



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:50 am BST

PDB ID : 6MXX  
Title : Structure of 53BP1 tandem Tudor domains in complex with small molecule UNC2991  
Authors : Cui, G.; Botuyan, M.V.; Mer, G.  
Deposited on : 2018-10-31  
Resolution : 2.30 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.

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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 : 2.11  
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) : 2.11

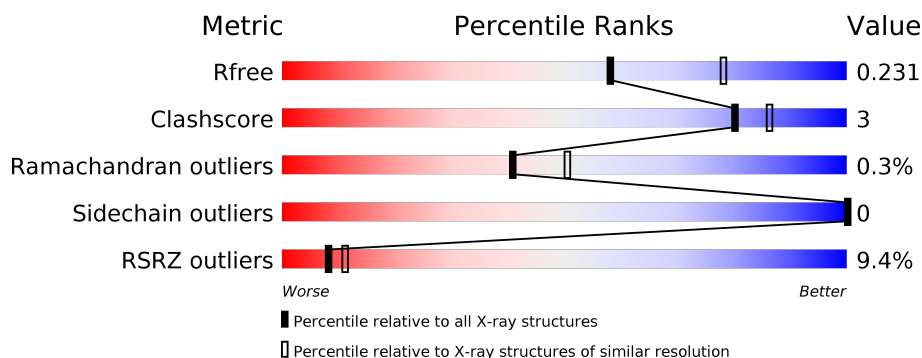
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on 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	123	<div> <div>3%</div> <div>91%</div> <div>7%</div> </div>
1	B	123	<div> <div>7%</div> <div>88%</div> <div>9%</div> </div>
1	C	123	<div> <div>7%</div> <div>93%</div> <div>5%</div> </div>
1	D	123	<div> <div>8%</div> <div>88%</div> <div>10%</div> </div>
1	E	123	<div> <div>14%</div> <div>89%</div> <div>9%</div> </div>
1	F	123	<div> <div>7%</div> <div>91%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	123	
1	H	123	
1	I	123	
1	J	123	

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
2	PO4	B	1703	-	-	-	X
2	PO4	C	1702	-	-	-	X
2	PO4	D	1703	-	-	-	X
2	PO4	E	1702	-	-	-	X
3	K6P	B	1701[A]	-	-	-	X
3	K6P	B	1701[B]	-	-	-	X
3	K6P	J	1701[A]	-	-	-	X
3	K6P	J	1701[B]	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 20865 atoms, of which 10103 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 TP53-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	120	Total	C	H	N	O	S	6	13	0
			2051	659	1021	174	194	3			
1	B	119	Total	C	H	N	O	S	11	7	0
			1968	637	978	165	185	3			
1	C	121	Total	C	H	N	O	S	10	14	0
			2066	667	1026	175	195	3			
1	D	120	Total	C	H	N	O	S	11	13	0
			2045	659	1019	171	193	3			
1	E	120	Total	C	H	N	O	S	12	6	0
			1944	627	965	163	186	3			
1	F	120	Total	C	H	N	O	S	19	14	0
			2066	662	1031	176	193	4			
1	G	119	Total	C	H	N	O	S	21	13	0
			1974	644	966	165	195	4			
1	H	119	Total	C	H	N	O	S	8	10	0
			1993	643	990	167	188	5			
1	I	118	Total	C	H	N	O	S	16	2	0
			1831	596	901	157	174	3			
1	J	120	Total	C	H	N	O	S	23	10	0
			2005	648	992	170	192	3			

There are 30 discrepancies between the modelled and reference sequences:

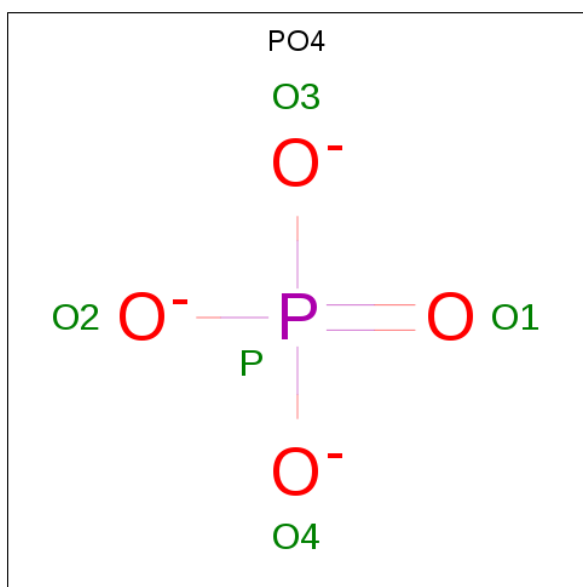
Chain	Residue	Modelled	Actual	Comment	Reference
A	1481	GLY	-	expression tag	UNP Q12888
A	1482	HIS	-	expression tag	UNP Q12888
A	1483	MET	-	expression tag	UNP Q12888
B	1481	GLY	-	expression tag	UNP Q12888
B	1482	HIS	-	expression tag	UNP Q12888
B	1483	MET	-	expression tag	UNP Q12888
C	1481	GLY	-	expression tag	UNP Q12888
C	1482	HIS	-	expression tag	UNP Q12888
C	1483	MET	-	expression tag	UNP Q12888

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1481	GLY	-	expression tag	UNP Q12888
D	1482	HIS	-	expression tag	UNP Q12888
D	1483	MET	-	expression tag	UNP Q12888
E	1481	GLY	-	expression tag	UNP Q12888
E	1482	HIS	-	expression tag	UNP Q12888
E	1483	MET	-	expression tag	UNP Q12888
F	1481	GLY	-	expression tag	UNP Q12888
F	1482	HIS	-	expression tag	UNP Q12888
F	1483	MET	-	expression tag	UNP Q12888
G	1481	GLY	-	expression tag	UNP Q12888
G	1482	HIS	-	expression tag	UNP Q12888
G	1483	MET	-	expression tag	UNP Q12888
H	1481	GLY	-	expression tag	UNP Q12888
H	1482	HIS	-	expression tag	UNP Q12888
H	1483	MET	-	expression tag	UNP Q12888
I	1481	GLY	-	expression tag	UNP Q12888
I	1482	HIS	-	expression tag	UNP Q12888
I	1483	MET	-	expression tag	UNP Q12888
J	1481	GLY	-	expression tag	UNP Q12888
J	1482	HIS	-	expression tag	UNP Q12888
J	1483	MET	-	expression tag	UNP Q12888

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



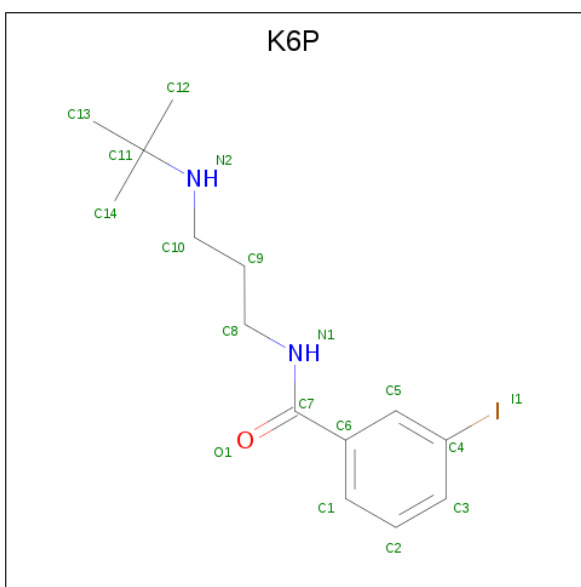
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

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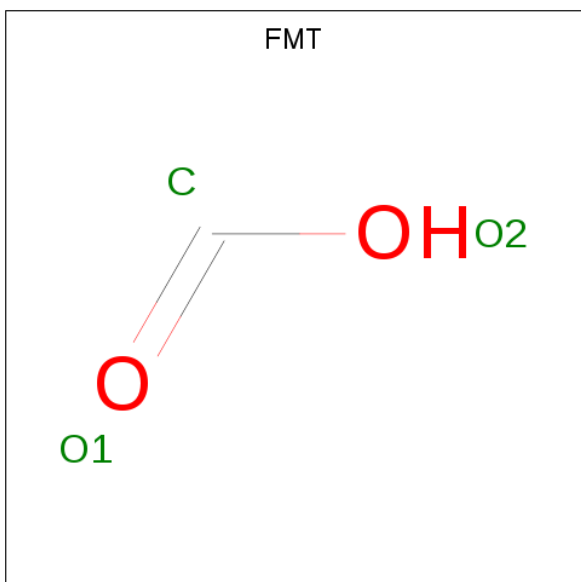
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is N-[3-(tert-butylamino)propyl]-3-iodobenzamide (three-letter code: K6P) (formula: C<sub>14</sub>H<sub>21</sub>IN<sub>2</sub>O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total 78	C 28	H 42	I 2	N 4	O 2	0	1
3	C	1	Total 78	C 28	H 42	I 2	N 4	O 2	0	1
3	E	1	Total 78	C 28	H 42	I 2	N 4	O 2	0	1
3	G	1	Total 78	C 28	H 42	I 2	N 4	O 2	0	1
3	J	1	Total 78	C 28	H 42	I 2	N 4	O 2	0	1

- Molecule 4 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

- Molecule 5 is water.

