



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2026 – 05:21 PM EDT

PDB ID : 7I9A / pdb\_00007i9a  
Title : Crystal Structure of 24 bound to the PH domain of Btk  
Authors : Brear, P.; West, R.M.; Nicolescu, R.C.B.; Blaszczyk, B.K.; Anwar, A.; Deingruber, T.; Sanders, M.G.; Perez-Areales, F.J.; Stephens, L.R.; Hawkins, P.T.; Spring, D.R.; Hyvonen, M.  
Deposited on : 2025-03-24  
Resolution : 2.11 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

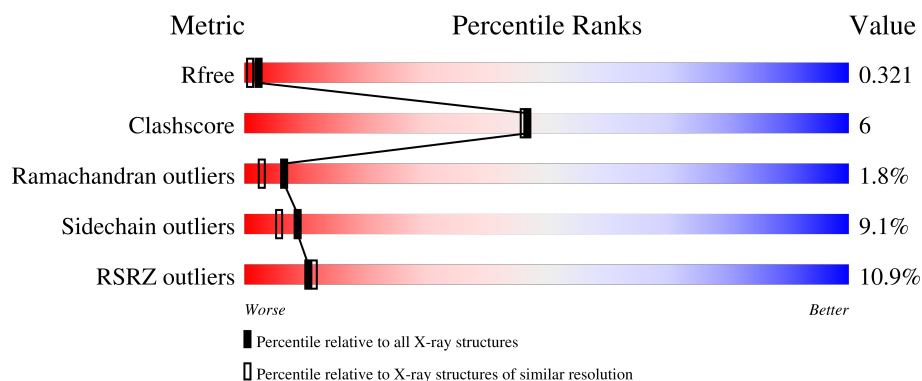
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.11 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	169	<div> <div>8%</div> <div>80%</div> <div>15%</div> <div>..</div> </div>
1	C	169	<div> <div>8%</div> <div>78%</div> <div>17%</div> <div>..</div> </div>
1	H	169	<div> <div>16%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	K	169	<div> <div>12%</div> <div>78%</div> <div>18%</div> <div>..</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5848 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.

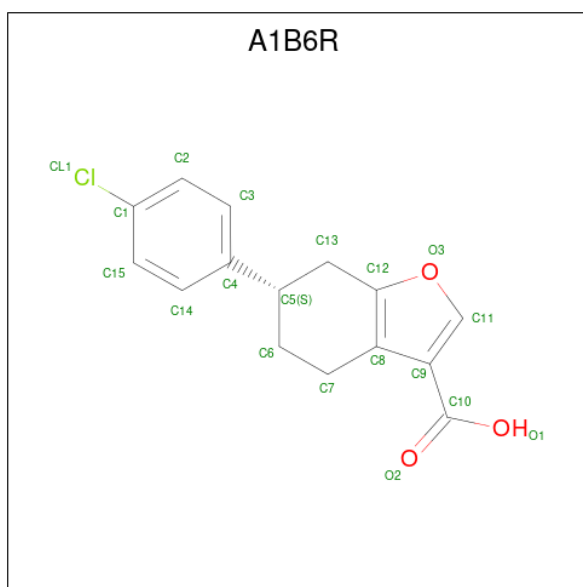
- Molecule 1 is a protein called Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	2	0
			1404	900	245	253	6			
1	C	167	Total	C	N	O	S	0	2	0
			1409	903	248	252	6			
1	H	167	Total	C	N	O	S	0	2	0
			1405	900	246	253	6			
1	K	167	Total	C	N	O	S	0	2	0
			1405	900	246	253	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	145	SER	CYS	engineered mutation	UNP Q06187
C	145	SER	CYS	engineered mutation	UNP Q06187
H	145	SER	CYS	engineered mutation	UNP Q06187
K	145	SER	CYS	engineered mutation	UNP Q06187

- Molecule 2 is (6S)-6-(4-chlorophenyl)-4,5,6,7-tetrahydro-1-benzofuran-3-carboxylic acid (CCD ID: A1B6R) (formula: C<sub>15</sub>H<sub>13</sub>ClO<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	O	0	0
			19	15	1	3		
2	C	1	Total	C	Cl	O	0	0
			19	15	1	3		
2	H	1	Total	C	Cl	O	0	0
			19	15	1	3		
2	K	1	Total	C	Cl	O	0	0
			19	15	1	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	1	0
			1	1		
3	C	1	Total	Zn	1	0
			1	1		
3	H	1	Total	Zn	1	0
			1	1		
3	K	1	Total	Zn	1	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	1	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Mg	1	0
			1	1		
4	K	2	Total	Mg	2	0
			2	2		

