain	Res	Type
1	D	161	GLN
1	D	236	GLN
1	D	286	HIS
1	D	405	GLN
1	D	470	GLN
1	D	503	GLN
1	D	544	HIS

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 62 ligands modelled in this entry, 14 are monoatomic - leaving 48 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
6	EDO	B	609	-	3,3,3	0.32	0	2,2,2	0.69	0
6	EDO	C	611	-	3,3,3	0.56	0	2,2,2	0.43	0
6	EDO	A	613	-	3,3,3	0.72	0	2,2,2	0.18	0
6	EDO	A	610	-	3,3,3	0.86	0	2,2,2	0.72	0
7	PEG	D	615	-	6,6,6	0.68	0	5,5,5	0.63	0
2	FBP	B	601	-	18,20,20	0.77	0	21,32,32	1.39	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PG4	A	616	-	12,12,12	0.61	0	11,11,11	0.97	1 (9%)
6	EDO	C	608	-	3,3,3	0.56	0	2,2,2	0.52	0
6	EDO	C	613	-	3,3,3	0.65	0	2,2,2	0.21	0
6	EDO	B	611	-	3,3,3	0.46	0	2,2,2	0.18	0
6	EDO	D	611	-	3,3,3	0.40	0	2,2,2	0.62	0
2	FBP	A	601	-	18,20,20	0.96	1 (5%)	21,32,32	1.24	2 (9%)
4	ATP	B	606	3	32,33,33	1.71	8 (25%)	48,52,52	1.73	12 (25%)
6	EDO	B	617	-	3,3,3	0.44	0	2,2,2	0.64	0
9	PGE	B	608	-	9,9,9	0.91	0	8,8,8	1.21	1 (12%)
6	EDO	A	611	-	3,3,3	0.40	0	2,2,2	0.47	0
5	OXL	B	607	3	5,5,5	2.47	1 (20%)	6,6,6	3.83	4 (66%)
4	ATP	A	606	3	32,33,33	1.98	7 (21%)	48,52,52	1.96	12 (25%)
5	OXL	A	607	3	5,5,5	2.51	2 (40%)	6,6,6	1.70	1 (16%)
6	EDO	B	612	-	3,3,3	0.39	0	2,2,2	0.65	0
6	EDO	B	610	-	3,3,3	0.52	0	2,2,2	0.29	0
6	EDO	B	614	-	3,3,3	0.38	0	2,2,2	0.91	0
6	EDO	D	612	-	3,3,3	0.38	0	2,2,2	0.82	0
6	EDO	D	610	-	3,3,3	0.22	0	2,2,2	0.88	0
6	EDO	D	614	-	3,3,3	0.38	0	2,2,2	0.50	0
6	EDO	A	612	-	3,3,3	0.71	0	2,2,2	0.42	0
5	OXL	C	604	3	5,5,5	2.02	2 (40%)	6,6,6	2.75	3 (50%)
2	FBP	C	601	-	18,20,20	0.67	0	21,32,32	1.12	1 (4%)
7	PEG	A	615	-	6,6,6	1.16	0	5,5,5	1.08	0
6	EDO	B	615	-	3,3,3	0.35	0	2,2,2	0.59	0
6	EDO	C	606	-	3,3,3	0.26	0	2,2,2	0.52	0
6	EDO	C	612	-	3,3,3	0.52	0	2,2,2	0.19	0
6	EDO	A	609	-	3,3,3	0.54	0	2,2,2	0.34	0
6	EDO	A	614	-	3,3,3	0.54	0	2,2,2	0.35	0
6	EDO	D	608	-	3,3,3	0.76	0	2,2,2	0.45	0
4	ATP	D	605	3	32,33,33	1.83	8 (25%)	48,52,52	1.94	13 (27%)
5	OXL	D	606	3	5,5,5	2.34	3 (60%)	6,6,6	1.24	1 (16%)
6	EDO	B	613	-	3,3,3	0.71	0	2,2,2	0.56	0
6	EDO	D	613	-	3,3,3	0.41	0	2,2,2	0.41	0
6	EDO	C	607	-	3,3,3	0.78	0	2,2,2	0.42	0
6	EDO	C	605	-	3,3,3	0.36	0	2,2,2	0.48	0
6	EDO	D	607	-	3,3,3	0.33	0	2,2,2	0.59	0
6	EDO	C	609	-	3,3,3	0.57	0	2,2,2	0.23	0
6	EDO	C	610	-	3,3,3	0.53	0	2,2,2	0.86	0
6	EDO	B	616	-	3,3,3	0.70	0	2,2,2	0.14	0
6	EDO	D	609	-	3,3,3	0.53	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FBP	D	601	-	18,20,20	0.94	0	21,32,32	1.66	5 (23%)
6	EDO	A	608	-	3,3,3	0.80	0	2,2,2	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
6	EDO	B	609	-	-	0/1/1/1	-
6	EDO	C	611	-	-	1/1/1/1	-
6	EDO	A	613	-	-	1/1/1/1	-
6	EDO	A	610	-	-	1/1/1/1	-
7	PEG	D	615	-	-	1/4/4/4	-
2	FBP	B	601	-	-	2/13/32/32	0/1/1/1
8	PG4	A	616	-	-	7/10/10/10	-
6	EDO	C	608	-	-	1/1/1/1	-
6	EDO	C	613	-	-	1/1/1/1	-
6	EDO	B	611	-	-	1/1/1/1	-
6	EDO	D	611	-	-	1/1/1/1	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
4	ATP	B	606	3	-	4/22/38/38	0/3/3/3
6	EDO	B	617	-	-	0/1/1/1	-
9	PGE	B	608	-	-	4/7/7/7	-
6	EDO	A	611	-	-	1/1/1/1	-
5	OXL	B	607	3	-	4/4/4/4	-
4	ATP	A	606	3	-	2/22/38/38	0/3/3/3
5	OXL	A	607	3	-	4/4/4/4	-
6	EDO	B	612	-	-	0/1/1/1	-
6	EDO	B	610	-	-	1/1/1/1	-
6	EDO	B	614	-	-	1/1/1/1	-
6	EDO	D	612	-	-	0/1/1/1	-
6	EDO	D	610	-	-	0/1/1/1	-
6	EDO	D	614	-	-	0/1/1/1	-
6	EDO	A	612	-	-	1/1/1/1	-
5	OXL	C	604	3	-	4/4/4/4	-
2	FBP	C	601	-	-	2/13/32/32	0/1/1/1
7	PEG	A	615	-	-	1/4/4/4	-
6	EDO	B	615	-	-	1/1/1/1	-
6	EDO	C	606	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	EDO	C	612	-	-	1/1/1/1	-
6	EDO	A	609	-	-	0/1/1/1	-
6	EDO	A	614	-	-	1/1/1/1	-
6	EDO	D	608	-	-	0/1/1/1	-
4	ATP	D	605	3	-	5/22/38/38	0/3/3/3
5	OXL	D	606	3	-	4/4/4/4	-
6	EDO	B	613	-	-	1/1/1/1	-
6	EDO	D	613	-	-	1/1/1/1	-
6	EDO	C	607	-	-	0/1/1/1	-
6	EDO	C	605	-	-	1/1/1/1	-
6	EDO	D	607	-	-	1/1/1/1	-
6	EDO	C	609	-	-	0/1/1/1	-
6	EDO	C	610	-	-	1/1/1/1	-
6	EDO	B	616	-	-	1/1/1/1	-
6	EDO	D	609	-	-	1/1/1/1	-
2	FBP	D	601	-	-	3/13/32/32	0/1/1/1
6	EDO	A	608	-	-	1/1/1/1	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	606	ATP	PB-O3A	5.89	1.65	1.59
4	B	606	ATP	C5-C4	5.19	1.48	1.39
4	D	605	ATP	C5-C4	4.91	1.47	1.39
5	B	607	OXL	C2-C1	-4.76	1.46	1.54
5	A	607	OXL	C2-C1	-4.56	1.46	1.54
4	A	606	ATP	C5-N7	-4.01	1.31	1.39
4	A	606	ATP	PA-O3A	3.93	1.63	1.59
4	D	605	ATP	PB-O3B	3.86	1.63	1.59
4	A	606	ATP	PB-O3B	3.75	1.63	1.59
4	D	605	ATP	PB-O3A	3.68	1.63	1.59
5	D	606	OXL	C2-C1	-3.66	1.48	1.54
4	D	605	ATP	C5-N7	-3.59	1.32	1.39
4	B	606	ATP	C4-N9	-3.50	1.30	1.37
4	B	606	ATP	C5-N7	-3.49	1.32	1.39
4	B	606	ATP	PA-O3A	3.44	1.63	1.59
4	D	605	ATP	PA-O3A	3.36	1.63	1.59
4	A	606	ATP	C5-C4	3.33	1.45	1.39
5	C	604	OXL	C2-C1	-3.24	1.49	1.54
4	A	606	ATP	C4-N9	-2.96	1.31	1.37
5	C	604	OXL	O1-C1	2.51	1.28	1.22
5	D	606	OXL	O1-C1	2.32	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	606	ATP	C5-C6	2.32	1.47	1.41
4	A	606	ATP	C8-N9	-2.28	1.33	1.37
4	B	606	ATP	C8-N7	2.19	1.35	1.31
4	D	605	ATP	C4-N3	2.17	1.38	1.34
2	A	601	FBP	O5-C2	-2.17	1.40	1.43
4	D	605	ATP	C8-N7	2.17	1.35	1.31
4	D	605	ATP	C5-C6	2.12	1.46	1.41
4	B	606	ATP	PB-O3B	2.06	1.61	1.59
5	D	606	OXL	O2-C2	2.02	1.27	1.22
5	A	607	OXL	O1-C1	2.02	1.27	1.22
4	B	606	ATP	PG-O1G	2.01	1.56	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	605	ATP	C5-C4-N3	-5.50	119.14	126.72
5	B	607	OXL	O3-C1-C2	5.35	123.22	112.83
5	B	607	OXL	O1-C1-C2	-5.27	109.64	120.63
4	D	605	ATP	N3-C4-N9	4.90	135.51	127.17
5	C	604	OXL	O4-C2-C1	4.89	122.31	112.83
5	B	607	OXL	O4-C2-C1	4.40	121.37	112.83
4	A	606	ATP	C5-C4-N3	-4.39	120.67	126.72
4	B	606	ATP	C5-C4-N3	-4.26	120.86	126.72
4	A	606	ATP	N3-C4-N9	3.99	133.95	127.17
4	D	605	ATP	N3-C2-N1	-3.88	122.70	128.58
4	A	606	ATP	O3G-PG-O2G	3.83	122.14	107.80
4	A	606	ATP	C4-N9-C8	3.77	109.69	105.74
5	C	604	OXL	O3-C1-C2	3.64	119.89	112.83
4	A	606	ATP	N3-C2-N1	-3.61	123.12	128.58
4	B	606	ATP	N3-C2-N1	-3.56	123.20	128.58
4	A	606	ATP	C2-N3-C4	3.39	120.12	111.83
4	D	605	ATP	C2-N3-C4	3.38	120.09	111.83
2	D	601	FBP	O6-P2-O4P	-3.35	97.39	106.44
4	A	606	ATP	O2A-PA-O1A	3.35	128.02	112.44
4	B	606	ATP	N3-C4-N9	3.28	132.74	127.17
5	B	607	OXL	O2-C2-C1	-3.19	113.99	120.63
2	D	601	FBP	O3P-P1-O2P	3.18	119.74	107.80
4	B	606	ATP	C2-N3-C4	3.14	119.50	111.83
4	D	605	ATP	O4'-C1'-N9	3.13	114.11	108.09
2	B	601	FBP	O2P-P1-O1P	3.13	123.02	110.83
4	A	606	ATP	N9-C8-N7	-3.07	109.59	113.94
4	B	606	ATP	C2-N1-C6	3.01	123.67	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	605	ATP	O3A-PA-O1A	-2.98	101.74	110.70
4	B	606	ATP	O2G-PG-O3B	-2.93	94.80	104.64
4	B	606	ATP	O3A-PA-O1A	-2.86	102.10	110.70
4	A	606	ATP	C5-N7-C8	2.86	107.94	103.45
4	A	606	ATP	C4-C5-N7	-2.80	107.38	110.58
4	D	605	ATP	C2-N1-C6	2.78	123.30	118.73
4	A	606	ATP	C6-C5-N7	2.77	137.43	132.09
4	B	606	ATP	C4-C5-N7	-2.63	107.57	110.58
4	B	606	ATP	O3G-PG-O2G	2.60	117.56	107.80
4	B	606	ATP	O2A-PA-O1A	2.58	124.44	112.44
2	D	601	FBP	O3P-P1-O1	-2.51	100.12	106.67
2	B	601	FBP	O1-P1-O1P	-2.47	99.76	106.44
2	A	601	FBP	O5P-P2-O6	-2.46	100.26	106.67
2	D	601	FBP	O3P-P1-O1P	2.44	120.35	110.83
4	B	606	ATP	O3G-PG-O1G	2.44	120.33	110.83
4	D	605	ATP	O2G-PG-O1G	2.37	120.08	110.83
4	A	606	ATP	C4-N9-C1'	-2.36	121.11	126.63
5	D	606	OXL	O2-C2-C1	2.34	125.52	120.63
5	C	604	OXL	O2-C2-C1	-2.32	115.79	120.63
4	B	606	ATP	N6-C6-N1	2.30	123.50	118.38
9	B	608	PGE	O3-C5-C6	2.27	120.12	110.11
2	C	601	FBP	O1-P1-O1P	-2.23	100.42	106.44
2	B	601	FBP	O6P-P2-O5P	2.23	116.15	107.80
4	D	605	ATP	N6-C6-N1	2.22	123.33	118.38
4	D	605	ATP	C4-C5-N7	-2.22	108.04	110.58
4	D	605	ATP	O2A-PA-O1A	2.19	122.62	112.44
2	D	601	FBP	O5P-P2-O6	2.16	112.31	106.67
4	D	605	ATP	C5-N7-C8	2.11	106.76	103.45
2	A	601	FBP	O1-P1-O1P	2.11	112.13	106.44
4	D	605	ATP	C4-N9-C8	2.08	107.92	105.74
5	A	607	OXL	O4-C2-C1	2.02	116.74	112.83
8	A	616	PG4	O2-C2-C1	2.02	119.00	110.11