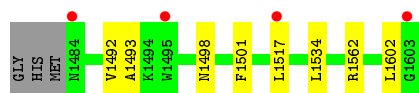
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	57	Total O 57 57	0	0
5	B	46	Total O 46 46	0	0
5	C	49	Total O 49 49	0	0
5	D	49	Total O 49 49	0	0
5	E	36	Total O 36 36	0	0
5	F	44	Total O 44 44	0	0
5	G	27	Total O 27 27	0	0
5	H	43	Total O 43 43	0	0
5	I	29	Total O 29 29	0	0
5	J	31	Total O 31 31	0	0



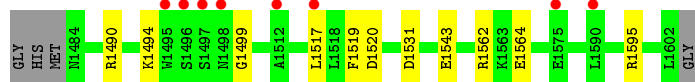
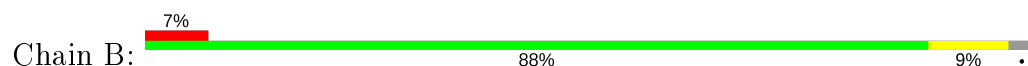
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

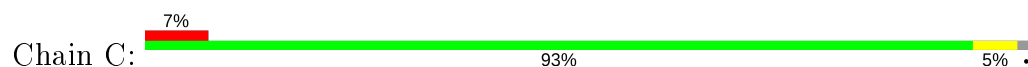
- Molecule 1: TP53-binding protein 1



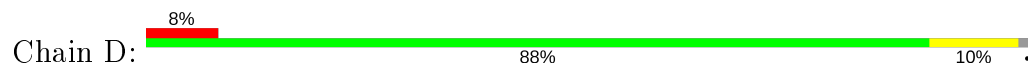
- Molecule 1: TP53-binding protein 1



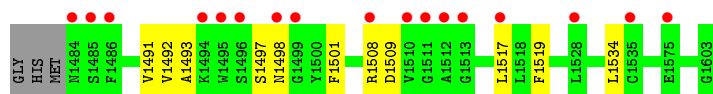
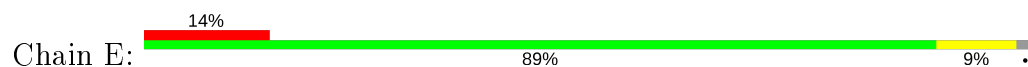
- Molecule 1: TP53-binding protein 1



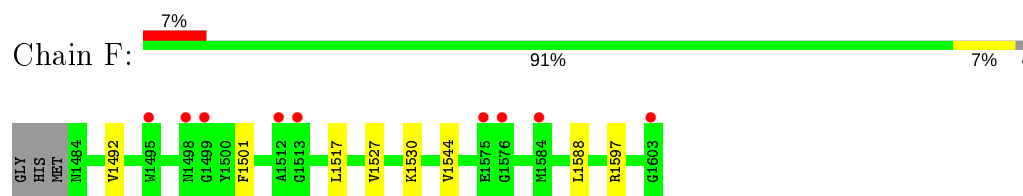
- Molecule 1: TP53-binding protein 1



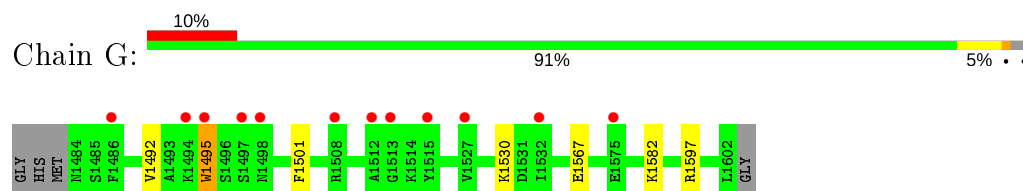
- Molecule 1: TP53-binding protein 1



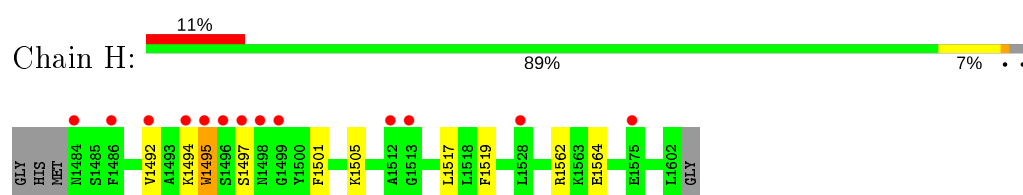
- Molecule 1: TP53-binding protein 1



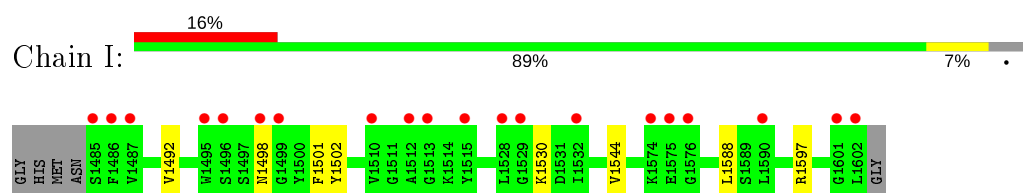
- Molecule 1: TP53-binding protein 1



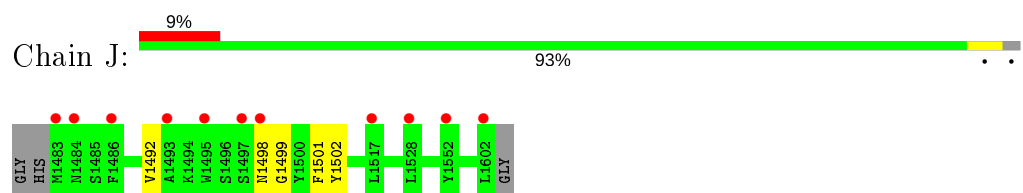
- Molecule 1: TP53-binding protein 1



- Molecule 1: TP53-binding protein 1



- Molecule 1: TP53-binding protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.94Å 159.43Å 181.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.30 48.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.14-2.30) 97.5 (48.14-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.45 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, $R_{free}$	0.206 , 0.232 0.206 , 0.231	Depositor DCC
$R_{free}$ test set	2000 reflections (2.29%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20865	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, PO4, K6P

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	0.26	0/1075	0.45	0/1444
1	B	0.25	0/1022	0.45	0/1375
1	C	0.28	0/1093	0.46	0/1472
1	D	0.26	0/1082	0.45	0/1454
1	E	0.25	0/1025	0.44	0/1378
1	F	0.25	0/1088	0.45	0/1460
1	G	0.25	0/1064	0.44	0/1436
1	H	0.25	0/1046	0.45	0/1409
1	I	0.25	0/954	0.44	0/1285
1	J	0.25	0/1055	0.43	0/1420
All	All	0.26	0/10504	0.45	0/14133

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 ⓘ

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	1030	1021	999	6	0
1	B	990	978	971	6	0
1	C	1040	1026	1004	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1026	1019	999	9	0
1	E	979	965	943	6	0
1	F	1035	1031	1003	5	0
1	G	1008	966	946	5	0
1	H	1003	990	978	6	0
1	I	930	901	898	5	0
1	J	1013	992	970	3	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	20	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
3	B	36	42	0	0	0
3	C	36	42	0	1	0
3	E	36	42	0	0	0
3	G	36	42	0	0	0
3	J	36	42	0	0	0
4	B	3	1	1	0	0
4	H	9	3	3	0	0
5	A	57	0	0	1	0
5	B	46	0	0	0	0
5	C	49	0	0	0	0
5	D	49	0	0	0	0
5	E	36	0	0	0	0
5	F	44	0	0	0	0
5	G	27	0	0	0	0
5	H	43	0	0	0	0
5	I	29	0	0	0	0
5	J	31	0	0	0	0
All	All	10762	10103	9715	55	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 3.