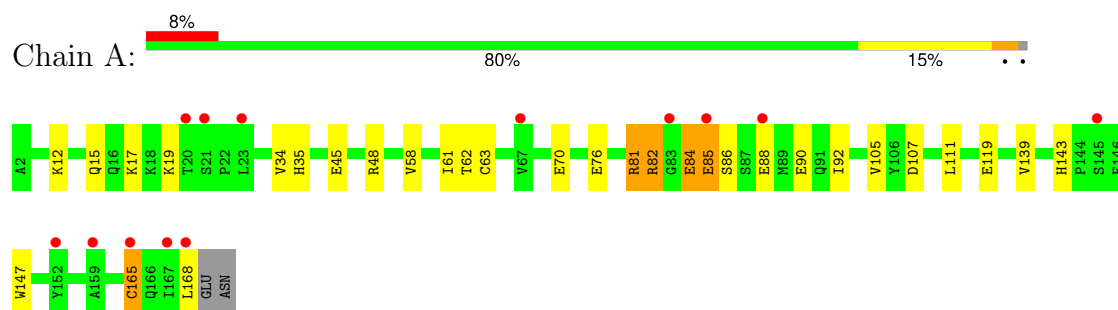
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	C	47	Total	O	0	0
			47	47		
5	H	17	Total	O	0	0
			17	17		
5	K	24	Total	O	0	0
			24	24		

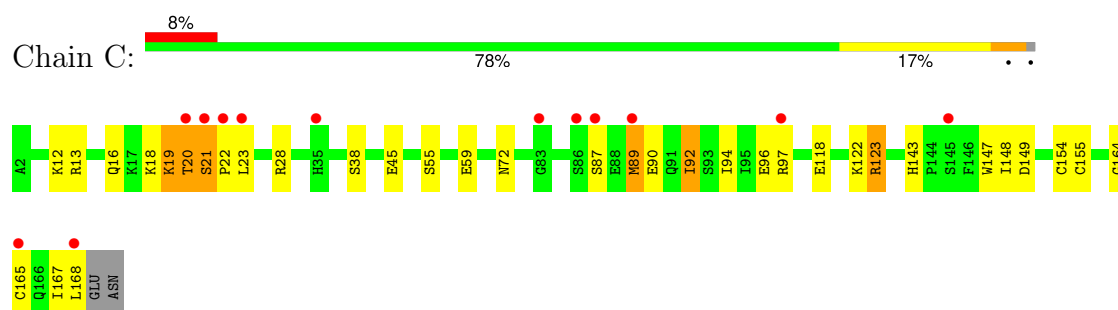
### 3 Residue-property plots [i](#)

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.

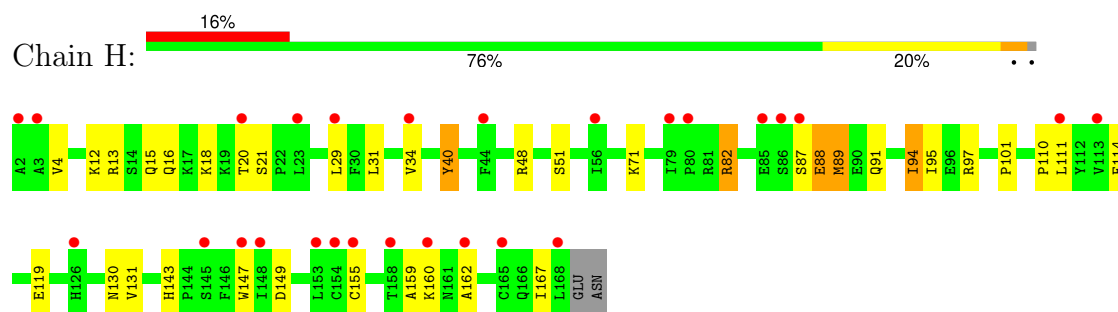
#### • Molecule 1: Tyrosine-protein kinase BTK



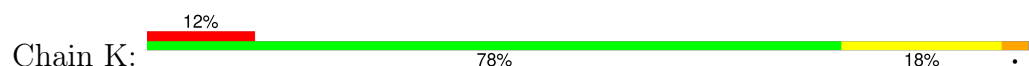
#### • Molecule 1: Tyrosine-protein kinase BTK

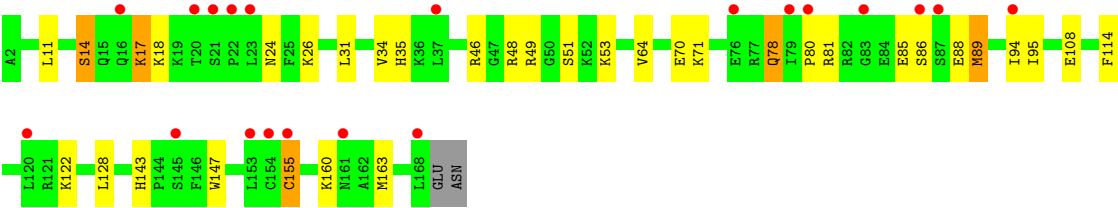


#### • Molecule 1: Tyrosine-protein kinase BTK



#### • Molecule 1: Tyrosine-protein kinase BTK





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.34Å 66.38Å 79.70Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	30.56 – 2.11 30.56 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.56-2.11) 99.6 (30.56-2.11)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, $R_{free}$	0.262 , 0.333 0.253 , 0.321	Depositor DCC
$R_{free}$ test set	2034 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.8	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	5848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.67% 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: ZN, MG, A1B6R

