



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:32 PM BST

PDB ID : 4ZY3  
Title : Crystal Structure of Keap1 in Complex with a small chemical compound, K67  
Authors : Fukutomi, T.; Iso, T.; Suzuki, T.; Takagi, K.; Mizushima, T.; Komatsu, M.; Yamamoto, M.  
Deposited on : 2015-05-21  
Resolution : 1.80 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 : 2.13.1  
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) : 2.13.1

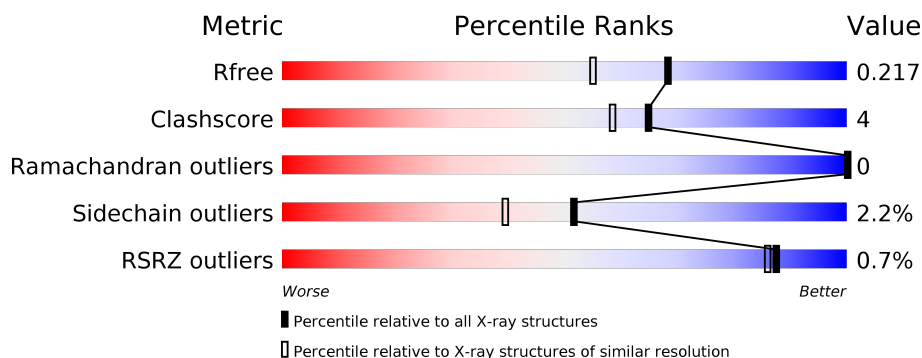
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	311	 82% 8% • 8%
1	B	311	 78% 12% • 8%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4712 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2189	1360	396	418	15			
1	B	285	Total	C	N	O	S	0	0	0
			2189	1360	396	418	15			

There are 44 discrepancies between the modelled and reference sequences:

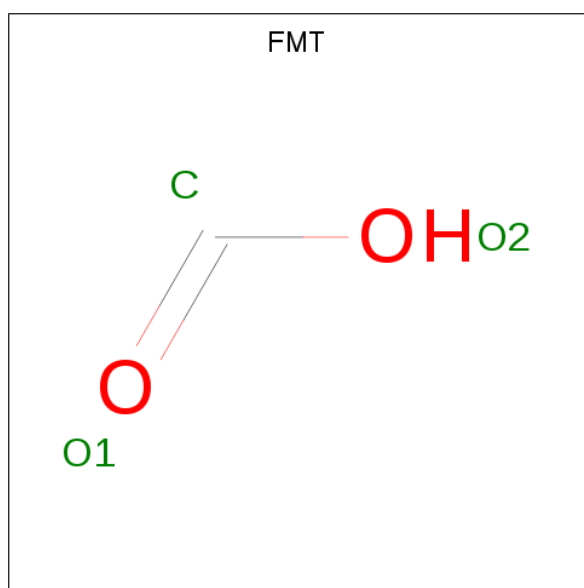
Chain	Residue	Modelled	Actual	Comment	Reference
A	299	MET	-	initiating methionine	UNP Q9Z2X8
A	300	GLY	-	expression tag	UNP Q9Z2X8
A	301	HIS	-	expression tag	UNP Q9Z2X8
A	302	HIS	-	expression tag	UNP Q9Z2X8
A	303	HIS	-	expression tag	UNP Q9Z2X8
A	304	HIS	-	expression tag	UNP Q9Z2X8
A	305	HIS	-	expression tag	UNP Q9Z2X8
A	306	HIS	-	expression tag	UNP Q9Z2X8
A	307	ASP	-	expression tag	UNP Q9Z2X8
A	308	TYR	-	expression tag	UNP Q9Z2X8
A	309	ASP	-	expression tag	UNP Q9Z2X8
A	310	ILE	-	expression tag	UNP Q9Z2X8
A	311	PRO	-	expression tag	UNP Q9Z2X8
A	312	THR	-	expression tag	UNP Q9Z2X8
A	313	THR	-	expression tag	UNP Q9Z2X8
A	314	GLU	-	expression tag	UNP Q9Z2X8
A	315	ASN	-	expression tag	UNP Q9Z2X8
A	316	LEU	-	expression tag	UNP Q9Z2X8
A	317	TYR	-	expression tag	UNP Q9Z2X8
A	318	PHE	-	expression tag	UNP Q9Z2X8
A	319	GLN	-	expression tag	UNP Q9Z2X8
A	320	GLY	-	expression tag	UNP Q9Z2X8
B	299	MET	-	initiating methionine	UNP Q9Z2X8
B	300	GLY	-	expression tag	UNP Q9Z2X8
B	301	HIS	-	expression tag	UNP Q9Z2X8

