



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2023 – 04:17 PM EST

PDB ID : 8TBS  
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator AG-946  
Authors : Jin, L.; Padyana, A.  
Deposited on : 2023-06-29  
Resolution : 2.35 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

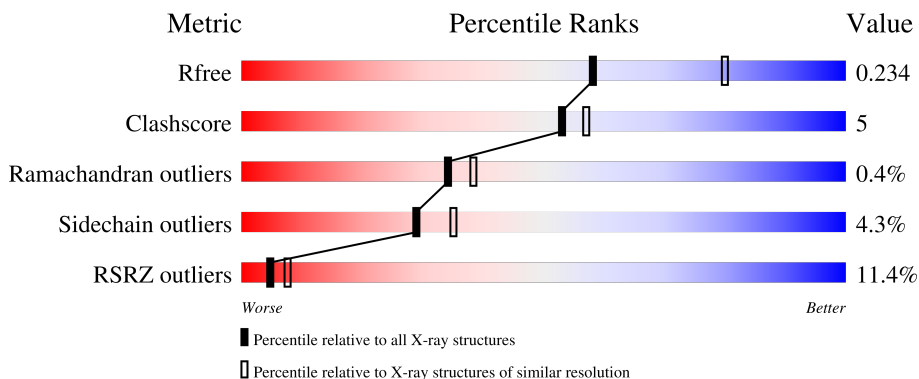
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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  $\geq 3$ , 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	544	 12% 78% 11% • 11%
1	B	544	 16% 84% 10% • 5%
1	C	544	 13% 82% 10% • 6%
1	D	544	 11% 74% 13% • 11%
1	E	544	 13% 72% 20% • 5%

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Mol	Chain	Length	Quality of chain
1	F	544	<p>4% 83% 12% • •</p>
1	G	544	<p>11% 75% 18% • 6%</p>
1	H	544	<p>3% 81% 13% • 5%</p>

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	MN	H	603	-	-	-	X
5	PYR	E	604	-	X	-	-
5	PYR	H	604	-	X	-	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 31741 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	485	Total 3693	C 2322	N 670	O 683	S 18	0	1	0
1	B	517	Total 3922	C 2468	N 708	O 728	S 18	0	0	0
1	C	512	Total 3895	C 2450	N 705	O 722	S 18	0	2	0
1	D	483	Total 3661	C 2303	N 664	O 676	S 18	0	0	0
1	E	515	Total 3908	C 2459	N 709	O 722	S 18	0	1	0
1	F	520	Total 3941	C 2479	N 712	O 732	S 18	0	0	0
1	G	509	Total 3901	C 2449	N 709	O 725	S 18	0	6	0
1	H	519	Total 3943	C 2480	N 712	O 733	S 18	0	1	0

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP P30613
A	32	GLY	-	expression tag	UNP P30613
A	33	SER	-	expression tag	UNP P30613
A	34	SER	-	expression tag	UNP P30613
A	35	HIS	-	expression tag	UNP P30613
A	36	HIS	-	expression tag	UNP P30613
A	37	HIS	-	expression tag	UNP P30613
A	38	HIS	-	expression tag	UNP P30613
A	39	HIS	-	expression tag	UNP P30613
A	40	HIS	-	expression tag	UNP P30613
A	41	SER	-	expression tag	UNP P30613
A	42	SER	-	expression tag	UNP P30613
A	43	GLY	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	44	LEU	-	expression tag	UNP P30613
A	45	VAL	-	expression tag	UNP P30613
A	46	PRO	-	expression tag	UNP P30613
A	47	ARG	-	expression tag	UNP P30613
A	48	GLY	-	expression tag	UNP P30613
A	49	SER	-	expression tag	UNP P30613
B	31	MET	-	initiating methionine	UNP P30613
B	32	GLY	-	expression tag	UNP P30613
B	33	SER	-	expression tag	UNP P30613
B	34	SER	-	expression tag	UNP P30613
B	35	HIS	-	expression tag	UNP P30613
B	36	HIS	-	expression tag	UNP P30613
B	37	HIS	-	expression tag	UNP P30613
B	38	HIS	-	expression tag	UNP P30613
B	39	HIS	-	expression tag	UNP P30613
B	40	HIS	-	expression tag	UNP P30613
B	41	SER	-	expression tag	UNP P30613
B	42	SER	-	expression tag	UNP P30613
B	43	GLY	-	expression tag	UNP P30613
B	44	LEU	-	expression tag	UNP P30613
B	45	VAL	-	expression tag	UNP P30613
B	46	PRO	-	expression tag	UNP P30613
B	47	ARG	-	expression tag	UNP P30613
B	48	GLY	-	expression tag	UNP P30613
B	49	SER	-	expression tag	UNP P30613
C	31	MET	-	initiating methionine	UNP P30613
C	32	GLY	-	expression tag	UNP P30613
C	33	SER	-	expression tag	UNP P30613
C	34	SER	-	expression tag	UNP P30613
C	35	HIS	-	expression tag	UNP P30613
C	36	HIS	-	expression tag	UNP P30613
C	37	HIS	-	expression tag	UNP P30613
C	38	HIS	-	expression tag	UNP P30613
C	39	HIS	-	expression tag	UNP P30613
C	40	HIS	-	expression tag	UNP P30613
C	41	SER	-	expression tag	UNP P30613
C	42	SER	-	expression tag	UNP P30613
C	43	GLY	-	expression tag	UNP P30613
C	44	LEU	-	expression tag	UNP P30613
C	45	VAL	-	expression tag	UNP P30613
C	46	PRO	-	expression tag	UNP P30613
C	47	ARG	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
C	48	GLY	-	expression tag	UNP P30613
C	49	SER	-	expression tag	UNP P30613
D	31	MET	-	initiating methionine	UNP P30613
D	32	GLY	-	expression tag	UNP P30613
D	33	SER	-	expression tag	UNP P30613
D	34	SER	-	expression tag	UNP P30613
D	35	HIS	-	expression tag	UNP P30613
D	36	HIS	-	expression tag	UNP P30613
D	37	HIS	-	expression tag	UNP P30613
D	38	HIS	-	expression tag	UNP P30613
D	39	HIS	-	expression tag	UNP P30613
D	40	HIS	-	expression tag	UNP P30613
D	41	SER	-	expression tag	UNP P30613
D	42	SER	-	expression tag	UNP P30613
D	43	GLY	-	expression tag	UNP P30613
D	44	LEU	-	expression tag	UNP P30613
D	45	VAL	-	expression tag	UNP P30613
D	46	PRO	-	expression tag	UNP P30613
D	47	ARG	-	expression tag	UNP P30613
D	48	GLY	-	expression tag	UNP P30613
D	49	SER	-	expression tag	UNP P30613
E	31	MET	-	initiating methionine	UNP P30613
E	32	GLY	-	expression tag	UNP P30613
E	33	SER	-	expression tag	UNP P30613
E	34	SER	-	expression tag	UNP P30613
E	35	HIS	-	expression tag	UNP P30613
E	36	HIS	-	expression tag	UNP P30613
E	37	HIS	-	expression tag	UNP P30613
E	38	HIS	-	expression tag	UNP P30613
E	39	HIS	-	expression tag	UNP P30613
E	40	HIS	-	expression tag	UNP P30613
E	41	SER	-	expression tag	UNP P30613
E	42	SER	-	expression tag	UNP P30613
E	43	GLY	-	expression tag	UNP P30613
E	44	LEU	-	expression tag	UNP P30613
E	45	VAL	-	expression tag	UNP P30613
E	46	PRO	-	expression tag	UNP P30613
E	47	ARG	-	expression tag	UNP P30613
E	48	GLY	-	expression tag	UNP P30613
E	49	SER	-	expression tag	UNP P30613
F	31	MET	-	initiating methionine	UNP P30613
F	32	GLY	-	expression tag	UNP P30613

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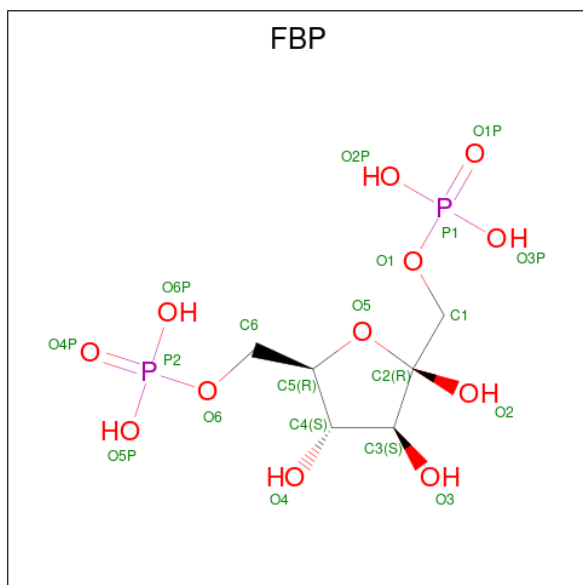
Chain	Residue	Modelled	Actual	Comment	Reference
F	33	SER	-	expression tag	UNP P30613
F	34	SER	-	expression tag	UNP P30613
F	35	HIS	-	expression tag	UNP P30613
F	36	HIS	-	expression tag	UNP P30613
F	37	HIS	-	expression tag	UNP P30613
F	38	HIS	-	expression tag	UNP P30613
F	39	HIS	-	expression tag	UNP P30613
F	40	HIS	-	expression tag	UNP P30613
F	41	SER	-	expression tag	UNP P30613
F	42	SER	-	expression tag	UNP P30613
F	43	GLY	-	expression tag	UNP P30613
F	44	LEU	-	expression tag	UNP P30613
F	45	VAL	-	expression tag	UNP P30613
F	46	PRO	-	expression tag	UNP P30613
F	47	ARG	-	expression tag	UNP P30613
F	48	GLY	-	expression tag	UNP P30613
F	49	SER	-	expression tag	UNP P30613
G	31	MET	-	initiating methionine	UNP P30613
G	32	GLY	-	expression tag	UNP P30613
G	33	SER	-	expression tag	UNP P30613
G	34	SER	-	expression tag	UNP P30613
G	35	HIS	-	expression tag	UNP P30613
G	36	HIS	-	expression tag	UNP P30613
G	37	HIS	-	expression tag	UNP P30613
G	38	HIS	-	expression tag	UNP P30613
G	39	HIS	-	expression tag	UNP P30613
G	40	HIS	-	expression tag	UNP P30613
G	41	SER	-	expression tag	UNP P30613
G	42	SER	-	expression tag	UNP P30613
G	43	GLY	-	expression tag	UNP P30613
G	44	LEU	-	expression tag	UNP P30613
G	45	VAL	-	expression tag	UNP P30613
G	46	PRO	-	expression tag	UNP P30613
G	47	ARG	-	expression tag	UNP P30613
G	48	GLY	-	expression tag	UNP P30613
G	49	SER	-	expression tag	UNP P30613
H	31	MET	-	initiating methionine	UNP P30613
H	32	GLY	-	expression tag	UNP P30613
H	33	SER	-	expression tag	UNP P30613
H	34	SER	-	expression tag	UNP P30613
H	35	HIS	-	expression tag	UNP P30613
H	36	HIS	-	expression tag	UNP P30613

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Chain	Residue	Modelled	Actual	Comment	Reference
H	37	HIS	-	expression tag	UNP P30613
H	38	HIS	-	expression tag	UNP P30613
H	39	HIS	-	expression tag	UNP P30613
H	40	HIS	-	expression tag	UNP P30613
H	41	SER	-	expression tag	UNP P30613
H	42	SER	-	expression tag	UNP P30613
H	43	GLY	-	expression tag	UNP P30613
H	44	LEU	-	expression tag	UNP P30613
H	45	VAL	-	expression tag	UNP P30613
H	46	PRO	-	expression tag	UNP P30613
H	47	ARG	-	expression tag	UNP P30613
H	48	GLY	-	expression tag	UNP P30613
H	49	SER	-	expression tag	UNP P30613

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	O	P	0	0
			20	6	12	2		
2	F	1	Total	C	O	P	0	0
			20	6	12	2		
2	G	1	Total	C	O	P	0	0
			20	6	12	2		
2	H	1	Total	C	O	P	0	0
			20	6	12	2		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		
3	F	1	Total	Mn	0	0
			1	1		
3	G	1	Total	Mn	0	0
			1	1		
3	H	1	Total	Mn	0	0
			1	1		

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

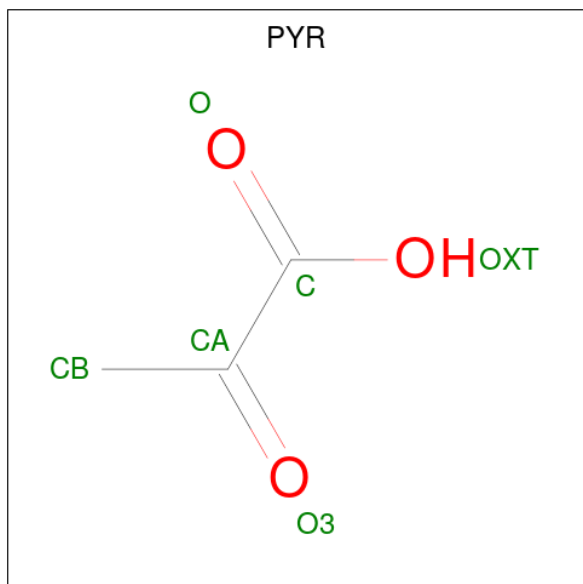
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	K	0	0
			1	1		
4	B	1	Total	K	0	0
			1	1		
4	C	1	Total	K	0	0
			1	1		
4	E	1	Total	K	0	0
			1	1		
4	F	1	Total	K	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total K 1 1	0	0

- Molecule 5 is PYRUVIC ACID (three-letter code: PYR) (formula: C<sub>3</sub>H<sub>4</sub>O<sub>3</sub>).

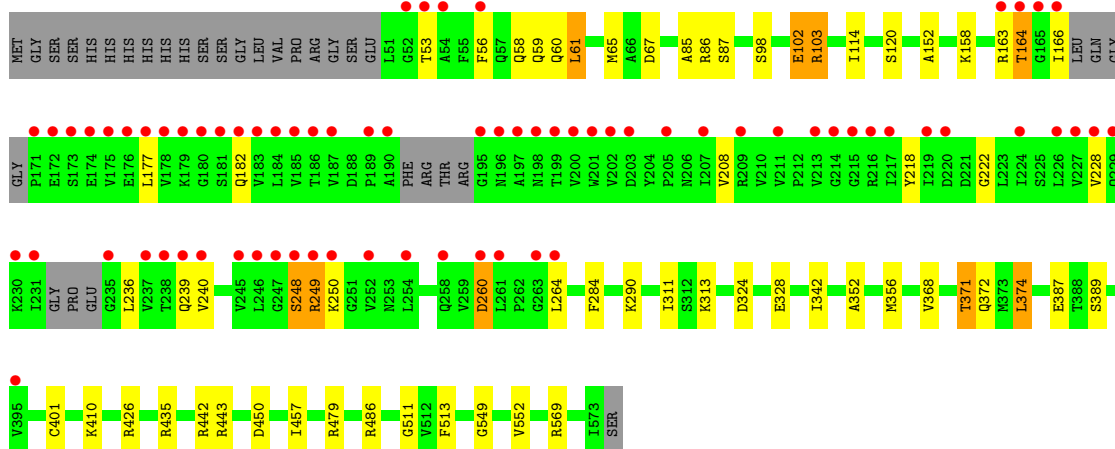
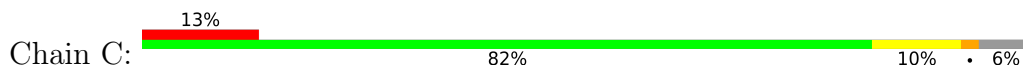


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0
5	F	1	Total C O 6 3 3	0	0
5	G	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0

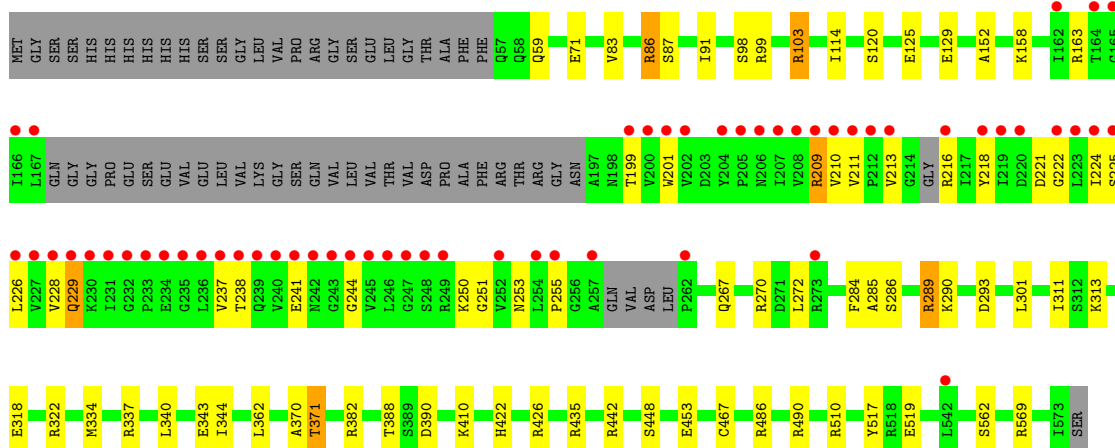
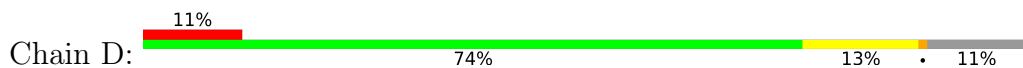
- Molecule 6 is 6-[(6-aminopyridin-2-yl)methyl]-4-methyl-2-[(1H-pyrazol-3-yl)methyl]-4,6-dihydro-5H-[1,3]thiazolo[5',4':4,5]pyrrolo[2,3-d]pyridazin-5-one (three-letter code: HVI) (formula: C<sub>18</sub>H<sub>16</sub>N<sub>8</sub>OS) (labeled as "Ligand of Interest" by depositor).