All (55) 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:G:1567:GLU:OE1	1:G:1582:LYS:NZ	2.27	0.68
1:H:1562:ARG:NH1	1:H:1564:GLU:OE2	2.27	0.67
1:I:1530:LYS:O	1:I:1597:ARG:NH1	2.30	0.65
1:A:1534[B]:LEU:HD11	1:A:1602:LEU:HD21	1.79	0.64
1:J:1492:VAL:HG12	1:J:1501:PHE:HB3	1.81	0.63
1:E:1492:VAL:HG12	1:E:1501:PHE:HB3	1.81	0.63
1:F:1492:VAL:HG12	1:F:1501:PHE:HB3	1.82	0.61
1:A:1492:VAL:HG12	1:A:1501:PHE:HB3	1.82	0.61
1:J:1498[A]:ASN:OD1	1:J:1499[A]:GLY:N	2.33	0.61
1:G:1492:VAL:HG12	1:G:1501:PHE:HB3	1.83	0.61
1:F:1530:LYS:O	1:F:1597:ARG:NH1	2.37	0.58
1:B:1490:ARG:NH2	1:B:1520:ASP:OD1	2.37	0.58
1:I:1492:VAL:HG22	1:I:1501:PHE:HB3	1.85	0.58
1:H:1492:VAL:HG12	1:H:1501:PHE:HB3	1.87	0.57
1:D:1505:LYS:O	1:D:1517[B]:LEU:HD12	2.06	0.56
1:B:1517[B]:LEU:HD23	1:B:1519:PHE:CZ	2.44	0.53
1:C:1517[B]:LEU:HD23	1:C:1519:PHE:CZ	2.44	0.52
1:G:1495[B]:TRP:HA	1:G:1495[B]:TRP:CE3	2.47	0.49
1:J:1498[A]:ASN:ND2	1:J:1502:TYR:OH	2.44	0.49
1:D:1517[A]:LEU:HD12	1:D:1527:VAL:HG21	1.95	0.48
1:A:1534[B]:LEU:CD1	1:A:1602:LEU:HD21	2.44	0.48
1:E:1497:SER:OG	1:E:1498:ASN:N	2.46	0.47
1:D:1517[B]:LEU:HD23	1:D:1519:PHE:CZ	2.50	0.46
1:A:1562:ARG:NH1	5:A:1803:HOH:O	2.48	0.46
1:B:1543:GLU:OE1	1:B:1595:ARG:NH1	2.47	0.46
1:F:1544:VAL:HG12	1:F:1588:LEU:CD2	2.46	0.46
1:B:1562:ARG:NH2	1:B:1564:GLU:OE2	2.50	0.45
1:G:1495[B]:TRP:HA	1:G:1495[B]:TRP:HE3	1.81	0.44
1:H:1505:LYS:O	1:H:1517[B]:LEU:HD12	2.17	0.44
1:D:1492[B]:VAL:HG22	1:D:1501:PHE:HB3	1.99	0.44
1:F:1544:VAL:HG12	1:F:1588:LEU:HD21	1.99	0.44
1:I:1498:ASN:ND2	1:I:1502:TYR:OH	2.51	0.44
1:D:1492[A]:VAL:HG12	1:D:1501:PHE:HB3	1.99	0.43
1:D:1493[B]:ALA:HB3	1:D:1517[B]:LEU:CD2	2.49	0.43
1:H:1494[B]:LYS:O	1:H:1495[B]:TRP:O	2.37	0.43
1:B:1494[B]:LYS:NZ	1:B:1499:GLY:O	2.46	0.43
1:C:1521:ASP:HB3	3:C:1701[A]:K6P:C4	2.49	0.42
1:E:1493:ALA:HB3	1:E:1517[A]:LEU:CD2	2.49	0.42
1:B:1494[B]:LYS:HB3	1:B:1531:ASP:HB3	2.01	0.42
1:E:1491:VAL:HG12	1:E:1534:LEU:HD12	2.00	0.42
1:D:1491:VAL:HG12	1:D:1534:LEU:HD12	2.02	0.42
1:H:1517[B]:LEU:HD23	1:H:1519:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1594:ASN:OD1	1:D:1597:ARG:NH2	2.47	0.41
1:I:1492:VAL:O	1:I:1492:VAL:HG13	2.19	0.41
1:E:1508[A]:ARG:HD3	1:E:1509:ASP:N	2.35	0.41
1:I:1544:VAL:HG12	1:I:1588:LEU:HD21	2.01	0.41
1:F:1517[A]:LEU:HD12	1:F:1527:VAL:HG21	2.02	0.41
1:A:1493[B]:ALA:HB3	1:A:1517[B]:LEU:CD2	2.50	0.41
1:G:1530:LYS:O	1:G:1597:ARG:NH1	2.54	0.40
1:C:1493[B]:ALA:HB3	1:C:1517[B]:LEU:CD2	2.52	0.40
1:C:1527[B]:VAL:HG23	1:C:1532:ILE:HD11	2.04	0.40
1:E:1517[A]:LEU:HD23	1:E:1519:PHE:CZ	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	131/123 (106%)	128 (98%)	3 (2%)	0	100	100
1	B	124/123 (101%)	120 (97%)	4 (3%)	0	100	100
1	C	133/123 (108%)	131 (98%)	2 (2%)	0	100	100
1	D	131/123 (106%)	120 (92%)	9 (7%)	2 (2%)	10	10
1	E	124/123 (101%)	119 (96%)	5 (4%)	0	100	100
1	F	132/123 (107%)	127 (96%)	5 (4%)	0	100	100
1	G	130/123 (106%)	122 (94%)	6 (5%)	2 (2%)	10	10
1	H	127/123 (103%)	120 (94%)	5 (4%)	2 (2%)	9	9
1	I	118/123 (96%)	114 (97%)	4 (3%)	0	100	100
1	J	128/123 (104%)	122 (95%)	6 (5%)	0	100	100
All	All	1278/1230 (104%)	1223 (96%)	49 (4%)	6 (0%)	41	35

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	1495[A]	TRP
1	H	1495[B]	TRP
1	G	1495[A]	TRP
1	G	1495[B]	TRP
1	D	1499[A]	GLY
1	D	1499[B]	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/103 (107%)	110 (100%)	0	100	100
1	B	104/103 (101%)	104 (100%)	0	100	100
1	C	112/103 (109%)	112 (100%)	0	100	100
1	D	109/103 (106%)	109 (100%)	0	100	100
1	E	104/103 (101%)	104 (100%)	0	100	100
1	F	110/103 (107%)	110 (100%)	0	100	100
1	G	106/103 (103%)	106 (100%)	0	100	100
1	H	108/103 (105%)	108 (100%)	0	100	100
1	I	94/103 (91%)	94 (100%)	0	100	100
1	J	107/103 (104%)	107 (100%)	0	100	100
All	All	1064/1030 (103%)	1064 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

35 ligands are modelled in this entry.

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	PO4	H	1704	-	4,4,4	0.92	0	6,6,6	0.43	0
3	K6P	J	1701[B]	-	18,18,18	0.18	0	23,24,24	0.34	0
3	K6P	J	1701[A]	-	18,18,18	0.18	0	23,24,24	0.45	0
3	K6P	C	1701[B]	-	18,18,18	0.17	0	23,24,24	0.34	0
4	FMT	H	1701	-	0,2,2	0.00	-	0,1,1	0.00	-
3	K6P	B	1701[B]	-	18,18,18	0.17	0	23,24,24	0.39	0
2	PO4	E	1703	-	4,4,4	0.91	0	6,6,6	0.43	0
3	K6P	B	1701[A]	-	18,18,18	0.19	0	23,24,24	0.45	0
3	K6P	C	1701[A]	-	18,18,18	0.20	0	23,24,24	0.58	0
2	PO4	I	1702	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	G	1702	-	4,4,4	0.93	0	6,6,6	0.41	0
2	PO4	C	1702	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	F	1702	-	4,4,4	0.92	0	6,6,6	0.42	0
2	PO4	D	1704	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	D	1703	-	4,4,4	0.92	0	6,6,6	0.45	0
2	PO4	B	1704	-	4,4,4	0.94	0	6,6,6	0.42	0
2	PO4	J	1702	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	I	1701	-	4,4,4	0.92	0	6,6,6	0.43	0
3	K6P	E	1701[A]	-	18,18,18	0.18	0	23,24,24	0.46	0
2	PO4	G	1703	-	4,4,4	0.92	0	6,6,6	0.43	0
3	K6P	E	1701[B]	-	18,18,18	0.18	0	23,24,24	0.35	0
3	K6P	G	1701[B]	-	18,18,18	0.18	0	23,24,24	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	K6P	G	1701[A]	-	18,18,18	0.17	0	23,24,24	0.45	0
4	FMT	H	1702	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PO4	A	1701	-	4,4,4	0.90	0	6,6,6	0.43	0
2	PO4	E	1702	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	J	1703	-	4,4,4	0.93	0	6,6,6	0.45	0
4	FMT	B	1702	-	0,2,2	0.00	-	0,1,1	0.00	-
2	PO4	B	1703	-	4,4,4	0.94	0	6,6,6	0.42	0
2	PO4	H	1705	-	4,4,4	0.95	0	6,6,6	0.44	0
2	PO4	C	1703	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	D	1701	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	F	1701	-	4,4,4	0.91	0	6,6,6	0.43	0
2	PO4	D	1702	-	4,4,4	0.92	0	6,6,6	0.43	0
4	FMT	H	1703	-	0,2,2	0.00	-	0,1,1	0.00	-

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
3	K6P	J	1701[B]	-	-	0/13/13/13	0/1/1/1
3	K6P	G	1701[B]	-	-	0/13/13/13	0/1/1/1
3	K6P	J	1701[A]	-	-	3/13/13/13	0/1/1/1
3	K6P	C	1701[B]	-	-	2/13/13/13	0/1/1/1
3	K6P	B	1701[B]	-	-	2/13/13/13	0/1/1/1
3	K6P	G	1701[A]	-	-	0/13/13/13	0/1/1/1
3	K6P	B	1701[A]	-	-	2/13/13/13	0/1/1/1
3	K6P	E	1701[A]	-	-	0/13/13/13	0/1/1/1
3	K6P	C	1701[A]	-	-	3/13/13/13	0/1/1/1
3	K6P	E	1701[B]	-	-	0/13/13/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	J	1701[A]	K6P	C6-C7-N1-C8
3	J	1701[A]	K6P	O1-C7-N1-C8
3	B	1701[A]	K6P	C6-C7-N1-C8

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Mol	Chain	Res	Type	Atoms
3	B	1701[A]	K6P	O1-C7-N1-C8
3	C	1701[A]	K6P	C6-C7-N1-C8
3	C	1701[A]	K6P	O1-C7-N1-C8
3	C	1701[A]	K6P	N1-C8-C9-C10
3	B	1701[B]	K6P	O1-C7-N1-C8
3	B	1701[B]	K6P	C6-C7-N1-C8
3	C	1701[B]	K6P	O1-C7-N1-C8
3	C	1701[B]	K6P	C6-C7-N1-C8
3	J	1701[A]	K6P	N1-C8-C9-C10

