



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2023 – 04:09 PM EST

PDB ID : 8TBT  
Title : Structure of human erythrocyte pyruvate kinase in complex with an allosteric activator Compound 2  
Authors : Jin, L.; Padyana, A.  
Deposited on : 2023-06-29  
Resolution : 2.34 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)  
Xtrriage (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

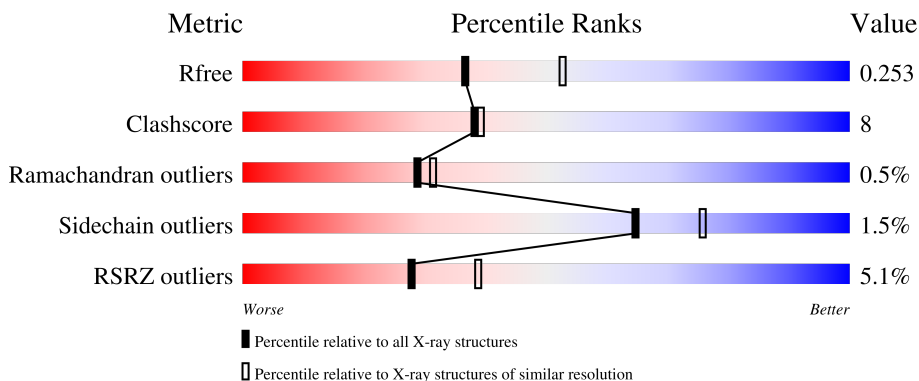
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	 5% 81% 13% 6%
1	B	544	 3% 80% 15% 5%
1	C	544	 7% 73% 19% 8%
1	D	544	 5% 81% 13% 6%

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	PYR	A	602	-	X	-	-
4	MN	B	604	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 16072 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	514	3894	2446	705	725	18	0	0	0
1	B	518	3918	2460	710	730	18	0	0	0
1	C	503	3806	2391	688	709	18	0	0	0
1	D	512	3877	2435	702	722	18	0	0	0

There are 76 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
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

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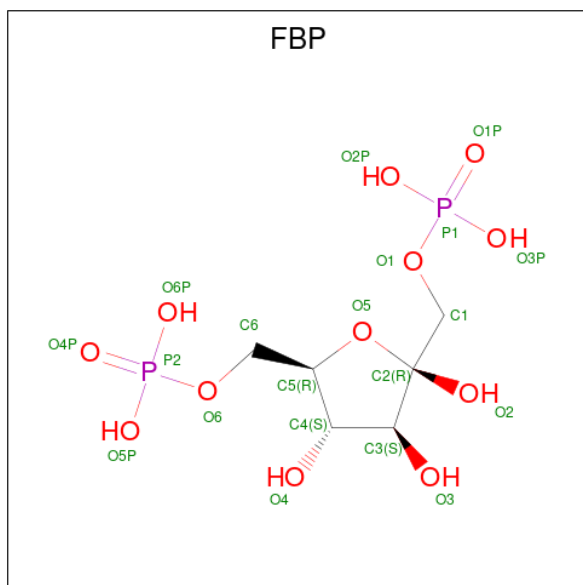
Chain	Residue	Modelled	Actual	Comment	Reference
B	33	SER	-	expression tag	UNP P30613
B	34	SER	-	expression tag	UNP P30613
B	35	HIS	-	expression tag	UNP P30613
B	36	HIS	-	expression tag	UNP P30613
B	37	HIS	-	expression tag	UNP P30613
B	38	HIS	-	expression tag	UNP P30613
B	39	HIS	-	expression tag	UNP P30613
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
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

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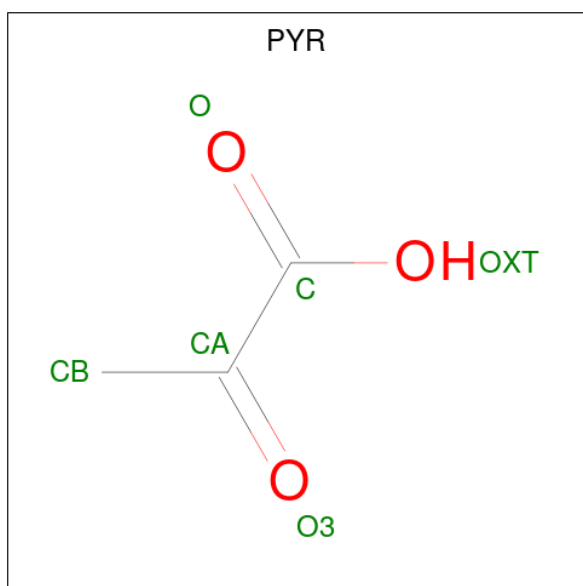
Chain	Residue	Modelled	Actual	Comment	Reference
D	37	HIS	-	expression tag	UNP P30613
D	38	HIS	-	expression tag	UNP P30613
D	39	HIS	-	expression tag	UNP P30613
D	40	HIS	-	expression tag	UNP P30613
D	41	SER	-	expression tag	UNP P30613
D	42	SER	-	expression tag	UNP P30613
D	43	GLY	-	expression tag	UNP P30613
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

- 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	20	6	12	2	0	0
2	B	1	20	6	12	2	0	0
2	C	1	20	6	12	2	0	0
2	D	1	20	6	12	2	0	0

- Molecule 3 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
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

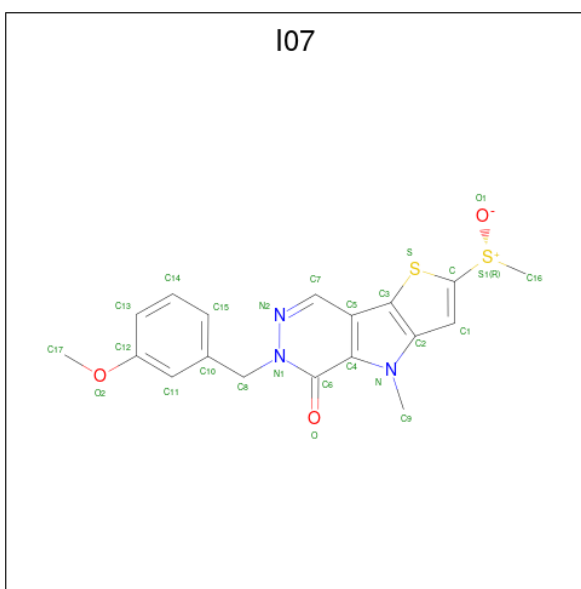
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total K 1 1	0	0
5	C	1	Total K 1 1	0	0
5	D	1	Total K 1 1	0	0

- Molecule 6 is {6-[(3-methoxyphenyl)methyl]-4-methyl-5-oxo-5,6-dihydro-4H-thieno[2',3':4,5]pyrrolo[2,3-d]pyridazin-2-yl}(methyl)sulfaniumolate (three-letter code: I07) (formula: C<sub>18</sub>H<sub>17</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C N O S 52 36 6 6 4	0	1
6	D	1	Total C N O S 52 36 6 6 4	0	1

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	91	Total O 91 91	0	0
7	B	92	Total O 92 92	0	0
7	C	70	Total O 70 70	0	0

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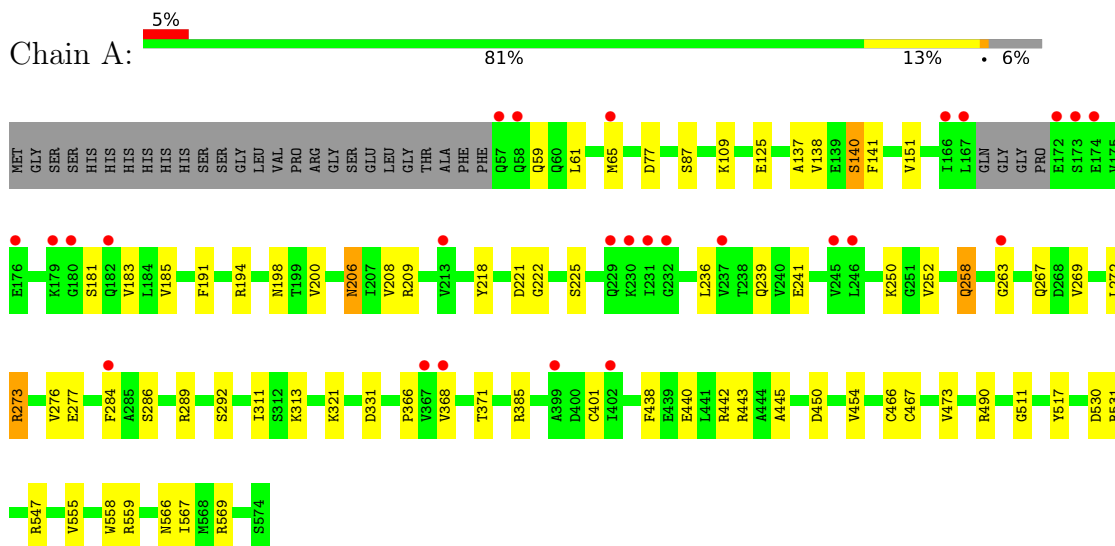
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	D	108	Total 108	O 108	0	0

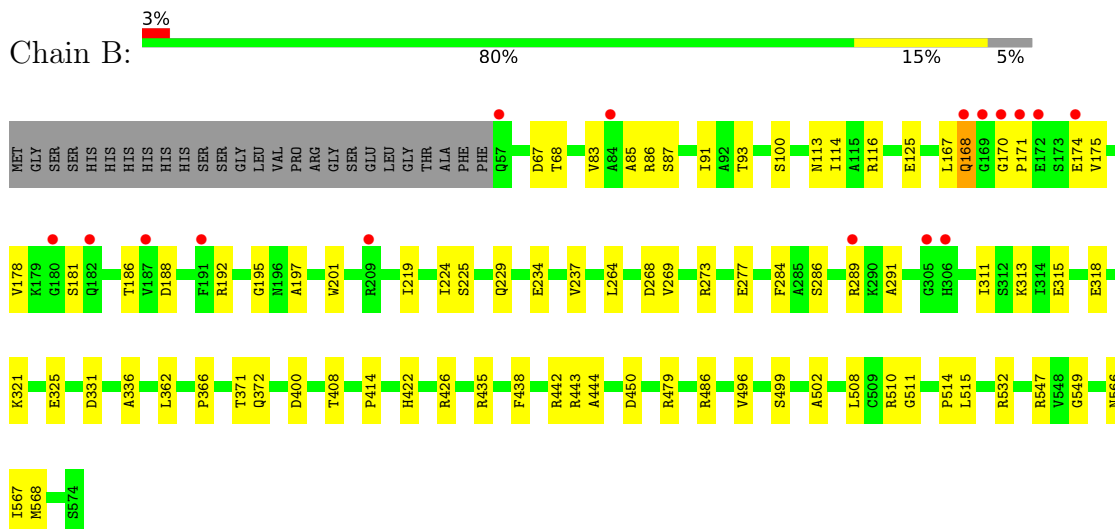
### 3 Residue-property plots [i](#)