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	0.77	0/1439	1.08	4/1940 (0.2%)
1	C	0.80	0/1444	1.11	6/1946 (0.3%)
1	H	0.68	0/1439	0.98	2/1939 (0.1%)
1	K	2.21	2/1439 (0.1%)	2.61	6/1939 (0.3%)
All	All	1.28	2/5761 (0.0%)	1.59	18/7764 (0.2%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	14[A]	SER	C-N	-56.49	0.54	1.33
1	K	14[B]	SER	C-N	-56.49	0.54	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	14[A]	SER	O-C-N	-73.87	24.34	122.59
1	K	14[B]	SER	O-C-N	-73.87	24.34	122.59
1	K	14[A]	SER	CA-C-N	-10.44	101.60	121.54
1	K	14[A]	SER	C-N-CA	-10.44	101.60	121.54
1	K	14[B]	SER	CA-C-N	-10.44	101.60	121.54
1	K	14[B]	SER	C-N-CA	-10.44	101.60	121.54
1	A	84	GLU	CA-C-N	7.25	135.40	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	GLU	C-N-CA	7.25	135.40	121.54
1	C	167	ILE	CA-C-N	6.35	133.14	121.70
1	C	167	ILE	C-N-CA	6.35	133.14	121.70
1	C	72	ASN	CA-CB-CG	6.29	118.89	112.60
1	H	88	GLU	CA-C-N	6.00	132.99	121.54
1	H	88	GLU	C-N-CA	6.00	132.99	121.54
1	C	164	GLY	CA-C-N	5.93	129.03	120.79
1	C	164	GLY	C-N-CA	5.93	129.03	120.79
1	A	147	TRP	N-CA-C	-5.70	100.53	109.25
1	C	147	TRP	N-CA-C	-5.67	99.94	108.96
1	A	86	SER	N-CA-C	-5.57	106.53	113.55

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	14[A]	SER	Mainchain
1	K	14[B]	SER	Mainchain

## 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	1404	0	1406	13	0
1	C	1409	0	1415	17	0
1	H	1405	0	1412	15	0
1	K	1405	0	1414	20	0
2	A	19	0	0	1	0
2	C	19	0	0	0	0
2	H	19	0	0	0	0
2	K	19	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	2	0	0	0	0
5	A	53	0	0	1	0
5	C	47	0	0	0	0
5	H	17	0	0	0	0
5	K	24	0	0	0	0
All	All	5848	0	5647	64	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 6.