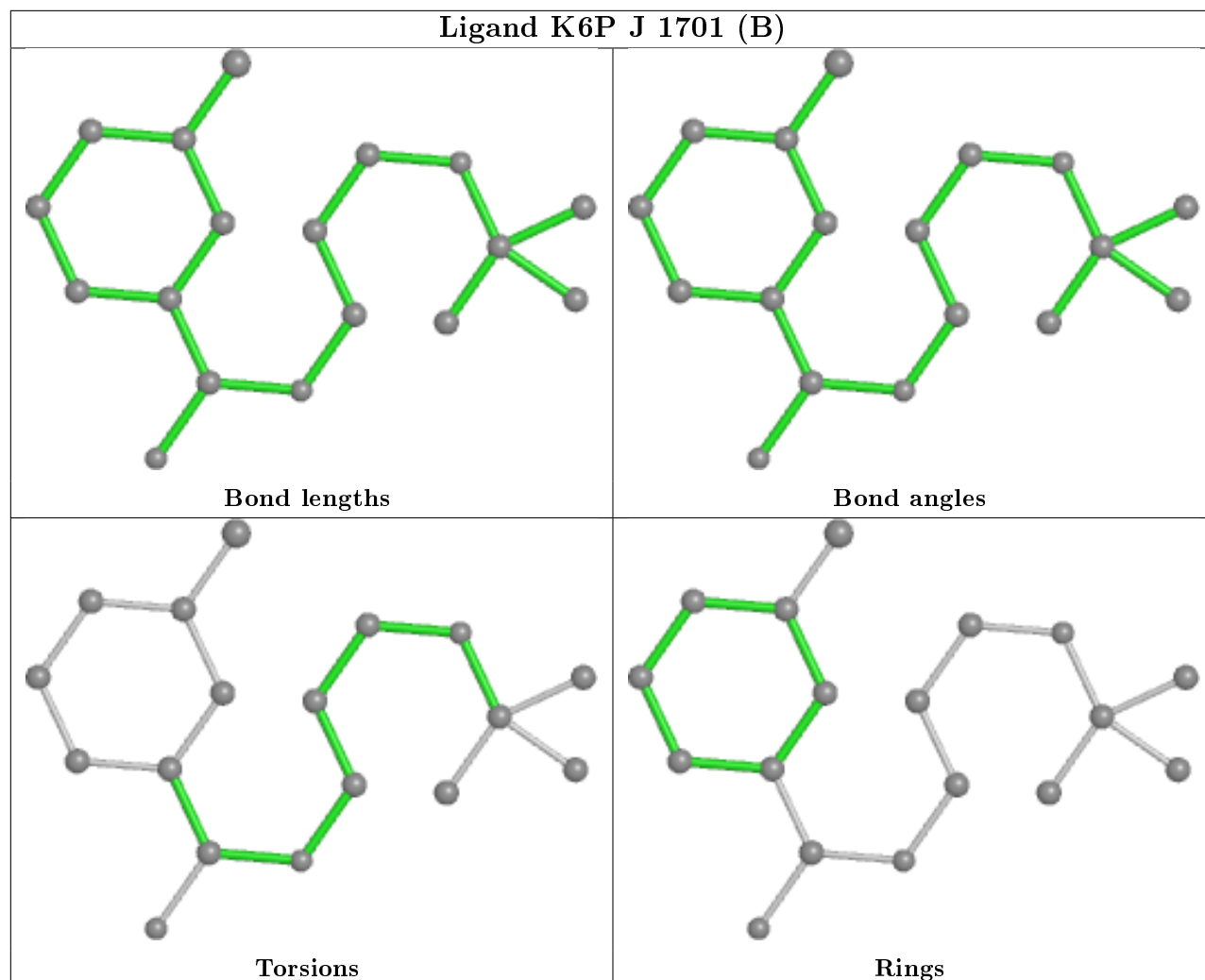
There are no ring outliers.

1 monomer is involved in 1 short contact:

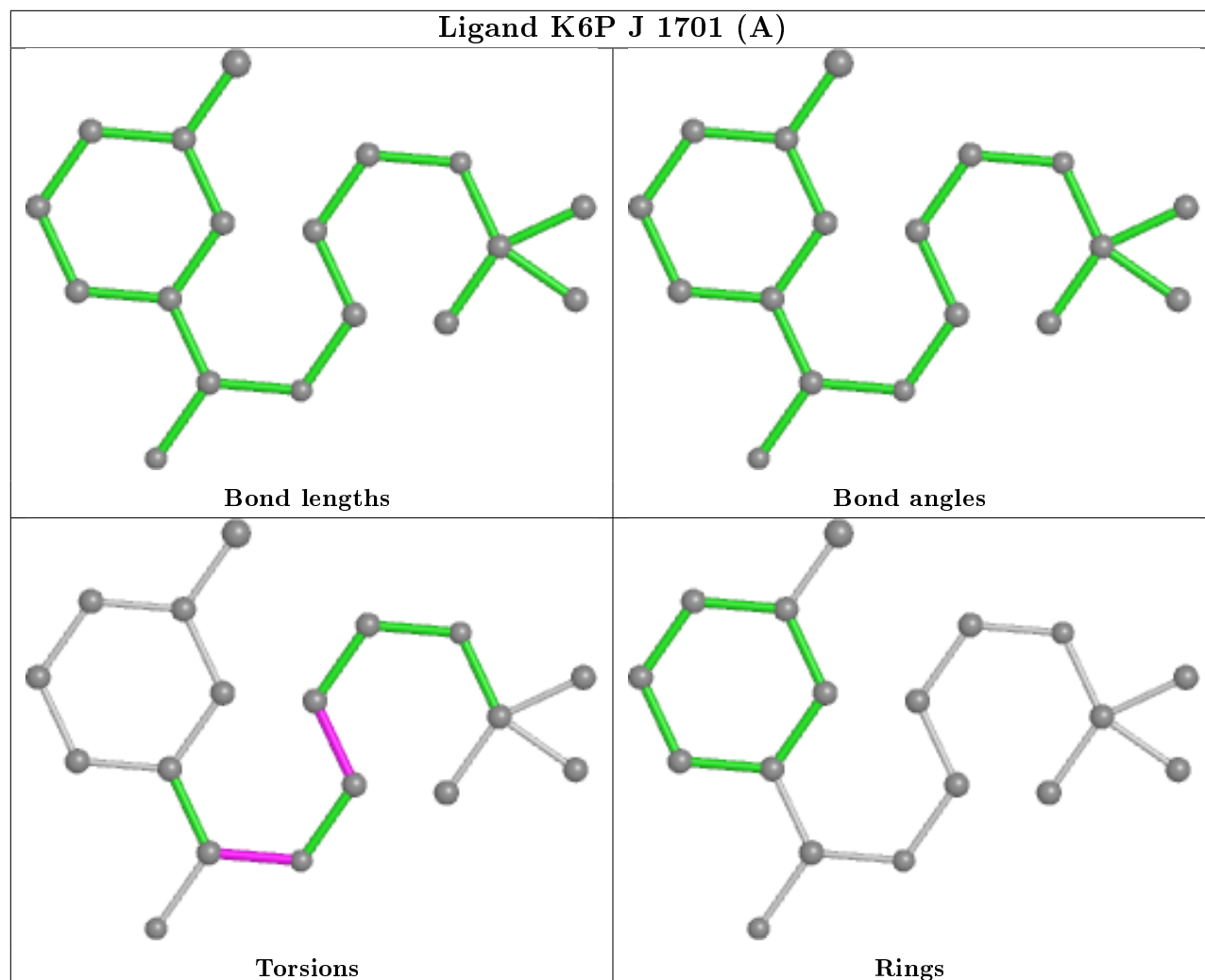
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1701[A]	K6P	1	0

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.