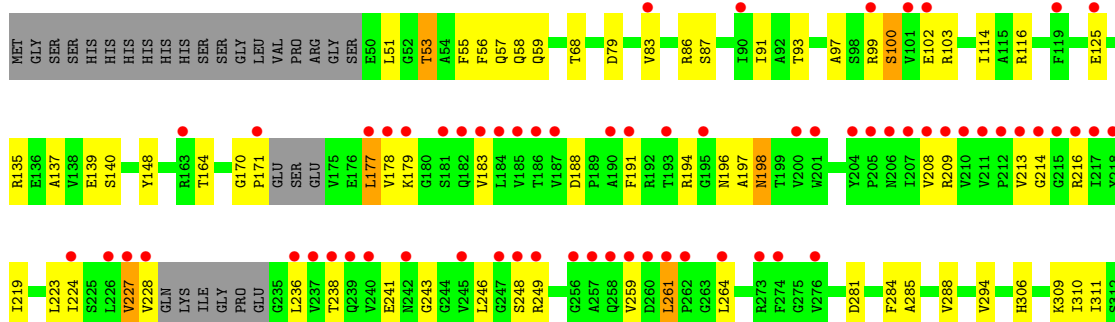




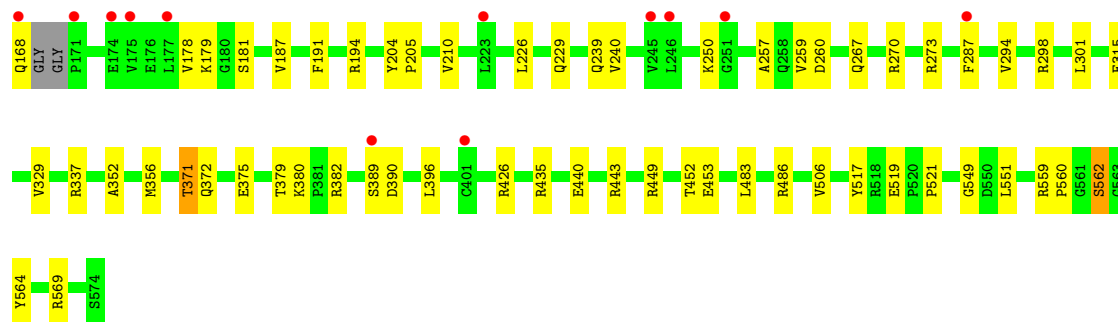
• Molecule 1: Pyruvate kinase PKLR



• 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, $\alpha$ , $\beta$ , $\gamma$	110.32Å 122.60Å 378.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.44 – 2.35 49.86 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.44-2.35) 99.5 (49.86-2.35)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.02 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.20_4459	Depositor
R, $R_{free}$	0.193 , 0.234 0.193 , 0.234	Depositor DCC
$R_{free}$ test set	10643 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtrriage
Anisotropy	0.052	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	31741	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.22 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2563e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN, HVI, FBP, K, PYR

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	0.27	0/3750	0.53	0/5076
1	B	0.28	0/3987	0.55	1/5403 (0.0%)
1	C	0.28	0/3956	0.56	2/5357 (0.0%)
1	D	0.27	0/3719	0.53	0/5035
1	E	0.28	0/3971	0.54	0/5380
1	F	0.29	0/4006	0.54	0/5428
1	G	0.27	0/3975	0.54	0/5381
1	H	0.29	0/4008	0.55	0/5431
All	All	0.28	0/31372	0.54	3/42491 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	LEU	CB-CG-CD2	7.79	124.24	111.00
1	C	61	LEU	CA-CB-CG	7.75	133.12	115.30
1	B	261	LEU	CA-CB-CG	6.28	129.74	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3693	0	3766	32	0
1	B	3922	0	3998	32	0
1	C	3895	0	3974	40	0
1	D	3661	0	3741	48	0
1	E	3908	0	3987	73	0
1	F	3941	0	4016	37	0
1	G	3901	0	3971	53	1
1	H	3943	0	4018	45	0
2	A	20	0	9	0	0
2	B	20	0	9	0	0
2	C	20	0	9	0	0
2	D	20	0	9	0	0
2	E	20	0	9	0	0
2	F	20	0	9	0	0
2	G	20	0	9	0	0
2	H	20	0	9	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
5	C	6	0	0	0	0
5	D	6	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	6	0	0	1	0
5	H	6	0	0	0	0
6	B	28	0	0	0	0
6	D	28	0	0	0	0
6	F	28	0	0	0	0
6	H	28	0	0	0	0
7	A	73	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	64	0	0	0	0
7	C	62	0	0	2	0
7	D	55	0	0	0	0
7	E	41	0	0	3	0
7	F	91	0	0	6	0
7	G	48	0	0	1	0
7	H	109	0	0	0	0
All	All	31741	0	31543	337	1

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 (337) 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:E:179:LYS:HB2	1:E:243:GLY:HA3	1.55	0.87
1:G:99:ARG:NH2	1:G:126:TYR:O	2.12	0.82
1:E:59:GLN:O	1:E:490[A]:ARG:NH2	2.10	0.82
1:F:486:ARG:NH1	7:F:701:HOH:O	2.11	0.79
1:G:185:VAL:N	1:G:200:VAL:O	2.18	0.77
1:F:549:GLY:O	1:G:449:ARG:NH2	2.18	0.77
1:B:228:VAL:HG22	1:B:236:LEU:HD11	1.66	0.75
1:E:449:ARG:NH2	1:H:549:GLY:O	2.20	0.74
1:C:120:SER:HA	1:C:158:LYS:HG3	1.69	0.74
1:F:559:ARG:HD2	1:F:560:PRO:O	1.88	0.74
1:E:213:VAL:HA	1:E:228:VAL:HG21	1.70	0.73
1:G:267:GLN:OE1	1:G:270:ARG:NH2	2.22	0.72
1:F:191:PHE:HA	1:F:194:ARG:HG3	1.73	0.71
1:E:86:ARG:HB2	1:E:426:ARG:HG2	1.72	0.71
1:F:146:LEU:HD23	1:F:542:LEU:HG	1.72	0.71
1:E:426:ARG:NH1	7:E:702:HOH:O	2.23	0.70
1:C:450:ASP:OD2	1:C:479[A]:ARG:NH2	2.25	0.69
1:E:288:VAL:HG12	1:E:326:ILE:HD13	1.75	0.68
1:A:449:ARG:NH2	1:C:549:GLY:O	2.26	0.68
1:D:229:GLN:H	1:D:237:VAL:HG21	1.60	0.67
1:B:225:SER:HB3	1:B:242:ASN:HB2	1.77	0.66
1:D:86:ARG:HB3	1:D:426:ARG:HG3	1.75	0.66
1:G:315:GLU:HG2	1:G:336:ALA:HB3	1.76	0.66
1:H:371:THR:HG22	1:H:372:GLN:HG3	1.76	0.66
1:F:449:ARG:NH2	1:G:549:GLY:O	2.26	0.66
1:C:328:GLU:OE1	7:C:701:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:ARG:NH2	7:E:701:HOH:O	2.18	0.66
1:F:328:GLU:OE1	7:F:702:HOH:O	2.14	0.65
1:E:450:ASP:OD2	1:E:479:ARG:NH2	2.29	0.65
1:B:382:ARG:NH2	1:B:385:ARG:HH12	1.94	0.65
1:F:204:TYR:OH	1:F:260:ASP:OD1	2.10	0.64
1:H:86:ARG:HB2	1:H:426:ARG:HG2	1.80	0.64
1:E:435:ARG:HH11	1:H:443:ARG:HE	1.45	0.63
1:B:187:VAL:HG21	1:B:205:PRO:HA	1.79	0.63
1:D:229:GLN:HG2	1:D:237:VAL:HG21	1.79	0.63
1:G:371:THR:HG22	1:G:372:GLN:HG3	1.79	0.63
1:A:306:HIS:CD2	1:A:306:HIS:H	2.18	0.62
1:D:199:THR:HG23	1:D:238:THR:HG21	1.82	0.62
1:H:379:THR:HG23	1:H:380:LYS:HG2	1.82	0.62
1:B:382:ARG:HH21	1:B:385:ARG:HH12	1.46	0.62
1:C:87:SER:HB2	1:C:511:GLY:HA2	1.80	0.62
1:F:149:ARG:NH2	7:F:703:HOH:O	2.33	0.62
1:C:67:ASP:OD2	7:C:702:HOH:O	2.16	0.61
1:E:371:THR:HG22	1:E:372:GLN:HG3	1.83	0.61
1:C:58:GLN:O	1:C:60:GLN:N	2.33	0.61
1:A:315:GLU:HG2	1:A:336:ALA:HB3	1.83	0.61
1:E:443:ARG:NH2	7:E:703:HOH:O	2.24	0.61
1:E:53:THR:O	1:E:57:GLN:NE2	2.34	0.60
1:E:435:ARG:NH1	1:H:443:ARG:HE	1.99	0.60
1:B:450:ASP:OD2	1:B:479:ARG:NH2	2.35	0.60
1:E:177:LEU:HD12	1:E:197:ALA:HA	1.85	0.59
1:D:86:ARG:HD3	1:D:422:HIS:ND1	2.18	0.59
1:D:337:ARG:NH2	1:D:390:ASP:OD1	2.34	0.59
1:G:313:LYS:HD2	1:G:334:MET:SD	2.42	0.59
1:B:273:ARG:O	1:B:277:GLU:HG3	2.03	0.58
1:C:218:TYR:HB3	1:C:222:GLY:HA2	1.85	0.58
1:E:178:VAL:HG12	1:E:179:LYS:H	1.67	0.58
1:G:99:ARG:NH2	1:G:130:SER:OG	2.36	0.58
1:C:368:VAL:HG22	1:C:401:CYS:HB2	1.86	0.58
1:A:185:VAL:HG12	1:A:200:VAL:HG23	1.85	0.58
1:E:91:ILE:HB	1:E:403:MET:HG3	1.84	0.58
1:E:437:LEU:HD21	1:E:488:ARG:HG2	1.86	0.58
1:E:313:LYS:HD2	1:E:334:MET:SD	2.43	0.57
1:A:207:ILE:HD11	1:A:254:LEU:HD13	1.85	0.57
1:E:51:LEU:HD12	1:H:449:ARG:HG3	1.87	0.57
1:A:372:GLN:NE2	7:A:701:HOH:O	2.30	0.57
1:H:229:GLN:HE21	1:H:239:GLN:HB2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:GLN:HG3	1:A:61:LEU:HD23	1.87	0.56
1:B:59:GLN:HG3	1:B:61:LEU:HD22	1.87	0.56
1:H:178:VAL:O	1:H:181:SER:OG	2.16	0.56
1:A:179:LYS:N	1:A:239:GLN:OE1	2.38	0.56
1:D:267:GLN:OE1	1:D:270:ARG:NH2	2.38	0.56
1:F:442:ARG:HG2	1:F:457:ILE:HD11	1.88	0.56
1:H:167:LEU:O	1:H:168:GLN:HB2	2.06	0.56
1:A:337:ARG:NH2	1:A:390:ASP:OD1	2.31	0.56
1:E:284:PHE:HD1	1:E:311:ILE:HB	1.71	0.56
1:H:226:LEU:HD22	1:H:240:VAL:HG12	1.88	0.55
1:C:182:GLN:HG2	1:C:239:GLN:HG3	1.86	0.55
1:H:337:ARG:NH2	1:H:390:ASP:OD1	2.36	0.55
1:H:372:GLN:HA	1:H:375:GLU:HG2	1.87	0.55
1:E:208:VAL:HA	1:E:236:LEU:HD21	1.87	0.55
1:G:54:ALA:O	1:G:58:GLN:NE2	2.39	0.55
1:G:93:THR:OG1	1:G:116:ARG:NH1	2.37	0.55
1:G:224:ILE:HB	1:G:243:GLY:HA3	1.89	0.55
1:E:337:ARG:NH2	1:E:373:MET:HG2	2.21	0.55
1:E:97:ALA:O	1:E:103:ARG:NH2	2.36	0.55
1:G:304:GLU:OE2	1:G:304:GLU:N	2.26	0.54
1:A:453:GLU:HG2	1:A:483:LEU:HD13	1.88	0.54
1:D:218:TYR:HB3	1:D:222:GLY:HA2	1.88	0.54
1:F:443:ARG:CZ	1:G:435:ARG:HD3	2.38	0.54
1:D:224:ILE:HG12	1:D:244:GLY:HA3	1.88	0.54
1:E:473:VAL:HG13	1:E:555:VAL:HB	1.88	0.54
1:B:382:ARG:HH21	1:B:385:ARG:NH1	2.06	0.54
1:C:371:THR:HG22	1:C:372:GLN:HG3	1.89	0.54
1:A:352:ALA:O	1:A:356:MET:HG3	2.08	0.54
1:D:218:TYR:CE2	1:D:255:PRO:HG3	2.43	0.54
1:F:569:ARG:HG2	1:G:567:ILE:HG23	1.90	0.53
1:E:183:VAL:HG22	1:E:198:ASN:HA	1.91	0.53
1:G:185:VAL:N	1:G:200:VAL:H	2.06	0.53
1:H:59:GLN:HG3	1:H:61:LEU:HD22	1.90	0.53
1:B:442:ARG:HG2	1:B:457:ILE:HD11	1.91	0.53
1:F:120:SER:HA	1:F:158:LYS:HG3	1.91	0.53
1:E:79:ASP:OD2	1:F:321:LYS:HE3	2.09	0.53
1:D:313:LYS:HD2	1:D:334:MET:SD	2.49	0.52
1:H:204:TYR:OH	1:H:260:ASP:OD1	2.20	0.52
1:G:266:GLU:HG3	1:G:270:ARG:HH12	1.75	0.52
1:D:125:GLU:O	1:D:129:GLU:HG3	2.09	0.52
1:D:209:ARG:HA	1:D:209:ARG:HH11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:368:VAL:HG22	1:E:401:CYS:HB2	1.91	0.52
1:E:135:ARG:O	1:E:139:GLU:HG2	2.10	0.52
1:F:86:ARG:HB2	1:F:426:ARG:HG2	1.92	0.52
1:E:177:LEU:HB3	1:E:246:LEU:HB3	1.92	0.51
1:H:229:GLN:HE21	1:H:239:GLN:CB	2.23	0.51
1:F:230:LYS:HG2	1:F:231:ILE:N	2.26	0.51
1:G:135:ARG:O	1:G:139:GLU:HG2	2.10	0.51
1:E:400:ASP:HA	1:E:510:ARG:HB2	1.92	0.51
1:F:486:ARG:HG2	7:F:701:HOH:O	2.11	0.51
1:B:167:LEU:HD21	1:B:175:VAL:HG23	1.91	0.51
1:F:101:VAL:HG12	1:F:105:LYS:HD2	1.92	0.51
1:B:227:VAL:HG23	1:B:241:GLU:HB2	1.93	0.51
1:G:259:VAL:HG22	1:G:261:LEU:H	1.76	0.51
1:A:204:TYR:HD1	1:A:205:PRO:HD2	1.76	0.51
1:G:211:VAL:HG13	1:G:215:GLY:HA3	1.93	0.51
1:G:217:ILE:HB	1:G:226:LEU:HD23	1.93	0.50
1:G:442:ARG:NH1	7:G:704:HOH:O	2.40	0.50
1:C:284:PHE:HB3	1:C:313:LYS:HD2	1.92	0.50
1:G:284:PHE:HD1	1:G:311:ILE:HB	1.76	0.50
1:H:57:GLN:O	1:H:80:SER:OG	2.17	0.50
1:H:125:GLU:O	1:H:129:GLU:HG3	2.12	0.50
1:E:398:GLY:O	1:E:488:ARG:NH2	2.44	0.50
1:G:208:VAL:HG22	1:G:237:VAL:HG11	1.93	0.50
1:C:166:ILE:HG13	1:C:249:ARG:HG3	1.93	0.50
1:G:224:ILE:HG22	1:G:244:GLY:H	1.76	0.50
1:A:196:ASN:HD21	1:A:198:ASN:HB2	1.77	0.50
1:C:442[A]:ARG:HB2	1:C:457:ILE:HD11	1.94	0.50
1:G:372:GLN:HG2	1:G:375:GLU:OE1	2.11	0.50
1:A:567:ILE:HG12	1:C:569:ARG:HG2	1.94	0.50
1:G:195:GLY:O	1:G:197:ALA:N	2.45	0.50
1:E:341:GLY:HA3	1:F:385:ARG:HE	1.76	0.49
1:H:147[A]:SER:O	1:H:149:ARG:NH1	2.45	0.49
1:G:336:ALA:HB1	5:G:604:PYR:C	2.42	0.49
1:H:559:ARG:HD2	1:H:560:PRO:O	2.13	0.49
1:G:266:GLU:HG3	1:G:270:ARG:NH1	2.27	0.49
1:D:225:SER:OG	1:D:241:GLU:OE1	2.29	0.49
1:E:214:GLY:H	1:E:228:VAL:CG2	2.24	0.49
1:H:187:VAL:HG11	1:H:205:PRO:HA	1.94	0.49
1:C:164:THR:HG23	1:C:250:LYS:O	2.13	0.49
1:B:114:ILE:HG12	1:B:152:ALA:HB3	1.95	0.49
1:C:352:ALA:O	1:C:356:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:THR:OG1	1:E:116:ARG:NH1	2.40	0.49
1:E:125:GLU:OE2	1:E:125:GLU:N	2.43	0.49
1:C:177:LEU:CD2	1:C:240:VAL:HG21	2.43	0.48
1:E:219:ILE:HB	1:E:224:ILE:HD11	1.95	0.48
1:B:91:ILE:HG12	1:B:114:ILE:HB	1.95	0.48
1:B:567:ILE:HG12	1:D:569:ARG:HG2	1.95	0.48
1:C:61:LEU:O	1:C:65:MET:HG2	2.13	0.48
1:D:286:SER:HA	1:D:313:LYS:HE2	1.94	0.48
1:B:461:GLU:OE2	1:D:442:ARG:HD2	2.13	0.48
1:C:260:ASP:OD1	1:C:260:ASP:N	2.37	0.48
1:E:228:VAL:HA	1:E:238:THR:HA	1.95	0.48
1:E:294:VAL:HG23	1:E:310:ILE:HG21	1.96	0.48
1:F:125:GLU:O	1:F:129:GLU:HG3	2.13	0.48
1:C:166:ILE:HG23	1:C:248:SER:HB3	1.96	0.48
1:A:368:VAL:HG22	1:A:401:CYS:HB2	1.96	0.48
1:A:284:PHE:HD1	1:A:311:ILE:HB	1.79	0.48
1:D:362:LEU:O	1:D:486:ARG:NH2	2.47	0.47
1:G:87:SER:HB2	1:G:511:GLY:HA2	1.95	0.47
1:E:148:TYR:O	1:E:543:ARG:NH2	2.47	0.47
1:E:177:LEU:HD13	1:E:246:LEU:HD23	1.96	0.47
1:E:554:VAL:HG21	1:E:571:LEU:HD12	1.96	0.47
1:A:354:LYS:HB3	1:B:73:LEU:HD22	1.96	0.47
1:A:204:TYR:CE2	1:A:207:ILE:HG12	2.49	0.47
1:G:156:ASP:HA	1:G:284:PHE:HB2	1.96	0.47
1:D:229:GLN:H	1:D:237:VAL:CG2	2.27	0.47
1:D:213:VAL:HG23	1:D:229:GLN:HA	1.97	0.47
1:E:216:ARG:NH1	1:E:241:GLU:OE2	2.47	0.47
1:F:228:VAL:HA	1:F:238:THR:HG22	1.96	0.47
1:F:246:LEU:HD13	1:F:247:GLY:O	2.14	0.47
1:F:476:THR:HG23	7:F:756:HOH:O	2.14	0.47
1:G:321:LYS:HA	1:G:321:LYS:HD3	1.63	0.47
1:E:322:ARG:NH1	1:E:325:GLU:OE1	2.48	0.47
1:G:177:LEU:O	1:G:178:VAL:HB	2.15	0.47
1:D:59:GLN:HG2	1:D:83:VAL:HB	1.98	0.46
1:B:97:ALA:O	1:B:103:ARG:NH1	2.46	0.46
1:C:208:VAL:HA	1:C:236:LEU:HD21	1.96	0.46
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.79	0.46
1:E:53:THR:C	1:E:57:GLN:HE21	2.16	0.46
1:E:188:ASP:HB3	1:E:191:PHE:HD2	1.81	0.46
1:G:373:MET:HE2	1:G:402:ILE:HB	1.97	0.46
1:B:216:ARG:NH2	1:B:255:PRO:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:PHE:HZ	1:C:65:MET:HG3	1.80	0.46
1:B:371:THR:HG22	1:B:372:GLN:HG3	1.98	0.46
1:E:91:ILE:HG12	1:E:114:ILE:HB	1.97	0.46
1:G:225:SER:OG	1:G:242:ASN:OD1	2.30	0.46
1:A:452:THR:HG22	1:A:483:LEU:HD12	1.97	0.46
1:E:100:SER:OG	1:E:102:GLU:HG2	2.16	0.46
1:F:298:ARG:HD2	7:F:771:HOH:O	2.16	0.46
1:G:61:LEU:O	1:G:65:MET:HG2	2.16	0.46
1:G:171:PRO:O	1:G:174:GLU:HG2	2.16	0.46
1:C:102:GLU:H	1:C:102:GLU:CD	2.19	0.45
1:A:120:SER:HA	1:A:158:LYS:HG3	1.97	0.45
1:D:114:ILE:HG12	1:D:152:ALA:HB3	1.97	0.45
1:D:490:ARG:HE	1:D:490:ARG:HB2	1.57	0.45
1:F:102:GLU:O	1:F:106:GLU:HG3	2.16	0.45
1:F:103:ARG:HD3	1:F:103:ARG:HA	1.71	0.45
1:G:81[B]:GLU:H	1:G:81[B]:GLU:CD	2.16	0.45
1:C:102:GLU:OE1	1:C:102:GLU:N	2.40	0.45
1:C:324:ASP:O	1:C:328:GLU:HG2	2.16	0.45
1:D:120:SER:HA	1:D:158:LYS:HG3	1.98	0.45
1:E:137:ALA:O	1:E:140:SER:OG	2.35	0.45
1:H:210:VAL:CG1	1:H:257:ALA:HB1	2.46	0.45
1:D:99:ARG:NH2	1:D:129:GLU:OE1	2.49	0.45
1:H:559:ARG:NH2	1:H:564:TYR:OH	2.49	0.45
1:A:181:SER:HA	1:A:239:GLN:HB3	1.97	0.45
1:E:324:ASP:O	1:E:328:GLU:HG3	2.17	0.45
1:A:91:ILE:HG12	1:A:114:ILE:HB	1.98	0.45
1:A:374:LEU:HD23	1:A:387:GLU:HB3	1.97	0.45
1:C:87:SER:HB2	1:C:511:GLY:CA	2.43	0.45
1:C:163:ARG:HG2	1:C:249:ARG:NE	2.32	0.45
1:E:323:PHE:HE1	1:E:333:ILE:HG21	1.82	0.44
1:B:294:VAL:HG13	1:B:310:ILE:HG21	2.00	0.44
1:D:250:LYS:HD2	1:D:250:LYS:HA	1.79	0.44
1:G:320:VAL:HG11	1:H:78:ILE:HD13	1.98	0.44
1:B:231:ILE:HA	1:B:236:LEU:HD22	1.99	0.44
1:C:86:ARG:HB2	1:C:426:ARG:HG2	1.99	0.44
1:C:374:LEU:HD12	1:C:387:GLU:HB3	1.99	0.44
1:D:253:ASN:ND2	1:D:343:GLU:OE1	2.45	0.44
1:E:337:ARG:HH21	1:E:373:MET:HG2	1.83	0.44
1:F:287:PHE:CE2	1:F:289:ARG:HD3	2.52	0.44
1:D:163:ARG:HH11	1:D:251:GLY:N	2.15	0.44
1:D:255:PRO:HB3	1:D:343:GLU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:SER:HB2	1:E:511:GLY:HA2	2.00	0.44
1:E:170:GLY:HA3	1:E:171:PRO:HD3	1.83	0.44
1:E:374:LEU:HD23	1:E:387:GLU:HB3	2.00	0.44
1:D:272:LEU:HD22	1:D:301:LEU:HD21	1.99	0.44
1:D:284:PHE:HB3	1:D:313:LYS:HD3	1.98	0.44
1:D:289:ARG:HG2	1:D:293:ASP:OD1	2.18	0.44
1:F:56:PHE:O	1:F:62:PRO:HD3	2.18	0.44
1:A:164:THR:HG1	1:A:250:LYS:H	1.55	0.44
1:E:567:ILE:HG23	1:H:569:ARG:HG2	1.99	0.44
1:D:517:TYR:CE2	1:D:519:GLU:HB2	2.53	0.44
1:E:58:GLN:NE2	1:E:83:VAL:HG21	2.32	0.44
1:E:285:ALA:O	1:E:313:LYS:HG3	2.17	0.44
1:H:147[B]:SER:O	1:H:149:ARG:NH1	2.50	0.44
1:H:191:PHE:HA	1:H:194:ARG:HG3	2.00	0.44
1:A:225:SER:OG	1:A:240:VAL:HG13	2.18	0.44
1:C:264:LEU:HD12	1:C:264:LEU:HA	1.83	0.44
1:D:213:VAL:HA	1:D:228:VAL:HG23	2.00	0.44
1:C:85:ALA:HB1	1:C:513:PHE:CZ	2.52	0.44
1:F:146:LEU:HB2	1:F:542:LEU:HD21	1.99	0.44
1:A:179:LYS:C	1:A:239:GLN:HE22	2.20	0.43
1:B:554:VAL:HG21	1:B:571:LEU:HD12	2.00	0.43
1:F:125:GLU:CD	1:F:125:GLU:H	2.20	0.43
1:H:287:PHE:N	1:H:315:GLU:OE2	2.50	0.43
1:D:210:VAL:HG23	1:D:211:VAL:HG23	1.98	0.43
1:F:354:LYS:NZ	1:F:397:ASP:OD2	2.41	0.43
1:H:91:ILE:HG12	1:H:114:ILE:HB	2.00	0.43
1:E:373:MET:CE	1:E:402:ILE:HB	2.48	0.43
1:E:435:ARG:HD3	1:H:443:ARG:NH2	2.33	0.43
1:C:98:SER:HA	1:C:103:ARG:HG2	2.00	0.43
1:C:410:LYS:HE2	1:C:410:LYS:HB2	1.92	0.43
1:F:466:CYS:HB2	1:F:551:LEU:HD12	2.01	0.43
1:B:192:ARG:HG3	1:B:201:TRP:CZ2	2.54	0.43
1:D:99:ARG:HH22	1:D:129:GLU:HB2	1.83	0.43
1:E:281:ASP:CG	1:E:504:ARG:HE	2.22	0.43
1:H:562:SER:OG	2:H:602:FBP:O6P	2.37	0.43
1:A:266:GLU:O	1:A:270:ARG:HG3	2.19	0.42
1:C:435:ARG:HE	1:C:435:ARG:HB2	1.64	0.42
1:E:309:LYS:NZ	1:E:505:GLN:OE1	2.50	0.42
1:E:549:GLY:O	1:H:449:ARG:NH2	2.47	0.42
1:H:179:LYS:HA	1:H:240:VAL:HG23	2.01	0.42
1:C:114:ILE:HG12	1:C:152:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LYS:HD2	1:G:250:LYS:HA	1.80	0.42
1:D:98:SER:HA	1:D:103:ARG:HG2	2.00	0.42
1:G:218:TYR:HB3	1:G:222:GLY:HA2	2.01	0.42
1:D:250:LYS:HE3	1:D:251:GLY:H	1.83	0.42
1:E:322:ARG:O	1:E:326:ILE:HG13	2.20	0.42
1:H:250:LYS:HA	1:H:250:LYS:HD3	1.63	0.42
1:H:267:GLN:HE21	1:H:270:ARG:HH21	1.67	0.42
1:H:382:ARG:HA	1:H:382:ARG:HD2	1.79	0.42
1:A:225:SER:O	1:A:226:LEU:HD23	2.20	0.42
1:E:352:ALA:O	1:E:356:MET:HG3	2.20	0.42
1:G:368:VAL:HG22	1:G:401:CYS:HB2	2.01	0.42
1:D:209:ARG:HA	1:D:209:ARG:HD2	1.56	0.42
1:D:216:ARG:HA	1:D:226:LEU:O	2.20	0.42
1:E:56:PHE:HB2	1:E:57:GLN:NE2	2.35	0.42
1:G:68:THR:HB	1:H:440:GLU:CD	2.40	0.42
1:H:517:TYR:CZ	1:H:519:GLU:HB2	2.55	0.42
1:A:476[B]:THR:OG1	1:A:562:SER:HB3	2.19	0.42
1:H:56:PHE:O	1:H:62:PRO:HD3	2.19	0.42
1:D:87:SER:HB2	1:D:510:ARG:HG2	2.02	0.42
1:F:284:PHE:HD1	1:F:311:ILE:HB	1.84	0.42
1:G:164:THR:OG1	1:G:250:LYS:N	2.52	0.42
1:D:318:GLU:O	1:D:322:ARG:HG3	2.19	0.42
1:E:68:THR:HB	1:F:440:GLU:CD	2.40	0.42
1:G:83:VAL:O	1:G:426:ARG:HD2	2.19	0.42
1:A:114:ILE:HG12	1:A:152:ALA:HB3	2.00	0.41
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.89	0.41
1:G:185:VAL:HG22	1:G:237:VAL:O	2.20	0.41
1:E:261:LEU:HD12	1:E:261:LEU:HA	1.85	0.41
1:G:165:GLY:N	1:G:201:TRP:O	2.54	0.41
1:G:383:PRO:HG3	1:G:420:MET:HG2	2.03	0.41
1:G:435:ARG:HE	1:G:435:ARG:HB2	1.68	0.41
1:H:352:ALA:O	1:H:356:MET:HG3	2.20	0.41
1:H:517:TYR:CE2	1:H:519:GLU:HB2	2.54	0.41
1:A:457:ILE:HD12	1:A:487:TYR:CE1	2.56	0.41
1:B:87:SER:HB3	1:B:511:GLY:HA2	2.02	0.41
1:B:160:PRO:HD2	1:B:287:PHE:HB2	2.02	0.41
1:F:551:LEU:HD23	1:F:551:LEU:HA	1.82	0.41
1:B:228:VAL:HG22	1:B:236:LEU:CD1	2.46	0.41
1:D:285:ALA:O	1:D:313:LYS:HG3	2.20	0.41
1:B:194:ARG:O	1:B:194:ARG:HG3	2.21	0.41
1:D:91:ILE:HG12	1:D:114:ILE:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ILE:HG12	1:D:382:ARG:HH22	1.86	0.41
1:D:340:LEU:O	1:D:344:ILE:HG12	2.21	0.41
1:G:525:TRP:CD1	1:G:560:PRO:HG3	2.56	0.41
1:H:452:THR:HG22	1:H:483:LEU:HD12	2.03	0.41
1:B:566:ASN:OD1	1:B:567:ILE:HG13	2.21	0.41
1:E:164:THR:O	1:E:249:ARG:HA	2.21	0.41
1:E:485:SER:HB2	1:E:510:ARG:O	2.20	0.41
1:B:87:SER:CB	1:B:511:GLY:HA2	2.51	0.40
1:C:177:LEU:HD22	1:C:240:VAL:HG21	2.03	0.40
1:C:284:PHE:HD1	1:C:311:ILE:HB	1.84	0.40
1:C:250:LYS:HD3	1:C:250:LYS:HA	1.85	0.40
1:G:442:ARG:HG2	1:G:457:ILE:HD11	2.03	0.40
1:D:370:ALA:O	1:D:371:THR:HB	2.22	0.40
1:E:449:ARG:CZ	1:H:551:LEU:HD23	2.50	0.40
1:H:267:GLN:NE2	1:H:270:ARG:HH21	2.19	0.40
1:H:435:ARG:HE	1:H:435:ARG:HB2	1.70	0.40
1:A:204:TYR:HE2	1:A:207:ILE:HG12	1.87	0.40
1:B:83:VAL:O	1:B:426:ARG:HD2	2.22	0.40
1:F:86:ARG:HD3	1:F:422:HIS:HA	2.03	0.40
1:F:91:ILE:HG12	1:F:114:ILE:HB	2.04	0.40
1:G:125:GLU:O	1:G:129:GLU:HG3	2.21	0.40
1:G:204:TYR:CE1	1:G:206:ASN:HB2	2.57	0.40
1:B:99:ARG:NH2	1:B:129:GLU:HB3	2.36	0.40
1:E:177:LEU:HG	1:E:178:VAL:N	2.37	0.40