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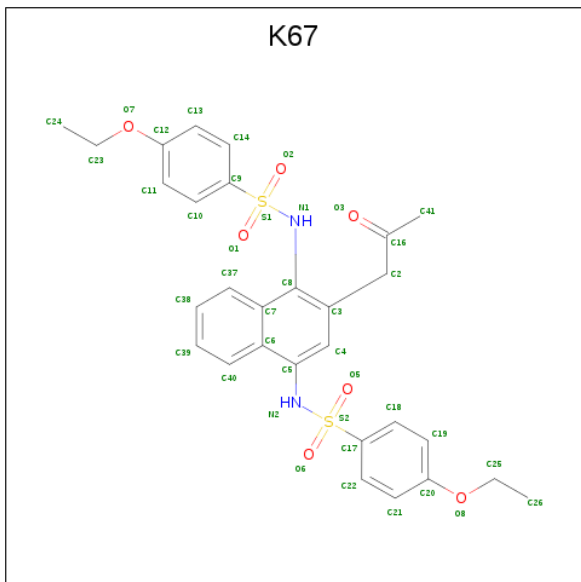
Chain	Residue	Modelled	Actual	Comment	Reference
B	302	HIS	-	expression tag	UNP Q9Z2X8
B	303	HIS	-	expression tag	UNP Q9Z2X8
B	304	HIS	-	expression tag	UNP Q9Z2X8
B	305	HIS	-	expression tag	UNP Q9Z2X8
B	306	HIS	-	expression tag	UNP Q9Z2X8
B	307	ASP	-	expression tag	UNP Q9Z2X8
B	308	TYR	-	expression tag	UNP Q9Z2X8
B	309	ASP	-	expression tag	UNP Q9Z2X8
B	310	ILE	-	expression tag	UNP Q9Z2X8
B	311	PRO	-	expression tag	UNP Q9Z2X8
B	312	THR	-	expression tag	UNP Q9Z2X8
B	313	THR	-	expression tag	UNP Q9Z2X8
B	314	GLU	-	expression tag	UNP Q9Z2X8
B	315	ASN	-	expression tag	UNP Q9Z2X8
B	316	LEU	-	expression tag	UNP Q9Z2X8
B	317	TYR	-	expression tag	UNP Q9Z2X8
B	318	PHE	-	expression tag	UNP Q9Z2X8
B	319	GLN	-	expression tag	UNP Q9Z2X8
B	320	GLY	-	expression tag	UNP Q9Z2X8

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			3	1	2		
2	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 3 is N,N'-[2-(2-oxopropyl)naphthalene-1,4-diyl]bis(4-ethoxybenzenesulfonamide) (three-letter code: K67) (formula: C<sub>29</sub>H<sub>30</sub>N<sub>2</sub>O<sub>7</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			40	29	2	7	2		
3	B	1	Total	C	N	O	S	0	0
			40	29	2	7	2		


- Molecule 4 is water.

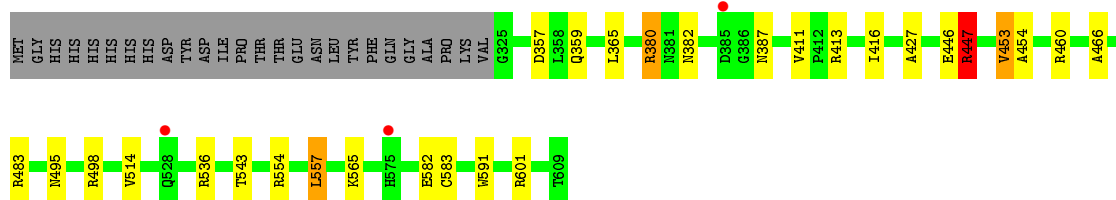
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	130	Total	O	0	0
			130	130		
4	B	118	Total	O	0	0
			118	118		

### 3 Residue-property plots


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.