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	606	ATP	PB-O3B-PG-O3G
8	A	616	PG4	C1-C2-O2-C3
2	A	601	FBP	C4-C5-C6-O6
2	B	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	608	PGE	O2-C3-C4-O3
2	A	601	FBP	O5-C5-C6-O6
2	D	601	FBP	C4-C5-C6-O6
7	A	615	PEG	O1-C1-C2-O2
9	B	608	PGE	O3-C5-C6-O4
9	B	608	PGE	C3-C4-O3-C5
6	A	610	EDO	O1-C1-C2-O2
6	A	612	EDO	O1-C1-C2-O2
6	C	608	EDO	O1-C1-C2-O2
6	C	611	EDO	O1-C1-C2-O2
6	D	613	EDO	O1-C1-C2-O2
2	C	601	FBP	O5-C5-C6-O6
7	D	615	PEG	O1-C1-C2-O2
2	B	601	FBP	O5-C5-C6-O6
6	C	606	EDO	O1-C1-C2-O2
6	C	612	EDO	O1-C1-C2-O2
6	D	607	EDO	O1-C1-C2-O2
6	D	611	EDO	O1-C1-C2-O2
4	B	606	ATP	PB-O3A-PA-O1A
4	D	605	ATP	PA-O3A-PB-O1B
5	D	606	OXL	O3-C1-C2-O4
6	B	616	EDO	O1-C1-C2-O2
8	A	616	PG4	O2-C3-C4-O3
9	B	608	PGE	C1-C2-O2-C3
4	A	606	ATP	PB-O3B-PG-O2G
4	D	605	ATP	PB-O3B-PG-O2G
8	A	616	PG4	C8-C7-O4-C6
8	A	616	PG4	C3-C4-O3-C5
5	C	604	OXL	O3-C1-C2-O4
6	B	613	EDO	O1-C1-C2-O2
6	C	605	EDO	O1-C1-C2-O2
4	D	605	ATP	PB-O3A-PA-O2A
5	C	604	OXL	O1-C1-C2-O2
5	A	607	OXL	O3-C1-C2-O4
5	B	607	OXL	O3-C1-C2-O4
5	A	607	OXL	O1-C1-C2-O2
5	B	607	OXL	O1-C1-C2-O2
5	D	606	OXL	O1-C1-C2-O2
6	A	611	EDO	O1-C1-C2-O2
2	D	601	FBP	O5-C5-C6-O6
8	A	616	PG4	O1-C1-C2-O2
5	D	606	OXL	O1-C1-C2-O4