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

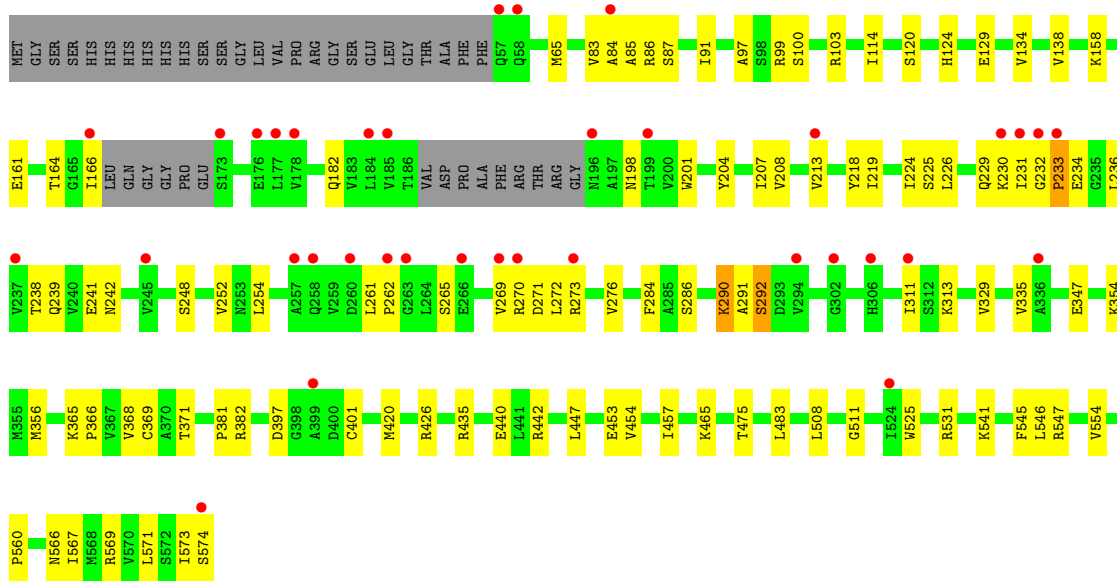


- Molecule 1: Pyruvate kinase PKLR

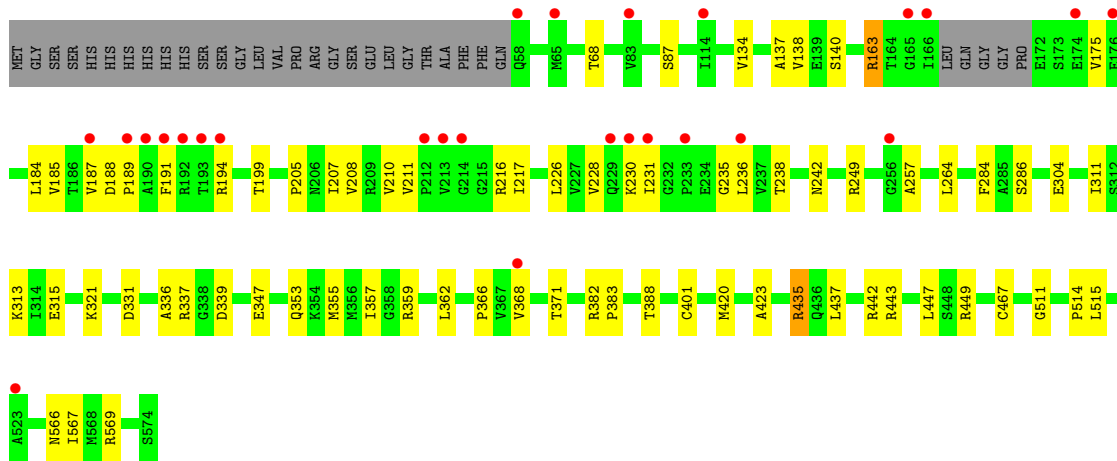
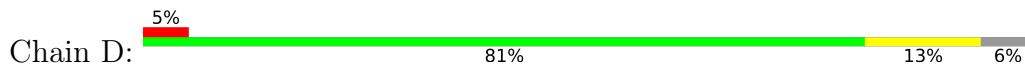


- Molecule 1: Pyruvate kinase PKLR





● Molecule 1: Pyruvate kinase PKLR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.35Å 174.04Å 87.34Å 90.00° 94.29° 90.00°	Depositor
Resolution (Å)	33.77 – 2.34 33.77 – 2.34	Depositor EDS
% Data completeness (in resolution range)	97.2 (33.77-2.34) 97.2 (33.77-2.34)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.30 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.198 , 0.253 0.198 , 0.253	Depositor DCC
$R_{free}$ test set	4551 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.3	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16072	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: I07, MN, K, FBP, 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	0.42	0/3956	0.58	0/5361
1	B	0.42	0/3982	0.57	0/5398
1	C	0.42	0/3865	0.57	0/5236
1	D	0.44	0/3939	0.57	0/5338
All	All	0.42	0/15742	0.57	0/21333

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3894	0	3974	48	0
1	B	3918	0	3996	57	0
1	C	3806	0	3886	102	0
1	D	3877	0	3955	59	0
2	A	20	0	10	0	0
2	B	20	0	10	0	0
2	C	20	0	10	2	0
2	D	20	0	10	0	0
3	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	52	0	0	0	0
6	D	52	0	0	1	0
7	A	91	0	0	1	0
7	B	92	0	0	1	0
7	C	70	0	0	0	0
7	D	108	0	0	2	0
All	All	16072	0	15851	240	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 8.