All (1) 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)
1:G:53:THR:OG1	1:G:304:GLU:OE1[4_544]	2.16	0.04

## 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	476/544 (88%)	458 (96%)	16 (3%)	2 (0%)	34	38
1	B	513/544 (94%)	498 (97%)	13 (2%)	2 (0%)	34	38
1	C	506/544 (93%)	489 (97%)	12 (2%)	5 (1%)	15	15
1	D	475/544 (87%)	460 (97%)	14 (3%)	1 (0%)	47	56
1	E	510/544 (94%)	491 (96%)	17 (3%)	2 (0%)	34	38
1	F	516/544 (95%)	505 (98%)	10 (2%)	1 (0%)	47	56
1	G	507/544 (93%)	485 (96%)	18 (4%)	4 (1%)	19	20
1	H	516/544 (95%)	507 (98%)	8 (2%)	1 (0%)	47	56
All	All	4019/4352 (92%)	3893 (97%)	108 (3%)	18 (0%)	34	38

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	G	178	VAL
1	E	227	VAL
1	G	196	ASN
1	C	164	THR
1	D	371	THR
1	E	371	THR
1	B	371	THR
1	C	249	ARG
1	C	371	THR
1	F	371	THR
1	G	371	THR
1	B	233	PRO
1	G	249	ARG
1	H	371	THR
1	A	228	VAL
1	C	228	VAL
1	A	227	VAL

### 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	391/436 (90%)	376 (96%)	15 (4%)	33	41
1	B	416/436 (95%)	400 (96%)	16 (4%)	33	41
1	C	412/436 (94%)	401 (97%)	11 (3%)	44	55
1	D	386/436 (88%)	370 (96%)	16 (4%)	30	37
1	E	412/436 (94%)	388 (94%)	24 (6%)	20	22
1	F	417/436 (96%)	401 (96%)	16 (4%)	33	41
1	G	413/436 (95%)	387 (94%)	26 (6%)	18	19
1	H	418/436 (96%)	399 (96%)	19 (4%)	27	33
All	All	3265/3488 (94%)	3122 (96%)	143 (4%)	29	34

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	MET
1	A	164	THR
1	A	183	VAL
1	A	202	VAL
1	A	207	ILE
1	A	209	ARG
1	A	227	VAL
1	A	230	LYS
1	A	246	LEU
1	A	273	ARG
1	A	321	LYS
1	A	389	SER
1	A	448	SER
1	A	453	GLU
1	A	572	SER
1	B	56	PHE
1	B	61	LEU
1	B	65	MET
1	B	163	ARG
1	B	194	ARG
1	B	198	ASN
1	B	216	ARG
1	B	231	ILE
1	B	236	LEU
1	B	289	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	290	LYS
1	B	325	GLU
1	B	396	LEU
1	B	486	ARG
1	B	531	ARG
1	B	572	SER
1	C	53	THR
1	C	102	GLU
1	C	103	ARG
1	C	248	SER
1	C	260	ASP
1	C	290	LYS
1	C	374	LEU
1	C	389	SER
1	C	443	ARG
1	C	486	ARG
1	C	552	VAL
1	D	71	GLU
1	D	86	ARG
1	D	103	ARG
1	D	201	TRP
1	D	209	ARG
1	D	221	ASP
1	D	229	GLN
1	D	289	ARG
1	D	290	LYS
1	D	388	THR
1	D	410	LYS
1	D	435	ARG
1	D	448	SER
1	D	453	GLU
1	D	467	CYS
1	D	562	SER
1	E	53	THR
1	E	55	PHE
1	E	99	ARG
1	E	100	SER
1	E	177	LEU
1	E	194	ARG
1	E	196	ASN
1	E	198	ASN
1	E	209	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	223	LEU
1	E	227	VAL
1	E	248	SER
1	E	259	VAL
1	E	261	LEU
1	E	306	HIS
1	E	313	LYS
1	E	389	SER
1	E	473	VAL
1	E	485	SER
1	E	486	ARG
1	E	506	VAL
1	E	518	ARG
1	E	530	ASP
1	E	531	ARG
1	F	65	MET
1	F	103	ARG
1	F	104	LEU
1	F	211	VAL
1	F	213	VAL
1	F	216	ARG
1	F	230	LYS
1	F	258	GLN
1	F	294	VAL
1	F	301	LEU
1	F	389	SER
1	F	531	ARG
1	F	552	VAL
1	F	559	ARG
1	F	568	MET
1	F	574	SER
1	G	100	SER
1	G	103	ARG
1	G	144	SER
1	G	172	GLU
1	G	185	VAL
1	G	186	THR
1	G	200	VAL
1	G	210	VAL
1	G	238	THR
1	G	240	VAL
1	G	294	VAL

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Mol	Chain	Res	Type
1	G	322	ARG
1	G	330	SER
1	G	389	SER
1	G	410	LYS
1	G	443	ARG
1	G	485	SER
1	G	486	ARG
1	G	488	ARG
1	G	490[A]	ARG
1	G	490[B]	ARG
1	G	531[A]	ARG
1	G	531[B]	ARG
1	G	552	VAL
1	G	562[A]	SER
1	G	562[B]	SER
1	H	61	LEU
1	H	104	LEU
1	H	125	GLU
1	H	139	GLU
1	H	147[A]	SER
1	H	147[B]	SER
1	H	259	VAL
1	H	273	ARG
1	H	294	VAL
1	H	298	ARG
1	H	301	LEU
1	H	329	VAL
1	H	389	SER
1	H	396	LEU
1	H	453	GLU
1	H	486	ARG
1	H	506	VAL
1	H	521	PRO
1	H	562	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	HIS
1	B	242	ASN
1	E	57	GLN
1	E	58	GLN