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Mol	Chain	Res	Type	Atoms
4	B	606	ATP	PB-O3A-PA-O2A
6	A	613	EDO	O1-C1-C2-O2
6	B	615	EDO	O1-C1-C2-O2
6	C	613	EDO	O1-C1-C2-O2
5	B	607	OXL	O1-C1-C2-O4
8	A	616	PG4	O3-C5-C6-O4
6	B	610	EDO	O1-C1-C2-O2
6	B	614	EDO	O1-C1-C2-O2
6	C	610	EDO	O1-C1-C2-O2
4	D	605	ATP	PB-O3A-PA-O1A
5	C	604	OXL	O1-C1-C2-O4
5	C	604	OXL	O3-C1-C2-O2
6	A	614	EDO	O1-C1-C2-O2
5	A	607	OXL	O3-C1-C2-O2
5	B	607	OXL	O3-C1-C2-O2
2	D	601	FBP	C6-O6-P2-O4P
5	A	607	OXL	O1-C1-C2-O4
5	D	606	OXL	O3-C1-C2-O2
6	D	609	EDO	O1-C1-C2-O2
4	D	605	ATP	PA-O3A-PB-O2B
4	B	606	ATP	PB-O3B-PG-O1G
6	B	611	EDO	O1-C1-C2-O2
6	A	608	EDO	O1-C1-C2-O2
8	A	616	PG4	O4-C7-C8-O5
4	A	606	ATP	PA-O3A-PB-O2B

There are no ring outliers.

16 monomers are involved in 37 short contacts:

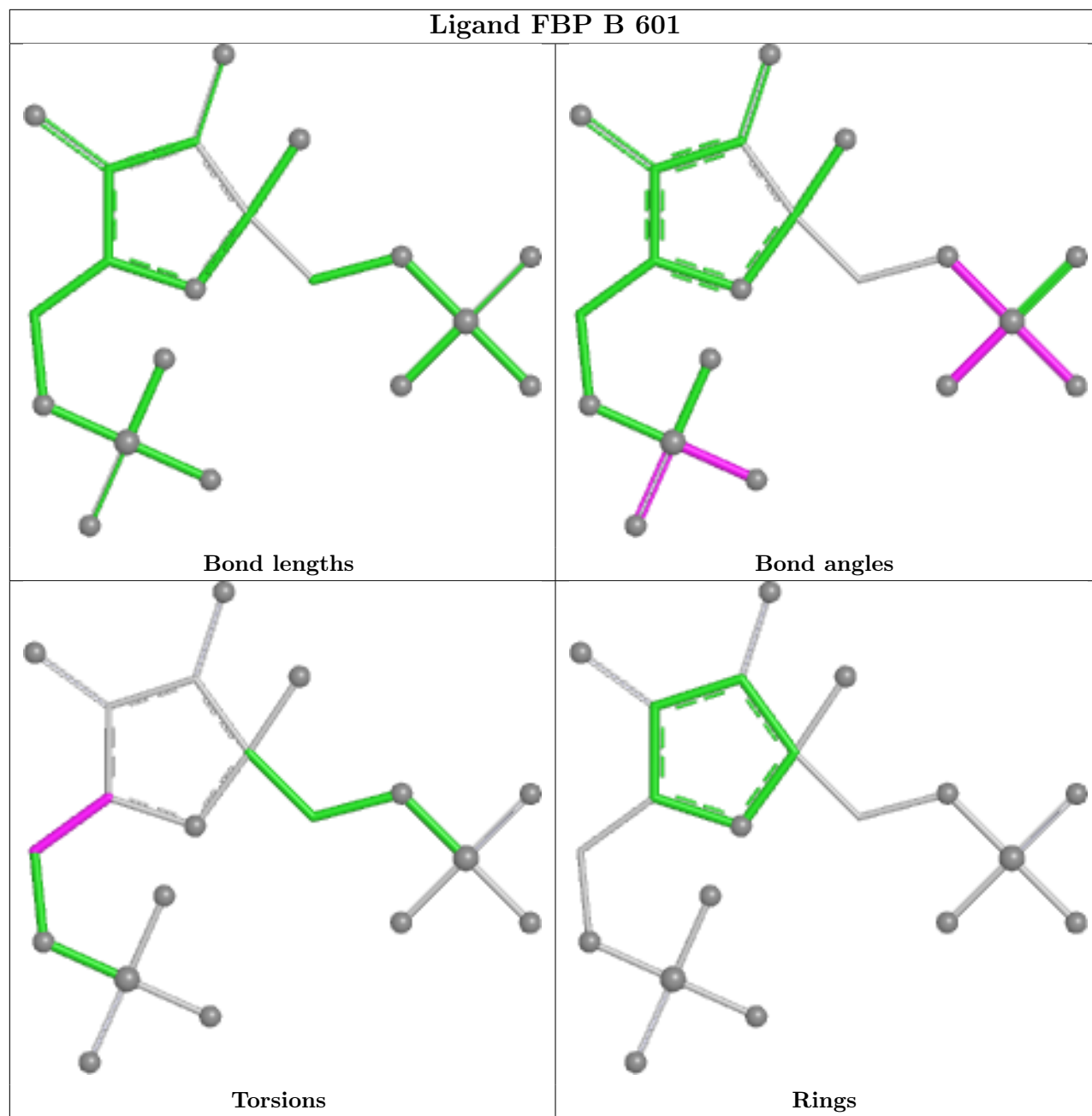
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	611	EDO	5	0
6	A	613	EDO	1	0
6	A	610	EDO	1	0
2	B	601	FBP	2	0
8	A	616	PG4	2	0
6	C	608	EDO	2	0
6	B	611	EDO	2	0
9	B	608	PGE	5	0
6	A	611	EDO	2	0
5	A	607	OXL	1	0
6	B	610	EDO	3	0
6	A	612	EDO	3	0