All (240) 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:C:290:LYS:CD	1:C:292:SER:H	1.31	1.40
1:C:290:LYS:HD3	1:C:292:SER:H	1.03	1.11
1:C:290:LYS:HD2	1:C:292:SER:HB3	1.30	1.07
1:C:290:LYS:CD	1:C:292:SER:N	2.17	1.06
1:C:290:LYS:HD2	1:C:292:SER:H	1.21	0.99
1:C:229:GLN:OE1	1:C:238:THR:C	2.02	0.97
1:C:290:LYS:HD3	1:C:292:SER:N	1.75	0.95
1:C:381:PRO:HB2	1:C:382:ARG:HH11	1.34	0.92
1:C:290:LYS:HD3	1:C:291:ALA:N	1.88	0.89
1:C:290:LYS:HD2	1:C:292:SER:CB	2.03	0.88
1:C:381:PRO:CB	1:C:382:ARG:HH11	1.86	0.87
1:C:381:PRO:CG	1:C:382:ARG:HH11	1.90	0.84
1:C:381:PRO:CG	1:C:382:ARG:NH1	2.41	0.82
1:D:355:MET:SD	1:D:359:ARG:CZ	2.69	0.81
1:C:381:PRO:HB2	1:C:382:ARG:NH1	1.97	0.79
1:C:475:THR:HA	2:C:601:FBP:H61	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD12	1:C:262:PRO:HD2	1.64	0.79
1:B:567:ILE:HG12	1:D:569:ARG:HG2	1.64	0.78
1:A:263:GLY:HA2	1:A:289:ARG:HH22	1.47	0.78
1:C:290:LYS:HD2	1:C:292:SER:N	1.89	0.77
1:B:549:GLY:O	1:D:449:ARG:NH2	2.19	0.75
1:C:231:ILE:HG22	1:C:233:PRO:HD3	1.71	0.73
1:A:286:SER:HA	1:A:313:LYS:HE2	1.68	0.73
1:C:381:PRO:CB	1:C:382:ARG:NH1	2.52	0.73
1:C:442:ARG:HG2	1:C:457:ILE:HD11	1.73	0.69
1:C:213:VAL:HG11	1:C:230:LYS:HA	1.73	0.69
1:B:186:THR:HG22	1:B:188:ASP:H	1.55	0.68
1:B:178:VAL:HG13	1:B:181:SER:HB2	1.75	0.67
1:C:541:LYS:NZ	1:C:574:SER:O	2.27	0.67
1:C:83:VAL:HG12	1:C:85:ALA:H	1.58	0.66
1:D:228:VAL:HA	1:D:238:THR:HG22	1.78	0.66
1:D:230:LYS:HZ2	1:D:231:ILE:H	1.44	0.66
1:A:206:ASN:HD21	1:A:209:ARG:HB2	1.62	0.65
1:D:315:GLU:HG2	1:D:336:ALA:HB3	1.79	0.65
1:B:435:ARG:NH2	1:D:443:ARG:NH1	2.44	0.65
1:A:225:SER:HB2	1:A:241:GLU:HB3	1.79	0.65
1:C:368:VAL:HG22	1:C:401:CYS:HB2	1.78	0.64
1:C:225:SER:OG	1:C:241:GLU:OE1	2.16	0.64
1:C:229:GLN:OE1	1:C:238:THR:CA	2.46	0.64
1:A:191:PHE:HA	1:A:194:ARG:HG3	1.79	0.63
1:A:206:ASN:ND2	1:A:209:ARG:HB2	2.13	0.63
1:C:265:SER:O	1:C:269:VAL:HG23	1.98	0.63
1:B:168:GLN:HG3	1:B:195:GLY:O	1.97	0.62
1:B:435:ARG:NH2	1:D:443:ARG:HH11	1.98	0.62
1:C:381:PRO:HG2	1:C:382:ARG:HH11	1.61	0.62
1:C:381:PRO:HG2	1:C:382:ARG:NH1	2.13	0.62
1:C:233:PRO:HB2	1:C:234:GLU:OE1	2.00	0.62
1:B:167:LEU:HD23	1:B:195:GLY:HA3	1.81	0.62
1:A:569:ARG:HG2	1:C:567:ILE:HG12	1.81	0.62
1:D:447:LEU:HD22	1:D:447:LEU:H	1.66	0.60
1:A:284:PHE:HD1	1:A:311:ILE:HB	1.67	0.59
1:D:187:VAL:HG11	1:D:205:PRO:HA	1.84	0.59
1:B:83:VAL:HG12	1:B:85:ALA:H	1.68	0.59
1:C:290:LYS:CD	1:C:292:SER:HB3	2.20	0.58
3:D:603:PYR:O	4:D:604:MN:MN	1.60	0.58
1:B:273:ARG:O	1:B:277:GLU:HG3	2.04	0.58
1:D:87:SER:HB2	1:D:511:GLY:HA2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:ILE:HG12	1:C:569:ARG:HG2	1.85	0.57
1:C:347:GLU:HG2	1:D:423:ALA:HB1	1.85	0.57
1:B:435:ARG:NH2	1:D:443:ARG:HD2	2.20	0.57
1:A:442:ARG:HH22	1:C:442:ARG:HD3	1.70	0.56
1:A:263:GLY:HA2	1:A:289:ARG:NH2	2.17	0.56
1:B:87:SER:HB2	1:B:511:GLY:HA2	1.87	0.56
1:C:290:LYS:HD3	1:C:291:ALA:CA	2.36	0.56
1:B:435:ARG:HH22	1:D:443:ARG:NH1	2.02	0.56
1:C:366:PRO:HB3	1:C:508:LEU:O	2.06	0.56
1:D:566:ASN:OD1	1:D:567:ILE:HG13	2.06	0.56
1:B:234:GLU:H	1:B:234:GLU:CD	2.10	0.55
1:A:517:TYR:OH	1:A:531:ARG:HD2	2.07	0.55
1:B:86:ARG:HD3	1:B:422:HIS:ND1	2.22	0.54
1:B:566:ASN:OD1	1:B:567:ILE:HG13	2.08	0.54
1:C:225:SER:HB3	1:C:242:ASN:N	2.22	0.54
1:C:290:LYS:HD2	1:C:292:SER:CA	2.37	0.54
1:D:210:VAL:HG22	1:D:257:ALA:HB1	1.89	0.54
1:B:219:ILE:HB	1:B:224:ILE:HB	1.90	0.53
1:B:67:ASP:OD1	7:B:701:HOH:O	2.18	0.53
1:A:61:LEU:O	1:A:65:MET:HG3	2.09	0.53
1:B:264:LEU:HD22	1:B:269:VAL:HG22	1.90	0.53
1:B:289:ARG:HB3	1:B:318:GLU:HG2	1.91	0.52
1:B:450:ASP:OD2	1:B:479:ARG:NH2	2.39	0.52
1:C:87:SER:HB2	1:C:511:GLY:HA2	1.92	0.52
1:D:207:ILE:HA	1:D:210:VAL:HG12	1.91	0.52
1:C:525:TRP:CE2	1:C:560:PRO:HG3	2.45	0.52
1:D:184:LEU:HD12	1:D:199:THR:HG23	1.92	0.51
1:C:286:SER:HA	1:C:313:LYS:HE2	1.91	0.51
1:A:385:ARG:HG2	1:B:372:GLN:OE1	2.11	0.51
1:B:284:PHE:HD1	1:B:311:ILE:HB	1.75	0.51
1:C:83:VAL:O	1:C:426:ARG:HD2	2.11	0.51
1:C:208:VAL:HG12	1:C:236:LEU:HG	1.92	0.51
1:A:267:GLN:NE2	7:A:703:HOH:O	2.43	0.50
1:B:86:ARG:NH2	1:B:113:ASN:OD1	2.44	0.50
1:A:77:ASP:OD1	1:B:321:LYS:NZ	2.44	0.50
1:D:304:GLU:CD	1:D:304:GLU:H	2.14	0.50
1:D:339:ASP:OD2	3:D:603:PYR:O	2.29	0.50
1:B:86:ARG:HB2	1:B:426:ARG:HG3	1.94	0.50
1:C:134:VAL:O	1:C:138:VAL:HG23	2.11	0.50
1:C:219:ILE:HG12	1:C:252:VAL:HG22	1.92	0.50
1:A:61:LEU:HD11	1:A:490:ARG:CZ	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:LEU:HD13	1:D:184:LEU:C	2.32	0.49
1:A:181:SER:O	1:A:239:GLN:HG3	2.12	0.49
1:D:188:ASP:HB3	1:D:191:PHE:CD2	2.47	0.49
1:A:440:GLU:CD	1:B:68:THR:HB	2.32	0.49
1:B:315:GLU:HG2	1:B:336:ALA:HB3	1.94	0.49
1:D:284:PHE:HD1	1:D:311:ILE:HB	1.77	0.49
1:B:435:ARG:HH21	1:D:443:ARG:HD2	1.77	0.49
1:C:120:SER:OG	1:C:161:GLU:OE2	2.30	0.49
1:D:163:ARG:HD3	1:D:249:ARG:NH1	2.26	0.49
1:A:218:TYR:HD2	1:A:222:GLY:HA2	1.78	0.49
1:C:229:GLN:OE1	1:C:239:GLN:N	2.45	0.49
1:D:304:GLU:O	7:D:701:HOH:O	2.20	0.48
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.78	0.48
1:A:208:VAL:HA	1:A:236:LEU:HD21	1.96	0.48
1:C:335:VAL:CG2	1:C:369:CYS:HA	2.44	0.48
1:D:514:PRO:O	1:D:515:LEU:HD23	2.13	0.48
1:B:438:PHE:CE2	1:B:442:ARG:HD2	2.49	0.48
1:D:368:VAL:HG22	1:D:401:CYS:HB2	1.95	0.48
1:A:138:VAL:HG21	1:A:151:VAL:HB	1.96	0.47
1:B:86:ARG:HD2	1:B:422:HIS:HA	1.97	0.47
1:C:84:ALA:HA	1:C:426:ARG:HH11	1.79	0.47
1:C:99:ARG:NH2	1:C:129:GLU:HB2	2.29	0.47
1:C:225:SER:HB2	1:C:242:ASN:HB2	1.96	0.47
1:C:290:LYS:CE	1:C:292:SER:H	2.16	0.47
1:C:546:LEU:HD13	1:C:573:ILE:CD1	2.45	0.47
1:D:210:VAL:HG13	1:D:211:VAL:HG13	1.96	0.47
1:C:120:SER:HA	1:C:158:LYS:HG3	1.96	0.47
1:C:291:ALA:HB1	1:C:329:VAL:HG21	1.97	0.47
1:A:125:GLU:CD	1:A:125:GLU:H	2.19	0.47
1:A:368:VAL:HG22	1:A:401:CYS:HB2	1.97	0.46
1:B:229:GLN:HB2	1:B:237:VAL:HG23	1.97	0.46
1:C:86:ARG:HB2	1:C:426:ARG:HG2	1.97	0.46
1:A:250:LYS:HA	1:A:250:LYS:HD3	1.61	0.46
1:A:438:PHE:CE2	1:A:442:ARG:HD3	2.51	0.46
1:C:204:TYR:CE1	1:C:261:LEU:HB2	2.50	0.46
1:C:229:GLN:OE1	1:C:238:THR:HA	2.16	0.46
1:D:208:VAL:HA	1:D:236:LEU:HD11	1.96	0.46
1:A:109:LYS:HE3	1:A:141:PHE:HE1	1.79	0.46
1:A:221:ASP:N	1:A:221:ASP:OD1	2.49	0.46
1:B:186:THR:CG2	1:B:188:ASP:H	2.26	0.46
1:D:331:ASP:O	1:D:366:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:GLN:N	1:A:258:GLN:OE1	2.49	0.45
1:D:355:MET:SD	1:D:359:ARG:NH1	2.89	0.45
1:B:291:ALA:HB2	1:B:325:GLU:HG3	1.98	0.45
1:A:443:ARG:NE	1:C:435:ARG:HH11	2.14	0.45
1:C:218:TYR:O	1:C:252:VAL:HA	2.17	0.45
1:B:192:ARG:HA	1:B:201:TRP:CG	2.52	0.45
1:B:435:ARG:NH2	1:D:443:ARG:CD	2.80	0.45
1:B:499:SER:HB3	1:B:502:ALA:HB3	1.98	0.45
1:B:93:THR:HA	1:B:116:ARG:HB3	1.97	0.45
1:C:91:ILE:HG12	1:C:114:ILE:HB	1.99	0.45
1:B:442:ARG:HH11	1:D:442:ARG:NH2	2.14	0.45
1:C:166:ILE:HA	1:C:248:SER:HB3	1.99	0.45
1:D:184:LEU:HD13	1:D:185:VAL:N	2.32	0.44
1:D:230:LYS:NZ	1:D:231:ILE:HG22	2.33	0.44
1:A:269:VAL:O	1:A:273:ARG:HG3	2.17	0.44
1:A:87:SER:HB2	1:A:511:GLY:HA2	2.00	0.44
1:B:83:VAL:CG1	1:B:85:ALA:H	2.30	0.44
1:A:59:GLN:HB3	1:A:61:LEU:HD13	1.99	0.44
1:D:362:LEU:HD22	7:D:750:HOH:O	2.18	0.44
1:C:164:THR:HA	1:C:201:TRP:O	2.17	0.44
1:D:383:PRO:HG3	1:D:420:MET:HG2	1.99	0.44
1:A:185:VAL:HA	1:A:200:VAL:HG23	1.99	0.43
1:D:353:GLN:O	1:D:357:ILE:HG13	2.18	0.43
1:A:273:ARG:O	1:A:277:GLU:HG3	2.17	0.43
1:A:331:ASP:O	1:A:366:PRO:HD2	2.18	0.43
1:C:84:ALA:HA	1:C:426:ARG:NH1	2.34	0.43
1:C:232:GLY:N	1:C:233:PRO:HD3	2.33	0.43
1:C:269:VAL:O	1:C:273:ARG:HG2	2.18	0.43
1:B:286:SER:HA	1:B:313:LYS:HD3	2.00	0.43
1:D:337:ARG:HD3	1:D:353:GLN:OE1	2.17	0.43
1:A:466:CYS:HB3	1:C:454:VAL:HG21	2.01	0.43
1:B:331:ASP:O	1:B:366:PRO:HD2	2.19	0.43
1:C:207:ILE:HG13	1:C:254:LEU:HD11	2.01	0.43
1:C:525:TRP:CD1	1:C:560:PRO:HG3	2.54	0.43
1:C:382:ARG:HH22	1:D:242:ASN:CB	2.32	0.43
1:A:185:VAL:HB	1:A:236:LEU:HB2	2.00	0.43
1:D:137:ALA:O	1:D:140:SER:HB3	2.19	0.43
1:A:442:ARG:HH22	1:C:442:ARG:CD	2.30	0.43
1:A:558:TRP:CE3	1:A:559:ARG:HB2	2.53	0.42
1:B:125:GLU:CD	1:B:125:GLU:H	2.20	0.42
1:C:85:ALA:HB2	1:C:545:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:HIS:NE2	1:C:271:ASP:OD1	2.44	0.42
1:D:264:LEU:HD12	1:D:264:LEU:HA	1.85	0.42
1:B:83:VAL:HG12	1:B:85:ALA:N	2.32	0.42
1:C:420:MET:HE2	1:C:420:MET:O	2.20	0.42
1:B:443:ARG:HD3	1:D:435:ARG:HH11	1.83	0.42
1:B:91:ILE:HG12	1:B:114:ILE:HB	2.02	0.42
1:B:496:VAL:HG11	1:B:532:ARG:HB3	2.01	0.42
1:B:408:THR:HA	1:B:414:PRO:HB3	2.01	0.42
1:A:183:VAL:HG22	1:A:198:ASN:HA	2.01	0.42
1:C:554:VAL:HG21	1:C:571:LEU:HD12	2.00	0.42
1:C:182:GLN:O	1:C:198:ASN:ND2	2.48	0.42
1:C:208:VAL:HA	1:C:236:LEU:HD21	2.01	0.42
1:B:234:GLU:OE2	1:B:234:GLU:N	2.45	0.42
1:D:134:VAL:O	1:D:138:VAL:HG23	2.19	0.42
1:A:272:LEU:O	1:A:276:VAL:HG23	2.20	0.42
1:C:83:VAL:CG1	1:C:85:ALA:H	2.29	0.42
1:C:225:SER:O	1:C:226:LEU:HD23	2.19	0.42
1:C:231:ILE:HG22	1:C:233:PRO:CD	2.46	0.42
1:A:218:TYR:O	1:A:252:VAL:HA	2.20	0.41
1:B:400:ASP:HA	1:B:510:ARG:HB2	2.01	0.41
1:D:184:LEU:HD21	1:D:235:GLY:HA3	2.02	0.41
1:C:83:VAL:HG12	1:C:85:ALA:N	2.31	0.41
1:C:347:GLU:HG2	1:D:423:ALA:CB	2.50	0.41
1:D:388:THR:HG22	1:D:420:MET:HE2	2.02	0.41
1:B:175:VAL:HG11	1:B:197:ALA:N	2.35	0.41
1:C:447:LEU:HD22	1:C:447:LEU:H	1.85	0.41
1:D:87:SER:HB2	1:D:511:GLY:CA	2.49	0.41
1:D:286:SER:HA	1:D:313:LYS:HD3	2.02	0.41
1:A:445:ALA:HB3	1:C:465:LYS:NZ	2.35	0.41
1:C:97:ALA:O	1:C:103:ARG:HD2	2.21	0.41
1:C:284:PHE:HD1	1:C:311:ILE:HB	1.85	0.41
1:C:365:LYS:HA	1:C:366:PRO:HD3	1.96	0.41
1:D:188:ASP:HA	1:D:189:PRO:HD3	1.91	0.41
1:C:382:ARG:HH22	1:D:242:ASN:HB3	1.86	0.41
1:D:211:VAL:HG21	1:D:217:ILE:HD11	2.02	0.41
1:B:264:LEU:HD23	1:B:268:ASP:HB2	2.03	0.41
1:C:442:ARG:CZ	1:C:442:ARG:HB3	2.51	0.41
1:A:137:ALA:O	1:A:140:SER:HB3	2.21	0.41
1:A:473:VAL:HG23	1:A:555:VAL:HB	2.03	0.41
1:A:547:ARG:HE	1:A:547:ARG:HB2	1.71	0.41
1:B:514:PRO:O	1:B:515:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ILE:HD13	1:C:224:ILE:HA	1.76	0.41
1:C:453:GLU:OE2	1:C:483:LEU:HD22	2.20	0.41
1:D:216:ARG:HA	1:D:226:LEU:O	2.21	0.41
1:A:450:ASP:O	1:A:454:VAL:HG23	2.21	0.40
1:B:547:ARG:HD2	1:B:547:ARG:HA	1.76	0.40
1:D:437:LEU:HB2	6:D:601[B]:I07:C16	2.50	0.40
1:C:382:ARG:NH2	1:D:242:ASN:CG	2.74	0.40
1:C:440:GLU:CD	1:D:68:THR:HB	2.41	0.40
1:B:362:LEU:HD11	1:B:444:ALA:HB1	2.03	0.40
1:C:272:LEU:O	1:C:276:VAL:HG23	2.20	0.40
1:C:335:VAL:HG12	1:C:356:MET:CE	2.52	0.40
1:C:525:TRP:HZ2	2:C:601:FBP:H12	1.86	0.40
1:B:366:PRO:HB3	1:B:508:LEU:O	2.22	0.40
1:C:354:LYS:NZ	1:C:397:ASP:OD1	2.52	0.40
1:C:453:GLU:HG2	1:C:483:LEU:HD13	2.03	0.40
1:D:321:LYS:HD2	1:D:321:LYS:HA	1.76	0.40
1:C:290:LYS:CD	1:C:292:SER:CB	2.88	0.40
1:C:420:MET:HE1	1:D:347:GLU:HB3	2.03	0.40
1:C:525:TRP:NE1	1:C:560:PRO:HG3	2.37	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	510/544 (94%)	498 (98%)	10 (2%)	2 (0%)	34 38
1	B	516/544 (95%)	503 (98%)	9 (2%)	4 (1%)	19 20
1	C	497/544 (91%)	484 (97%)	10 (2%)	3 (1%)	25 26
1	D	508/544 (93%)	492 (97%)	14 (3%)	2 (0%)	34 38
All	All	2031/2176 (93%)	1977 (97%)	43 (2%)	11 (0%)	29 31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	PRO
1	C	233	PRO
1	B	168	GLN
1	B	371	THR
1	C	371	THR
1	D	175	VAL
1	D	371	THR
1	A	566	ASN
1	B	170	GLY
1	A	371	THR
1	C	566	ASN