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Mol	Chain	Res	Type
1	E	482	GLN
1	F	198	ASN
1	H	229	GLN
1	H	239	GLN
1	H	267	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 14 are monoatomic - leaving 20 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
5	PYR	G	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.75	1 (33%)
6	HVI	B	601	-	25,32,32	2.47	8 (32%)	26,47,47	2.55	9 (34%)
6	HVI	F	601	-	25,32,32	2.35	7 (28%)	26,47,47	2.50	9 (34%)
6	HVI	D	601	-	25,32,32	2.40	7 (28%)	26,47,47	2.53	8 (30%)
2	FBP	E	601	-	18,20,20	3.40	6 (33%)	23,32,32	0.74	0
2	FBP	G	601	-	18,20,20	3.41	5 (27%)	23,32,32	0.79	0
5	PYR	A	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.75	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PYR	F	605	-	5,5,5	2.93	3 (60%)	3,6,6	1.57	1 (33%)
2	FBP	F	602	-	18,20,20	3.38	5 (27%)	23,32,32	0.63	0
5	PYR	B	605	3	5,5,5	3.01	3 (60%)	3,6,6	1.34	0
2	FBP	A	601	-	18,20,20	3.42	5 (27%)	23,32,32	0.71	0
2	FBP	B	602	-	18,20,20	3.42	5 (27%)	23,32,32	0.74	0
2	FBP	H	602	-	18,20,20	3.43	6 (33%)	23,32,32	0.66	0
2	FBP	D	602	-	18,20,20	3.43	5 (27%)	23,32,32	0.82	1 (4%)
5	PYR	E	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.81	2 (66%)
2	FBP	C	601	-	18,20,20	3.59	6 (33%)	23,32,32	1.53	6 (26%)
6	HVI	H	601	-	25,32,32	2.36	8 (32%)	26,47,47	2.55	10 (38%)
5	PYR	C	604	3	5,5,5	3.00	3 (60%)	3,6,6	1.43	1 (33%)
5	PYR	H	604	-	5,5,5	2.91	3 (60%)	3,6,6	1.49	1 (33%)
5	PYR	D	604	3	5,5,5	2.88	3 (60%)	3,6,6	1.85	1 (33%)

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
5	PYR	G	604	3	-	0/4/4/4	-
6	HVI	B	601	-	-	2/4/8/8	0/5/5/5
6	HVI	F	601	-	-	2/4/8/8	0/5/5/5
6	HVI	D	601	-	-	2/4/8/8	0/5/5/5
2	FBP	E	601	-	-	4/13/32/32	0/1/1/1
2	FBP	G	601	-	-	4/13/32/32	0/1/1/1
5	PYR	A	604	3	-	0/4/4/4	-
5	PYR	F	605	-	-	0/4/4/4	-
2	FBP	F	602	-	-	2/13/32/32	0/1/1/1
5	PYR	B	605	3	-	0/4/4/4	-
2	FBP	A	601	-	-	2/13/32/32	0/1/1/1
2	FBP	B	602	-	-	2/13/32/32	0/1/1/1
2	FBP	H	602	-	-	2/13/32/32	0/1/1/1
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
5	PYR	E	604	3	-	3/4/4/4	-
2	FBP	C	601	-	-	3/13/32/32	0/1/1/1
6	HVI	H	601	-	-	2/4/8/8	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PYR	C	604	3	-	0/4/4/4	-
5	PYR	H	604	-	-	4/4/4/4	-
5	PYR	D	604	3	-	0/4/4/4	-

All (97) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	FBP	O5-C2	-8.83	1.29	1.43
2	C	601	FBP	O5-C5	8.71	1.62	1.43
2	C	601	FBP	O5-C2	-8.46	1.30	1.43
2	A	601	FBP	O5-C5	8.41	1.62	1.43
6	B	601	HVI	C03-N02	8.37	1.41	1.33
6	D	601	HVI	C03-N02	8.35	1.41	1.33
2	B	602	FBP	O5-C2	-8.22	1.30	1.43
2	G	601	FBP	O5-C5	8.21	1.61	1.43
2	H	602	FBP	O5-C5	8.19	1.61	1.43
2	F	602	FBP	O5-C2	-8.15	1.30	1.43
2	G	601	FBP	O5-C2	-8.13	1.30	1.43
2	E	601	FBP	O5-C2	-8.12	1.30	1.43
2	H	602	FBP	O5-C2	-8.10	1.30	1.43
2	B	602	FBP	O5-C5	8.10	1.61	1.43
2	E	601	FBP	O5-C5	8.00	1.61	1.43
2	F	602	FBP	O5-C5	7.97	1.61	1.43
2	A	601	FBP	O5-C2	-7.83	1.31	1.43
6	F	601	HVI	C03-N02	7.76	1.40	1.33
6	H	601	HVI	C03-N02	7.76	1.40	1.33
2	D	602	FBP	O5-C5	7.68	1.60	1.43
2	C	601	FBP	C4-C5	-7.30	1.34	1.53
2	F	602	FBP	C4-C5	-7.03	1.35	1.53
2	H	602	FBP	C4-C5	-7.00	1.35	1.53
2	D	602	FBP	C4-C5	-6.97	1.35	1.53
2	E	601	FBP	C4-C5	-6.89	1.35	1.53
2	G	601	FBP	C4-C5	-6.88	1.35	1.53
2	A	601	FBP	C4-C5	-6.86	1.35	1.53
2	B	602	FBP	C4-C5	-6.85	1.35	1.53
5	C	604	PYR	CA-C	-4.45	1.38	1.54
5	B	605	PYR	CA-C	-4.41	1.38	1.54
6	B	601	HVI	C12-N11	4.25	1.34	1.29
6	D	601	HVI	C12-N11	4.17	1.34	1.29
5	H	604	PYR	CA-C	-4.16	1.39	1.54
5	F	605	PYR	CA-C	-4.08	1.39	1.54
5	G	604	PYR	CA-C	-3.99	1.40	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	604	PYR	CA-C	-3.99	1.40	1.54
5	A	604	PYR	CA-C	-3.96	1.40	1.54
5	E	604	PYR	CA-C	-3.94	1.40	1.54
5	F	605	PYR	O3-CA	3.87	1.31	1.23
6	F	601	HVI	C12-N11	3.86	1.34	1.29
5	E	604	PYR	O3-CA	3.84	1.31	1.23
6	H	601	HVI	C12-N11	3.81	1.34	1.29
5	D	604	PYR	O3-CA	3.79	1.31	1.23
5	A	604	PYR	O3-CA	3.79	1.31	1.23
5	B	605	PYR	O3-CA	3.77	1.31	1.23
5	G	604	PYR	O3-CA	3.76	1.31	1.23
5	C	604	PYR	O3-CA	3.73	1.31	1.23
6	B	601	HVI	C17-C18	3.68	1.43	1.38
5	H	604	PYR	O3-CA	3.66	1.31	1.23
2	H	602	FBP	O3-C3	-3.51	1.35	1.42
6	F	601	HVI	C17-C18	3.49	1.42	1.38
2	A	601	FBP	O3-C3	-3.44	1.35	1.42
2	B	602	FBP	O3-C3	-3.43	1.35	1.42
6	H	601	HVI	C17-C18	3.41	1.42	1.38
2	E	601	FBP	O3-C3	-3.39	1.36	1.42
5	B	605	PYR	O-C	3.37	1.31	1.22
5	H	604	PYR	O-C	3.37	1.31	1.22
5	A	604	PYR	O-C	3.37	1.31	1.22
5	F	605	PYR	O-C	3.35	1.31	1.22
5	E	604	PYR	O-C	3.34	1.31	1.22
5	G	604	PYR	O-C	3.34	1.31	1.22
5	C	604	PYR	O-C	3.33	1.31	1.22
2	G	601	FBP	O3-C3	-3.32	1.36	1.42
5	D	604	PYR	O-C	3.31	1.31	1.22
2	D	602	FBP	O3-C3	-3.26	1.36	1.42
6	D	601	HVI	C17-C18	3.16	1.42	1.38
2	F	602	FBP	O3-C3	-3.14	1.36	1.42
2	C	601	FBP	O3-C3	-3.05	1.36	1.42
6	H	601	HVI	C09-N10	-3.02	1.34	1.37
6	F	601	HVI	C09-N10	-2.99	1.34	1.37
2	A	601	FBP	O4-C4	2.80	1.49	1.43
2	C	601	FBP	P1-O1	2.80	1.69	1.60
2	B	602	FBP	O4-C4	2.79	1.49	1.43
6	D	601	HVI	N19-N20	-2.76	1.31	1.37
6	B	601	HVI	N10-N11	-2.70	1.31	1.36
2	E	601	FBP	O4-C4	2.70	1.49	1.43
6	F	601	HVI	N10-N11	-2.69	1.31	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FBP	O4-C4	2.64	1.49	1.43
6	H	601	HVI	N10-N11	-2.63	1.31	1.36
6	H	601	HVI	N19-N20	-2.59	1.32	1.37
2	F	602	FBP	O4-C4	2.59	1.49	1.43
2	H	602	FBP	O4-C4	2.56	1.49	1.43
6	F	601	HVI	N19-N20	-2.52	1.32	1.37
6	B	601	HVI	C26-N28	2.52	1.42	1.35
6	H	601	HVI	C26-N28	2.50	1.42	1.35
2	D	602	FBP	O4-C4	2.49	1.48	1.43
6	B	601	HVI	N19-N20	-2.48	1.32	1.37
6	D	601	HVI	N10-N11	-2.48	1.32	1.36
6	B	601	HVI	C09-N10	-2.47	1.34	1.37
6	D	601	HVI	C26-N28	2.45	1.42	1.35
6	F	601	HVI	C26-N28	2.44	1.42	1.35
2	C	601	FBP	O4-C4	2.41	1.48	1.43
6	D	601	HVI	C09-N10	-2.20	1.35	1.37
2	E	601	FBP	P1-O1	2.16	1.67	1.60
6	H	601	HVI	C21-C22	2.10	1.54	1.51
6	B	601	HVI	C15-C01	2.08	1.53	1.50
2	H	602	FBP	P1-O1	2.05	1.66	1.60

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	HVI	C12-N11-N10	6.75	122.55	117.12
6	F	601	HVI	C12-N11-N10	6.46	122.32	117.12
6	H	601	HVI	C12-N11-N10	6.46	122.32	117.12
6	B	601	HVI	C12-N11-N10	6.43	122.29	117.12
6	D	601	HVI	C08-C12-N11	-4.88	119.45	125.87
6	H	601	HVI	C07-C09-N10	4.74	119.73	113.76
6	B	601	HVI	C07-C09-N10	4.73	119.72	113.76
6	D	601	HVI	C07-C09-N10	4.71	119.69	113.76
6	B	601	HVI	C26-N27-C22	4.69	121.65	118.10
6	F	601	HVI	C08-C12-N11	-4.67	119.73	125.87
6	B	601	HVI	C08-C12-N11	-4.61	119.80	125.87
6	B	601	HVI	C17-C16-N20	-4.60	105.61	110.44
6	H	601	HVI	C08-C12-N11	-4.60	119.82	125.87
6	F	601	HVI	C07-C09-N10	4.51	119.44	113.76
6	H	601	HVI	C26-N27-C22	4.38	121.42	118.10
6	F	601	HVI	C17-C16-N20	-3.97	106.27	110.44
6	D	601	HVI	C26-N27-C22	3.97	121.11	118.10
6	H	601	HVI	C17-C16-N20	-3.91	106.33	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601	HVI	C17-C16-N20	-3.73	106.52	110.44
6	H	601	HVI	C21-N10-N11	3.69	118.90	114.40
2	C	601	FBP	O2-C2-O5	3.56	116.38	109.50
6	F	601	HVI	C26-N27-C22	3.45	120.72	118.10
6	F	601	HVI	C21-N10-N11	3.44	118.60	114.40
6	B	601	HVI	O13-C09-C07	-3.17	120.12	125.33
6	D	601	HVI	O13-C09-C07	-3.15	120.14	125.33
6	D	601	HVI	C21-N10-N11	2.77	117.78	114.40
6	F	601	HVI	C25-C24-C23	-2.76	116.33	120.25
6	B	601	HVI	C21-N10-N11	2.73	117.74	114.40
2	C	601	FBP	P1-O1-C1	2.65	125.61	118.30
5	D	604	PYR	OXT-C-CA	2.57	121.00	113.97
2	C	601	FBP	O1-P1-O1P	2.55	113.61	106.47
6	F	601	HVI	O13-C09-C07	-2.54	121.16	125.33
6	H	601	HVI	C25-C24-C23	-2.51	116.68	120.25
2	C	601	FBP	O3-C3-C4	-2.44	104.91	113.32
6	H	601	HVI	O13-C09-C07	-2.40	121.39	125.33
5	G	604	PYR	OXT-C-CA	2.36	120.42	113.97
2	C	601	FBP	C6-C5-C4	-2.34	106.40	115.18
5	E	604	PYR	OXT-C-CA	2.34	120.37	113.97
6	D	601	HVI	C25-C24-C23	-2.31	116.97	120.25
5	A	604	PYR	OXT-C-CA	2.23	120.06	113.97
5	F	605	PYR	OXT-C-CA	2.18	119.94	113.97
6	H	601	HVI	O13-C09-N10	-2.18	118.87	120.69
2	D	602	FBP	P1-O1-C1	-2.14	112.40	118.30
5	C	604	PYR	OXT-C-CA	2.12	119.76	113.97
6	F	601	HVI	C17-C18-N19	-2.07	106.12	111.33
5	E	604	PYR	OXT-C-O	-2.07	118.87	123.61
5	H	604	PYR	OXT-C-CA	2.07	119.64	113.97
5	A	604	PYR	OXT-C-O	-2.06	118.90	123.61
6	B	601	HVI	C25-C24-C23	-2.05	117.34	120.25
2	C	601	FBP	O3P-P1-O1	2.04	112.16	106.73
6	B	601	HVI	C17-C18-N19	-2.03	106.21	111.33
6	H	601	HVI	C17-C18-N19	-2.01	106.27	111.33

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	C	601	FBP	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	E	601	FBP	O1-C1-C2-O2
2	E	601	FBP	O1-C1-C2-O5
2	E	601	FBP	C4-C5-C6-O6
2	G	601	FBP	O1-C1-C2-O2
2	G	601	FBP	C4-C5-C6-O6
5	E	604	PYR	O-C-CA-CB
5	E	604	PYR	OXT-C-CA-CB
5	H	604	PYR	O-C-CA-O3
5	H	604	PYR	OXT-C-CA-O3
2	B	602	FBP	C4-C5-C6-O6
2	H	602	FBP	C4-C5-C6-O6
2	F	602	FBP	C4-C5-C6-O6
2	G	601	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	602	FBP	O5-C5-C6-O6
2	D	602	FBP	O5-C5-C6-O6
2	E	601	FBP	O5-C5-C6-O6
2	F	602	FBP	O5-C5-C6-O6
2	H	602	FBP	O5-C5-C6-O6
2	D	602	FBP	C4-C5-C6-O6
5	H	604	PYR	O-C-CA-CB
2	G	601	FBP	O1-C1-C2-O5
5	H	604	PYR	OXT-C-CA-CB
6	B	601	HVI	N10-C21-C22-N27
6	D	601	HVI	N10-C21-C22-N27
6	F	601	HVI	N10-C21-C22-N27
6	H	601	HVI	N10-C21-C22-N27
5	E	604	PYR	OXT-C-CA-O3
6	B	601	HVI	N10-C21-C22-C23
6	D	601	HVI	N10-C21-C22-C23
6	F	601	HVI	N10-C21-C22-C23
6	H	601	HVI	N10-C21-C22-C23
2	C	601	FBP	O1-C1-C2-C3

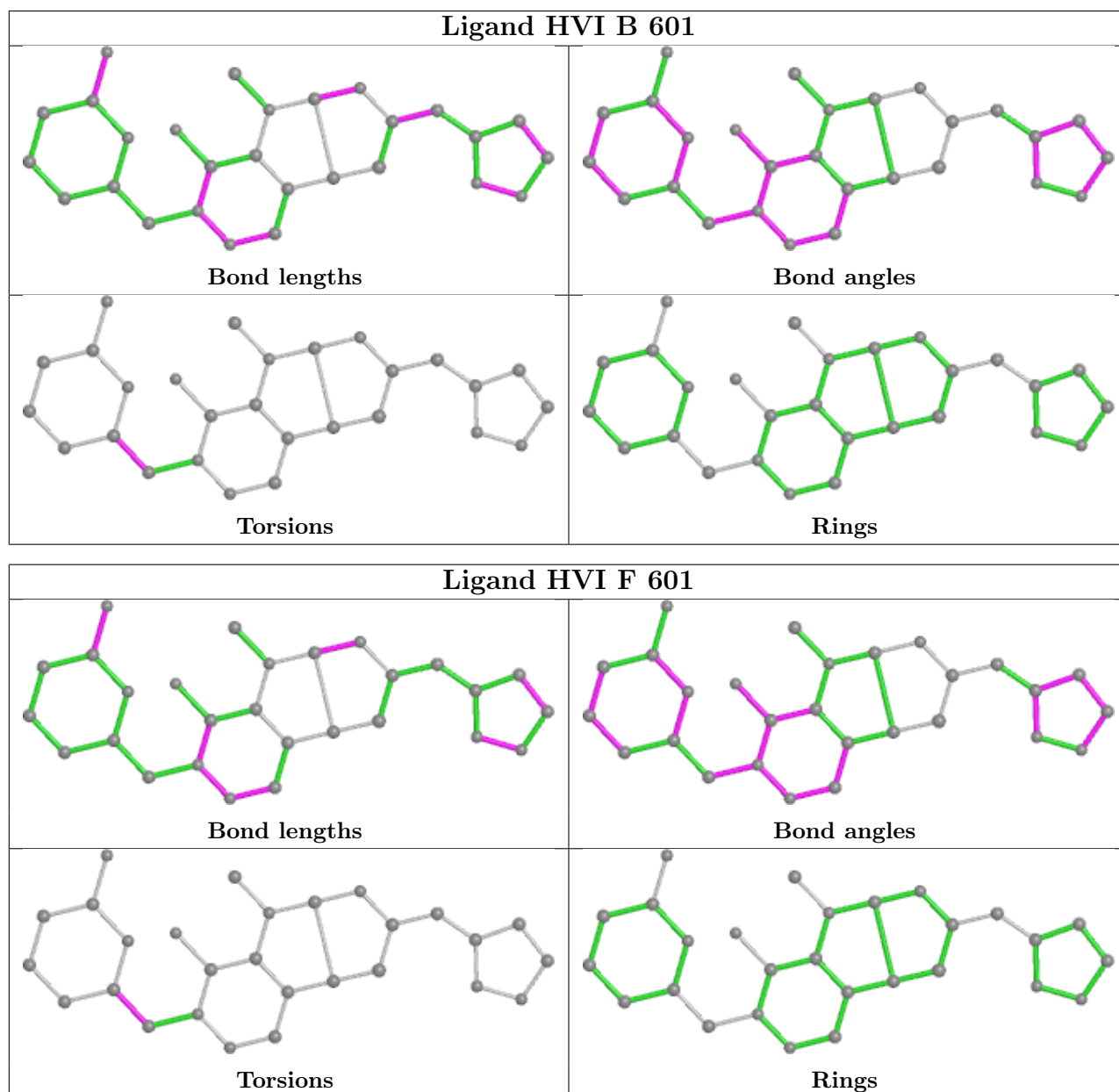
There are no ring outliers.