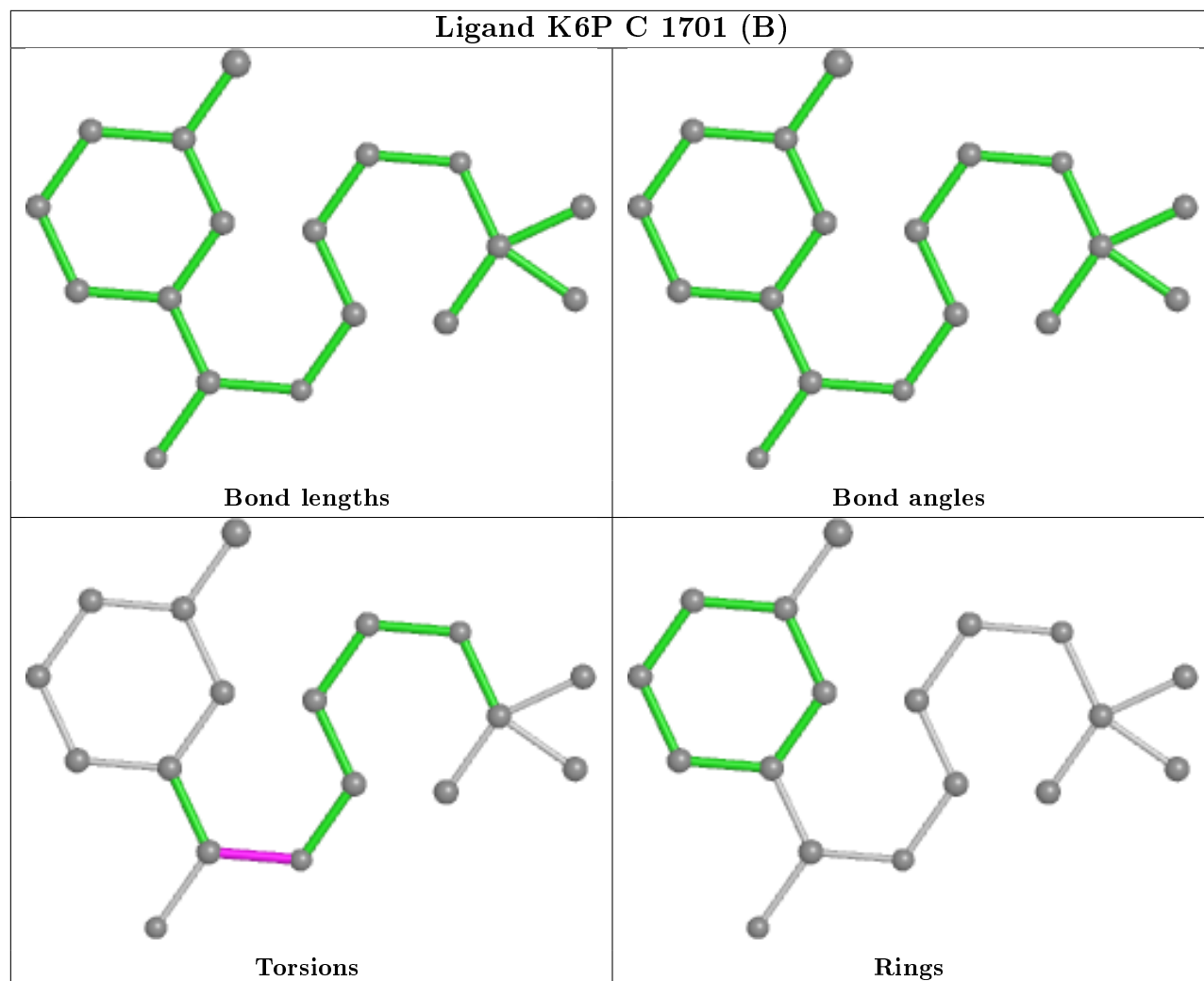
## Ligand K6P J 1701 (B)



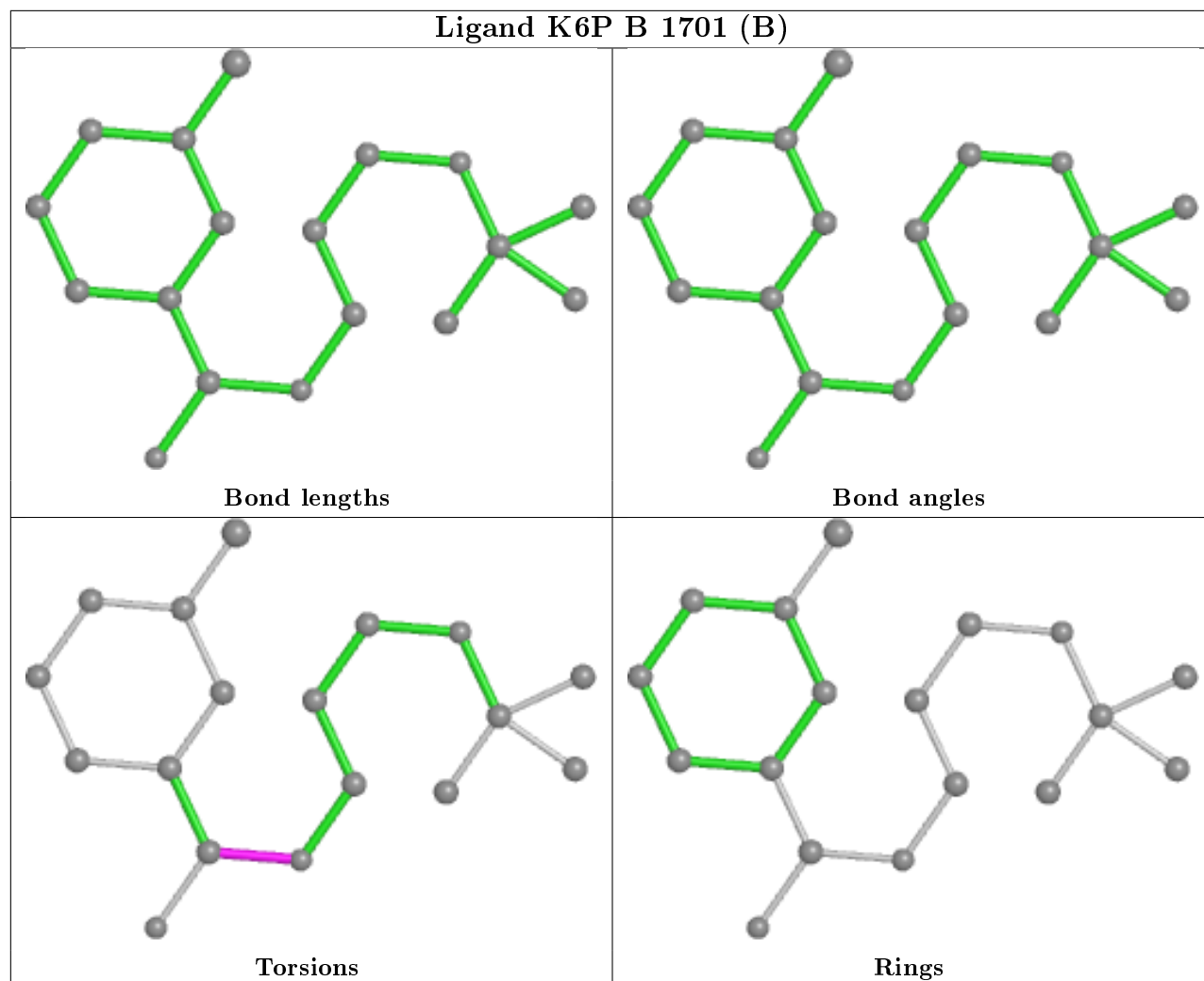
## Ligand K6P J 1701 (A)



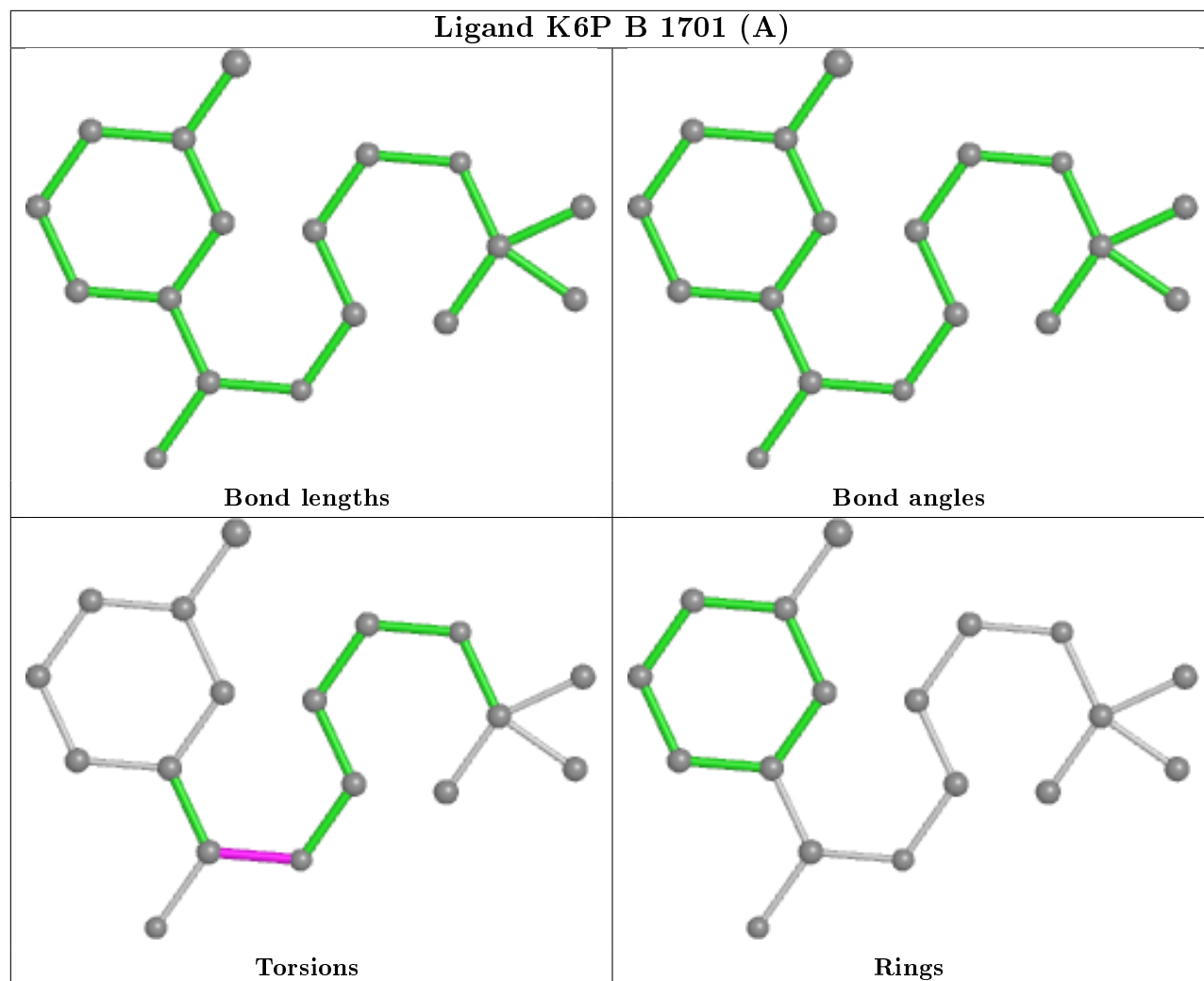
## Ligand K6P C 1701 (B)