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/436 (95%)	405 (98%)	8 (2%)	57	68
1	B	415/436 (95%)	410 (99%)	5 (1%)	71	82
1	C	404/436 (93%)	397 (98%)	7 (2%)	60	72
1	D	411/436 (94%)	406 (99%)	5 (1%)	71	82
All	All	1643/1744 (94%)	1618 (98%)	25 (2%)	65	76

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	SER
1	A	206	ASN
1	A	258	GLN
1	A	273	ARG
1	A	292	SER
1	A	321	LYS
1	A	467	CYS
1	A	530	ASP
1	B	100	SER

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Mol	Chain	Res	Type
1	B	174	GLU
1	B	225	SER
1	B	486	ARG
1	B	568	MET
1	C	65	MET
1	C	100	SER
1	C	270	ARG
1	C	290	LYS
1	C	292	SER
1	C	531	ARG
1	C	547	ARG
1	D	163	ARG
1	D	194	ARG
1	D	382	ARG
1	D	435	ARG
1	D	467	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	D	121	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 monosaccharides in this entry.

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

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FBP	C	601	-	18,20,20	1.01	1 (5%)	23,32,32	1.26	2 (8%)
3	PYR	B	603	4	5,5,5	2.77	3 (60%)	3,6,6	1.76	2 (66%)
3	PYR	D	603	4	5,5,5	2.65	3 (60%)	3,6,6	2.56	1 (33%)
6	I07	B	601[B]	-	21,29,29	3.85	7 (33%)	23,43,43	2.41	8 (34%)
6	I07	D	601[B]	-	21,29,29	3.60	7 (33%)	23,43,43	2.70	9 (39%)
2	FBP	D	602	-	18,20,20	0.84	1 (5%)	23,32,32	1.14	2 (8%)
6	I07	D	601[A]	-	21,29,29	3.80	6 (28%)	23,43,43	2.29	7 (30%)
3	PYR	C	602	4	5,5,5	2.83	3 (60%)	3,6,6	3.13	2 (66%)
6	I07	B	601[A]	-	21,29,29	3.82	6 (28%)	23,43,43	2.43	9 (39%)
3	PYR	A	602	4	5,5,5	2.71	3 (60%)	3,6,6	3.70	3 (100%)
2	FBP	A	601	-	18,20,20	0.88	1 (5%)	23,32,32	1.11	1 (4%)
2	FBP	B	602	-	18,20,20	0.91	1 (5%)	23,32,32	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FBP	C	601	-	-	8/13/32/32	0/1/1/1
3	PYR	B	603	4	-	0/4/4/4	-
3	PYR	D	603	4	-	0/4/4/4	-
6	I07	B	601[B]	-	-	0/6/10/10	0/4/4/4
6	I07	D	601[B]	-	-	0/6/10/10	0/4/4/4
2	FBP	D	602	-	-	2/13/32/32	0/1/1/1
6	I07	D	601[A]	-	-	0/6/10/10	0/4/4/4
3	PYR	C	602	4	-	0/4/4/4	-
6	I07	B	601[A]	-	-	0/6/10/10	0/4/4/4
3	PYR	A	602	4	-	0/4/4/4	-
2	FBP	A	601	-	-	5/13/32/32	0/1/1/1
2	FBP	B	602	-	-	3/13/32/32	0/1/1/1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	601[B]	I07	C7-N2	8.83	1.39	1.29
6	B	601[B]	I07	C7-N2	8.58	1.39	1.29
6	B	601[A]	I07	C7-N2	8.54	1.39	1.29
6	B	601[B]	I07	C-S	-8.50	1.57	1.72
6	D	601[A]	I07	C5-C7	-8.42	1.33	1.44
6	B	601[A]	I07	C5-C7	-8.37	1.33	1.44
6	B	601[B]	I07	C5-C7	-8.30	1.33	1.44
6	D	601[B]	I07	C5-C7	-8.14	1.33	1.44
6	D	601[A]	I07	C7-N2	8.00	1.38	1.29
6	D	601[A]	I07	C-S1	-7.83	1.68	1.80
6	B	601[A]	I07	C-S	-7.22	1.59	1.72
6	B	601[A]	I07	C8-C10	-6.55	1.39	1.51
6	D	601[A]	I07	C4-C6	-5.87	1.33	1.46
6	D	601[A]	I07	C8-C10	-5.83	1.41	1.51
6	D	601[B]	I07	C4-C6	-5.74	1.34	1.46
6	D	601[B]	I07	C-S1	-5.64	1.71	1.80
6	B	601[A]	I07	C4-C6	-5.59	1.34	1.46
6	D	601[B]	I07	C8-C10	-5.58	1.41	1.51
6	B	601[B]	I07	C8-C10	-5.35	1.41	1.51
6	B	601[B]	I07	C4-C6	-5.29	1.35	1.46
6	D	601[A]	I07	C-S	-4.99	1.63	1.72
6	B	601[B]	I07	C-S1	-4.97	1.72	1.80
6	B	601[A]	I07	C-S1	-4.97	1.72	1.80
3	C	602	PYR	O3-CA	4.48	1.33	1.23
6	D	601[B]	I07	C-S	-4.29	1.64	1.72
3	A	602	PYR	O3-CA	3.87	1.31	1.23
3	B	603	PYR	CA-C	-3.84	1.40	1.54
3	B	603	PYR	O3-CA	3.79	1.31	1.23
3	D	603	PYR	O-C	3.59	1.32	1.22
3	A	602	PYR	O-C	3.55	1.32	1.22
3	D	603	PYR	CA-C	-3.50	1.41	1.54
3	C	602	PYR	O-C	3.22	1.31	1.22
3	C	602	PYR	CA-C	-3.08	1.43	1.54
3	D	603	PYR	O3-CA	3.07	1.30	1.23
3	B	603	PYR	O-C	3.01	1.30	1.22
3	A	602	PYR	CA-C	-2.96	1.43	1.54
2	A	601	FBP	O2-C2	2.86	1.45	1.40
2	C	601	FBP	O2-C2	2.68	1.45	1.40
2	D	602	FBP	O2-C2	2.50	1.45	1.40
2	B	602	FBP	O2-C2	2.45	1.45	1.40
6	B	601[B]	I07	C6-N1	-2.34	1.34	1.37
6	D	601[B]	I07	C6-N1	-2.11	1.35	1.37



All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	601[B]	I07	C9-N-C4	7.21	132.39	124.49
6	D	601[B]	I07	C4-C6-N1	5.48	120.67	113.76
6	B	601[A]	I07	C9-N-C4	5.41	130.42	124.49
6	B	601[B]	I07	C4-C6-N1	5.32	120.46	113.76
6	D	601[A]	I07	C5-C7-N2	-5.18	119.06	125.87
6	B	601[A]	I07	C5-C7-N2	-5.13	119.12	125.87
6	B	601[A]	I07	C4-C6-N1	5.08	120.16	113.76
6	D	601[A]	I07	C4-C6-N1	4.90	119.94	113.76
6	B	601[B]	I07	C5-C7-N2	-4.85	119.50	125.87
6	D	601[B]	I07	C5-C7-N2	-4.75	119.62	125.87
3	A	602	PYR	OXT-C-O	-4.50	113.31	123.61
6	B	601[B]	I07	C8-N1-N2	4.39	119.76	114.40
6	D	601[A]	I07	C9-N-C4	4.35	129.26	124.49
6	D	601[B]	I07	C8-N1-N2	4.23	119.56	114.40
6	B	601[B]	I07	O-C6-N1	-4.22	117.17	120.69
2	C	601	FBP	P2-O6-C6	3.96	129.20	118.30
3	C	602	PYR	OXT-C-O	-3.93	114.62	123.61
3	D	603	PYR	OXT-C-CA	3.57	123.75	113.97
6	D	601[A]	I07	C10-C8-N1	-3.51	107.22	112.81
6	D	601[B]	I07	C10-C8-N1	-3.49	107.25	112.81
3	A	602	PYR	OXT-C-CA	3.46	123.43	113.97
2	D	602	FBP	P2-O6-C6	3.42	127.73	118.30
6	B	601[B]	I07	C10-C8-N1	-3.38	107.43	112.81
3	C	602	PYR	OXT-C-CA	3.35	123.12	113.97
2	A	601	FBP	O6-P2-O4P	3.31	115.77	106.47
6	D	601[A]	I07	C8-N1-N2	3.23	118.35	114.40
6	B	601[B]	I07	C9-N-C4	3.18	127.97	124.49
6	B	601[A]	I07	C8-N1-N2	3.00	118.06	114.40
3	A	602	PYR	O3-CA-CB	-2.97	113.15	119.73
6	D	601[A]	I07	O-C6-C4	-2.93	120.52	125.33
6	B	601[A]	I07	C17-O2-C12	-2.87	111.28	117.51
6	B	601[B]	I07	C2-C3-S	-2.84	108.17	111.84
6	B	601[A]	I07	O-C6-C4	-2.80	120.73	125.33
6	D	601[B]	I07	O-C6-C4	-2.74	120.83	125.33
6	D	601[B]	I07	O-C6-N1	-2.63	118.50	120.69
6	D	601[B]	I07	C17-O2-C12	-2.53	112.02	117.51
6	D	601[A]	I07	C7-N2-N1	2.39	119.04	117.12
6	D	601[B]	I07	C2-C3-S	-2.36	108.79	111.84
6	B	601[A]	I07	C2-C3-S	-2.34	108.82	111.84
6	B	601[A]	I07	C10-C8-N1	-2.33	109.09	112.81
2	C	601	FBP	O6P-P2-O6	2.20	112.58	106.73
2	D	602	FBP	O2P-P1-O1	2.19	112.56	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	PYR	OXT-C-CA	2.16	119.88	113.97
6	B	601[A]	I07	C7-N2-N1	2.16	118.86	117.12
3	B	603	PYR	OXT-C-O	-2.15	118.69	123.61
6	B	601[B]	I07	C7-N2-N1	2.09	118.80	117.12