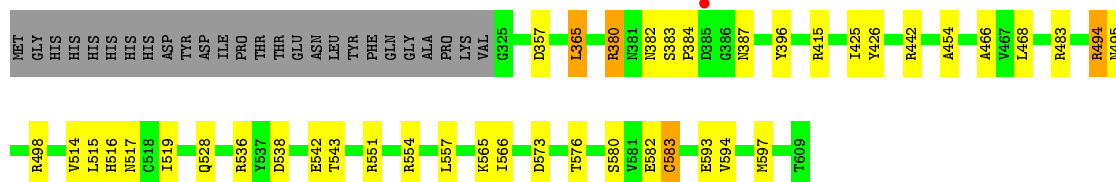
- Molecule 1: Kelch-like ECH-associated protein 1

Chain A: 



- Molecule 1: Kelch-like ECH-associated protein 1

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.40Å 75.19Å 109.80Å 90.00° 105.35° 90.00°	Depositor
Resolution (Å)	33.46 – 1.80 33.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (33.46-1.80) 99.6 (33.46-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.55 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.190 , 0.212 0.197 , 0.217	Depositor DCC
$R_{free}$ test set	4623 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 42.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4712	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.24% 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: K67, FMT

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	1.23	2/2243 (0.1%)	1.20	18/3053 (0.6%)
1	B	1.29	8/2243 (0.4%)	1.41	18/3053 (0.6%)
All	All	1.26	10/4486 (0.2%)	1.31	36/6106 (0.6%)

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	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	582	GLU	CG-CD	7.08	1.62	1.51
1	B	593	GLU	CD-OE1	-7.05	1.17	1.25
1	B	517	ASN	N-CA	6.24	1.58	1.46
1	A	591	TRP	CB-CG	-5.48	1.40	1.50
1	B	583	CYS	CA-CB	5.41	1.65	1.53
1	B	542	GLU	CD-OE2	-5.40	1.19	1.25
1	B	494	ARG	CD-NE	-5.35	1.37	1.46
1	B	582	GLU	CG-CD	5.17	1.59	1.51
1	B	396	TYR	CD1-CE1	5.16	1.47	1.39
1	B	580	SER	CB-OG	5.00	1.48	1.42

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	NE-CZ-NH2	-29.22	105.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	494	ARG	NE-CZ-NH1	23.49	132.04	120.30
1	B	494	ARG	CD-NE-CZ	12.68	141.34	123.60
1	B	516	HIS	C-N-CA	-10.92	94.39	121.70
1	A	483	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	413	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	380	ARG	NE-CZ-NH2	7.89	124.24	120.30
1	A	453	VAL	CG1-CB-CG2	7.60	123.06	110.90
1	B	516	HIS	O-C-N	-7.23	111.13	122.70
1	B	357	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	536	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	554	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	498	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	468	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	A	357	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	380	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	A	357	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	538	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	593	GLU	CG-CD-OE2	6.20	130.71	118.30
1	A	536	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	498	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	483	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	601	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	B	554	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	453	VAL	N-CA-CB	-5.67	99.02	111.50
1	A	447	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	B	597	MET	CG-SD-CE	-5.55	91.32	100.20
1	A	536	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	B	380	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	453	VAL	CA-CB-CG1	5.26	118.79	110.90
1	B	483	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	A	460	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	516	HIS	CA-C-N	5.16	128.54	117.20
1	B	536	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	415	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	365	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	494	ARG	Sidechain

## 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	2189	0	2075	16	0
1	B	2189	0	2075	19	0
2	A	3	0	1	0	0
2	B	3	0	1	0	0
3	A	40	0	0	0	0
3	B	40	0	0	0	0
4	A	130	0	0	4	0
4	B	118	0	0	0	0
All	All	4712	0	4152	35	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 4.