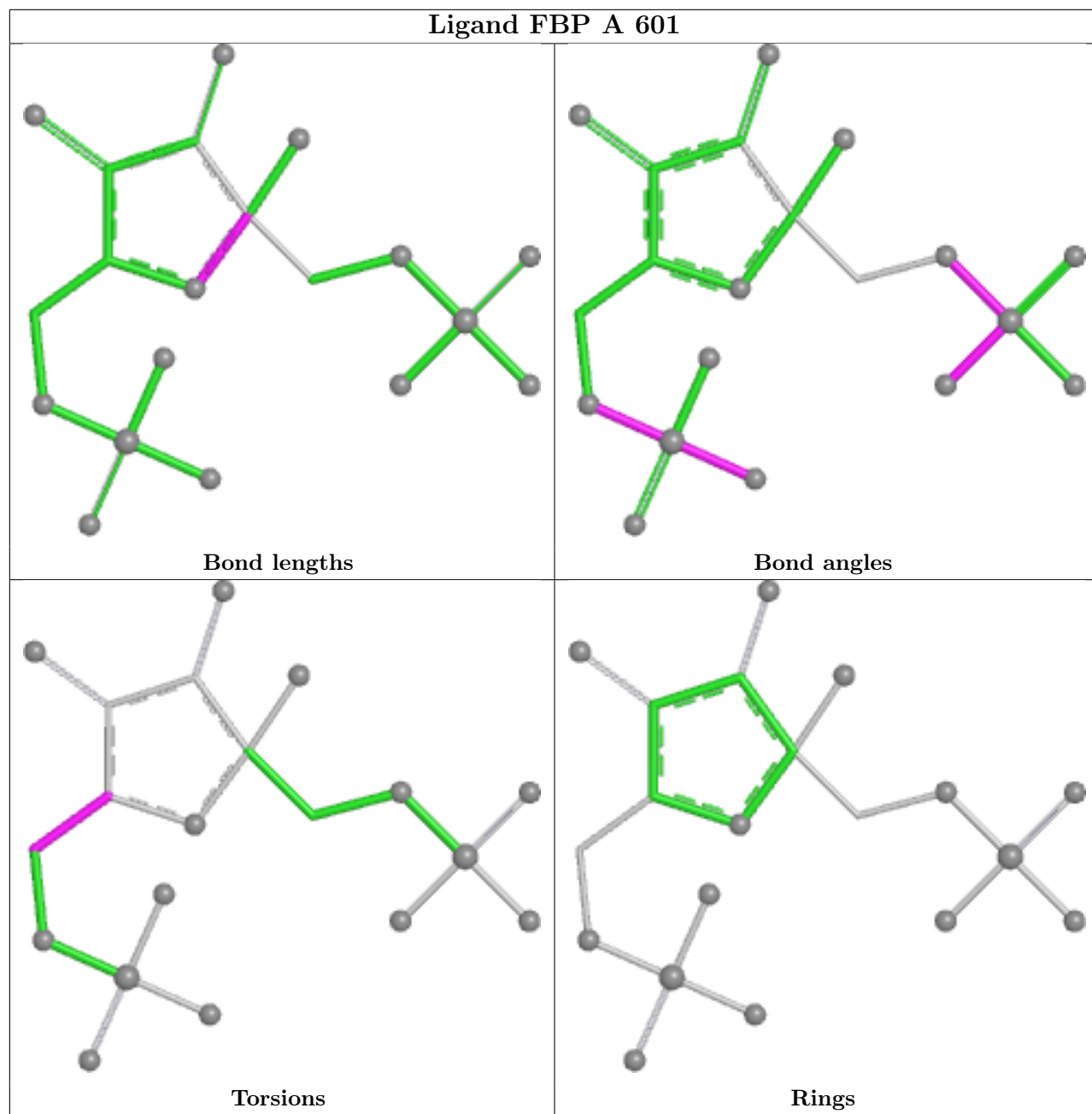
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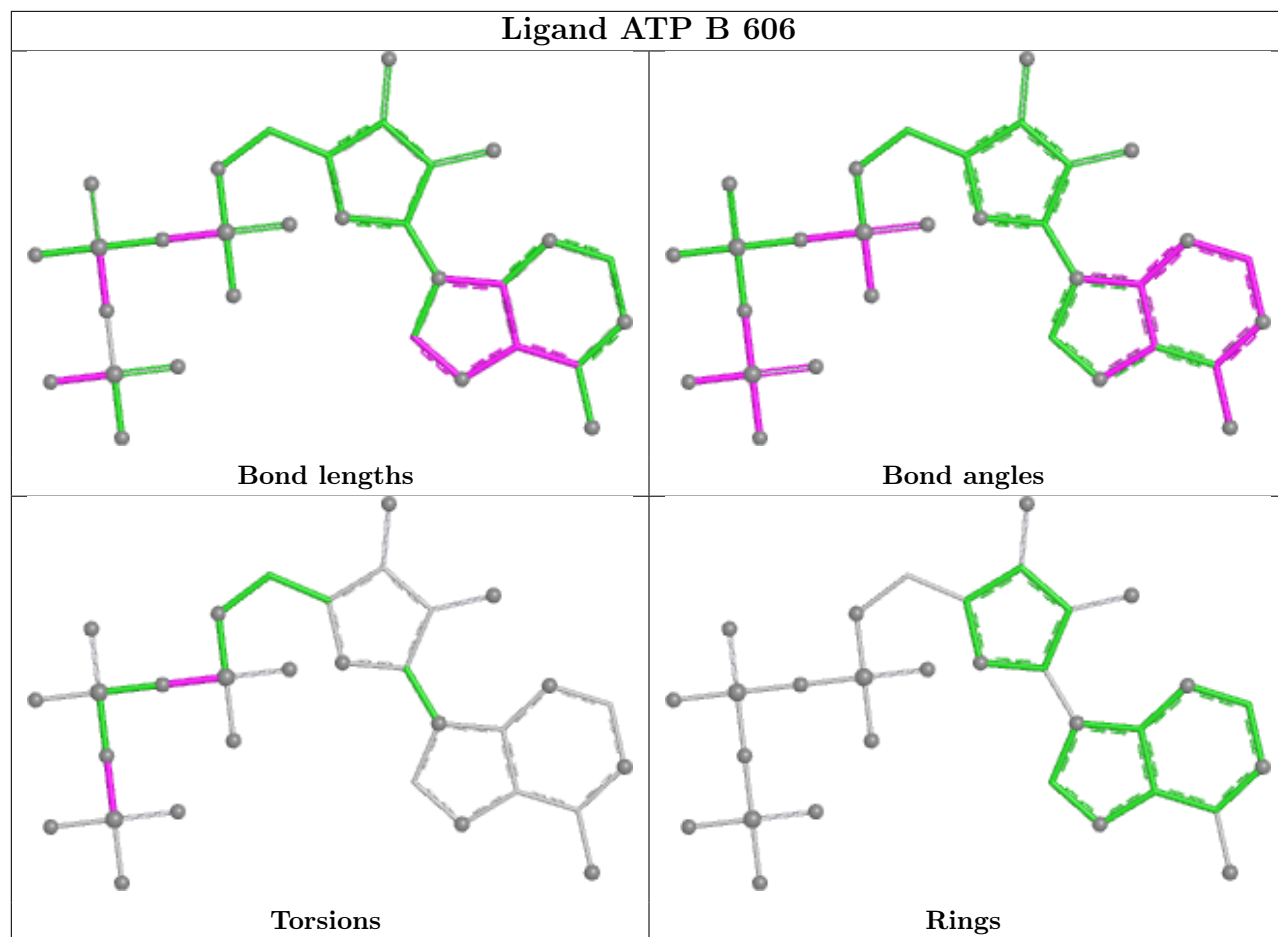
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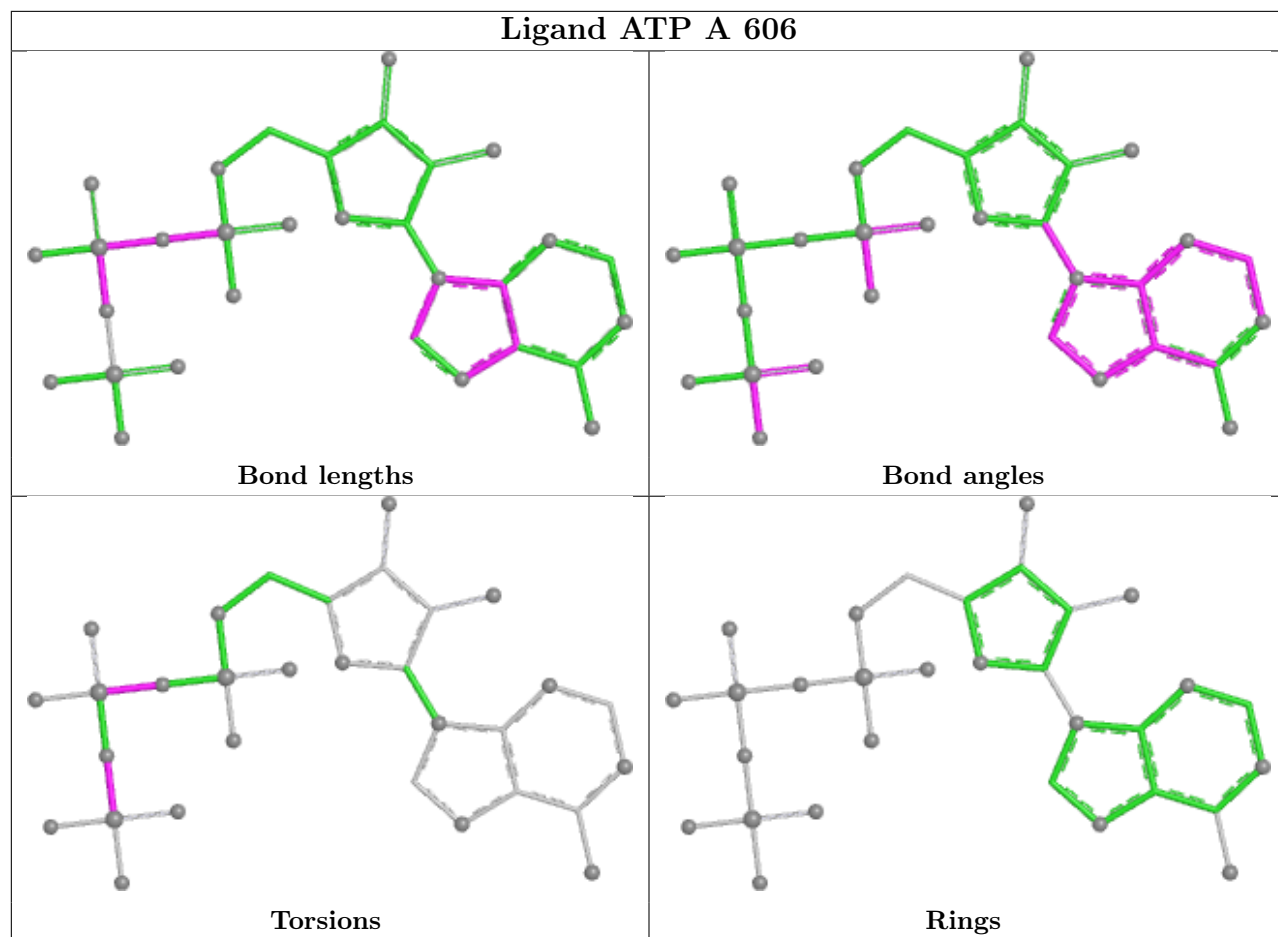
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	615	PEG	3	0
6	D	613	EDO	2	0
6	D	607	EDO	1	0
6	A	608	EDO	3	0