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FBP	C1-O1-P1-O2P
2	A	601	FBP	C1-O1-P1-O3P
2	A	601	FBP	C4-C5-C6-O6
2	B	602	FBP	C1-O1-P1-O3P
2	B	602	FBP	C4-C5-C6-O6
2	C	601	FBP	C1-O1-P1-O1P
2	C	601	FBP	C1-O1-P1-O3P
2	C	601	FBP	O5-C5-C6-O6
2	C	601	FBP	C6-O6-P2-O4P
2	C	601	FBP	C6-O6-P2-O5P
2	C	601	FBP	C6-O6-P2-O6P
2	D	602	FBP	C4-C5-C6-O6
2	C	601	FBP	C4-C5-C6-O6
2	D	602	FBP	O5-C5-C6-O6
2	A	601	FBP	O5-C5-C6-O6
2	B	602	FBP	O5-C5-C6-O6
2	A	601	FBP	C1-O1-P1-O1P
2	C	601	FBP	C1-O1-P1-O2P

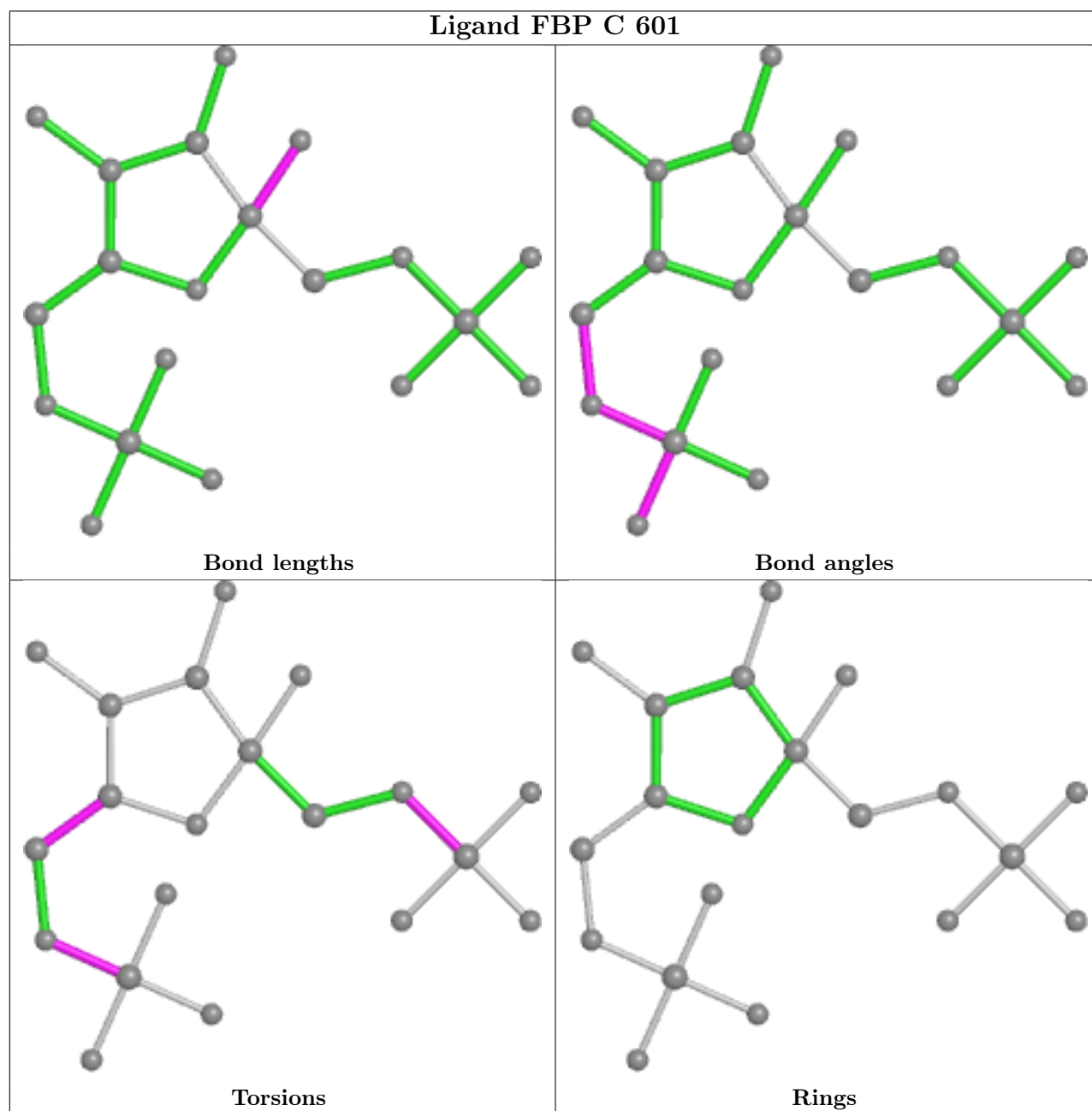
There are no ring outliers.

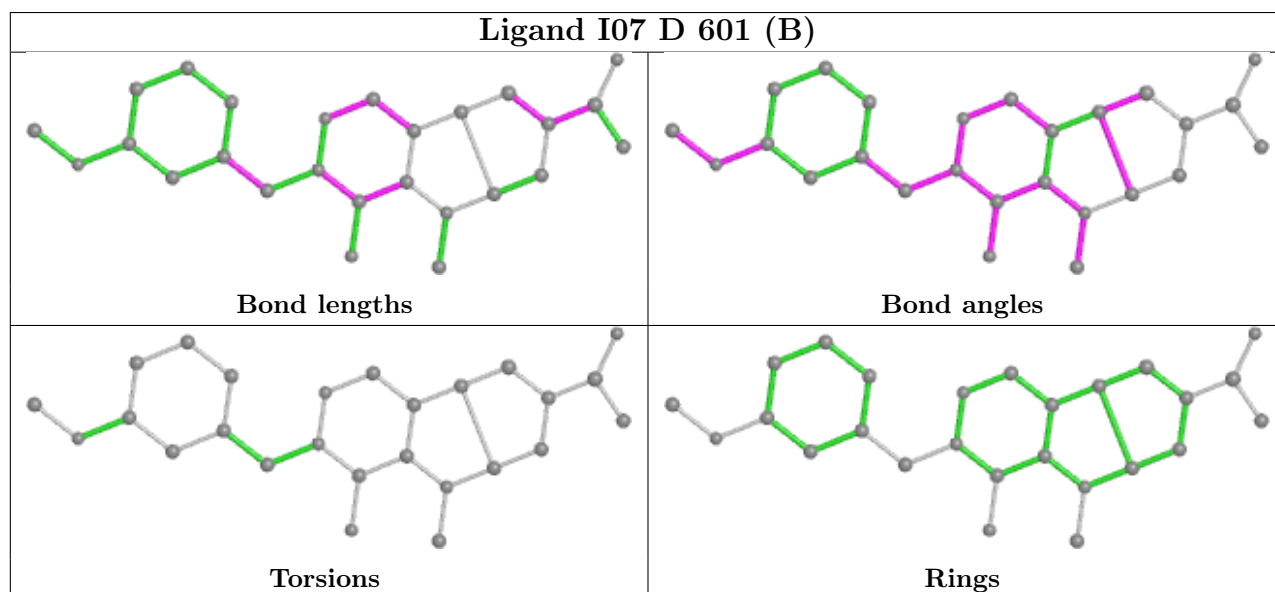
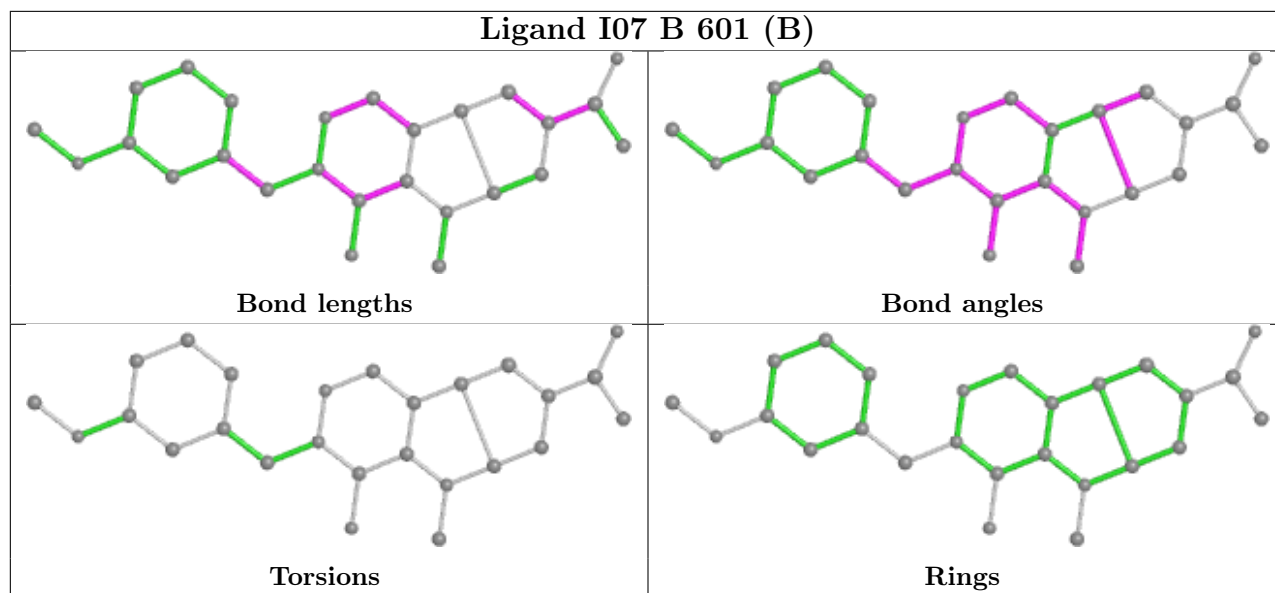
3 monomers are involved in 5 short contacts:

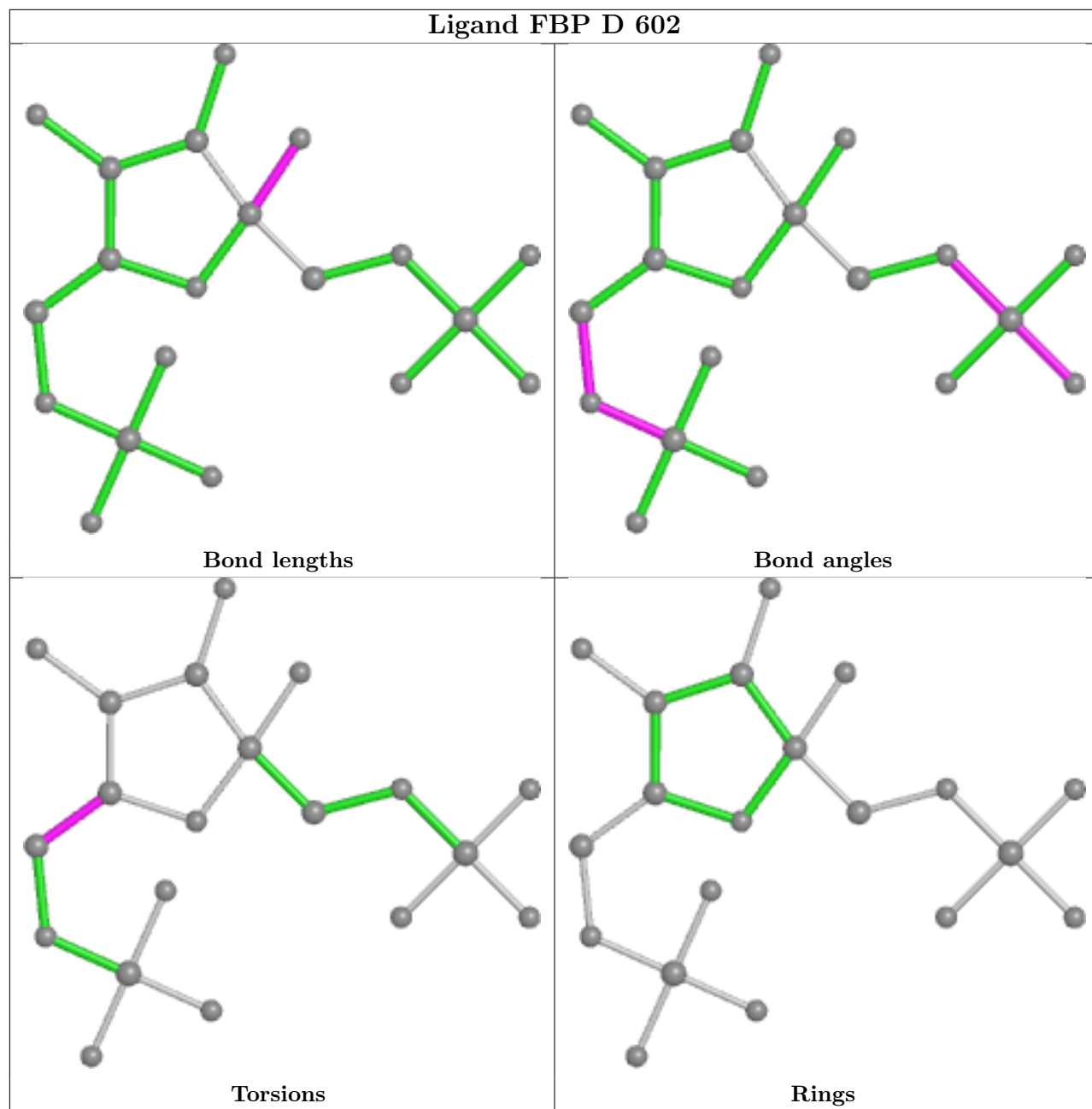
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	FBP	2	0
3	D	603	PYR	2	0
6	D	601[B]	I07	1	0