2 monomers are involved in 2 short contacts:

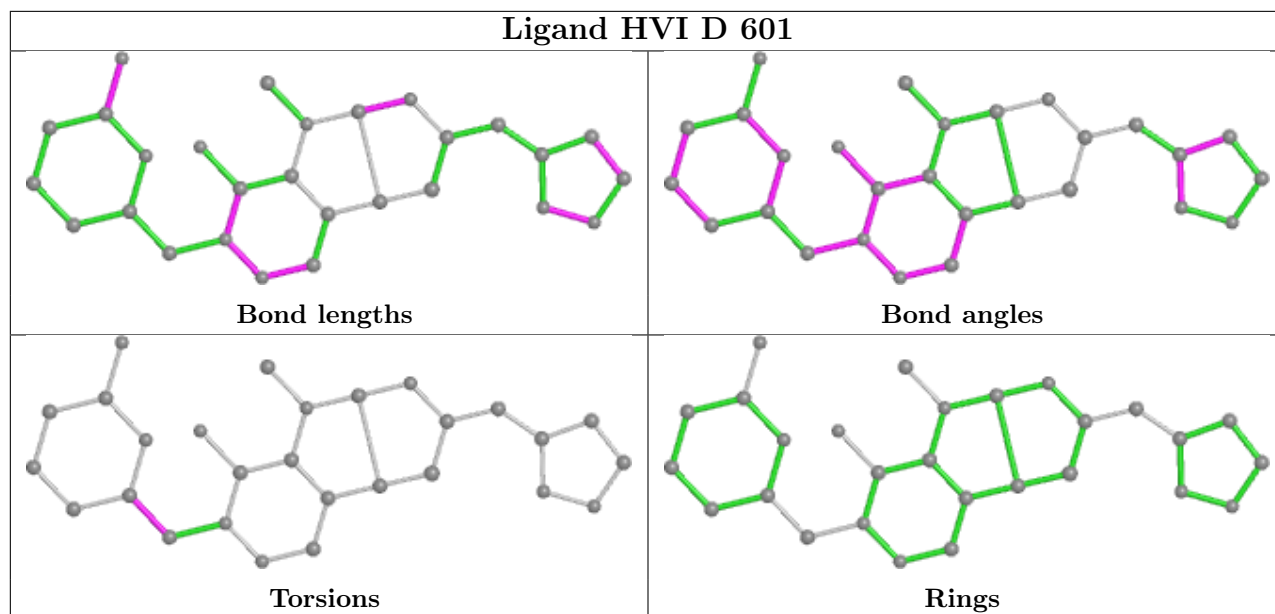
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	604	PYR	1	0
2	H	602	FBP	1	0

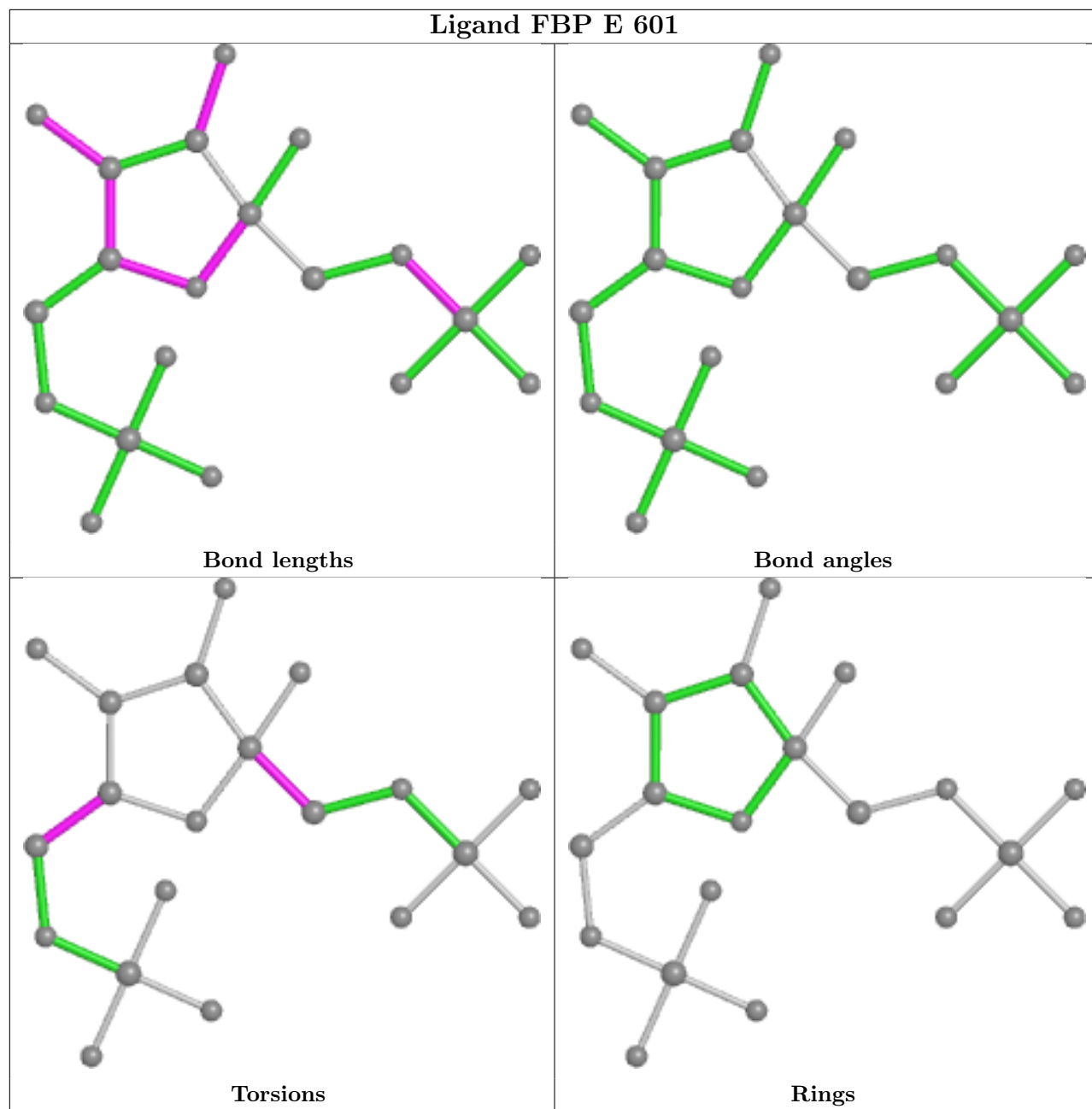
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

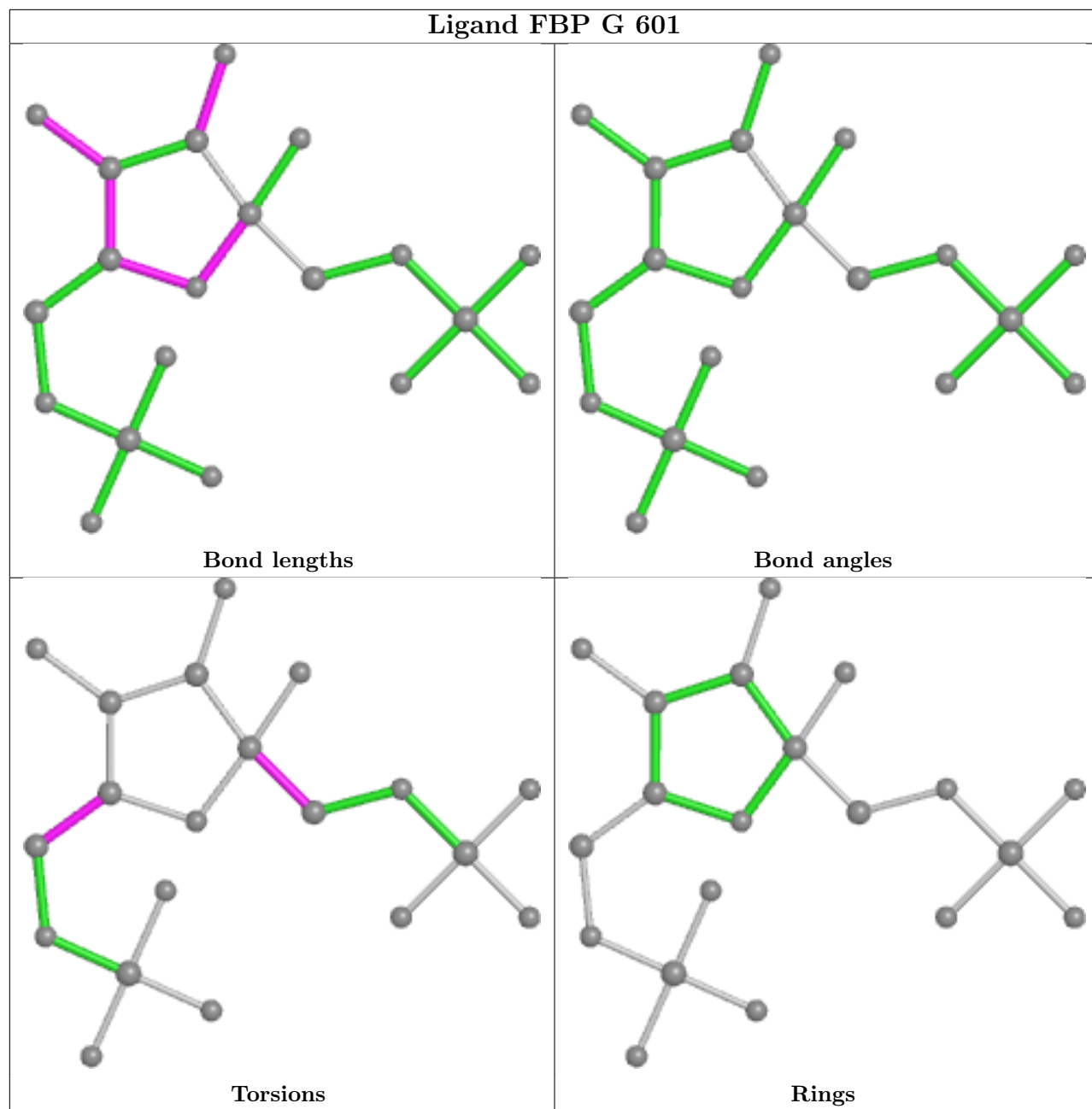
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