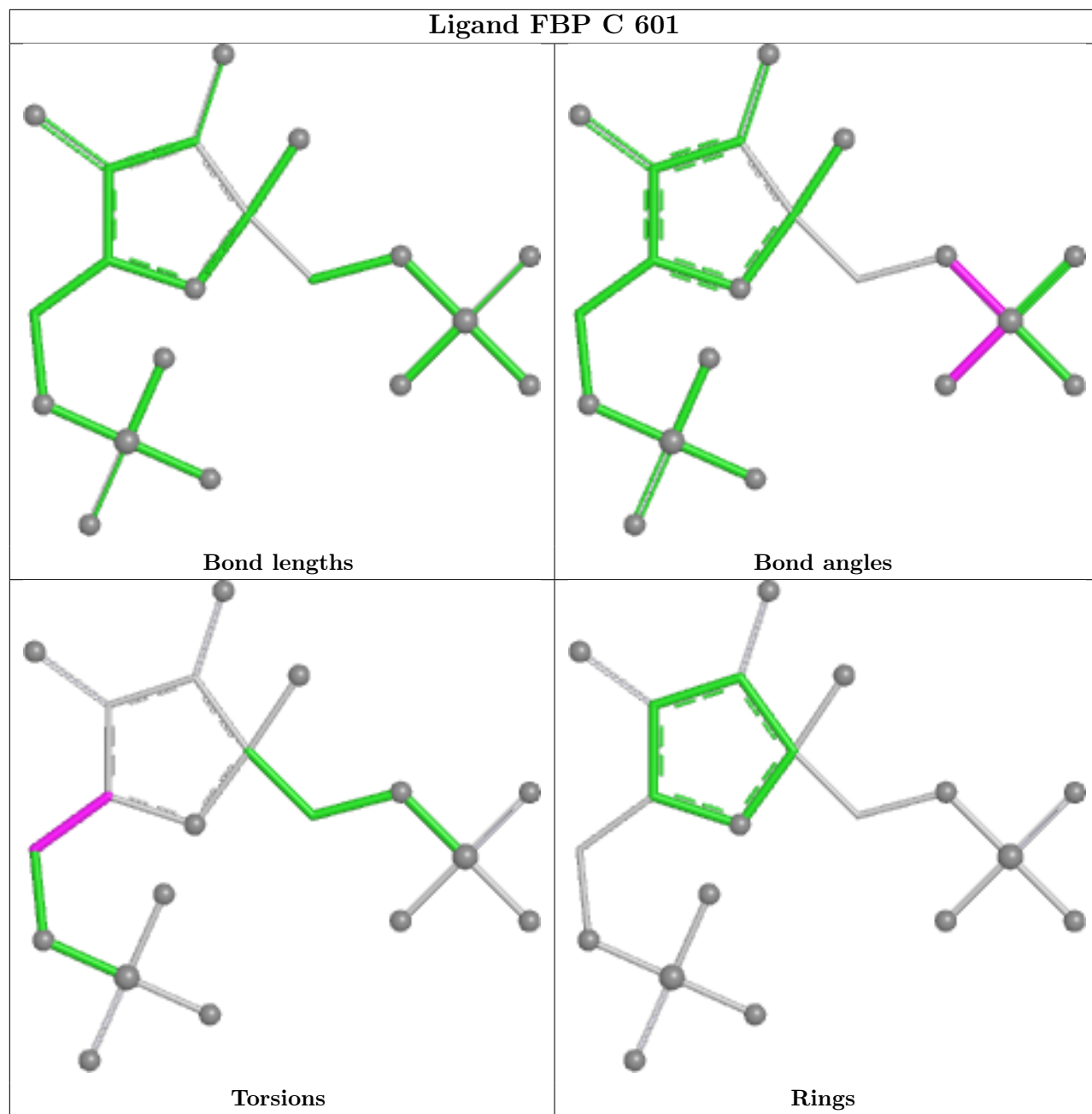
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