All (64) 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:K:17:LYS:HZ3	1:K:18:LYS:H	1.15	0.91
1:C:143:HIS:HD1	1:C:165:CYS:HG	1.22	0.80
1:K:24:ASN:HD22	1:K:26:LYS:HZ1	1.36	0.74
1:K:143:HIS:ND1	1:K:155:CYS:SG	2.60	0.71
1:K:51:SER:HB3	1:K:53:LYS:NZ	2.07	0.69
1:H:18:LYS:HB2	1:H:21:SER:HB3	1.75	0.69
1:H:143:HIS:ND1	1:H:155:CYS:SG	2.66	0.68
1:C:16:GLN:HG2	1:C:19:LYS:HA	1.76	0.68
1:K:24:ASN:ND2	1:K:26:LYS:NZ	2.42	0.67
1:C:23:LEU:HD21	1:C:148:ILE:HD11	1.77	0.67
1:C:143:HIS:ND1	1:C:165:CYS:SG	2.57	0.67
1:H:159:ALA:HB3	1:H:162:ALA:HB2	1.77	0.66
1:K:24:ASN:ND2	1:K:26:LYS:HZ1	1.93	0.66
1:H:15:GLN:HG3	1:H:160:LYS:NZ	2.12	0.64
1:A:81:ARG:HB2	1:A:84:GLU:HB2	1.79	0.63
1:K:17:LYS:HG2	1:K:18:LYS:HG3	1.81	0.63
1:H:91:GLN:HG3	1:K:94:ILE:HG13	1.83	0.60
1:A:34:VAL:HG23	1:A:35[A]:HIS:CE1	2.37	0.59
1:C:12:LYS:HD3	1:C:28:ARG:HG3	1.85	0.58
1:K:51:SER:HB3	1:K:53:LYS:HZ3	1.69	0.58
1:C:16:GLN:HE22	1:C:149:ASP:H	1.50	0.58
1:A:34:VAL:HG23	1:A:35[A]:HIS:ND1	2.22	0.55
1:C:155:CYS:SG	1:C:165:CYS:SG	3.05	0.55
1:K:64:VAL:HG21	1:K:128:LEU:HB3	1.90	0.54
1:C:122:LYS:HZ3	1:C:123:ARG:CD	2.21	0.54
1:A:143:HIS:ND1	1:A:165:CYS:SG	2.82	0.52
1:K:51:SER:HB3	1:K:53:LYS:HZ1	1.75	0.51
1:A:12:LYS:HE2	1:A:111:LEU:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:51:SER:CB	1:K:53:LYS:HZ3	2.23	0.50
1:A:76:GLU:HB2	5:A:319:HOH:O	2.10	0.50
1:C:23:LEU:HD22	1:C:23:LEU:N	2.26	0.49
1:A:81:ARG:HB2	1:A:84:GLU:H	1.78	0.49
1:H:34:VAL:HG12	1:H:131:VAL:HG12	1.94	0.49
1:C:23:LEU:HD21	1:C:148:ILE:CD1	2.43	0.48
1:C:92:ILE:O	1:C:96:GLU:HG3	2.14	0.48
1:A:58:VAL:HA	1:A:61:ILE:HD12	1.95	0.48
1:C:18:LYS:HB3	1:C:21:SER:HB3	1.95	0.48
1:H:31:LEU:HD12	1:H:40:TYR:CE1	2.49	0.48
1:C:122:LYS:NZ	1:C:123:ARG:CD	2.76	0.47
1:C:19:LYS:O	1:C:20:THR:C	2.58	0.46
1:K:94:ILE:HG23	1:K:95:ILE:HG23	1.98	0.46
1:H:12:LYS:HD2	1:H:111:LEU:HD11	1.99	0.45
1:K:78:GLN:O	1:K:80:PRO:HD3	2.17	0.45
1:K:17:LYS:H	1:K:17:LYS:NZ	2.15	0.45
1:A:63:CYS:HB3	1:A:105:VAL:HB	1.99	0.44
1:A:15:GLN:HB2	2:A:201:A1B6R:C13	2.47	0.44
1:A:62:THR:HB	1:A:139:VAL:HG13	1.99	0.44
1:A:81:ARG:CB	1:A:84:GLU:HB2	2.47	0.44
1:H:16:GLN:HE22	1:H:149:ASP:H	1.66	0.44
1:H:110:PRO:HD2	1:H:160:LYS:HE2	2.00	0.43
1:H:147:TRP:O	1:H:147:TRP:CG	2.70	0.43
1:H:88:GLU:O	1:H:89:MET:HB2	2.19	0.42
1:K:94:ILE:HD12	1:K:94:ILE:HA	1.93	0.42
1:K:31:LEU:HD11	1:K:49[B]:ARG:NE	2.34	0.42
1:H:15:GLN:CG	1:H:160:LYS:NZ	2.82	0.41
1:C:122:LYS:NZ	1:C:123:ARG:NE	2.67	0.41
1:C:90:GLU:O	1:C:94:ILE:HB	2.21	0.41
1:H:101:PRO:HB3	1:H:114:PHE:CE2	2.55	0.41
1:A:82:ARG:NE	1:A:82:ARG:H	2.19	0.40
1:H:94:ILE:HG23	1:H:95:ILE:HG23	2.04	0.40
1:C:92:ILE:HD13	1:C:92:ILE:HA	1.87	0.40
1:K:34:VAL:HG23	1:K:35:HIS:CE1	2.57	0.40
1:K:11:LEU:HB3	1:K:114:PHE:HB2	2.02	0.40
1:K:24:ASN:HD22	1:K:26:LYS:NZ	2.06	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	167/169 (99%)	154 (92%)	11 (7%)	2 (1%)	10	6
1	C	167/169 (99%)	158 (95%)	5 (3%)	4 (2%)	4	1
1	H	167/169 (99%)	152 (91%)	12 (7%)	3 (2%)	6	3
1	K	167/169 (99%)	151 (90%)	13 (8%)	3 (2%)	6	3
All	All	668/676 (99%)	615 (92%)	41 (6%)	12 (2%)	6	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	GLU
1	C	89	MET
1	H	89	MET
1	C	87	SER
1	H	4	VAL
1	K	89	MET
1	C	19	LYS
1	C	22	PRO
1	H	82	ARG
1	K	81	ARG
1	K	86	SER
1	A	17	LYS

### 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	158/158 (100%)	144 (91%)	14 (9%)	9	6
1	C	158/158 (100%)	143 (90%)	15 (10%)	8	5
1	H	158/158 (100%)	144 (91%)	14 (9%)	9	6
1	K	158/158 (100%)	143 (90%)	15 (10%)	8	5
All	All	632/632 (100%)	574 (91%)	58 (9%)	9	5

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	45	GLU
1	A	48	ARG
1	A	70	GLU
1	A	81	ARG
1	A	82	ARG
1	A	85	GLU
1	A	88	GLU
1	A	90	GLU
1	A	92	ILE
1	A	107	ASP
1	A	119	GLU
1	A	165	CYS
1	A	168	LEU
1	C	13	ARG
1	C	20	THR
1	C	21	SER
1	C	38	SER
1	C	45	GLU
1	C	55	SER
1	C	59	GLU
1	C	89	MET
1	C	92	ILE
1	C	97[A]	ARG
1	C	97[B]	ARG
1	C	118	GLU
1	C	123	ARG
1	C	154	CYS
1	C	168	LEU
1	H	13	ARG
1	H	20	THR
1	H	29	LEU
1	H	40	TYR