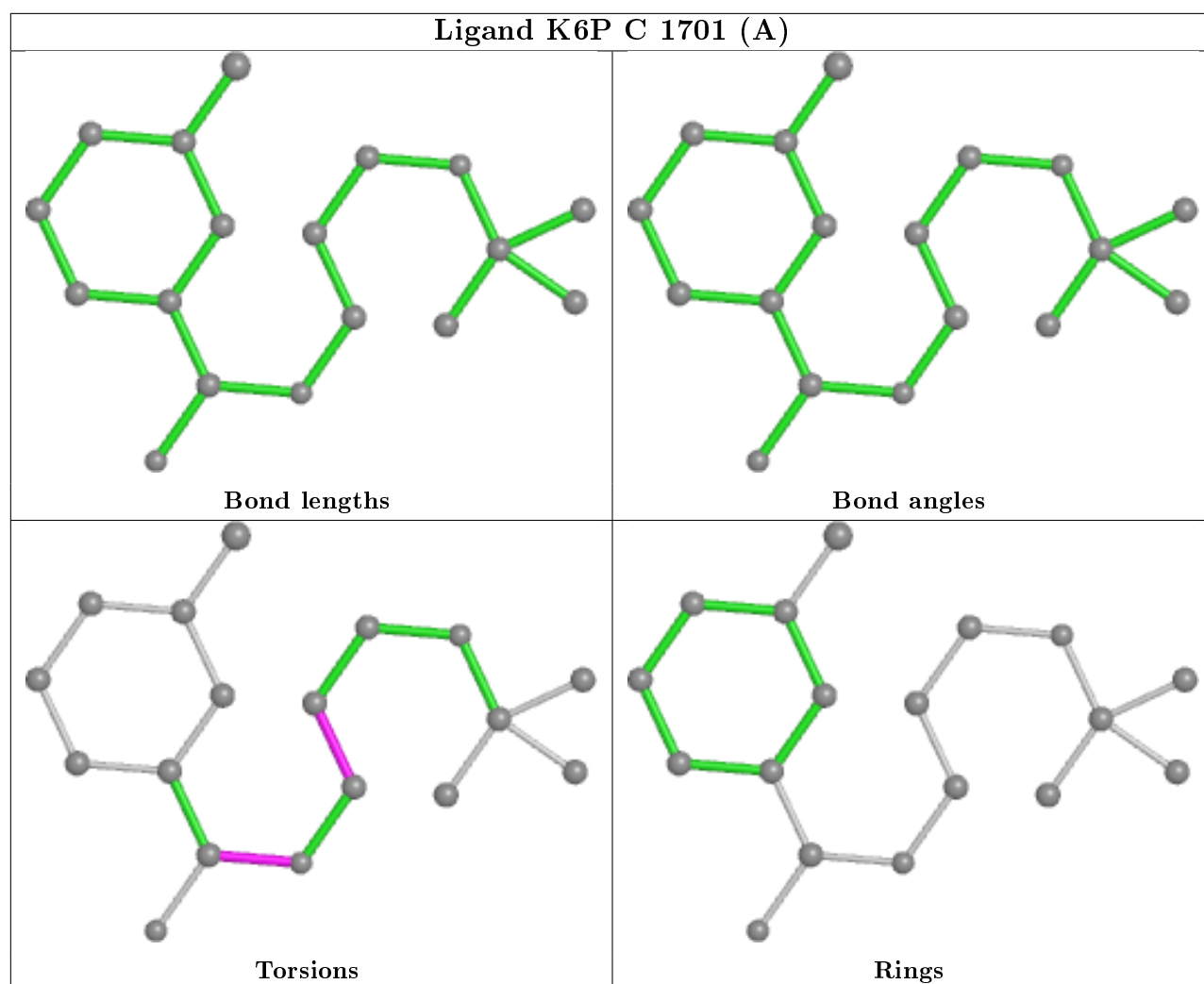
## Ligand K6P B 1701 (B)



## Ligand K6P B 1701 (A)







## 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	120/123 (97%)	0.40	4 (3%)	46 53	30, 44, 60, 132	2 (1%)
1	B	119/123 (96%)	0.47	8 (6%)	17 23	35, 49, 74, 101	3 (2%)
1	C	121/123 (98%)	0.53	8 (6%)	18 23	31, 47, 82, 139	1 (0%)
1	D	120/123 (97%)	0.53	10 (8%)	11 15	34, 51, 78, 101	2 (1%)
1	E	120/123 (97%)	0.68	17 (14%)	2 3	34, 51, 93, 115	3 (2%)
1	F	120/123 (97%)	0.43	9 (7%)	14 19	34, 50, 71, 108	5 (4%)
1	G	119/123 (96%)	0.70	12 (10%)	7 9	37, 56, 98, 121	5 (4%)
1	H	119/123 (96%)	0.54	13 (10%)	5 8	37, 53, 85, 123	2 (1%)
1	I	118/123 (95%)	0.90	20 (16%)	1 2	44, 67, 98, 135	3 (2%)
1	J	120/123 (97%)	0.53	11 (9%)	9 12	38, 56, 86, 129	5 (4%)
All	All	1196/1230 (97%)	0.57	112 (9%)	8 11	30, 52, 88, 139	31 (2%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	1484	ASN	6.1
1	I	1512	ALA	6.1
1	A	1603	GLY	6.0
1	H	1499	GLY	5.4
1	G	1495[A]	TRP	5.1
1	C	1495[A]	TRP	5.1
1	D	1603	GLY	5.0
1	E	1485	SER	5.0
1	G	1512	ALA	4.8
1	B	1498[A]	ASN	4.6
1	I	1602	LEU	4.6
1	G	1513	GLY	4.3
1	D	1499[A]	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	1482	HIS	4.1
1	F	1499[A]	GLY	4.0
1	E	1484	ASN	3.9
1	F	1603	GLY	3.9
1	F	1512	ALA	3.8
1	I	1529	GLY	3.7
1	I	1532	ILE	3.7
1	B	1497[A]	SER	3.7
1	I	1513	GLY	3.7
1	E	1511	GLY	3.6
1	E	1513	GLY	3.6
1	I	1528	LEU	3.5
1	I	1575	GLU	3.5
1	I	1510	VAL	3.5
1	G	1497[A]	SER	3.5
1	J	1528	LEU	3.4
1	J	1483	MET	3.4
1	E	1495	TRP	3.4
1	J	1495[A]	TRP	3.3
1	E	1512	ALA	3.3
1	G	1532	ILE	3.3
1	F	1498[A]	ASN	3.3
1	G	1494[A]	LYS	3.3
1	I	1486	PHE	3.3
1	J	1602	LEU	3.2
1	D	1498[A]	ASN	3.2
1	G	1498[A]	ASN	3.2
1	H	1495[A]	TRP	3.1
1	E	1575	GLU	3.0
1	E	1510	VAL	3.0
1	G	1527	VAL	3.0
1	I	1576	GLY	3.0
1	C	1512	ALA	3.0
1	B	1495[A]	TRP	2.9
1	C	1510	VAL	2.9
1	E	1486	PHE	2.9
1	D	1495[A]	TRP	2.9
1	G	1486	PHE	2.8
1	A	1484	ASN	2.8
1	G	1575[A]	GLU	2.8
1	I	1495	TRP	2.8
1	H	1498[A]	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	1496[A]	SER	2.8
1	H	1497[A]	SER	2.8
1	H	1575	GLU	2.8
1	G	1515	TYR	2.7
1	I	1485	SER	2.7
1	H	1513	GLY	2.7
1	I	1498	ASN	2.7
1	H	1528	LEU	2.7
1	J	1493[A]	ALA	2.7
1	D	1497[A]	SER	2.6
1	C	1497[A]	SER	2.6
1	A	1495[A]	TRP	2.6
1	I	1515	TYR	2.5
1	E	1494	LYS	2.5
1	H	1494[A]	LYS	2.4
1	B	1496[A]	SER	2.4
1	D	1496[A]	SER	2.4
1	I	1496	SER	2.4
1	B	1512	ALA	2.4
1	E	1508[A]	ARG	2.4
1	E	1528	LEU	2.4
1	I	1574	LYS	2.3
1	E	1499	GLY	2.3
1	I	1499	GLY	2.3
1	I	1601	GLY	2.3
1	H	1512	ALA	2.3
1	D	1574	LYS	2.3
1	E	1517[A]	LEU	2.3
1	I	1487	VAL	2.3
1	D	1492[A]	VAL	2.3
1	H	1486	PHE	2.3
1	A	1517[A]	LEU	2.3
1	E	1535	CYS	2.3
1	J	1552	TYR	2.3
1	C	1484	ASN	2.2
1	C	1517[A]	LEU	2.2
1	E	1498	ASN	2.2
1	E	1496	SER	2.2
1	J	1486	PHE	2.2
1	F	1495[A]	TRP	2.2
1	F	1576	GLY	2.2
1	I	1590	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	1517[A]	LEU	2.2
1	F	1584[A]	MET	2.2
1	B	1517[A]	LEU	2.1
1	J	1498[A]	ASN	2.1
1	F	1575	GLU	2.1
1	F	1513	GLY	2.1
1	H	1484	ASN	2.1
1	H	1492	VAL	2.1
1	C	1591	GLU	2.1
1	D	1517[A]	LEU	2.1
1	J	1497[A]	SER	2.0
1	G	1508	ARG	2.0
1	D	1494[A]	LYS	2.0
1	B	1590	LEU	2.0
1	B	1575	GLU	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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
2	PO4	D	1703	5/5	0.64	0.43	139,139,140,141	0
2	PO4	G	1703	5/5	0.67	0.29	141,142,143,143	0
2	PO4	I	1702	5/5	0.68	0.29	144,145,145,145	0
2	PO4	E	1702	5/5	0.68	0.84	260,260,261,262	0
2	PO4	B	1703	5/5	0.72	0.52	152,153,154,155	0
2	PO4	C	1702	5/5	0.75	0.47	173,173,174,175	0
3	K6P	J	1701[B]	18/18	0.76	0.52	149,183,212,212	39
3	K6P	J	1701[A]	18/18	0.76	0.52	148,183,203,205	39