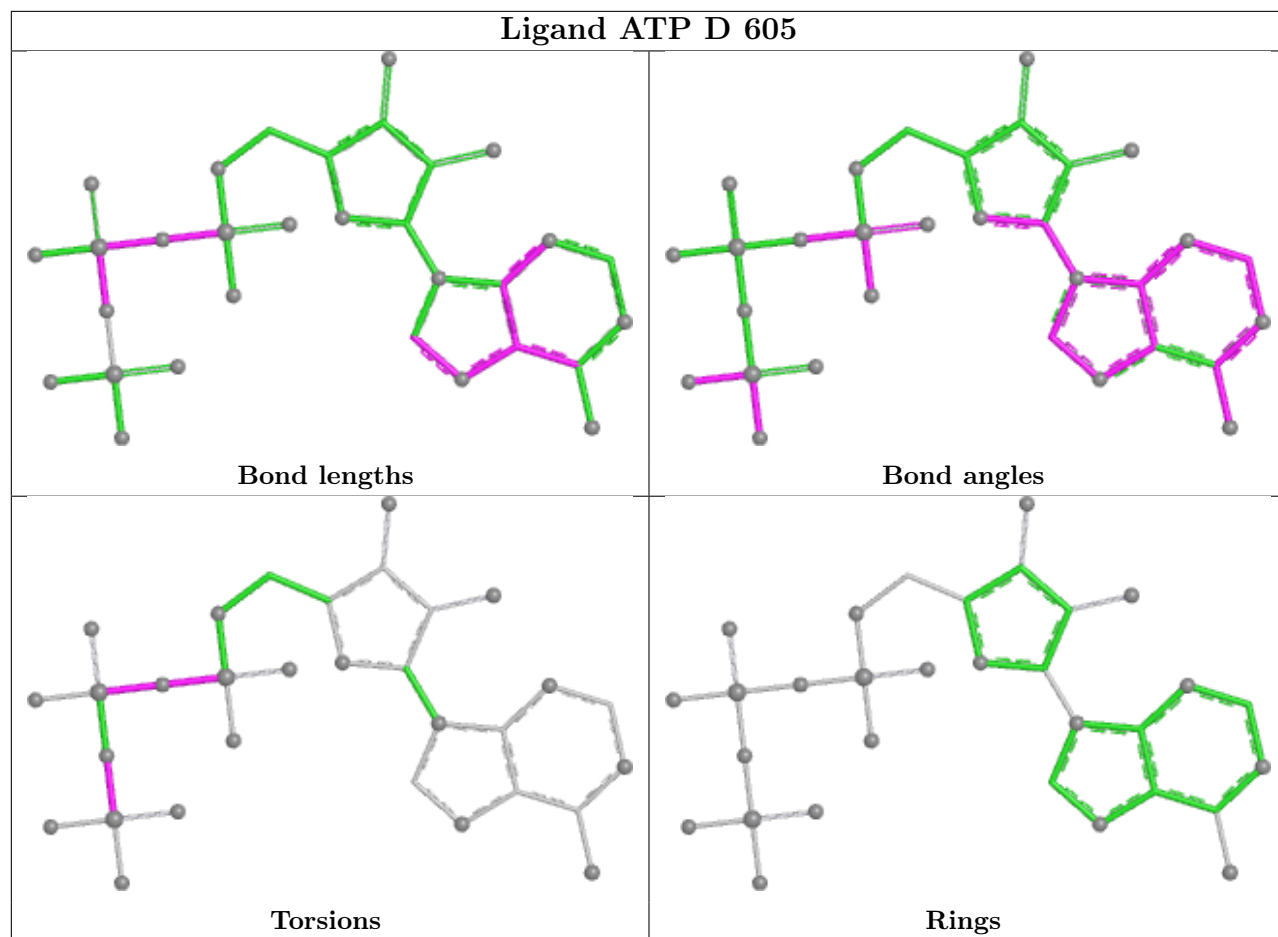


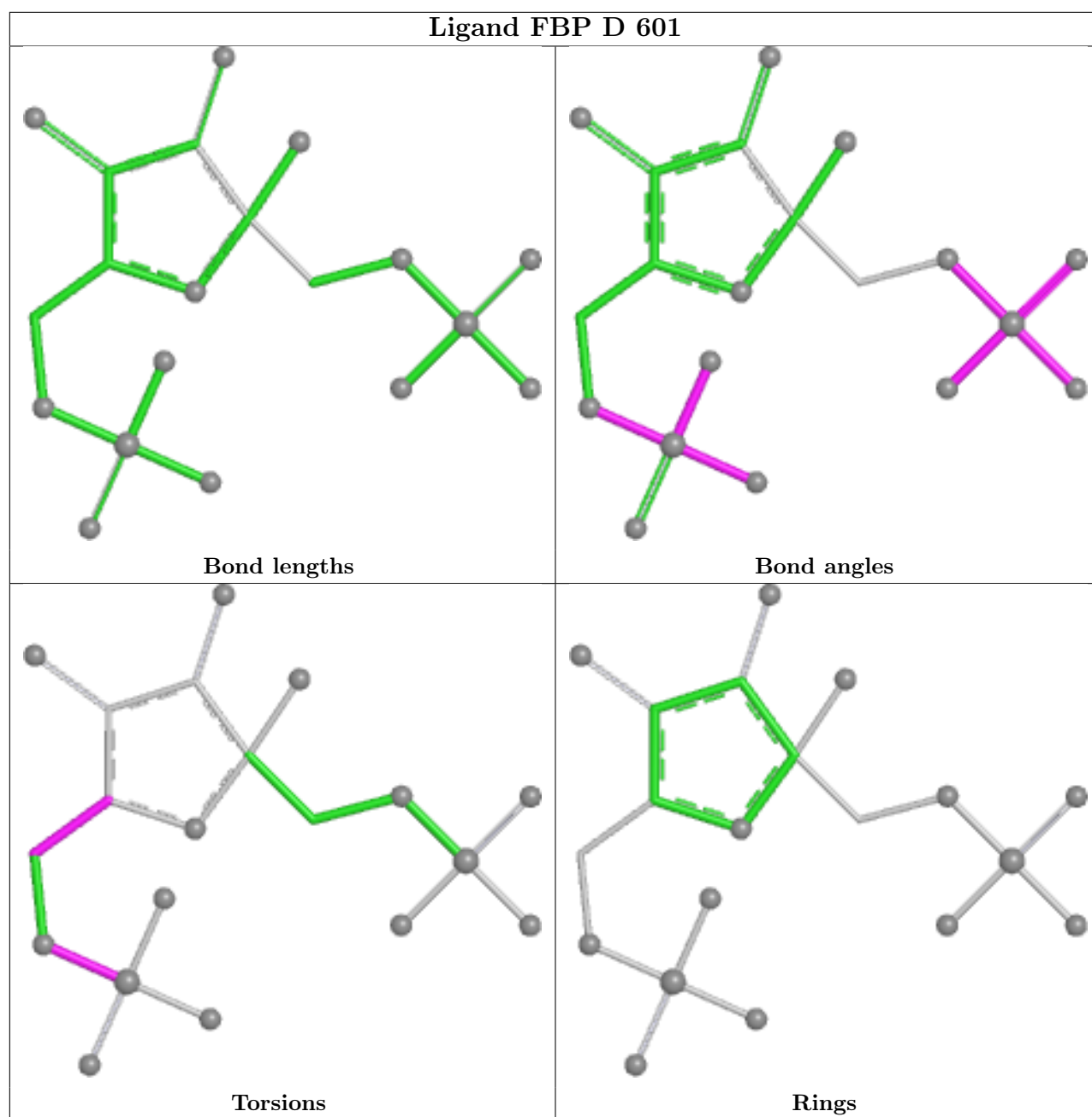












5.7 Other polymers [i](#)

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	528/550 (96%)	-0.12	7 (1%) 75 73	19, 40, 73, 110	2 (0%)
1	B	525/550 (95%)	-0.01	5 (0%) 79 77	21, 44, 70, 106	1 (0%)
1	C	528/550 (96%)	-0.03	6 (1%) 78 76	20, 42, 76, 123	2 (0%)
1	D	527/550 (95%)	0.04	14 (2%) 56 53	29, 44, 77, 124	0
All	All	2108/2200 (95%)	-0.03	32 (1%) 72 69	19, 43, 74, 124	5 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	114	PRO	5.6
1	A	115	LEU	5.3
1	D	115	LEU	4.4
1	C	25	PHE	3.9
1	A	116	SER	3.6
1	C	228	VAL	3.5
1	A	545	HIS	3.4
1	D	114	PRO	3.0
1	C	24	PHE	2.9
1	C	22	THR	2.9
1	D	511	LEU	2.6
1	B	514	PHE	2.6
1	D	113	SER	2.6
1	D	514	PHE	2.5
1	D	18	GLN	2.4
1	D	116	SER	2.4
1	D	112	THR	2.4
1	C	547[A]	HIS	2.4
1	B	20	LEU	2.3
1	B	232	GLY	2.3
1	D	202	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	544	HIS	2.2
1	D	21	GLY	2.2
1	D	20	LEU	2.2
1	B	23	ALA	2.1
1	A	176	ILE	2.1
1	A	21	GLY	2.1
1	D	111	ALA	2.1
1	B	25	PHE	2.0
1	D	23	ALA	2.0
1	C	229	ASP	2.0
1	A	22	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
7	PEG	A	615	7/7	0.68	0.28	48,63,77,78	0
3	MG	A	605	1/1	0.77	0.26	69,69,69,69	0
6	EDO	C	608	4/4	0.78	0.22	56,67,68,73	0
6	EDO	D	611	4/4	0.80	0.17	60,64,67,73	0
6	EDO	B	616	4/4	0.81	0.22	72,75,76,77	0
3	MG	C	602	1/1	0.81	0.14	47,47,47,47	0
6	EDO	C	609	4/4	0.82	0.21	75,82,85,88	0
6	EDO	B	617	4/4	0.82	0.15	66,67,68,69	0
3	MG	A	603	1/1	0.82	0.24	49,49,49,49	0
6	EDO	C	607	4/4	0.83	0.19	57,59,65,65	0
6	EDO	A	608	4/4	0.84	0.19	50,55,59,63	0
7	PEG	D	615	7/7	0.84	0.21	60,74,83,86	0