All (35) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:ARG:HE	1:A:382:ASN:HD21	1.25	0.84
1:A:359:GLN:HG3	4:A:925:HOH:O	1.78	0.81
1:B:454:ALA:H	1:B:495:ASN:HD21	1.39	0.70
1:A:454:ALA:H	1:A:495:ASN:HD21	1.41	0.69
1:B:380:ARG:HD3	1:B:382:ASN:ND2	2.08	0.69
1:A:380:ARG:HE	1:A:382:ASN:ND2	1.92	0.66
1:B:514:VAL:HG22	1:B:519:ILE:HD13	1.80	0.64
1:B:380:ARG:HD3	1:B:382:ASN:HD21	1.63	0.63
1:A:447:ARG:HH21	1:A:447:ARG:CG	2.12	0.63
4:A:812:HOH:O	1:B:576:THR:HG23	1.99	0.62
1:A:466:ALA:HB1	1:A:514:VAL:HG23	1.84	0.60
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.85	0.59
1:A:447:ARG:HG3	1:A:447:ARG:NH2	2.19	0.57
1:A:447:ARG:HH21	1:A:447:ARG:HG3	1.69	0.57
1:B:557:LEU:H	1:B:557:LEU:HD23	1.71	0.56
1:A:557:LEU:H	1:A:557:LEU:HD23	1.73	0.52
1:A:447:ARG:HH21	1:A:447:ARG:CB	2.23	0.50
1:A:565:LYS:HD2	1:A:583:CYS:SG	2.52	0.50
1:A:365:LEU:HD23	1:A:365:LEU:H	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:LYS:HE2	1:B:583:CYS:SG	2.53	0.49
1:B:426:TYR:CZ	1:B:442:ARG:HD3	2.48	0.48
1:A:411:VAL:CG2	4:A:916:HOH:O	2.60	0.48
1:A:380:ARG:NH1	1:A:387:ASN:HB3	2.29	0.48
1:A:416:ILE:HD11	1:A:427:ALA:HB1	1.98	0.44
1:B:383:SER:HB2	1:B:384:PRO:HD2	1.98	0.44
1:A:380:ARG:HH11	1:A:387:ASN:HD22	1.66	0.43
1:B:365:LEU:HD23	1:B:365:LEU:H	1.83	0.43
1:B:551:ARG:HG2	1:B:551:ARG:NH1	2.33	0.43
1:B:425:ILE:O	1:B:442:ARG:HA	2.19	0.42
1:B:466:ALA:HB1	1:B:514:VAL:CG2	2.49	0.42
4:A:812:HOH:O	1:B:576:THR:CG2	2.62	0.42
1:B:515:LEU:HD22	1:B:566:ILE:HG13	2.01	0.42
1:B:380:ARG:HH21	1:B:387:ASN:HB3	1.85	0.41
1:B:382:ASN:HA	1:B:387:ASN:HD22	1.85	0.41
1:B:382:ASN:HA	1:B:387:ASN:ND2	2.36	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	283/311 (91%)	276 (98%)	7 (2%)	0	100	100
1	B	283/311 (91%)	277 (98%)	6 (2%)	0	100	100
All	All	566/622 (91%)	553 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/255 (91%)	227 (98%)	5 (2%)	52	39
1	B	232/255 (91%)	227 (98%)	5 (2%)	52	39
All	All	464/510 (91%)	454 (98%)	10 (2%)	52	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	446	GLU
1	A	447	ARG
1	A	453	VAL
1	A	543	THR
1	A	557	LEU
1	B	498	ARG
1	B	528	GLN
1	B	543	THR
1	B	573	ASP
1	B	594	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	ASN
1	A	469	ASN
1	A	495	ASN
1	A	563	GLN
1	B	382	ASN
1	B	387	ASN
1	B	495	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

4 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	$\# Z  > 2$
3	K67	B	702	-	43,43,43	2.80	17 (39%)	57,62,62	2.56	22 (38%)
3	K67	A	702	-	43,43,43	2.67	16 (37%)	57,62,62	2.95	23 (40%)
2	FMT	B	701	-	0,2,2	0.00	-	0,1,1	0.00	-
2	FMT	A	701	-	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	K67	B	702	-	-	6/32/32/32	0/4/4/4
3	K67	A	702	-	-	8/32/32/32	0/4/4/4