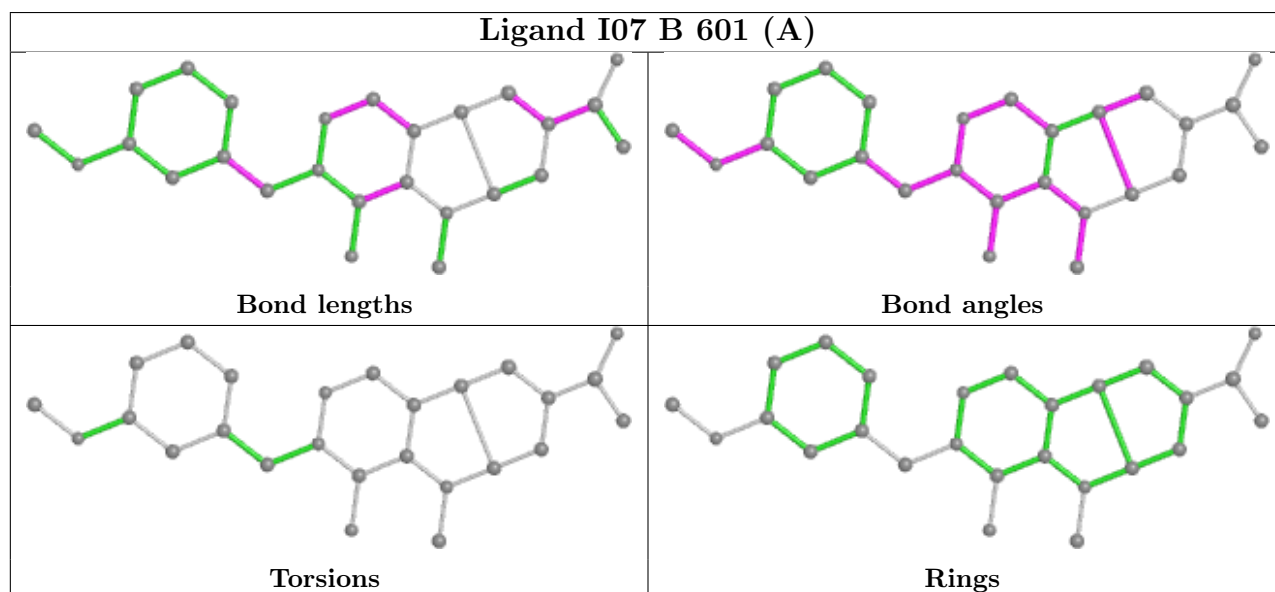
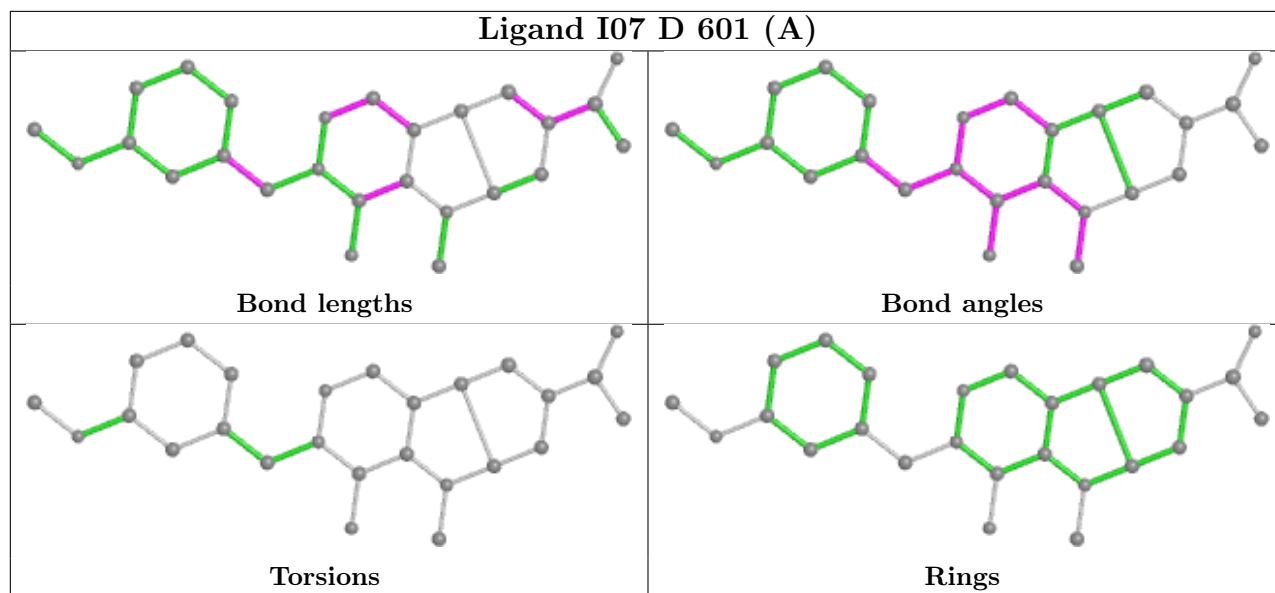
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

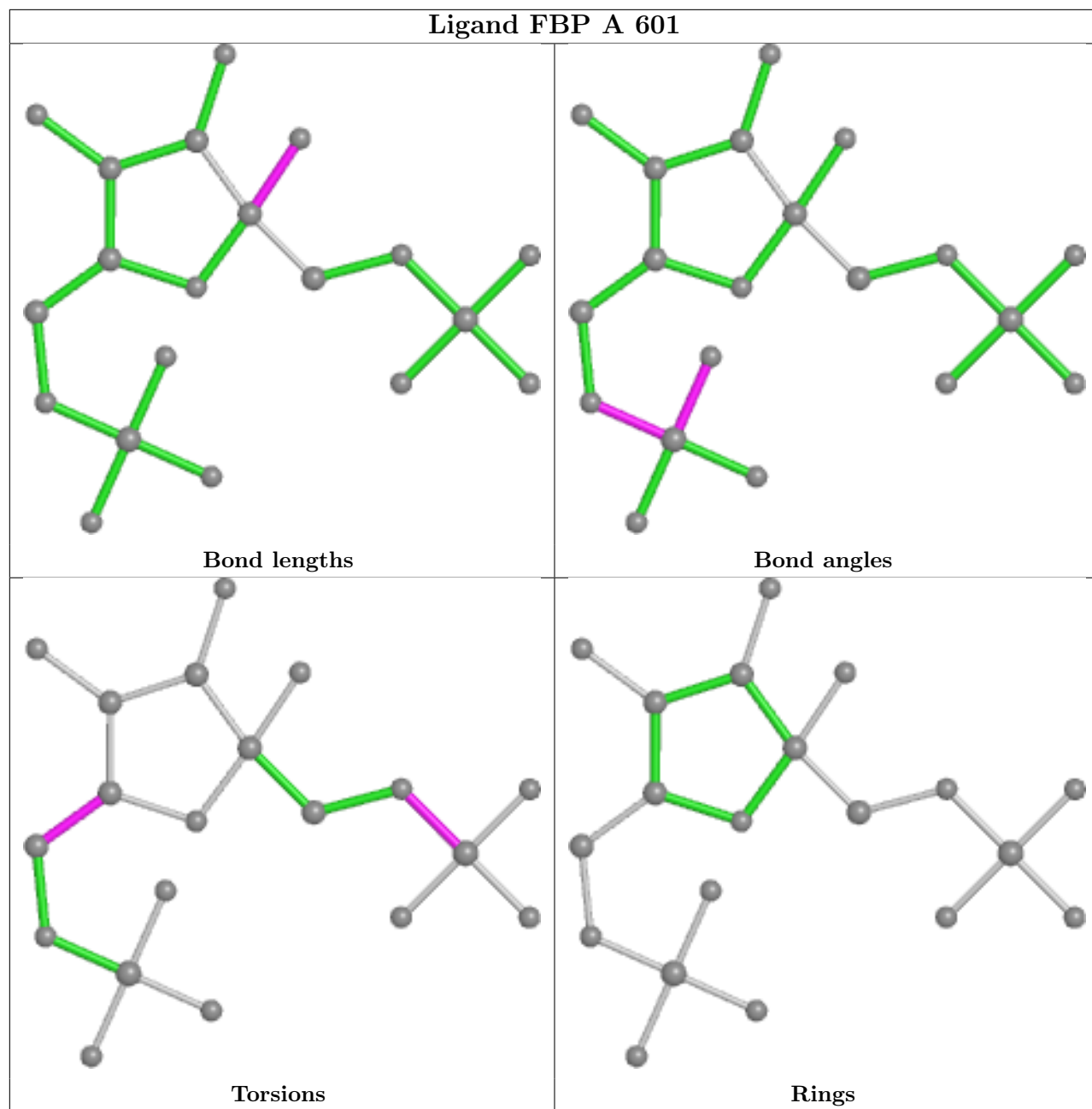
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.