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Mol	Chain	Res	Type
1	H	48	ARG
1	H	51	SER
1	H	71	LYS
1	H	82	ARG
1	H	87	SER
1	H	94	ILE
1	H	97	ARG
1	H	119	GLU
1	H	130	ASN
1	H	167	ILE
1	K	17	LYS
1	K	46	ARG
1	K	48	ARG
1	K	70	GLU
1	K	71	LYS
1	K	78	GLN
1	K	85	GLU
1	K	88	GLU
1	K	89	MET
1	K	108	GLU
1	K	122	LYS
1	K	147	TRP
1	K	155	CYS
1	K	160	LYS
1	K	163	MET

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	127	GLN
1	A	151	GLN
1	C	16	GLN
1	C	126	HIS
1	H	16	GLN
1	H	72	ASN
1	K	24	ASN
1	K	78	GLN
1	K	130	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	A1B6R	C	201	1	21,21,21	0.83	1 (4%)	24,30,30	1.40	4 (16%)
2	A1B6R	H	201	1	21,21,21	0.63	0	24,30,30	1.24	1 (4%)
2	A1B6R	K	201	1	21,21,21	0.86	1 (4%)	24,30,30	1.12	3 (12%)
2	A1B6R	A	201	1	21,21,21	0.66	0	24,30,30	1.30	3 (12%)

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	A1B6R	C	201	1	-	0/8/17/17	0/3/3/3
2	A1B6R	H	201	1	-	5/8/17/17	0/3/3/3
2	A1B6R	K	201	1	-	0/8/17/17	0/3/3/3
2	A1B6R	A	201	1	-	5/8/17/17	0/3/3/3



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	201	A1B6R	C7-C8	-2.47	1.46	1.51
2	C	201	A1B6R	C7-C8	-2.29	1.47	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	201	A1B6R	O3-C12-C13	4.48	124.30	119.88
2	A	201	A1B6R	O3-C12-C13	3.95	123.77	119.88
2	K	201	A1B6R	O3-C12-C13	3.67	123.50	119.88
2	C	201	A1B6R	O3-C12-C13	3.54	123.37	119.88
2	C	201	A1B6R	C13-C5-C4	2.95	119.75	112.47
2	C	201	A1B6R	O2-C10-C9	-2.64	117.22	122.67
2	C	201	A1B6R	O1-C10-C9	2.43	121.39	115.69
2	A	201	A1B6R	C6-C7-C8	-2.41	105.82	111.38
2	A	201	A1B6R	C13-C5-C4	2.26	118.05	112.47
2	K	201	A1B6R	O2-C10-C9	-2.14	118.25	122.67
2	K	201	A1B6R	O1-C10-C9	2.00	120.38	115.69

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	A1B6R	O1-C10-C9-C8
2	A	201	A1B6R	O1-C10-C9-C11
2	A	201	A1B6R	O2-C10-C9-C11
2	H	201	A1B6R	O1-C10-C9-C8
2	H	201	A1B6R	O1-C10-C9-C11
2	H	201	A1B6R	O2-C10-C9-C11
2	A	201	A1B6R	C3-C4-C5-C6
2	H	201	A1B6R	C14-C4-C5-C6
2	A	201	A1B6R	O2-C10-C9-C8
2	H	201	A1B6R	O2-C10-C9-C8