*Continued on next page...*

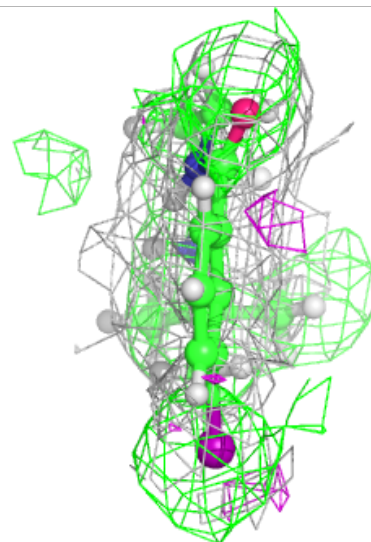
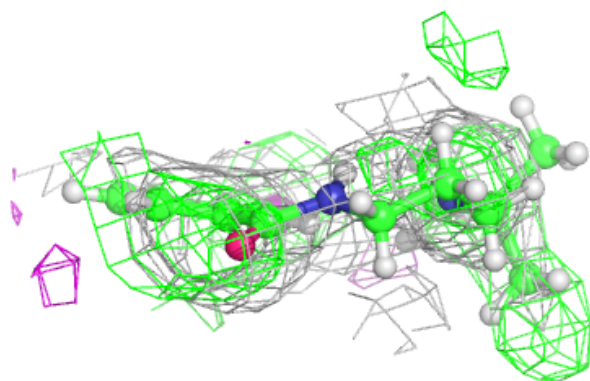
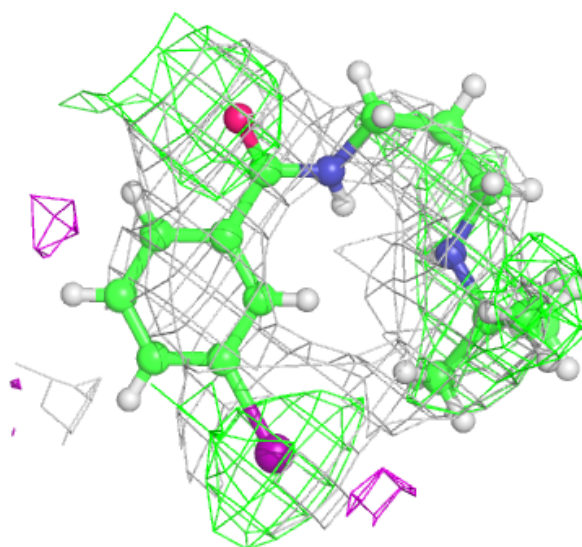
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FMT	H	1701	3/3	0.77	0.21	67,68,70,84	0
3	K6P	B	1701[B]	18/18	0.77	0.54	121,147,171,171	39
3	K6P	B	1701[A]	18/18	0.77	0.54	119,146,166,167	39
3	K6P	G	1701[B]	18/18	0.81	0.50	133,166,179,179	39
3	K6P	G	1701[A]	18/18	0.81	0.50	132,166,179,179	39
2	PO4	D	1701	5/5	0.82	0.35	130,131,131,133	0
2	PO4	J	1703	5/5	0.84	0.25	105,109,112,112	0
2	PO4	F	1701	5/5	0.84	0.53	196,198,198,199	0
2	PO4	J	1702	5/5	0.85	0.25	139,139,139,139	0
3	K6P	C	1701[A]	18/18	0.85	0.38	82,100,120,127	39
3	K6P	C	1701[B]	18/18	0.85	0.38	87,104,120,122	39
4	FMT	B	1702	3/3	0.86	0.13	72,73,74,87	0
2	PO4	B	1704	5/5	0.87	0.23	93,94,95,96	0
4	FMT	H	1703	3/3	0.87	0.18	79,80,81,97	0
2	PO4	C	1703	5/5	0.88	0.27	109,112,114,114	0
3	K6P	E	1701[A]	18/18	0.89	0.36	92,112,115,115	39
2	PO4	D	1702	5/5	0.89	0.53	180,181,182,184	0
3	K6P	E	1701[B]	18/18	0.89	0.36	92,111,114,116	39
2	PO4	D	1704	5/5	0.90	0.23	100,103,104,106	0
2	PO4	I	1701	5/5	0.90	0.18	98,98,98,101	0
2	PO4	E	1703	5/5	0.91	0.23	93,93,96,97	0
2	PO4	G	1702	5/5	0.91	0.24	96,96,97,101	0
2	PO4	A	1701	5/5	0.92	0.23	93,98,101,102	0
2	PO4	H	1705	5/5	0.93	0.27	88,89,92,93	0
2	PO4	F	1702	5/5	0.93	0.24	86,87,89,89	0
2	PO4	H	1704	5/5	0.93	0.19	121,121,122,122	0
4	FMT	H	1702	3/3	0.97	0.30	52,52,52,63	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.

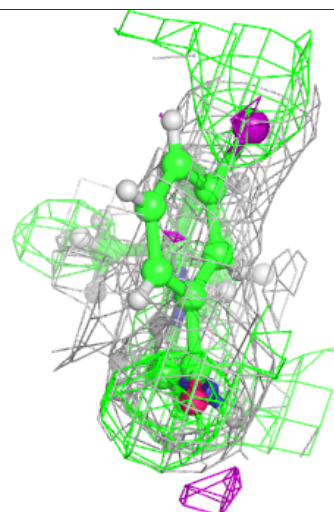
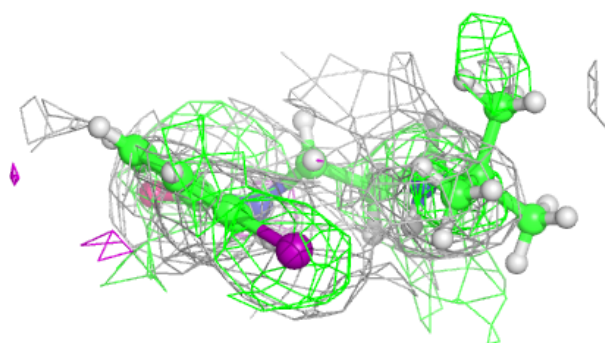
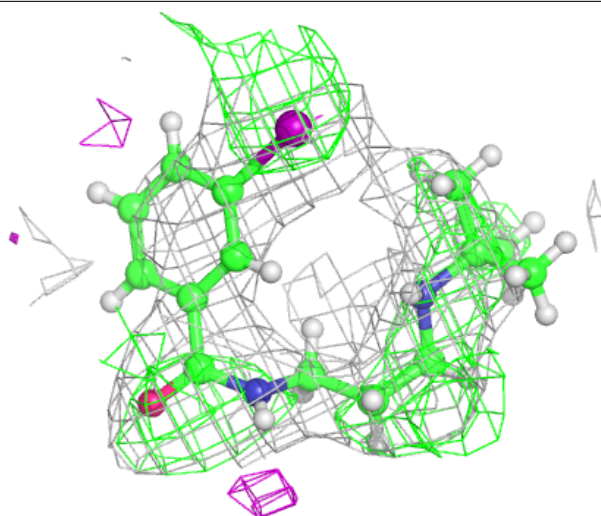
**Electron density around K6P J 1701 (B):**