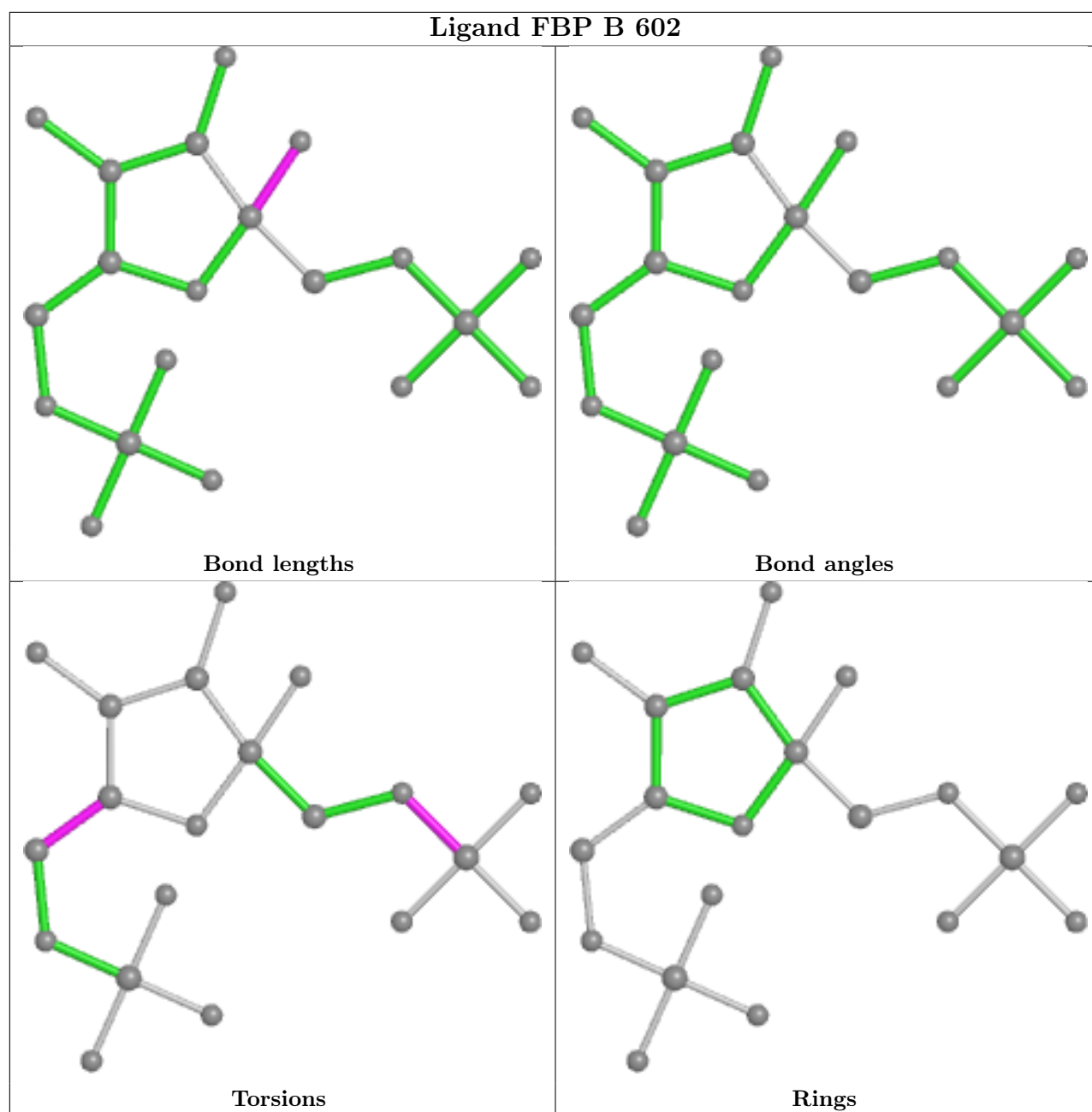












## 5.7 Other polymers [i](#)

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

### 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, 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	514/544 (94%)	0.21	26 (5%) 28 39	34, 49, 95, 119	0
1	B	518/544 (95%)	0.20	16 (3%) 49 59	32, 51, 84, 123	0
1	C	503/544 (92%)	0.41	36 (7%) 15 22	35, 55, 97, 141	0
1	D	512/544 (94%)	0.08	26 (5%) 28 39	31, 47, 92, 119	0
All	All	2047/2176 (94%)	0.22	104 (5%) 28 39	31, 51, 93, 141	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	ILE	7.7
1	B	171	PRO	5.8
1	A	230	LYS	5.5
1	D	230	LYS	5.4
1	B	170	GLY	5.2
1	D	193	THR	5.1
1	A	57	GLN	4.9
1	C	260	ASP	4.9
1	A	166	ILE	4.8
1	C	230	LYS	4.8
1	A	167	LEU	4.8
1	C	166	ILE	4.7
1	C	266	GLU	4.6
1	A	65	MET	4.5
1	D	194	ARG	4.4
1	C	262	PRO	4.2
1	B	191	PHE	4.2
1	C	270	ARG	4.2
1	D	166	ILE	4.2
1	D	231	ILE	4.2
1	D	190	ALA	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	213	VAL	4.0
1	D	165	GLY	4.0
1	C	306	HIS	3.9
1	A	176	GLU	3.8
1	A	213	VAL	3.8
1	C	574	SER	3.7
1	C	57	GLN	3.7
1	C	233	PRO	3.6
1	D	191	PHE	3.6
1	A	245	VAL	3.6
1	D	229	GLN	3.5
1	D	83	VAL	3.3
1	C	213	VAL	3.3
1	C	232	GLY	3.2
1	D	58	GLN	3.1
1	C	399	ALA	3.1
1	A	229	GLN	3.0
1	A	173	SER	3.0
1	B	168	GLN	3.0
1	A	231	ILE	2.9
1	D	65	MET	2.9
1	B	180	GLY	2.8
1	B	172	GLU	2.8
1	C	173	SER	2.8
1	D	174	GLU	2.7
1	A	263	GLY	2.7
1	D	212	PRO	2.7
1	D	256	GLY	2.7
1	B	57	GLN	2.7
1	C	237	VAL	2.7
1	C	184	LEU	2.7
1	B	182	GLN	2.6
1	A	179	LYS	2.6
1	C	178	VAL	2.5
1	D	233	PRO	2.5
1	C	257	ALA	2.5
1	D	214	GLY	2.5
1	C	185	VAL	2.4
1	D	189	PRO	2.4
1	D	192	ARG	2.4
1	D	236	LEU	2.4
1	C	258	GLN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	172	GLU	2.4
1	C	245	VAL	2.4
1	C	273	ARG	2.4
1	D	176	GLU	2.4
1	A	368	VAL	2.4
1	A	367	VAL	2.4
1	C	524	ILE	2.3
1	A	399	ALA	2.3
1	A	246	LEU	2.3
1	C	199	THR	2.3
1	A	174	GLU	2.3
1	C	302	GLY	2.3
1	B	187	VAL	2.3
1	A	232	GLY	2.2
1	C	177	LEU	2.2
1	D	187	VAL	2.2
1	A	402	ILE	2.2
1	D	368	VAL	2.2
1	B	84	ALA	2.2
1	D	523	ALA	2.2
1	C	196	ASN	2.2
1	A	180	GLY	2.2
1	B	169	GLY	2.2
1	B	209	ARG	2.2
1	A	58	GLN	2.1
1	A	182	GLN	2.1
1	C	269	VAL	2.1
1	A	284	PHE	2.1
1	A	237	VAL	2.1
1	C	294	VAL	2.1
1	C	336	ALA	2.1
1	B	305	GLY	2.1
1	B	174	GLU	2.0
1	B	289	ARG	2.0
1	C	311	ILE	2.0
1	D	114	ILE	2.0
1	C	84	ALA	2.0
1	C	263	GLY	2.0
1	C	176	GLU	2.0
1	C	58	GLN	2.0
1	B	306	HIS	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](#)

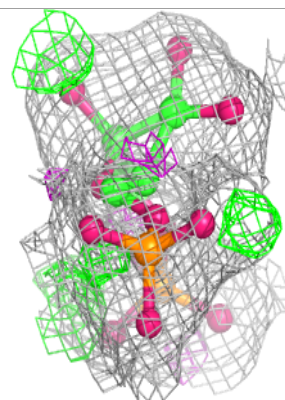
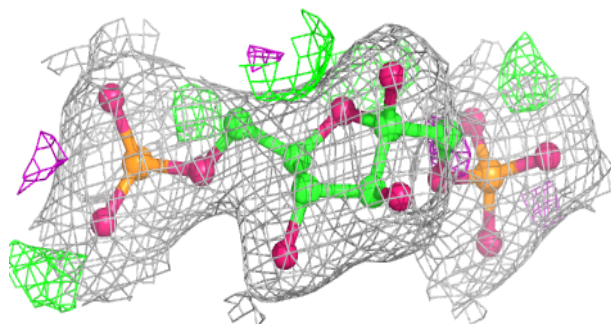
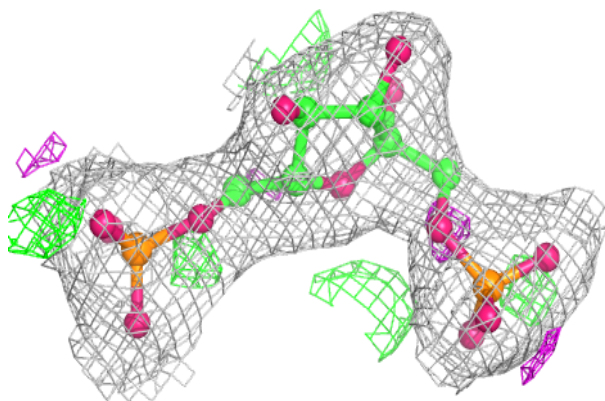
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
4	MN	B	604	1/1	0.78	0.51	163,163,163,163	0
5	K	C	604	1/1	0.87	0.11	73,73,73,73	0
3	PYR	B	603	6/6	0.91	0.29	51,65,85,120	0
4	MN	A	603	1/1	0.93	0.42	98,98,98,98	0
3	PYR	C	602	6/6	0.94	0.23	51,53,65,66	0
3	PYR	A	602	6/6	0.94	0.20	44,48,51,58	0
2	FBP	C	601	20/20	0.95	0.11	43,47,54,58	0
5	K	D	605	1/1	0.96	0.07	51,51,51,51	0
6	I07	B	601[A]	26/26	0.96	0.17	39,45,47,51	26
6	I07	B	601[B]	26/26	0.96	0.17	42,45,47,49	26
6	I07	D	601[A]	26/26	0.96	0.18	43,47,50,52	26
6	I07	D	601[B]	26/26	0.96	0.18	44,47,49,54	26
3	PYR	D	603	6/6	0.97	0.18	36,48,54,72	0
2	FBP	A	601	20/20	0.97	0.09	44,50,60,61	0
2	FBP	B	602	20/20	0.97	0.10	43,47,55,56	0
4	MN	C	603	1/1	0.97	0.13	57,57,57,57	0
4	MN	D	604	1/1	0.97	0.24	72,72,72,72	0
5	K	B	605	1/1	0.97	0.08	55,55,55,55	0
5	K	A	604	1/1	0.98	0.06	54,54,54,54	0
2	FBP	D	602	20/20	0.98	0.09	37,46,48,50	0

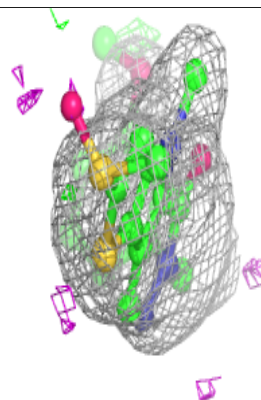
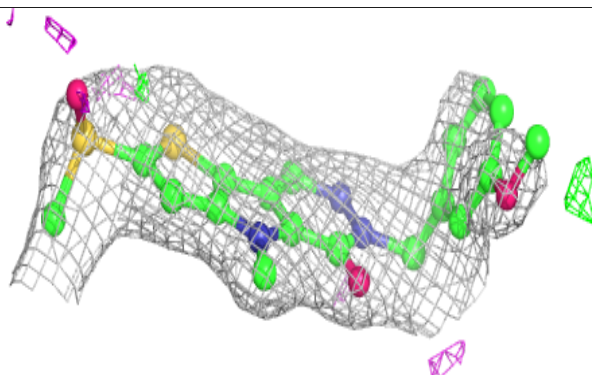
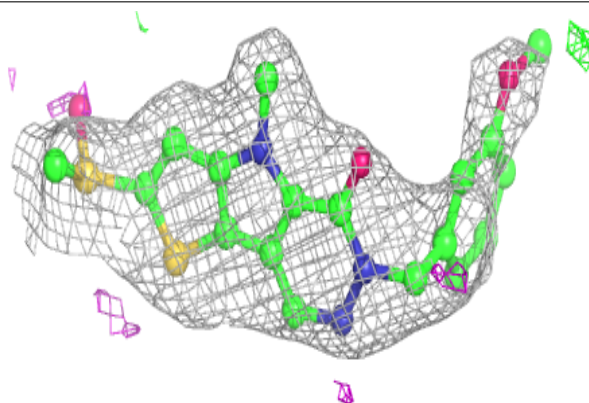
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