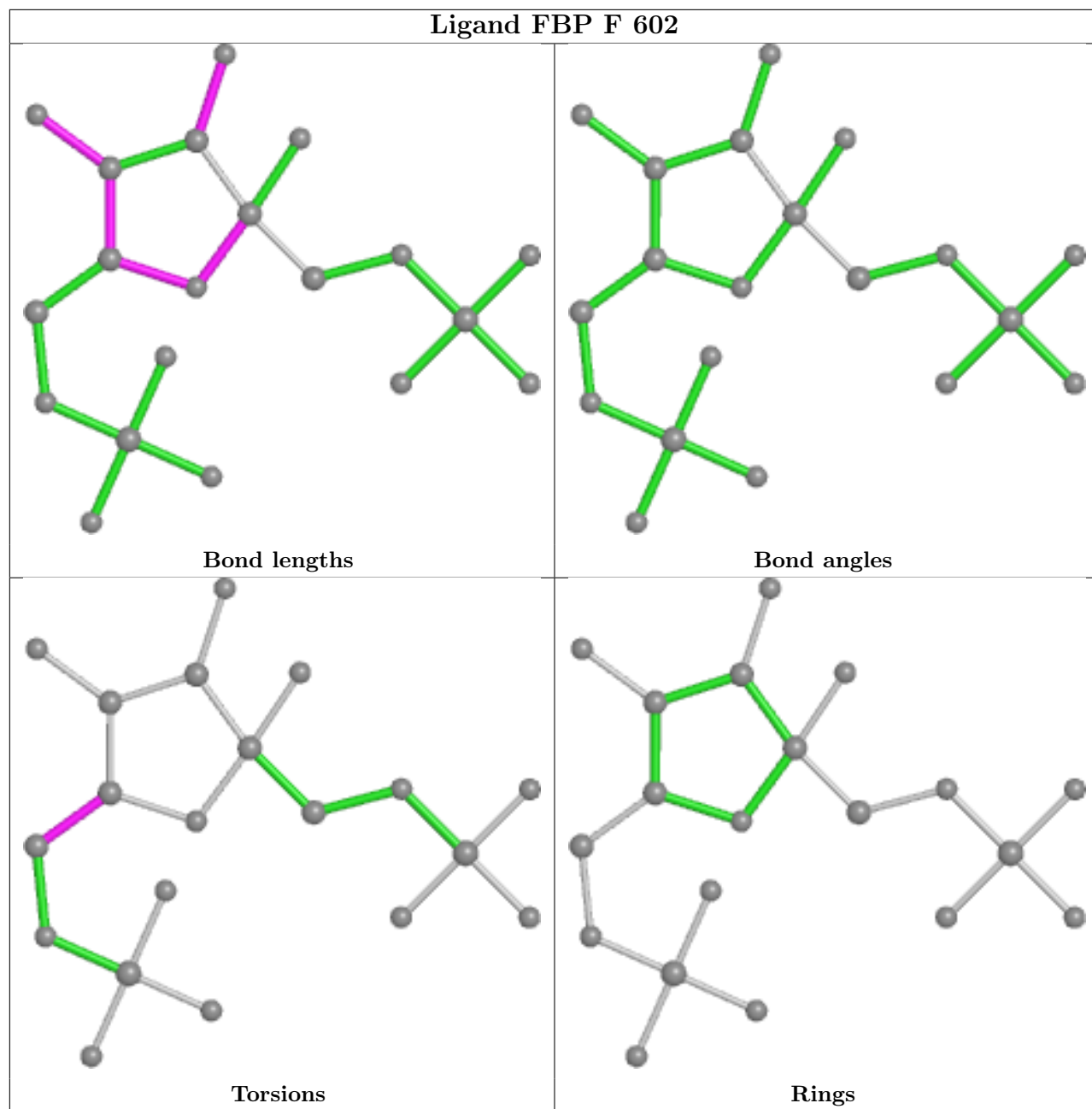


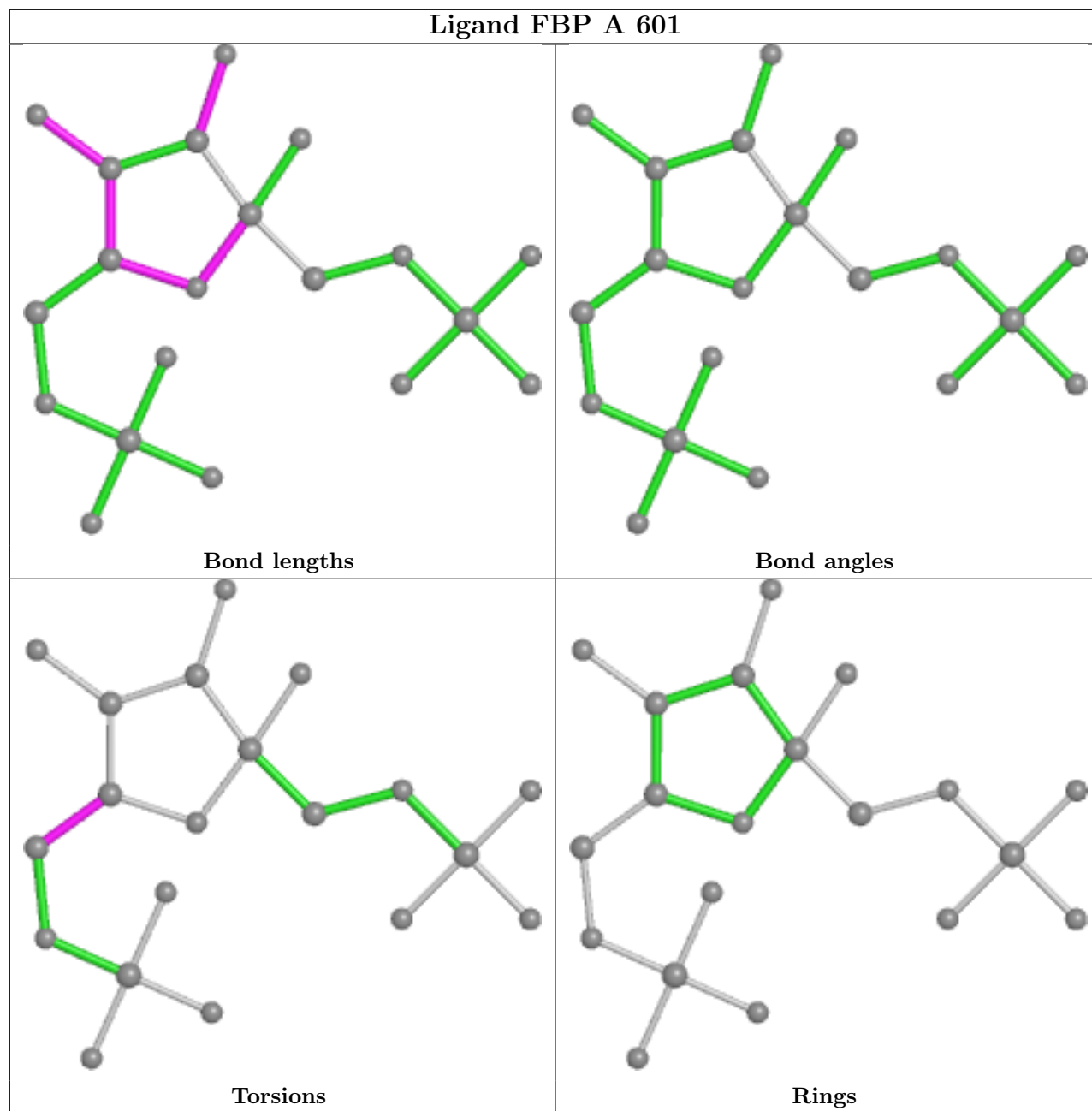


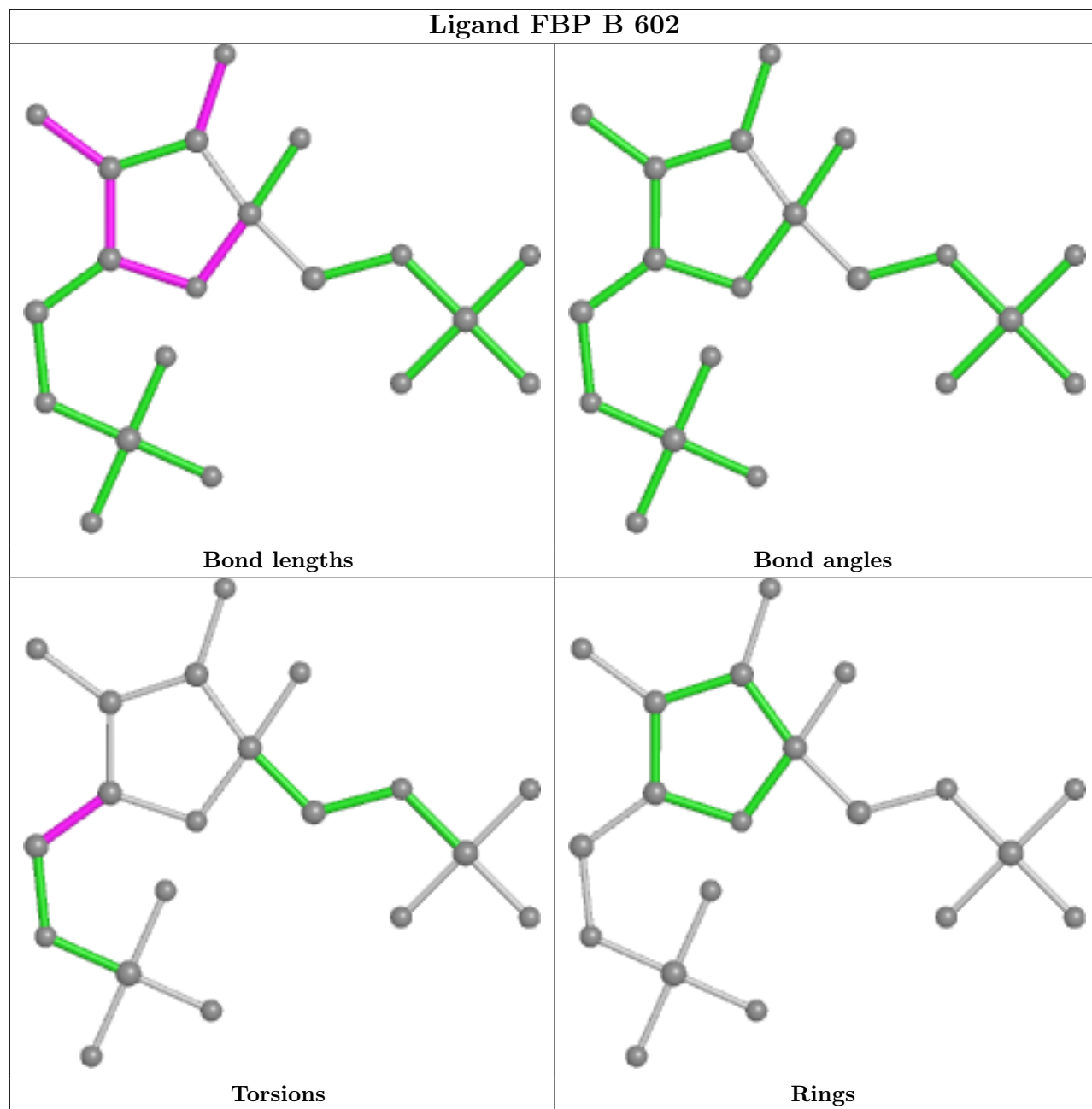


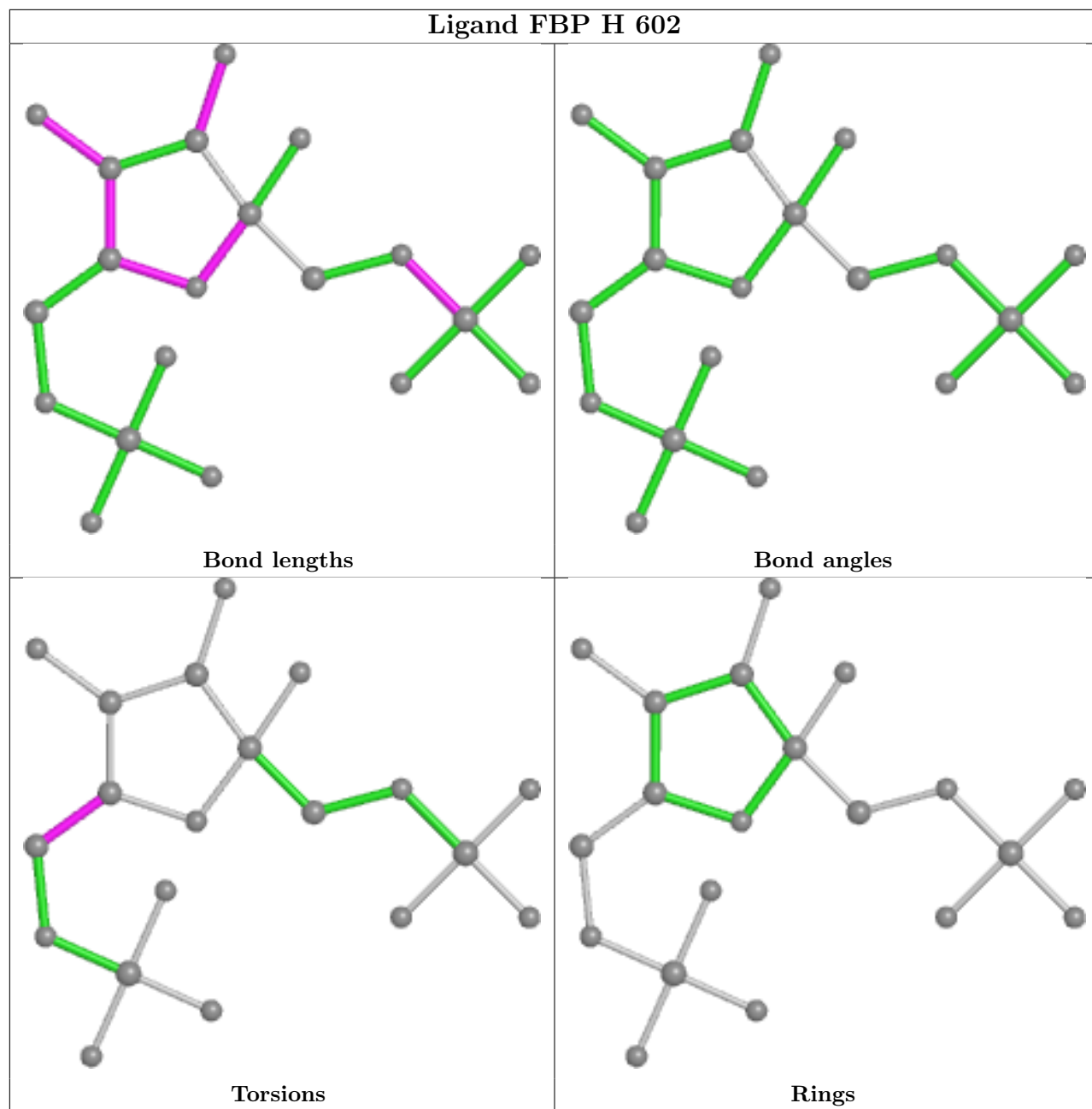


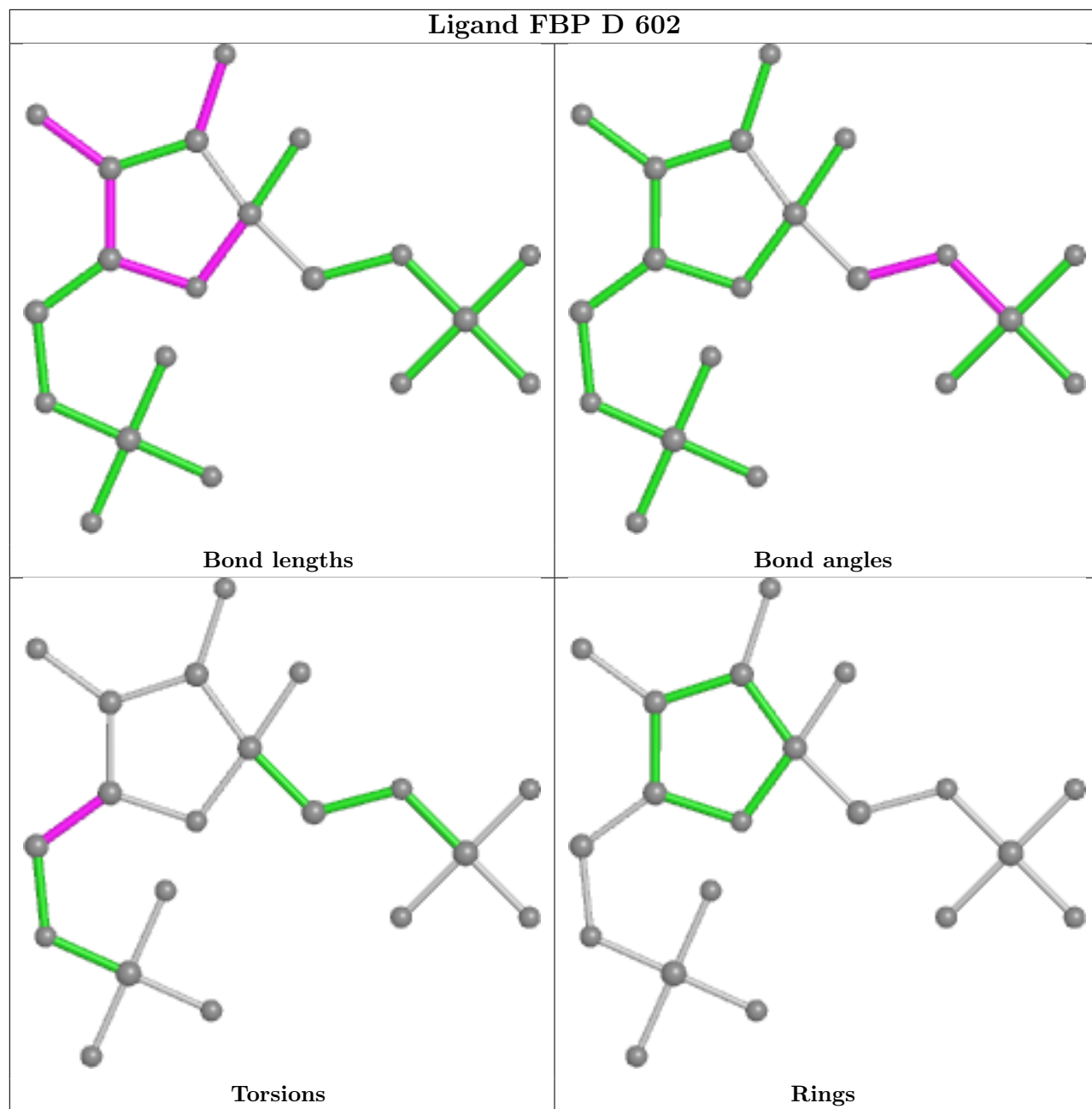




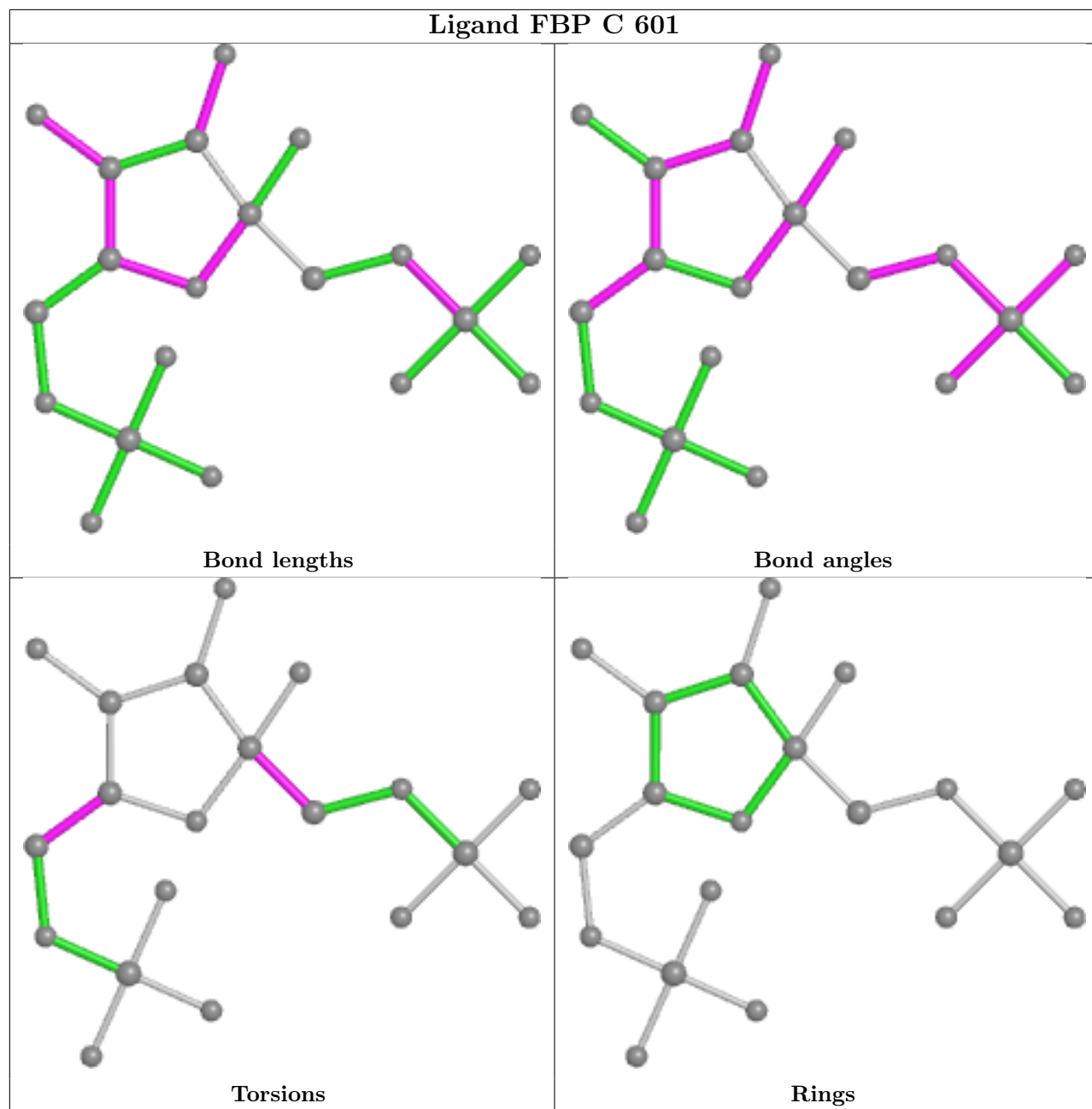


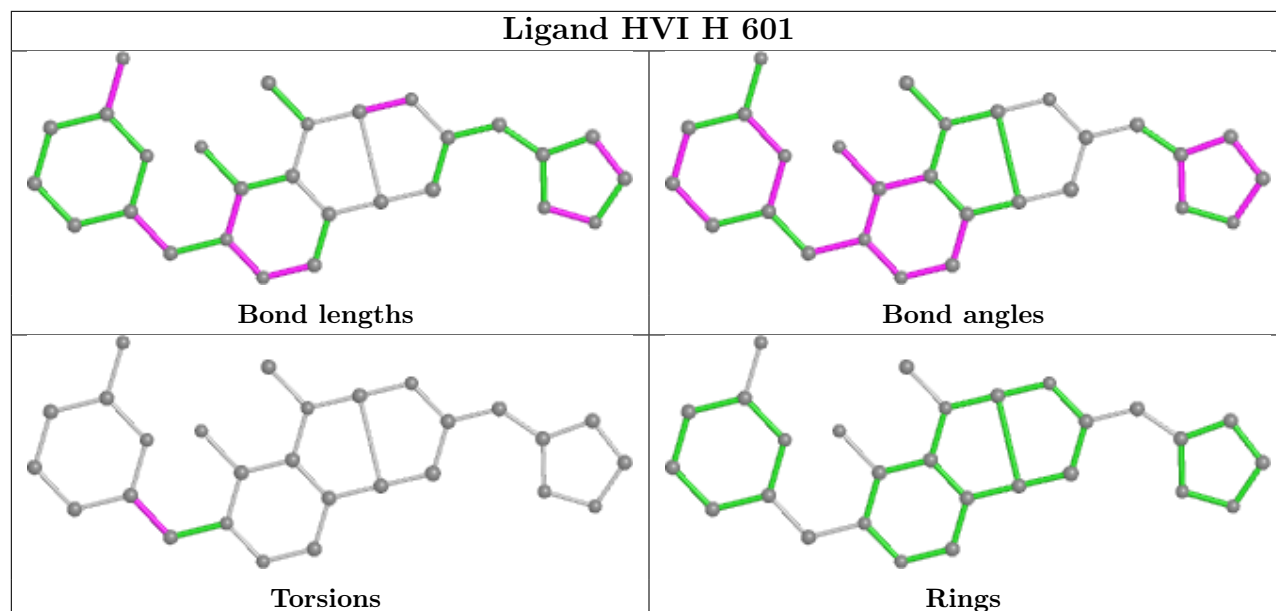












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	485/544 (89%)	0.76	67 (13%) 2 4	36, 51, 124, 158	0
1	B	517/544 (95%)	0.88	88 (17%) 1 2	35, 51, 132, 162	0
1	C	512/544 (94%)	0.78	73 (14%) 2 4	33, 50, 135, 181	0
1	D	483/544 (88%)	0.63	58 (12%) 4 7	36, 50, 110, 153	0
1	E	515/544 (94%)	0.75	73 (14%) 2 4	35, 62, 102, 155	0
1	F	520/544 (95%)	0.25	23 (4%) 34 46	31, 46, 75, 138	0
1	G	509/544 (93%)	0.74	60 (11%) 4 7	32, 61, 109, 155	0
1	H	519/544 (95%)	0.23	19 (3%) 41 54	29, 45, 73, 124	0
All	All	4060/4352 (93%)	0.63	461 (11%) 5 7	29, 51, 116, 181	0