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	K67	C8-C3	12.40	1.52	1.38
3	A	702	K67	C17-S2	-9.00	1.62	1.76
3	A	702	K67	C8-C3	8.30	1.47	1.38
3	A	702	K67	C9-S1	-4.93	1.68	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	K67	C17-S2	-4.88	1.68	1.76
3	B	702	K67	C8-C7	4.66	1.51	1.43
3	B	702	K67	C9-S1	-4.26	1.69	1.76
3	A	702	K67	C6-C7	3.82	1.50	1.43
3	B	702	K67	C5-N2	-3.72	1.36	1.42
3	A	702	K67	C8-N1	-3.53	1.36	1.43
3	A	702	K67	C8-C7	3.24	1.49	1.43
3	B	702	K67	C5-C6	3.23	1.49	1.43
3	B	702	K67	S2-N2	-3.06	1.58	1.63
3	B	702	K67	C39-C40	3.05	1.43	1.36
3	B	702	K67	C2-C3	2.99	1.56	1.51
3	B	702	K67	C14-C9	2.96	1.43	1.38
3	A	702	K67	O7-C12	2.96	1.44	1.37
3	A	702	K67	C5-N2	-2.90	1.37	1.42
3	B	702	K67	C6-C7	2.75	1.48	1.43
3	B	702	K67	C8-N1	-2.66	1.38	1.43
3	A	702	K67	C14-C9	2.65	1.43	1.38
3	B	702	K67	C22-C17	2.58	1.42	1.38
3	B	702	K67	C19-C20	2.56	1.43	1.38
3	A	702	K67	C39-C40	2.55	1.42	1.36
3	A	702	K67	C4-C3	2.37	1.43	1.39
3	B	702	K67	C18-C17	2.37	1.42	1.38
3	A	702	K67	C22-C17	2.34	1.42	1.38
3	A	702	K67	C38-C37	2.31	1.42	1.36
3	B	702	K67	O5-S2	-2.28	1.40	1.43
3	A	702	K67	C11-C10	2.22	1.42	1.38
3	B	702	K67	C38-C37	2.07	1.41	1.36
3	A	702	K67	C5-C6	2.03	1.47	1.43
3	A	702	K67	O1-S1	2.01	1.45	1.43

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	K67	C3-C8-N1	9.82	130.53	119.02
3	A	702	K67	C3-C8-N1	9.22	129.83	119.02
3	A	702	K67	O5-S2-O6	-8.89	108.63	119.55
3	A	702	K67	O5-S2-N2	7.34	125.09	106.73
3	B	702	K67	C17-S2-N2	-6.89	98.16	106.83
3	A	702	K67	O1-S1-O2	5.88	126.78	119.55
3	A	702	K67	C17-S2-N2	-5.81	99.53	106.83
3	B	702	K67	O2-S1-C9	4.71	113.77	107.97
3	B	702	K67	C2-C3-C4	-4.53	111.71	120.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	K67	C8-N1-S1	4.14	129.64	121.52
3	A	702	K67	C38-C37-C7	-4.11	115.19	120.89
3	A	702	K67	C23-O7-C12	3.92	128.02	117.99
3	B	702	K67	O6-S2-C17	3.76	112.60	107.97
3	A	702	K67	O6-S2-C17	3.73	112.56	107.97
3	B	702	K67	C14-C9-S1	-3.73	115.72	119.77
3	A	702	K67	C37-C7-C8	-3.65	118.21	124.78
3	A	702	K67	C5-C4-C3	3.52	127.77	121.92
3	A	702	K67	C9-S1-N1	3.28	110.96	106.83
3	B	702	K67	O5-S2-N2	3.22	114.79	106.73
3	B	702	K67	C8-N1-S1	3.13	127.65	121.52
3	B	702	K67	C40-C6-C5	-3.12	118.03	123.00
3	B	702	K67	O5-S2-C17	-3.10	104.14	107.97
3	A	702	K67	O7-C23-C24	3.10	118.81	108.21
3	B	702	K67	C37-C7-C8	-3.06	119.27	124.78
3	B	702	K67	C10-C9-S1	2.98	123.01	119.77
3	B	702	K67	C8-C7-C6	2.98	121.21	117.66
3	B	702	K67	C4-C5-N2	-2.97	114.15	120.98
3	A	702	K67	C4-C5-N2	-2.93	114.25	120.98
3	B	702	K67	C39-C40-C6	-2.78	117.04	120.89
3	A	702	K67	O1-S1-C9	-2.77	104.55	107.97
3	B	702	K67	O5-S2-O6	2.65	122.80	119.55
3	B	702	K67	O1-S1-N1	-2.54	100.37	106.73
3	B	702	K67	C38-C37-C7	-2.49	117.44	120.89
3	A	702	K67	C39-C40-C6	-2.49	117.44	120.89
3	A	702	K67	C4-C5-C6	-2.48	115.56	119.29
3	A	702	K67	C40-C6-C5	-2.46	119.08	123.00
3	A	702	K67	O2-S1-C9	-2.39	105.03	107.97
3	A	702	K67	C8-C7-C6	2.39	120.51	117.66
3	B	702	K67	C5-N2-S2	2.33	131.00	124.20
3	B	702	K67	C10-C11-C12	2.31	122.56	119.73
3	A	702	K67	C2-C3-C4	-2.30	115.82	120.08
3	A	702	K67	C25-O8-C20	2.27	123.81	117.99
3	B	702	K67	C40-C6-C7	2.17	121.15	118.45
3	B	702	K67	C11-C10-C9	-2.04	117.33	119.45
3	A	702	K67	C37-C7-C6	2.02	120.96	118.45