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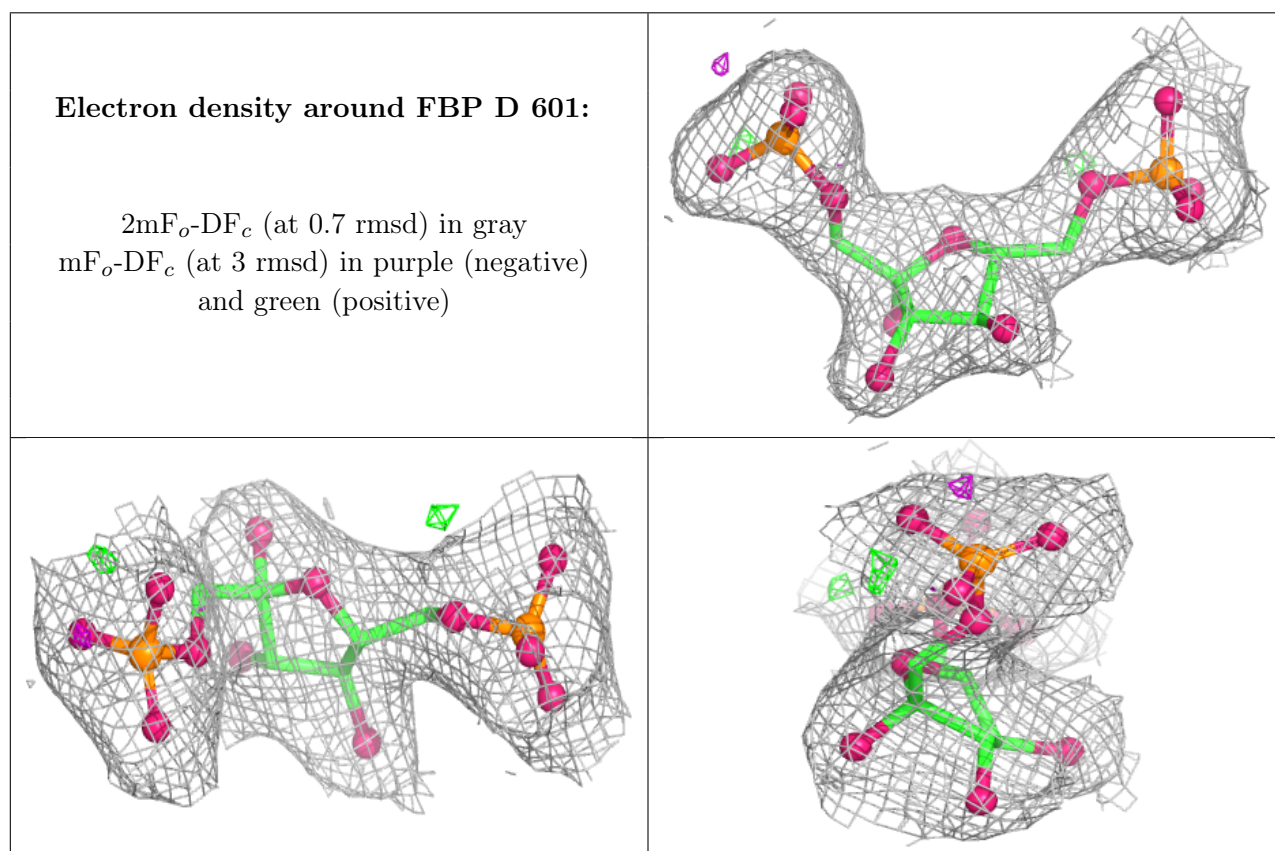
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	PGE	B	608	10/10	0.84	0.16	46,68,79,86	0
6	EDO	B	614	4/4	0.85	0.18	61,69,70,74	0
6	EDO	B	611	4/4	0.85	0.14	79,79,80,81	0
3	MG	D	602	1/1	0.86	0.18	41,41,41,41	0
8	PG4	A	616	13/13	0.86	0.16	58,75,86,90	0
6	EDO	C	613	4/4	0.86	0.15	63,70,73,73	0
3	MG	B	604	1/1	0.87	0.15	35,35,35,35	0
6	EDO	B	609	4/4	0.87	0.18	59,65,68,73	0
3	MG	B	605	1/1	0.87	0.09	44,44,44,44	0
6	EDO	C	610	4/4	0.88	0.15	40,41,52,53	0
3	MG	A	602	1/1	0.89	0.07	34,34,34,34	0
6	EDO	A	611	4/4	0.90	0.11	56,57,57,58	0
6	EDO	B	615	4/4	0.90	0.13	55,64,66,67	0
6	EDO	C	611	4/4	0.90	0.17	41,52,53,64	0
6	EDO	A	614	4/4	0.90	0.13	53,55,57,62	0
6	EDO	D	610	4/4	0.90	0.14	57,60,61,70	0
6	EDO	C	606	4/4	0.91	0.17	61,62,65,72	0
6	EDO	A	613	4/4	0.91	0.13	51,51,61,63	0
6	EDO	C	605	4/4	0.91	0.15	60,60,67,68	0
6	EDO	D	613	4/4	0.91	0.13	53,60,65,68	0
6	EDO	A	612	4/4	0.92	0.16	63,63,68,68	0
6	EDO	B	613	4/4	0.92	0.10	42,50,54,62	0
6	EDO	B	610	4/4	0.92	0.11	56,59,59,65	0
6	EDO	D	614	4/4	0.93	0.11	54,60,61,67	0
6	EDO	C	612	4/4	0.93	0.12	65,72,72,73	0
6	EDO	B	612	4/4	0.93	0.10	44,56,60,64	0
6	EDO	D	612	4/4	0.93	0.12	47,51,53,61	0
6	EDO	D	608	4/4	0.93	0.09	42,42,43,46	0
6	EDO	A	610	4/4	0.94	0.10	46,48,51,51	0
5	OXL	C	604	6/6	0.95	0.08	33,42,44,50	0
6	EDO	D	607	4/4	0.95	0.10	59,61,67,72	0
3	MG	B	602	1/1	0.95	0.07	38,38,38,38	0
3	MG	D	603	1/1	0.95	0.05	35,35,35,35	0
5	OXL	D	606	6/6	0.96	0.07	35,38,41,43	0
5	OXL	A	607	6/6	0.96	0.09	32,35,37,41	0
10	CL	D	616	1/1	0.96	0.14	62,62,62,62	0
2	FBP	D	601	20/20	0.97	0.06	37,42,45,49	0
5	OXL	B	607	6/6	0.97	0.06	33,36,44,45	0
6	EDO	A	609	4/4	0.97	0.09	43,44,44,44	0
2	FBP	B	601	20/20	0.97	0.06	39,43,47,48	0
6	EDO	D	609	4/4	0.97	0.08	41,46,46,48	0
3	MG	B	603	1/1	0.98	0.05	25,25,25,25	0

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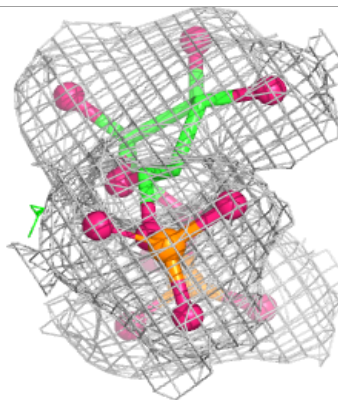
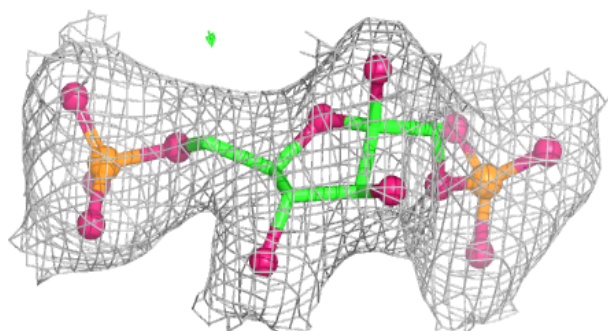
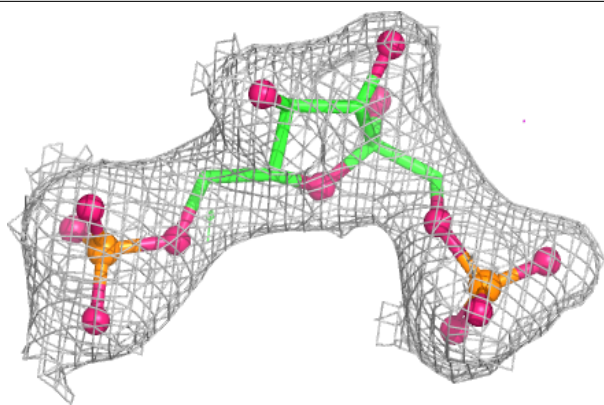
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FBP	C	601	20/20	0.98	0.05	32,35,39,40	0
3	MG	D	604	1/1	0.98	0.04	28,28,28,28	0
4	ATP	A	606	31/31	0.98	0.04	27,31,34,38	0
4	ATP	B	606	31/31	0.98	0.04	25,36,43,45	0
4	ATP	D	605	31/31	0.98	0.04	30,37,43,44	0
2	FBP	A	601	20/20	0.99	0.04	29,31,34,35	0
3	MG	A	604	1/1	0.99	0.05	24,24,24,24	0
3	MG	C	603	1/1	0.99	0.02	26,26,26,26	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.