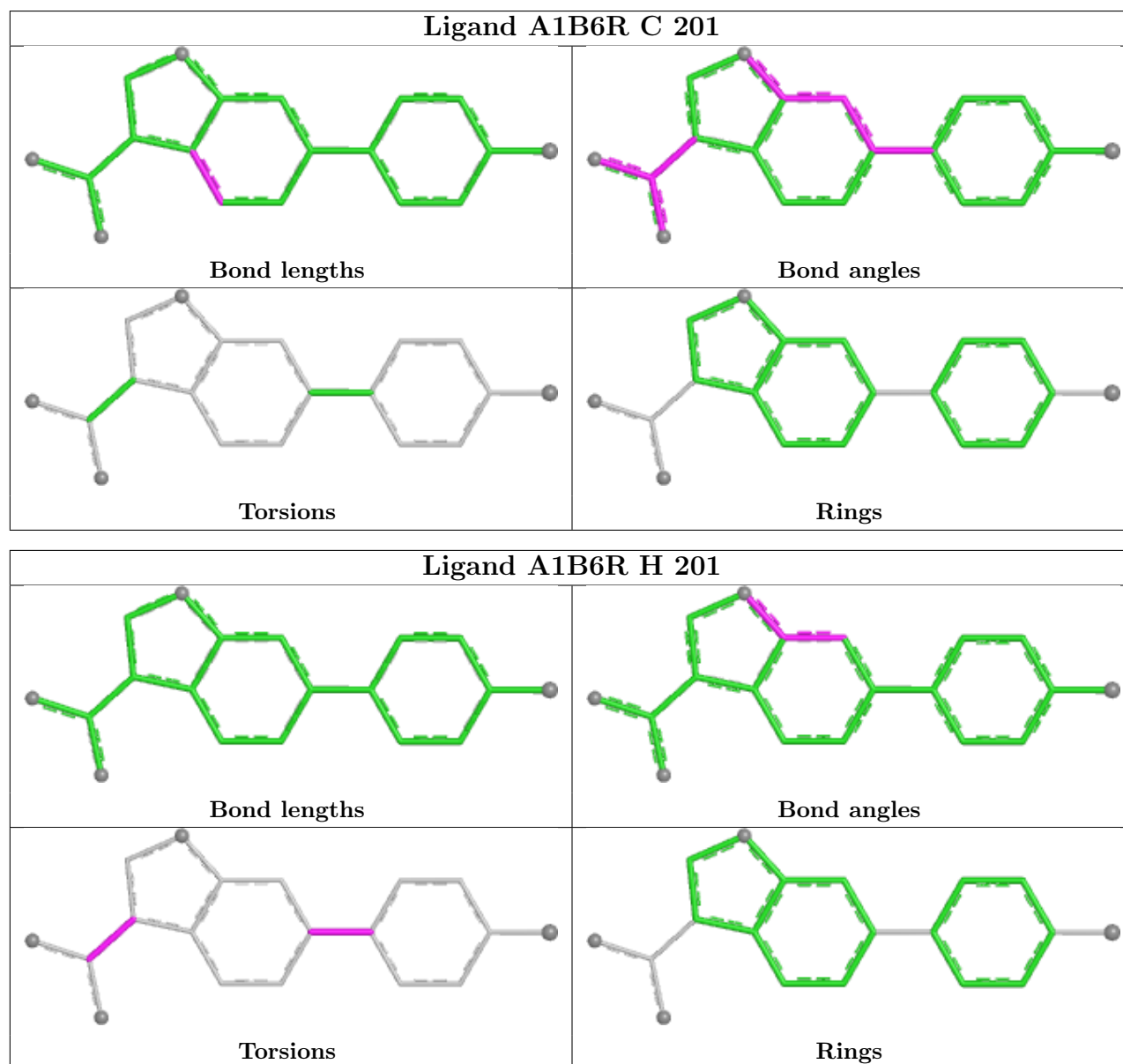
There are no ring outliers.

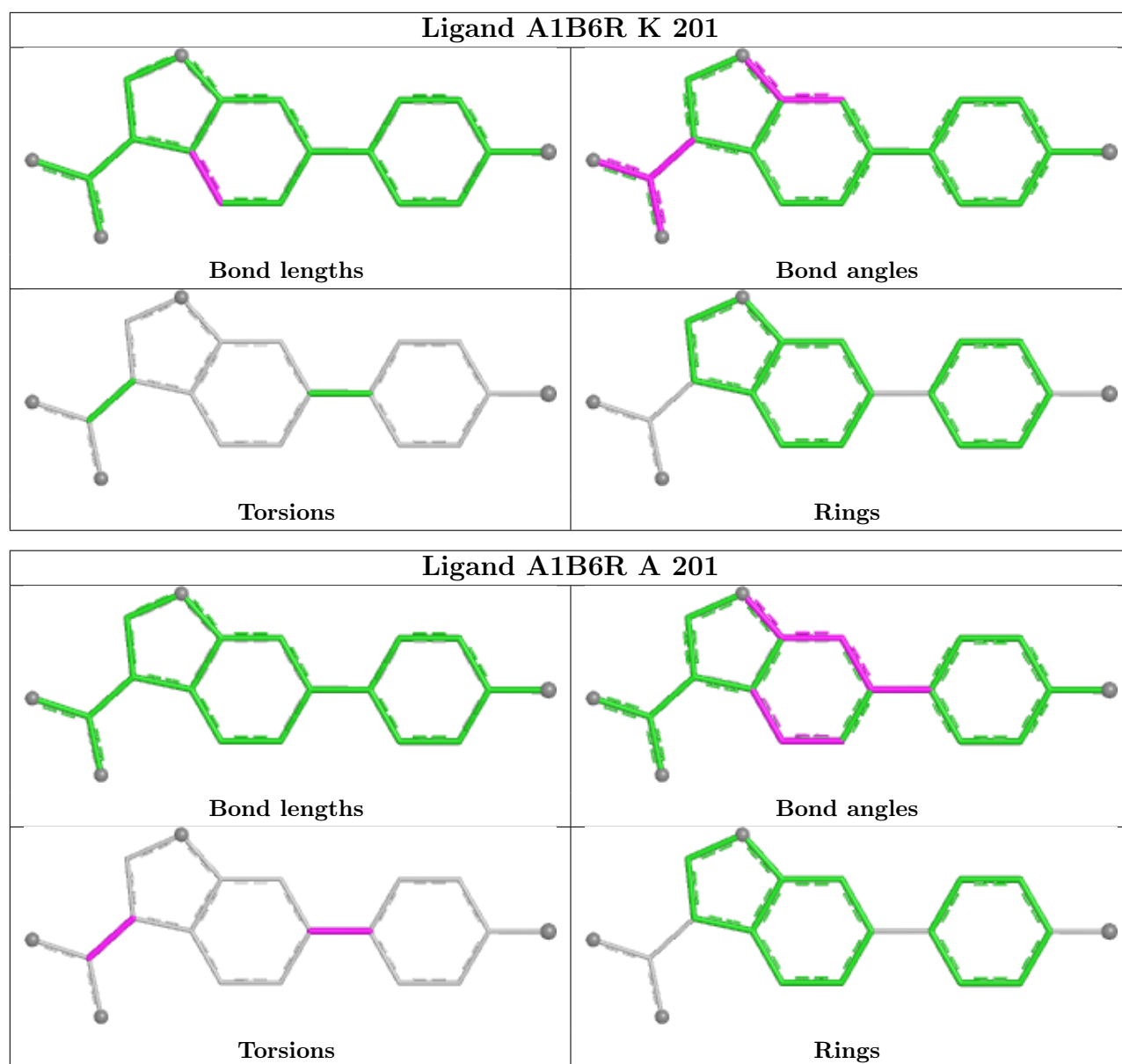
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	A1B6R	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	K	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	14[B]:SER	C	15:GLN	N	0.54
1	K	14[A]:SER	C	15:GLN	N	0.54