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	K67	C41-C16-C2-C3

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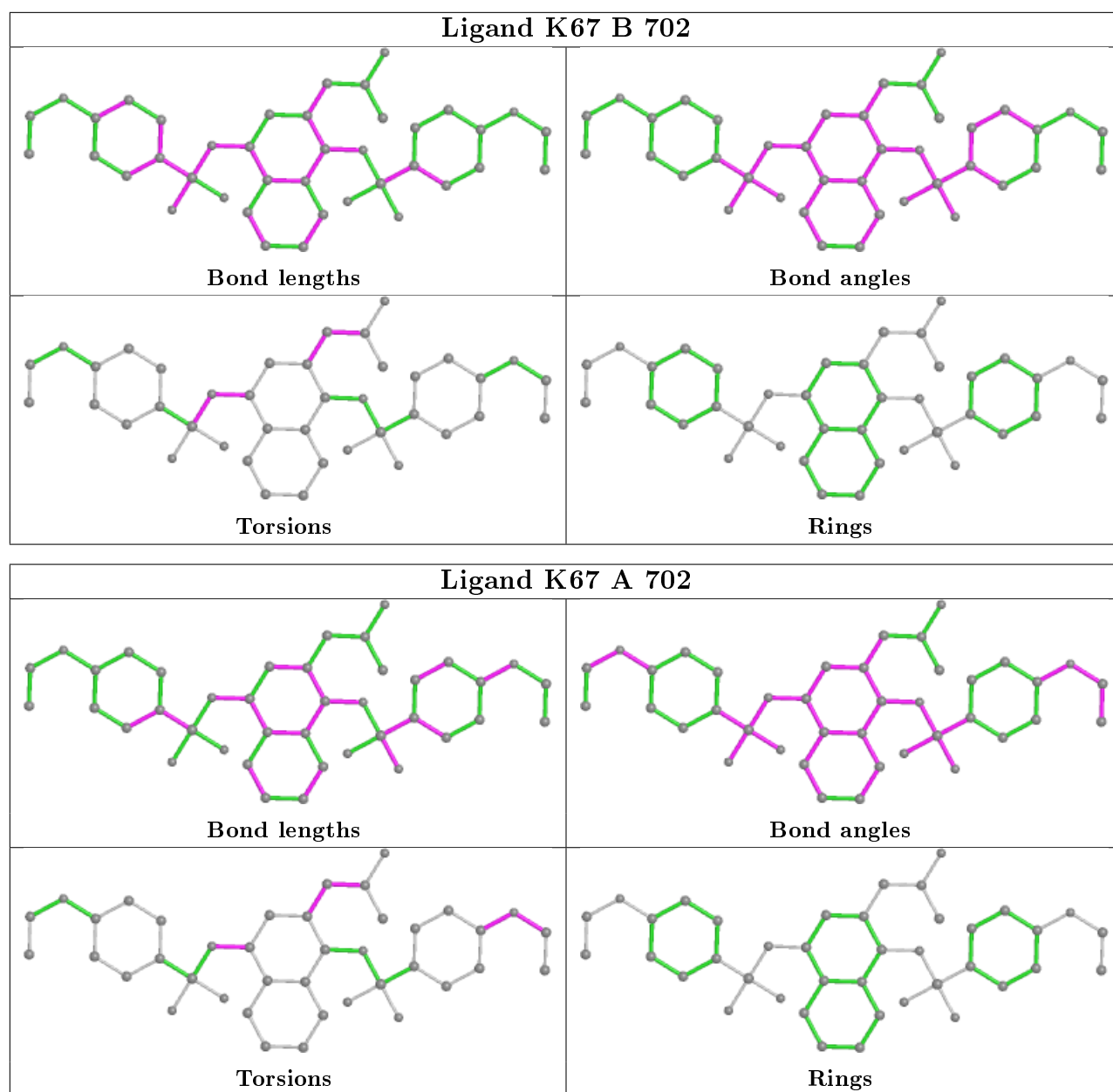
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Mol	Chain	Res	Type	Atoms
3	B	702	K67	C4-C5-N2-S2
3	B	702	K67	C6-C5-N2-S2
3	A	702	K67	C4-C5-N2-S2
3	A	702	K67	C6-C5-N2-S2
3	A	702	K67	C24-C23-O7-C12
3	A	702	K67	C13-C12-O7-C23
3	A	702	K67	C11-C12-O7-C23
3	B	702	K67	C16-C2-C3-C8
3	A	702	K67	O3-C16-C2-C3
3	A	702	K67	C16-C2-C3-C8
3	B	702	K67	C5-N2-S2-O5
3	A	702	K67	C41-C16-C2-C3