All (461) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	VAL	13.0
1	A	245	VAL	11.9
1	C	201	TRP	11.8
1	D	235	GLY	10.9
1	B	191	PHE	10.5
1	A	186	THR	10.5
1	A	201	TRP	10.3
1	C	197	ALA	10.3
1	D	247	GLY	10.1
1	C	186	THR	10.1
1	A	191	PHE	9.5
1	B	193	THR	9.4
1	D	245	VAL	9.2
1	A	187	VAL	9.1
1	B	167	LEU	9.1
1	B	171	PRO	9.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	166	ILE	8.8
1	D	236	LEU	8.6
1	B	194	ARG	8.6
1	B	201	TRP	8.6
1	A	189	PRO	8.5
1	B	237	VAL	8.4
1	B	165	GLY	8.2
1	A	190	ALA	8.1
1	A	197	ALA	8.0
1	B	169	GLY	8.0
1	A	183	VAL	7.9
1	D	241	GLU	7.9
1	A	215	GLY	7.9
1	B	168	GLN	7.8
1	C	178	VAL	7.8
1	B	190	ALA	7.8
1	C	229	GLN	7.5
1	D	208	VAL	7.5
1	C	190	ALA	7.4
1	B	235	GLY	7.4
1	D	246	LEU	7.4
1	C	200	VAL	7.3
1	C	165	GLY	7.3
1	G	241	GLU	7.2
1	B	211	VAL	7.2
1	G	259	VAL	7.2
1	C	228	VAL	7.2
1	G	258	GLN	7.0
1	A	212	PRO	7.0
1	B	192	ARG	6.9
1	E	207	ILE	6.9
1	D	166	ILE	6.9
1	E	208	VAL	6.8
1	C	246	LEU	6.7
1	B	195	GLY	6.6
1	E	258	GLN	6.6
1	G	211	VAL	6.6
1	B	178	VAL	6.6
1	B	213	VAL	6.6
1	B	183	VAL	6.5
1	D	244	GLY	6.5
1	A	196	ASN	6.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	215	GLY	6.3
1	D	213	VAL	6.3
1	B	166	ILE	6.3
1	C	166	ILE	6.2
1	D	201	TRP	6.2
1	A	182	GLN	6.2
1	B	238	THR	6.2
1	B	185	VAL	6.2
1	B	207	ILE	6.1
1	E	227	VAL	6.1
1	E	171	PRO	6.1
1	H	56	PHE	6.1
1	C	249	ARG	6.1
1	D	237	VAL	6.0
1	A	246	LEU	6.0
1	B	187	VAL	6.0
1	C	215	GLY	6.0
1	D	227	VAL	5.9
1	C	199	THR	5.9
1	B	186	THR	5.9
1	C	198	ASN	5.9
1	E	238	THR	5.8
1	C	227	VAL	5.8
1	C	230	LYS	5.8
1	C	245	VAL	5.8
1	B	184	LEU	5.8
1	C	202	VAL	5.8
1	E	183	VAL	5.8
1	C	196	ASN	5.7
1	A	205	PRO	5.7
1	C	171	PRO	5.7
1	D	226	LEU	5.6
1	G	208	VAL	5.6
1	B	182	GLN	5.6
1	C	177	LEU	5.6
1	C	237	VAL	5.6
1	A	165	GLY	5.6
1	B	246	LEU	5.5
1	B	198	ASN	5.5
1	B	233	PRO	5.5
1	B	234	GLU	5.5
1	C	164	THR	5.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	231	ILE	5.5
1	C	231	ILE	5.3
1	C	195	GLY	5.3
1	D	229	GLN	5.3
1	E	226	LEU	5.3
1	D	210	VAL	5.3
1	A	214	GLY	5.3
1	A	227	VAL	5.3
1	C	182	GLN	5.3
1	C	240	VAL	5.2
1	G	260	ASP	5.2
1	A	241	GLU	5.2
1	D	234	GLU	5.2
1	A	211	VAL	5.2
1	A	204	TYR	5.2
1	C	175	VAL	5.2
1	A	213	VAL	5.1
1	E	211	VAL	5.1
1	C	213	VAL	5.1
1	G	263	GLY	5.1
1	D	205	PRO	5.0
1	B	181	SER	5.0
1	G	210	VAL	5.0
1	C	247	GLY	5.0
1	A	207	ILE	5.0
1	B	248	SER	5.0
1	A	226	LEU	5.0
1	A	184	LEU	5.0
1	B	196	ASN	4.9
1	C	217	ILE	4.9
1	C	184	LEU	4.9
1	B	200	VAL	4.9
1	C	181	SER	4.9
1	G	207	ILE	4.9
1	G	186	THR	4.9
1	B	214	GLY	4.9
1	D	199	THR	4.8
1	D	238	THR	4.8
1	A	198	ASN	4.8
1	C	203	ASP	4.8
1	G	248	SER	4.8
1	B	175	VAL	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	209	ARG	4.8
1	G	178	VAL	4.8
1	A	242	ASN	4.8
1	B	239	GLN	4.7
1	C	185	VAL	4.7
1	C	248	SER	4.7
1	F	167	LEU	4.7
1	B	228	VAL	4.6
1	G	238	THR	4.6
1	F	56	PHE	4.6
1	G	240	VAL	4.6
1	B	229	GLN	4.6
1	A	210	VAL	4.6
1	D	228	VAL	4.6
1	D	223	LEU	4.6
1	B	173	SER	4.6
1	D	206	ASN	4.6
1	B	210	VAL	4.5
1	C	187	VAL	4.5
1	A	188	ASP	4.5
1	A	209	ARG	4.5
1	D	254	LEU	4.5
1	G	200	VAL	4.5
1	C	238	THR	4.4
1	A	208	VAL	4.4
1	C	226	LEU	4.4
1	H	167	LEU	4.4
1	B	208	VAL	4.4
1	D	257	ALA	4.4
1	D	233	PRO	4.4
1	B	170	GLY	4.4
1	G	195	GLY	4.4
1	G	202	VAL	4.4
1	D	165	GLY	4.4
1	G	262	PRO	4.4
1	A	254	LEU	4.3
1	E	185	VAL	4.3
1	E	184	LEU	4.3
1	G	181	SER	4.3
1	C	173	SER	4.3
1	D	209	ARG	4.3
1	B	227	VAL	4.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	214	GLY	4.3
1	C	183	VAL	4.3
1	C	54	ALA	4.2
1	A	179	LYS	4.2
1	E	210	VAL	4.2
1	G	213	VAL	4.2
1	C	263	GLY	4.2
1	D	240	VAL	4.2
1	E	237	VAL	4.2
1	A	217	ILE	4.2
1	B	180	GLY	4.2
1	D	220	ASP	4.2
1	B	250	LYS	4.1
1	C	260	ASP	4.1
1	C	52	GLY	4.1
1	D	204	TYR	4.1
1	D	252	VAL	4.1
1	A	216	ARG	4.1
1	B	179	LYS	4.0
1	A	202	VAL	4.0
1	A	244	GLY	4.0
1	C	239	GLN	4.0
1	E	178	VAL	4.0
1	A	185	VAL	4.0
1	D	218	TYR	3.9
1	G	261	LEU	3.9
1	E	186	THR	3.9
1	F	54	ALA	3.9
1	D	207	ILE	3.9
1	B	223	LEU	3.9
1	E	213	VAL	3.9
1	B	226	LEU	3.9
1	B	241	GLU	3.8
1	B	55	PHE	3.8
1	D	225	SER	3.8
1	F	246	LEU	3.8
1	D	167	LEU	3.8
1	B	172	GLU	3.7
1	B	574	SER	3.7
1	E	177	LEU	3.7
1	A	264	LEU	3.7
1	D	211	VAL	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	262	PRO	3.7
1	C	53	THR	3.7
1	G	201	TRP	3.6
1	A	199	THR	3.6
1	B	217	ILE	3.6
1	C	211	VAL	3.6
1	D	239	GLN	3.6
1	G	182	GLN	3.6
1	D	222	GLY	3.6
1	A	248	SER	3.6
1	C	219	ILE	3.6
1	E	224	ILE	3.6
1	B	164	THR	3.6
1	B	199	THR	3.6
1	F	55	PHE	3.5
1	E	260	ASP	3.5
1	B	57	GLN	3.5
1	B	197	ALA	3.5
1	B	251	GLY	3.5
1	E	261	LEU	3.5
1	C	176	GLU	3.5
1	A	206	ASN	3.5
1	C	252	VAL	3.5
1	B	216	ARG	3.5
1	C	209	ARG	3.5
1	D	224	ILE	3.4
1	B	202	VAL	3.4
1	E	190	ALA	3.4
1	G	197	ALA	3.4
1	A	252	VAL	3.4
1	B	264	LEU	3.4
1	C	250	LYS	3.4
1	E	217	ILE	3.4
1	D	212	PRO	3.4
1	D	262	PRO	3.4
1	F	177	LEU	3.4
1	D	216	ARG	3.4
1	F	251	GLY	3.4
1	F	174	GLU	3.4
1	H	174	GLU	3.3
1	E	259	VAL	3.3
1	H	57	GLN	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	G	204	TYR	3.3
1	D	249	ARG	3.3
1	H	54	ALA	3.3
1	G	164	THR	3.3
1	B	189	PRO	3.3
1	C	207	ILE	3.3
1	C	174	GLU	3.3
1	E	256	GLY	3.2
1	F	171	PRO	3.2
1	D	242	ASN	3.2
1	B	174	GLU	3.2
1	A	228	VAL	3.2
1	D	232	GLY	3.2
1	B	240	VAL	3.2
1	E	200	VAL	3.2
1	B	249	ARG	3.2
1	B	260	ASP	3.2
1	G	217	ILE	3.2
1	E	218	TYR	3.2
1	H	246	LEU	3.1
1	D	248	SER	3.1
1	H	168	GLN	3.1
1	B	230	LYS	3.1
1	B	188	ASP	3.1
1	G	424	ILE	3.1
1	D	230	LYS	3.1
1	C	179	LYS	3.1
1	G	237	VAL	3.1
1	C	189	PRO	3.1
1	E	209	ARG	3.1
1	E	236	LEU	3.0
1	F	245	VAL	3.0
1	B	263	GLY	3.0
1	A	240	VAL	3.0
1	A	218	TYR	3.0
1	C	172	GLU	2.9
1	D	202	VAL	2.9
1	A	203	ASP	2.9
1	E	394	ALA	2.9
1	B	219	ILE	2.9
1	H	166	ILE	2.9
1	E	191	PHE	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	247	GLY	2.9
1	F	168	GLN	2.8
1	B	236	LEU	2.8
1	B	231	ILE	2.8
1	G	277	GLU	2.8
1	H	251	GLY	2.8
1	E	264	LEU	2.8
1	E	182	GLN	2.8
1	F	57	GLN	2.8
1	A	180	GLY	2.8
1	G	247	GLY	2.8
1	D	164	THR	2.8
1	G	162	ILE	2.8
1	C	258	GLN	2.8
1	A	249	ARG	2.8
1	B	261	LEU	2.8
1	F	169	GLY	2.8
1	G	123	SER	2.8
1	B	176	GLU	2.8
1	C	180	GLY	2.7
1	H	245	VAL	2.7
1	B	224	ILE	2.7
1	C	224	ILE	2.7
1	E	242	ASN	2.7
1	C	205	PRO	2.7
1	E	392	ALA	2.7
1	E	101	VAL	2.7
1	D	219	ILE	2.7
1	E	214	GLY	2.7
1	G	199	THR	2.7
1	G	170	GLY	2.7
1	E	212	PRO	2.7
1	E	216	ARG	2.7
1	B	259	VAL	2.7
1	A	164	THR	2.7
1	F	176	GLU	2.7
1	G	245	VAL	2.7
1	A	251	GLY	2.7
1	G	256	GLY	2.7
1	E	187	VAL	2.6
1	E	248	SER	2.6
1	C	216	ARG	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	245	VAL	2.6
1	C	56	PHE	2.6
1	B	212	PRO	2.5
1	G	239	GLN	2.5
1	G	395	VAL	2.5
1	E	423	ALA	2.5
1	E	425	ALA	2.5
1	B	121	HIS	2.5
1	E	204	TYR	2.5
1	E	179	LYS	2.5
1	C	235	GLY	2.5
1	G	246	LEU	2.5
1	H	177	LEU	2.5
1	A	83	VAL	2.5
1	E	240	VAL	2.5
1	D	162	ILE	2.5
1	D	542	LEU	2.5
1	F	223	LEU	2.5
1	B	395	VAL	2.5
1	E	201	TRP	2.5
1	H	171	PRO	2.5
1	C	261	LEU	2.5
1	E	276	VAL	2.5
1	F	175	VAL	2.5
1	E	273	ARG	2.5
1	E	205	PRO	2.5
1	G	226	LEU	2.5
1	G	219	ILE	2.4
1	C	254	LEU	2.4
1	H	175	VAL	2.4
1	E	99	ARG	2.4
1	G	194	ARG	2.4
1	A	247	GLY	2.4
1	B	204	TYR	2.4
1	E	102	GLU	2.4
1	F	401	CYS	2.4
1	C	395	VAL	2.4
1	G	391	VAL	2.4
1	E	125	GLU	2.4
1	G	190	ALA	2.4
1	G	203	ASP	2.4
1	E	90	ILE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	239	GLN	2.4
1	G	57	GLN	2.4
1	A	230	LYS	2.3
1	D	255	PRO	2.3
1	D	273	ARG	2.3
1	A	396	LEU	2.3
1	B	161	GLU	2.3
1	E	395	VAL	2.3
1	G	125	GLU	2.3
1	C	214	GLY	2.3
1	D	200	VAL	2.3
1	A	160	PRO	2.3
1	H	223	LEU	2.3
1	F	65	MET	2.3
1	A	163	ARG	2.3
1	E	163	ARG	2.3
1	E	274	PHE	2.3
1	D	243	GLY	2.2
1	A	255	PRO	2.2
1	G	171	PRO	2.2
1	A	542	LEU	2.2
1	E	195	GLY	2.2
1	G	396	LEU	2.2
1	E	215	GLY	2.2
1	F	219	ILE	2.2
1	F	191	PHE	2.2
1	B	221	ASP	2.2
1	G	257	ALA	2.2
1	E	424	ILE	2.2
1	E	228	VAL	2.2
1	A	143	GLY	2.2
1	E	119	PHE	2.2
1	G	180	GLY	2.2
1	E	399	ALA	2.2
1	G	392	ALA	2.2
1	G	399	ALA	2.2
1	A	266	GLU	2.2
1	E	391	VAL	2.2
1	G	101	VAL	2.2
1	G	191	PHE	2.2
1	G	274	PHE	2.2
1	G	212	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	249	ARG	2.1
1	C	264	LEU	2.1
1	A	273	ARG	2.1
1	C	163	ARG	2.1
1	E	83	VAL	2.1
1	C	220	ASP	2.1
1	F	166	ILE	2.1
1	H	146	LEU	2.1
1	H	65	MET	2.1
1	A	239	GLN	2.1
1	B	205	PRO	2.1
1	E	181	SER	2.1
1	H	401	CYS	2.1
1	E	257	ALA	2.1
1	H	287	PHE	2.1
1	H	389	SER	2.1
1	B	84	ALA	2.1
1	B	177	LEU	2.0
1	F	402	ILE	2.0
1	B	391	VAL	2.0
1	E	206	ASN	2.0
1	A	392	ALA	2.0
1	F	391	VAL	2.0
1	A	225	SER	2.0
1	E	193	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

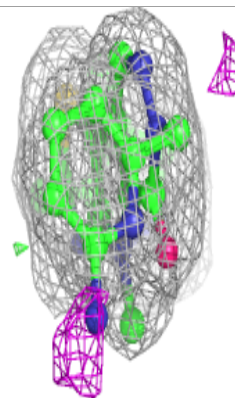
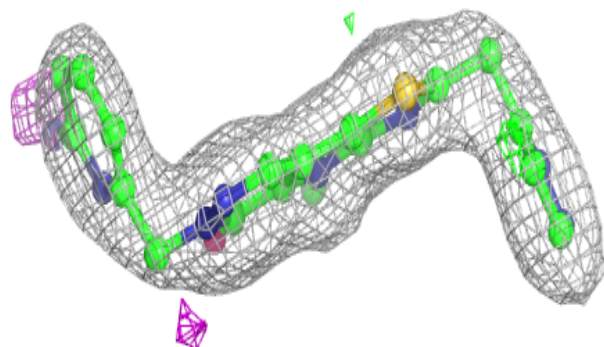
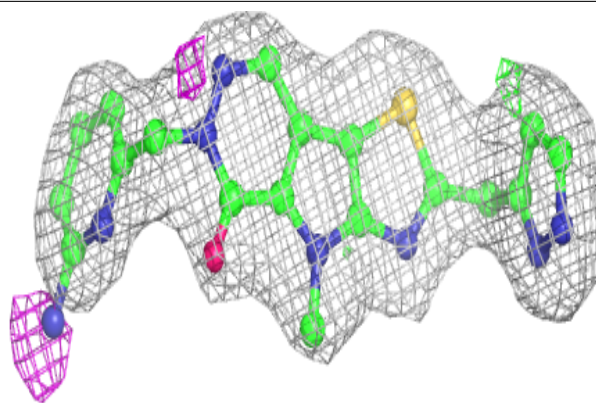
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MN	H	603	1/1	0.60	0.48	210,210,210,210	0
3	MN	F	603	1/1	0.69	0.34	160,160,160,160	0
4	K	E	603	1/1	0.73	0.29	140,140,140,140	0
4	K	C	603	1/1	0.75	0.15	102,102,102,102	0
4	K	B	604	1/1	0.79	0.21	98,98,98,98	0
5	PYR	F	605	6/6	0.81	0.14	74,75,85,90	0
4	K	G	603	1/1	0.84	0.10	119,119,119,119	0
5	PYR	D	604	6/6	0.89	0.19	58,68,78,84	0
4	K	A	603	1/1	0.89	0.17	90,90,90,90	0
5	PYR	E	604	6/6	0.90	0.16	61,75,77,84	0
3	MN	D	603	1/1	0.91	0.07	99,99,99,99	0
4	K	F	604	1/1	0.91	0.19	107,107,107,107	0
5	PYR	H	604	6/6	0.91	0.12	80,81,83,86	0
3	MN	G	602	1/1	0.93	0.23	133,133,133,133	0
5	PYR	G	604	6/6	0.94	0.10	63,70,75,78	0
5	PYR	B	605	6/6	0.94	0.15	51,72,77,78	0
6	HVI	B	601	28/28	0.94	0.16	31,46,52,58	0
2	FBP	G	601	20/20	0.96	0.13	38,47,58,61	0
2	FBP	C	601	20/20	0.96	0.17	37,42,56,57	0
2	FBP	E	601	20/20	0.96	0.13	41,48,56,61	0
6	HVI	H	601	28/28	0.96	0.14	31,38,45,48	0
2	FBP	D	602	20/20	0.97	0.12	40,49,55,62	0
6	HVI	D	601	28/28	0.97	0.14	33,45,55,59	0
6	HVI	F	601	28/28	0.97	0.15	31,38,46,50	0
3	MN	B	603	1/1	0.97	0.15	87,87,87,87	0
5	PYR	A	604	6/6	0.98	0.15	50,59,65,65	0
2	FBP	F	602	20/20	0.98	0.12	31,41,47,48	0
5	PYR	C	604	6/6	0.98	0.12	52,60,68,72	0
3	MN	C	602	1/1	0.98	0.15	67,67,67,67	0
2	FBP	A	601	20/20	0.98	0.10	39,46,56,61	0
2	FBP	H	602	20/20	0.98	0.11	35,41,51,51	0
3	MN	A	602	1/1	0.99	0.05	61,61,61,61	0
2	FBP	B	602	20/20	0.99	0.13	32,39,44,47	0
3	MN	E	602	1/1	0.99	0.13	93,93,93,93	0

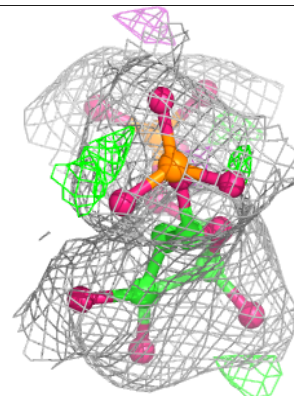
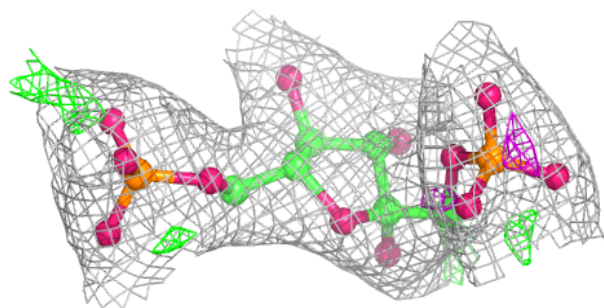
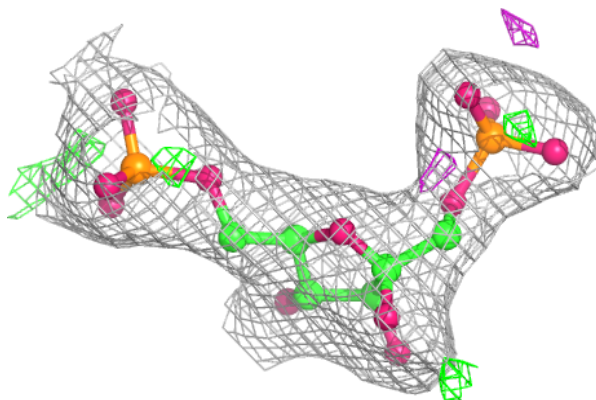
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around HVI 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 G 601:**