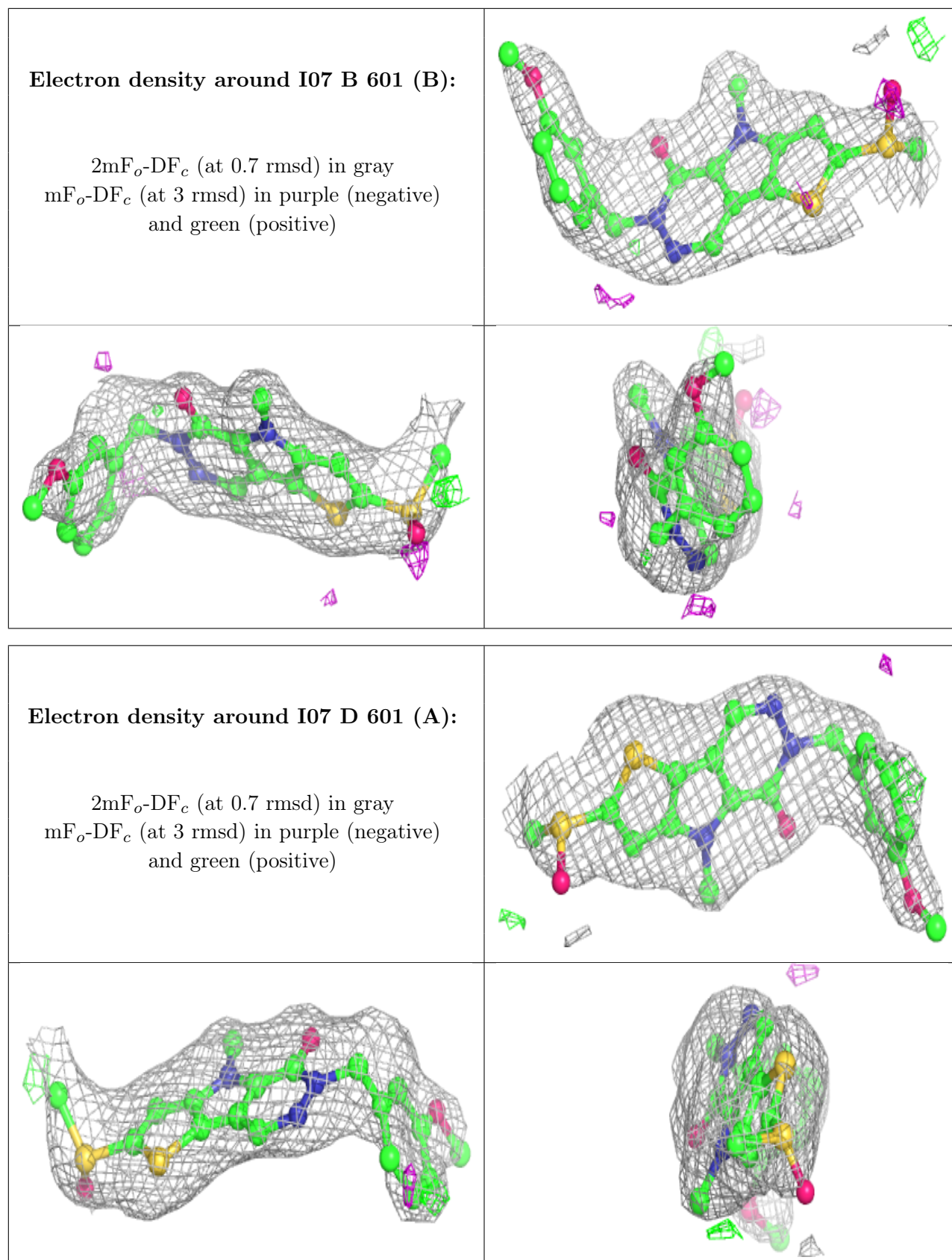
**Electron density around FBP C 601:**

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

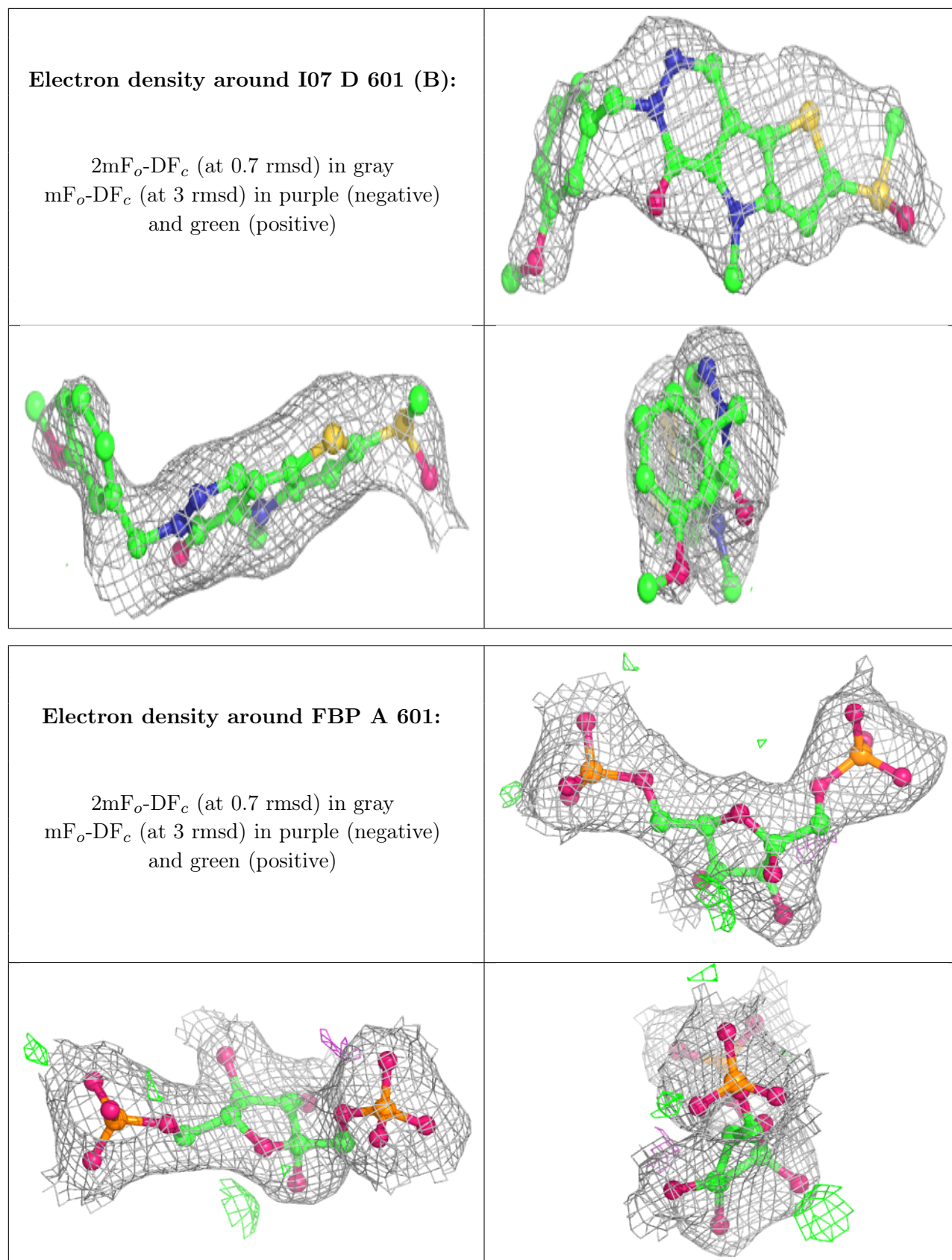
**Electron density around I07 B 601 (A):**

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



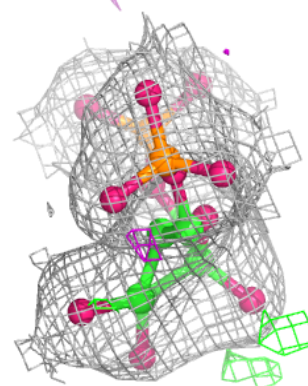
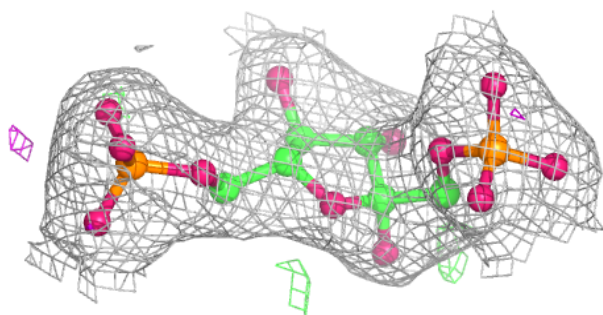
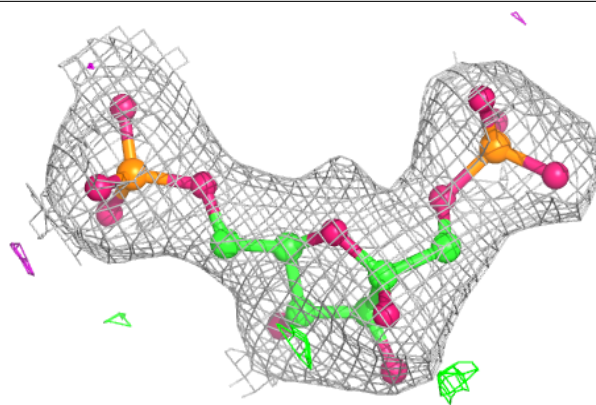




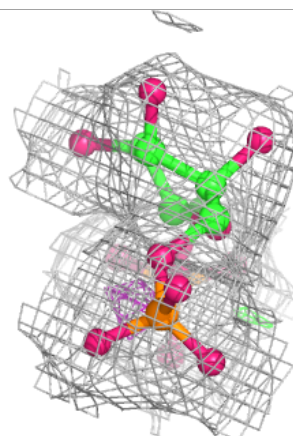
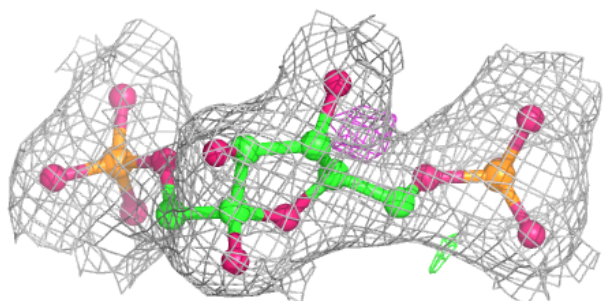
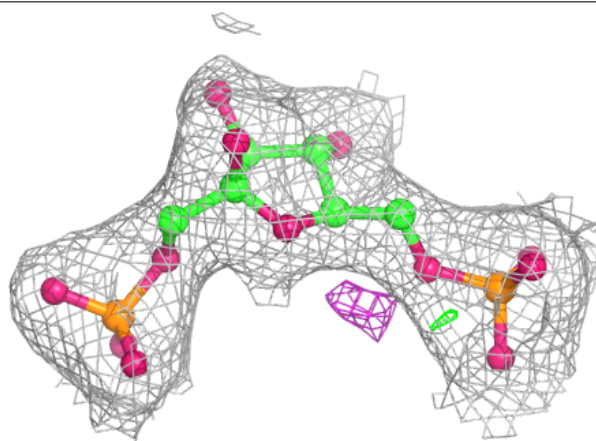


**Electron density around FBP B 602:**

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

**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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.