## 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	167/169 (98%)	0.76	13 (7%)	19 21	31, 60, 84, 104	2 (1%)
1	C	167/169 (98%)	0.53	13 (7%)	19 21	20, 51, 93, 103	2 (1%)
1	H	167/169 (98%)	1.19	27 (16%)	4 5	42, 78, 104, 120	2 (1%)
1	K	167/169 (98%)	0.98	20 (11%)	9 9	43, 73, 111, 121	2 (1%)
All	All	668/676 (98%)	0.86	73 (10%)	10 11	20, 68, 103, 121	8 (1%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	155	CYS	5.1
1	H	2	ALA	4.8
1	A	83	GLY	4.3
1	H	87	SER	4.3
1	K	22	PRO	4.3
1	K	155	CYS	4.2
1	C	20	THR	3.8
1	H	168	LEU	3.8
1	C	168	LEU	3.7
1	K	145	SER	3.7
1	K	161	ASN	3.6
1	A	88	GLU	3.6
1	A	20	THR	3.6
1	C	165	CYS	3.6
1	C	86	SER	3.4
1	H	147	TRP	3.4
1	K	23	LEU	3.4
1	K	20	THR	3.3
1	C	87	SER	3.3
1	C	22	PRO	3.3
1	H	148	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	K	79	ILE	3.1
1	K	94	ILE	3.1
1	K	168	LEU	3.0
1	H	165	CYS	2.8
1	H	145	SER	2.8
1	A	165	CYS	2.8
1	H	86	SER	2.8
1	C	89	MET	2.8
1	A	23	LEU	2.8
1	K	153	LEU	2.7
1	C	97[A]	ARG	2.7
1	K	83	GLY	2.6
1	H	3	ALA	2.6
1	K	80	PRO	2.6
1	A	21	SER	2.6
1	H	80	PRO	2.6
1	A	67	VAL	2.6
1	H	20	THR	2.6
1	A	168	LEU	2.6
1	K	21	SER	2.6
1	H	34	VAL	2.5
1	H	160	LYS	2.5
1	A	145	SER	2.5
1	K	154	CYS	2.4
1	K	16	GLN	2.4
1	C	23	LEU	2.4
1	A	167	ILE	2.3
1	C	21	SER	2.3
1	H	154	CYS	2.3
1	H	111	LEU	2.3
1	A	159	ALA	2.3
1	H	23	LEU	2.3
1	H	79	ILE	2.2
1	C	83	GLY	2.2
1	C	145	SER	2.2
1	H	158	THR	2.2
1	H	162	ALA	2.2
1	K	37	LEU	2.2
1	K	86	SER	2.2
1	C	35[A]	HIS	2.1
1	A	152	TYR	2.1
1	H	113	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	85	GLU	2.1
1	H	153	LEU	2.1
1	H	126	HIS	2.1
1	A	85	GLU	2.0
1	H	29	LEU	2.0
1	H	56	ILE	2.0
1	H	44	PHE	2.0
1	K	76	GLU	2.0
1	K	87	SER	2.0
1	K	120	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