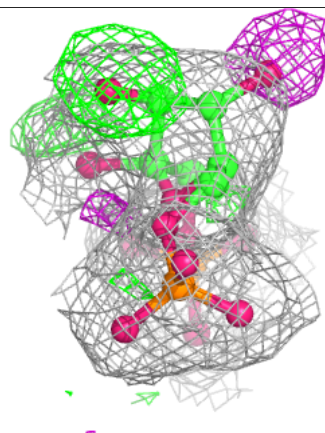
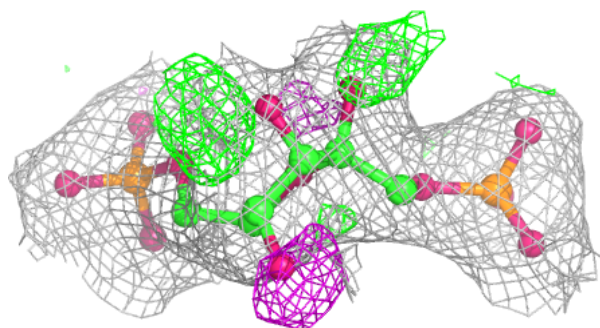
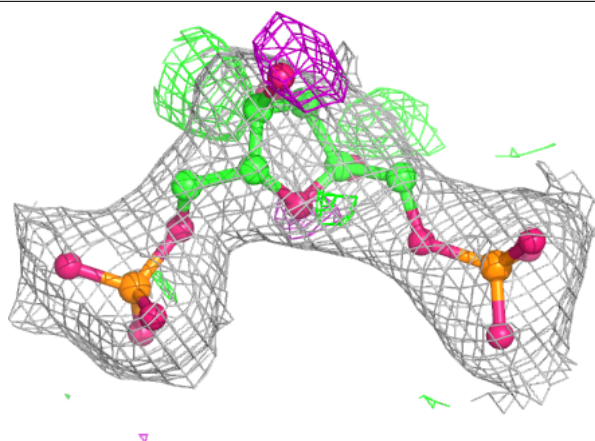
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



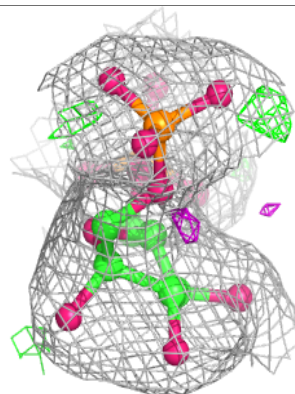
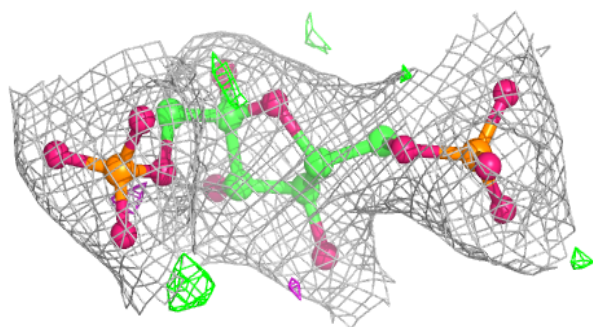
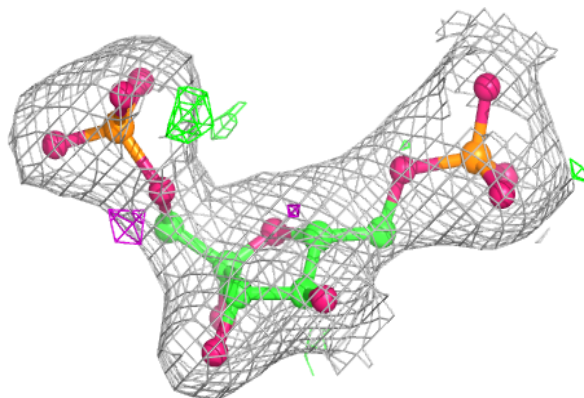


**Electron density around FBP C 601:**

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

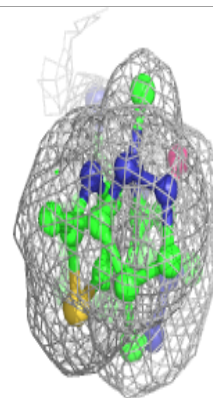
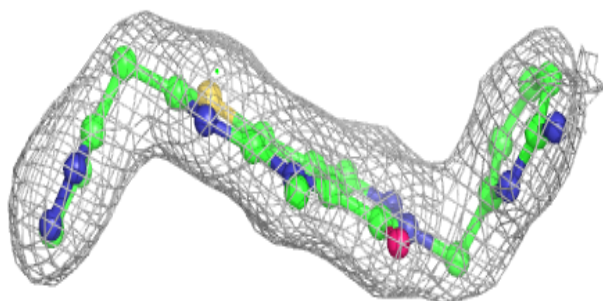
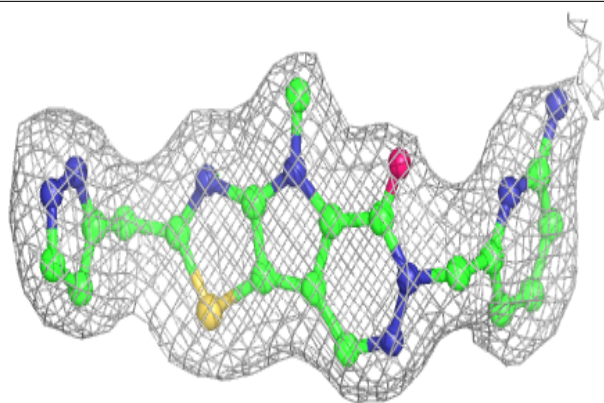
**Electron density around FBP E 601:**

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

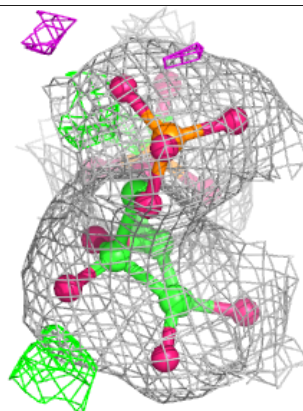
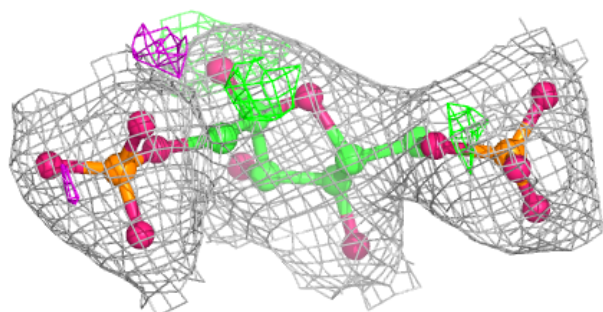
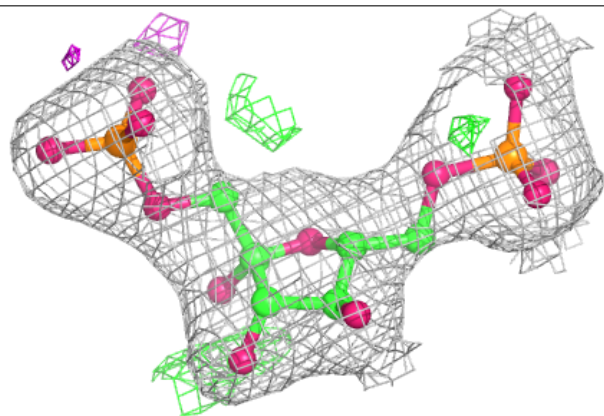


**Electron density around HVI H 601:**

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

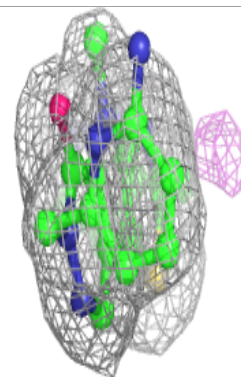
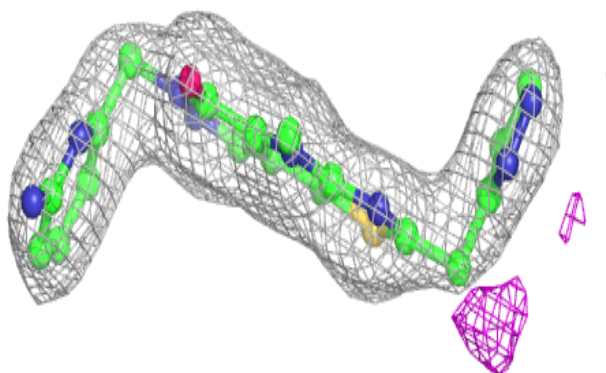
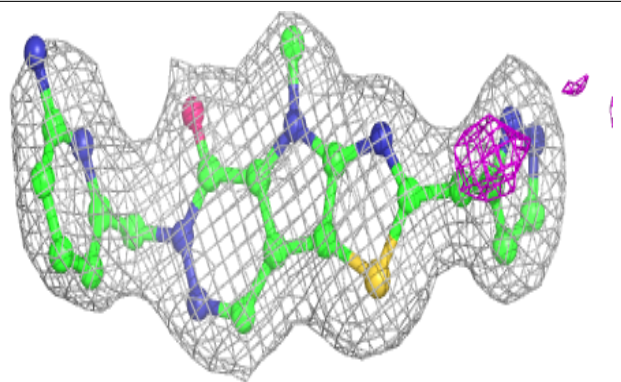
**Electron density around FBP D 602:**

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

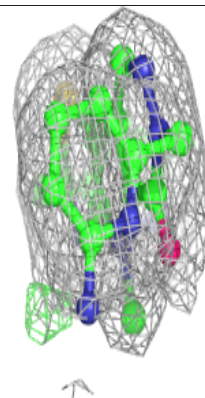
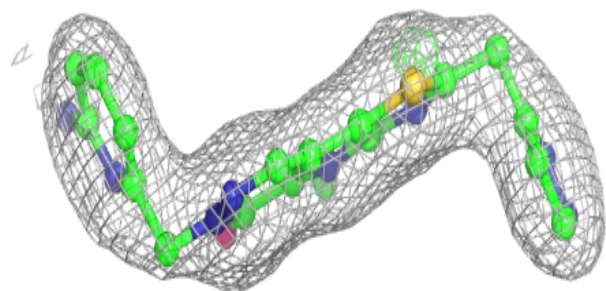
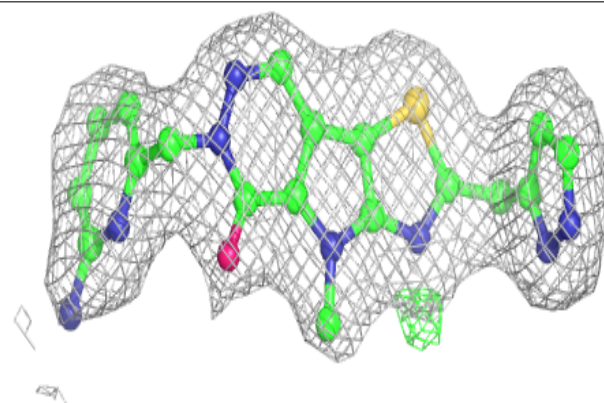


**Electron density around HVI D 601:**

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

**Electron density around HVI F 601:**

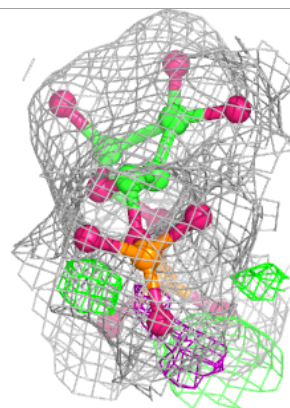
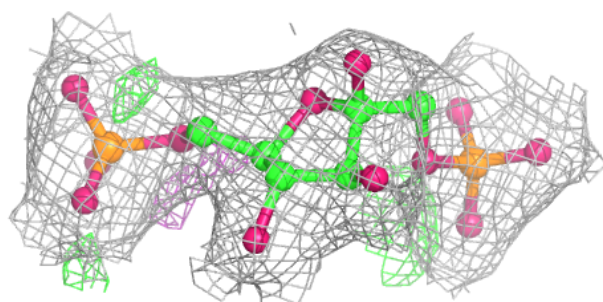
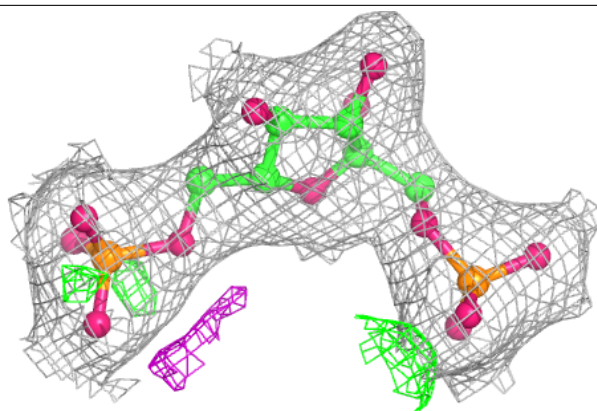
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



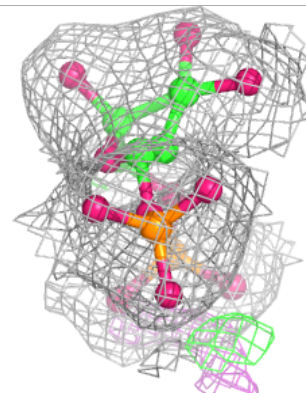
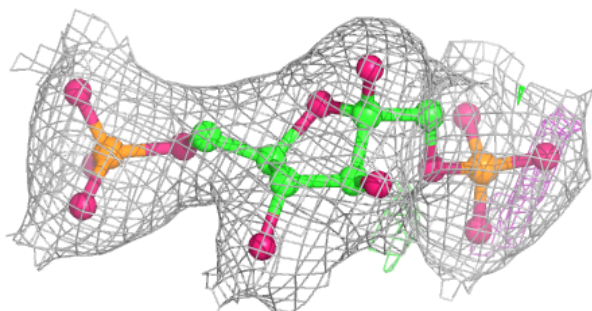
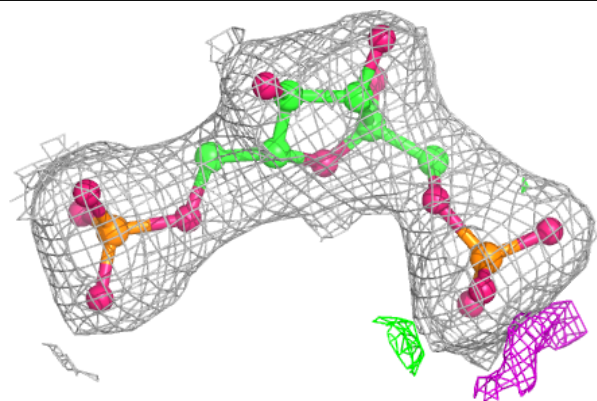


**Electron density around FBP F 602:**

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

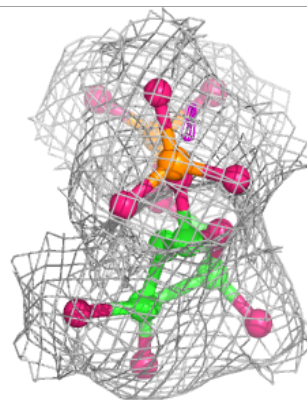
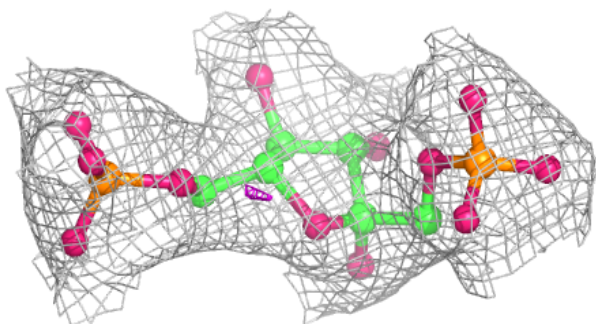
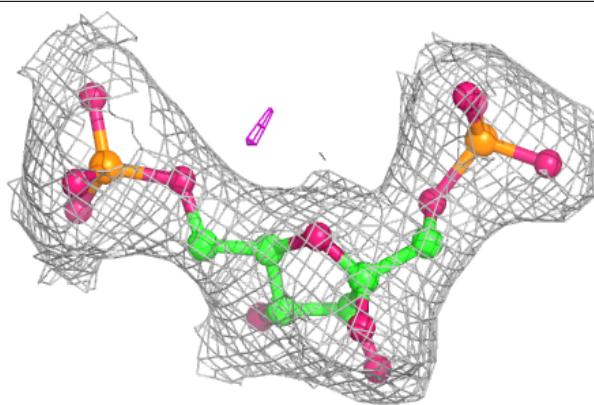
**Electron density around FBP A 601:**

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

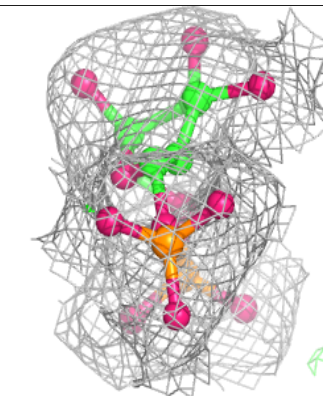
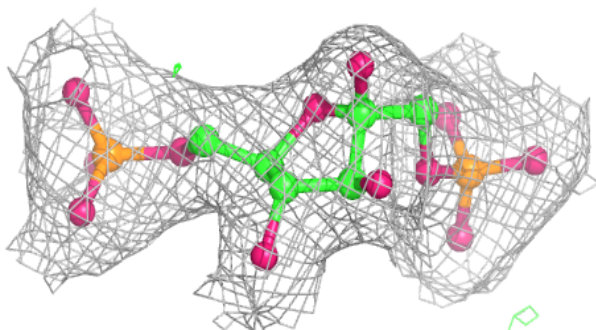
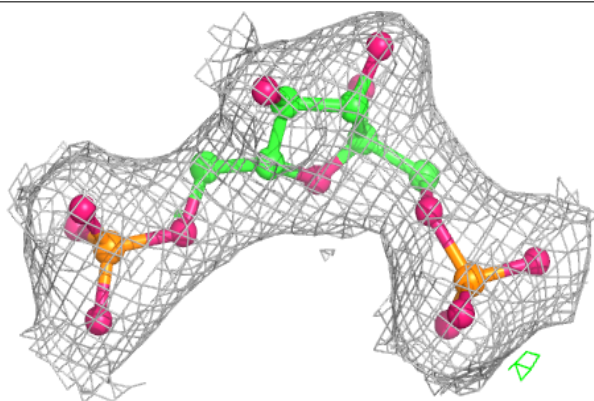


**Electron density around FBP H 602:**

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

**Electron density around FBP B 602:**

$2mF_o-DF_c$  (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.