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



**Electron density around K6P J 1701 (A):**

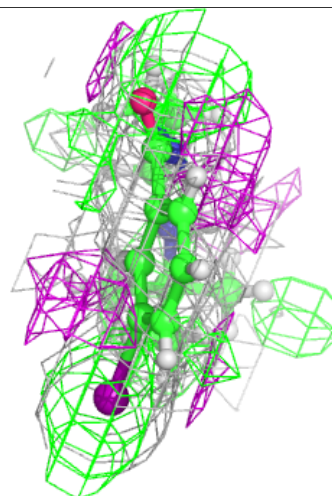
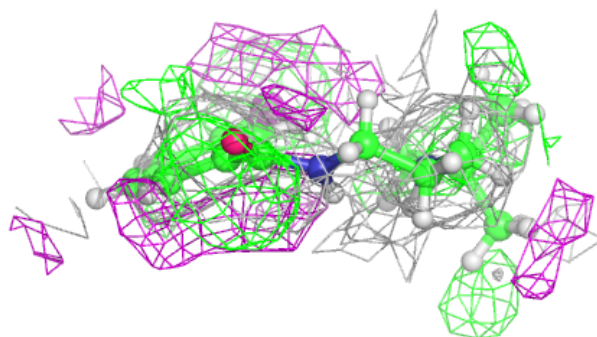
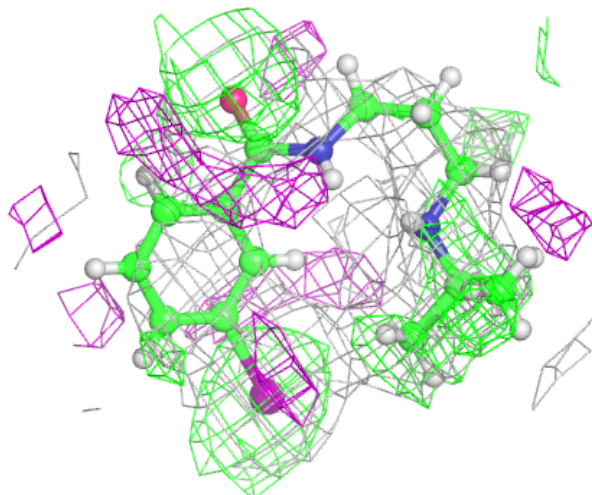
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





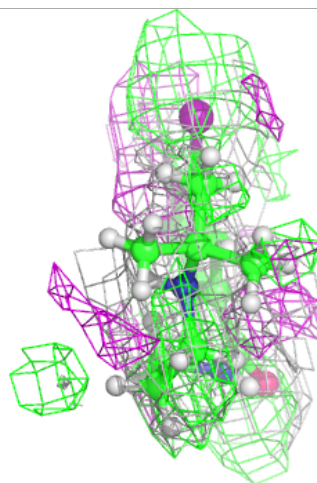
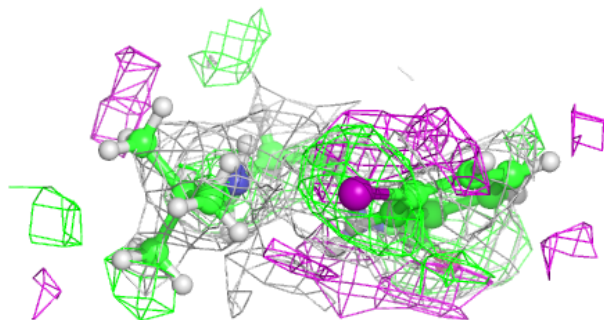
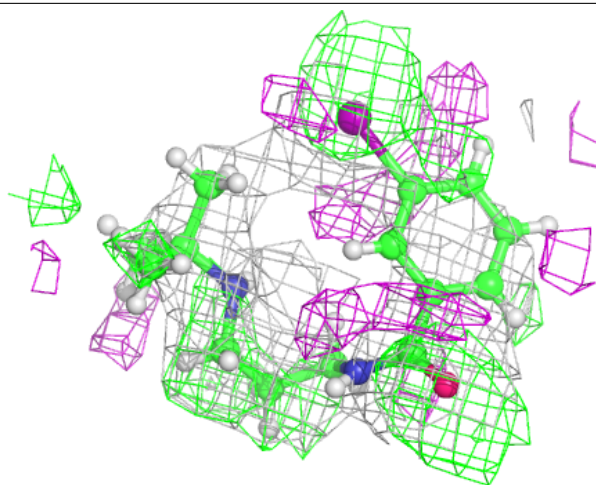
**Electron density around K6P B 1701 (B):**

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



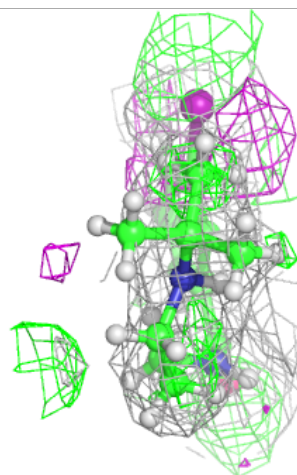
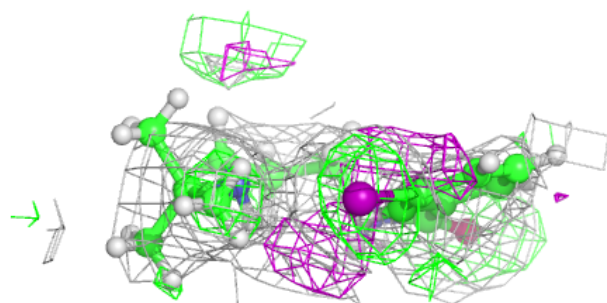
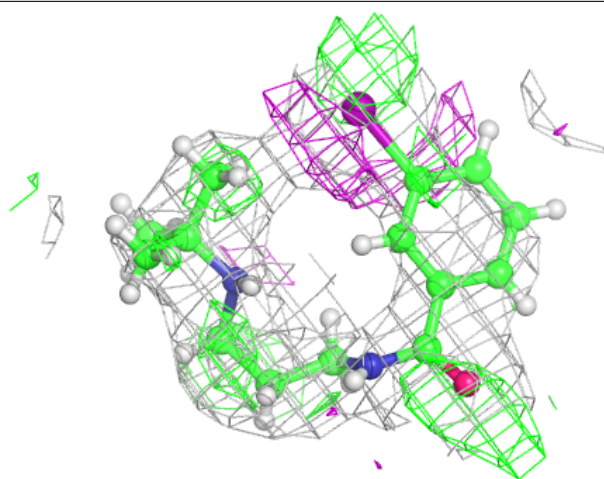
**Electron density around K6P B 1701 (A):**

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



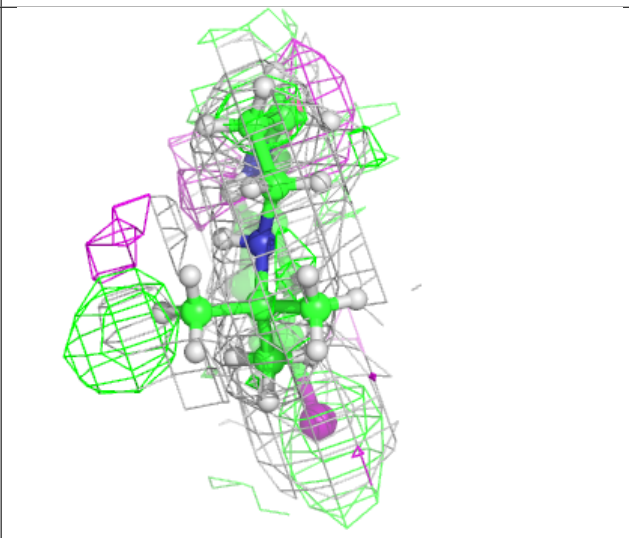
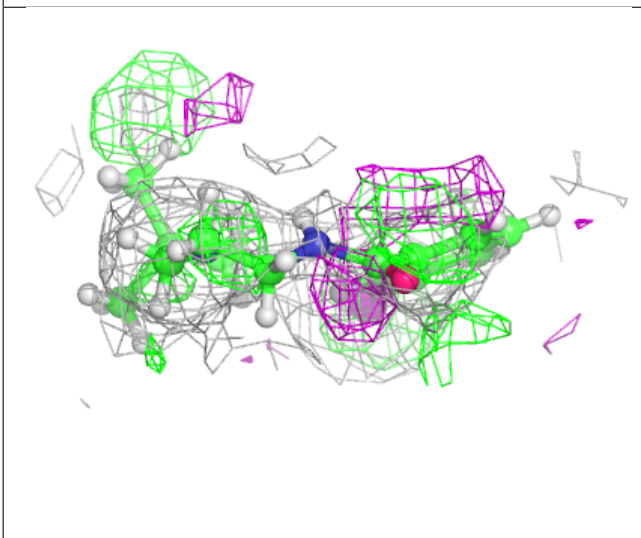
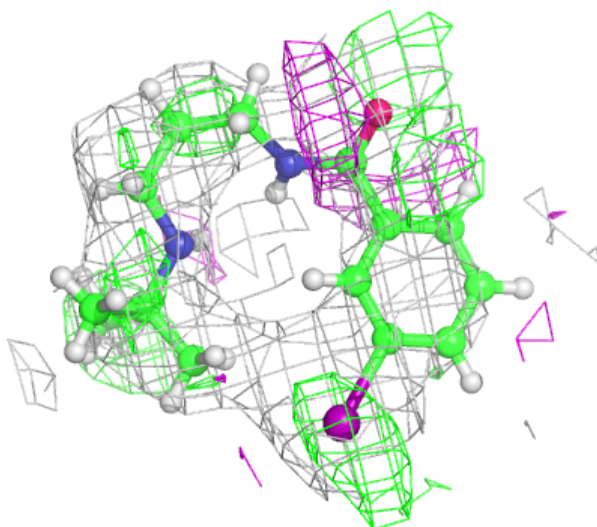
**Electron density around K6P C 1701 (A):**

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



**Electron density around K6P C 1701 (B):**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.