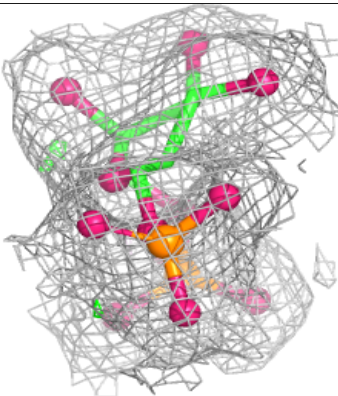
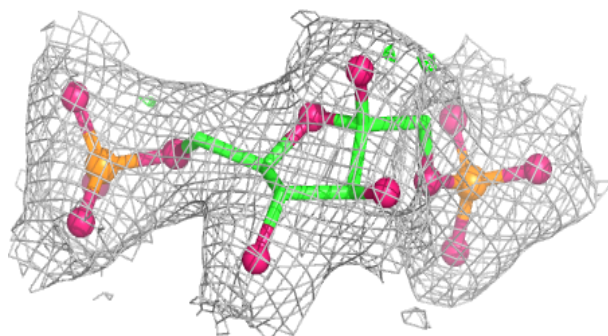
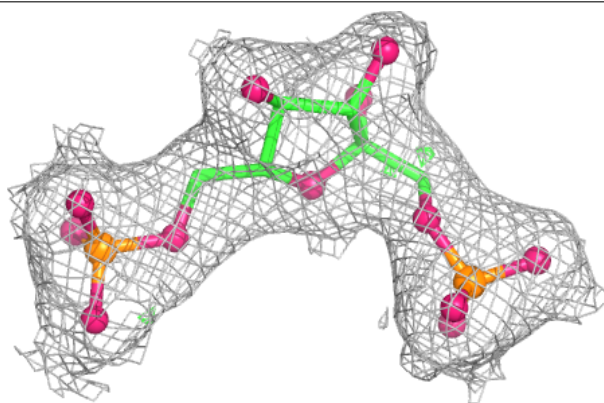


Electron density around FBP B 601:

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

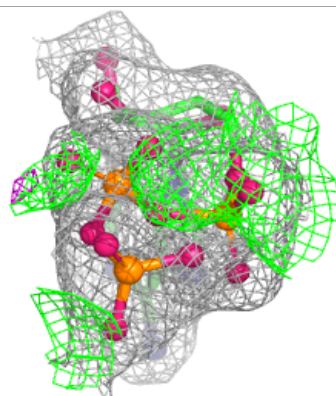
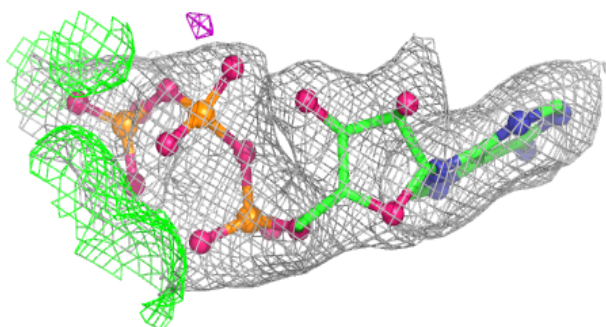
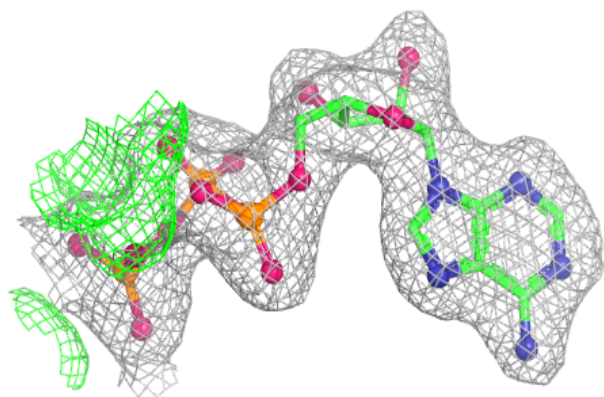
**Electron density around FBP C 601:**

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

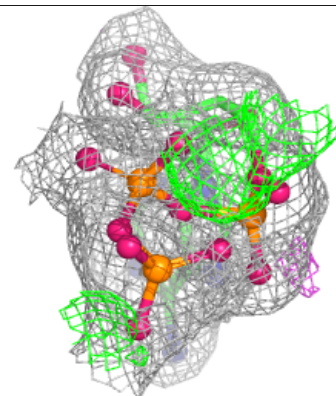
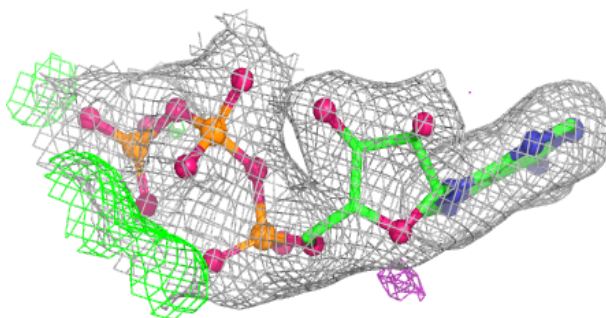
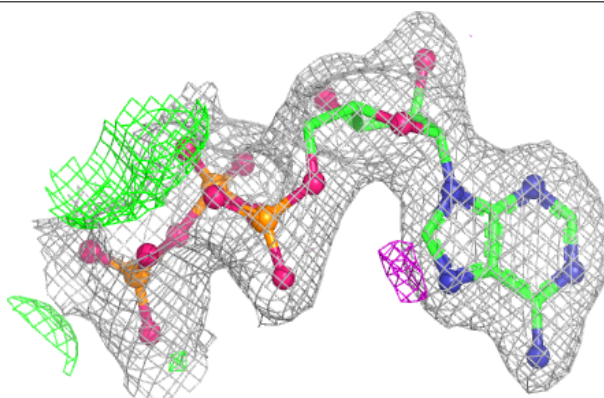


Electron density around ATP A 606:

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and green (positive)

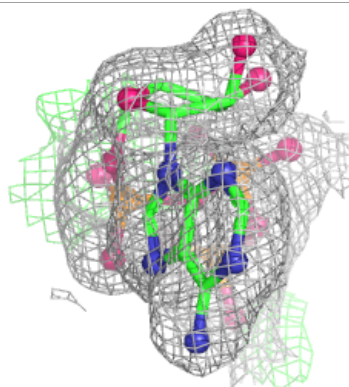
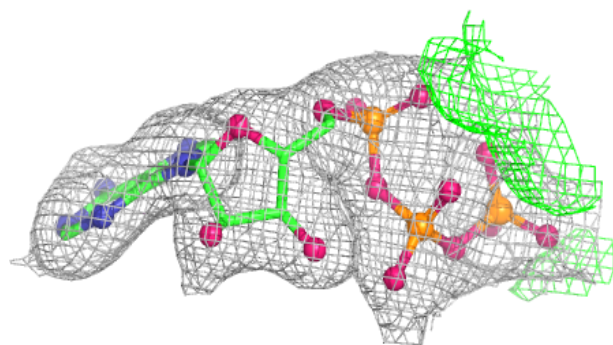
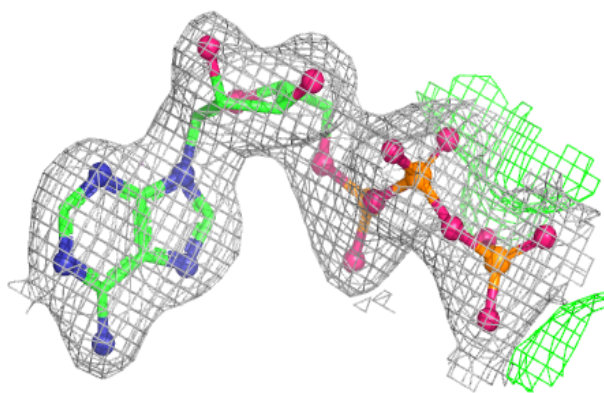
**Electron density around ATP B 606:**

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

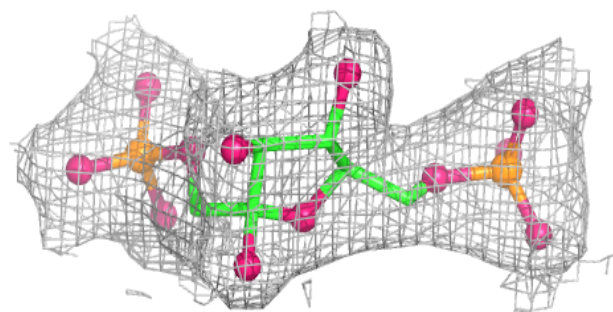
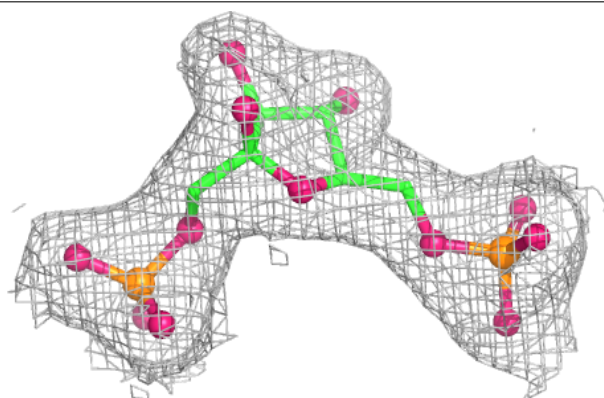


Electron density around ATP D 605:

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

**Electron density around FBP A 601:**

$2mF_o-DF_c$ (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.