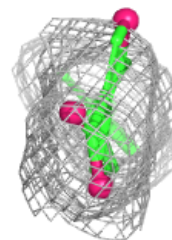
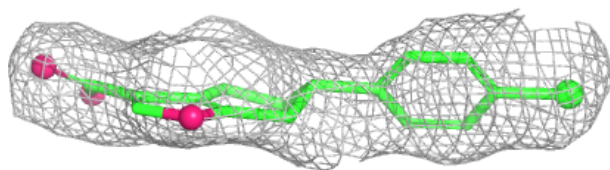
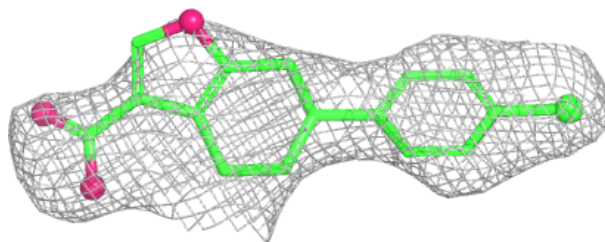
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	A1B6R	H	201	19/19	0.80	0.13	86,88,90,90	0
2	A1B6R	K	201	19/19	0.82	0.12	94,94,94,95	0
2	A1B6R	A	201	19/19	0.85	0.11	66,69,72,72	0
2	A1B6R	C	201	19/19	0.92	0.08	53,53,55,56	0
3	ZN	A	202	1/1	-	-	61,61,61,61	1
3	ZN	C	203	1/1	-	-	58,58,58,58	1
3	ZN	H	202	1/1	-	-	77,77,77,77	1
3	ZN	K	204	1/1	-	-	78,78,78,78	1
4	MG	A	203	1/1	-	-	54,54,54,54	1
4	MG	C	202	1/1	-	-	107,107,107,107	1
4	MG	K	202	1/1	-	-	79,79,79,79	1
4	MG	K	203	1/1	-	-	72,72,72,72	1

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 A1B6R H 201:**

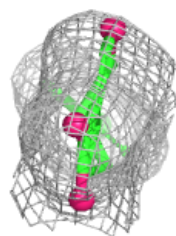
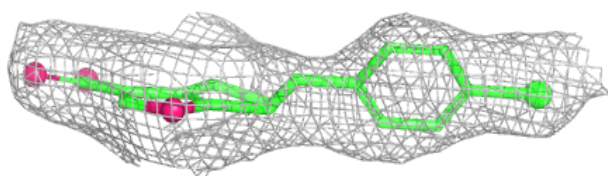
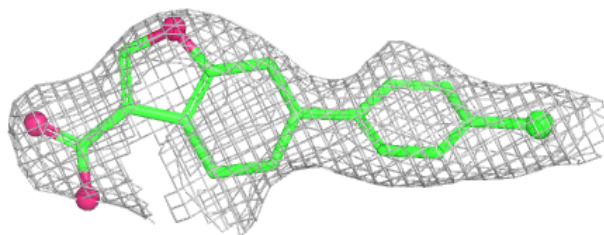
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



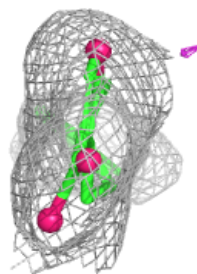
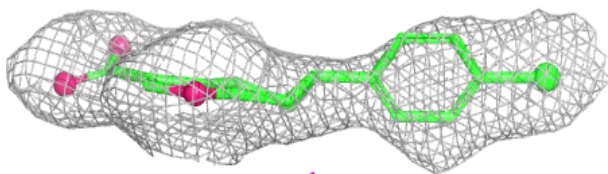
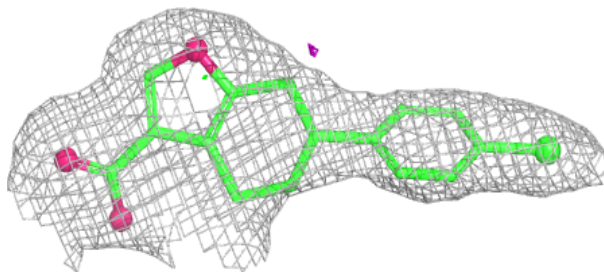


**Electron density around A1B6R K 201:**

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

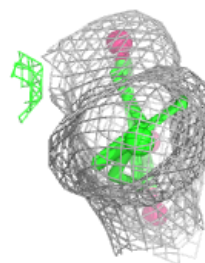
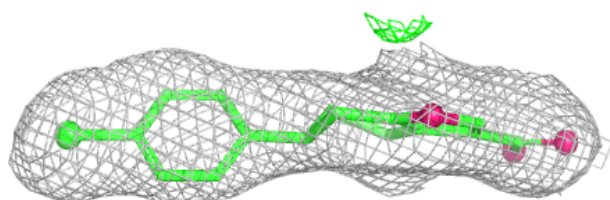
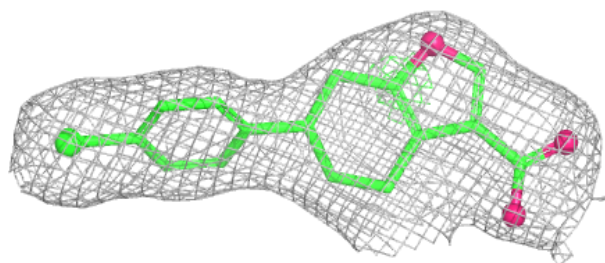
**Electron density around A1B6R A 201:**

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



**Electron density around A1B6R C 201:**

$2mF_o-DF_c$  (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.