3	B	702	K67	O3-C16-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	285/311 (91%)	-0.30	3 (1%) 80 78	17, 23, 39, 60	0
1	B	285/311 (91%)	-0.40	1 (0%) 92 90	15, 22, 38, 58	0
All	All	570/622 (91%)	-0.35	4 (0%) 87 86	15, 23, 39, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ASP	2.7
1	A	575	HIS	2.6
1	B	385	ASP	2.5
1	A	528	GLN	2.2

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	K67	A	702	40/40	0.94	0.12	22,34,57,58	0

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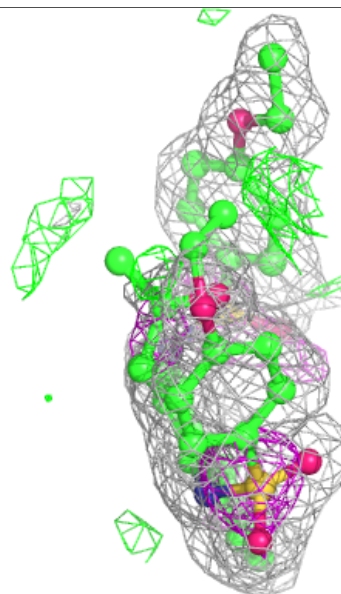
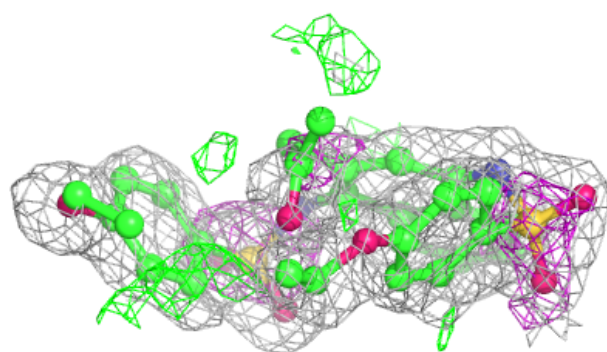
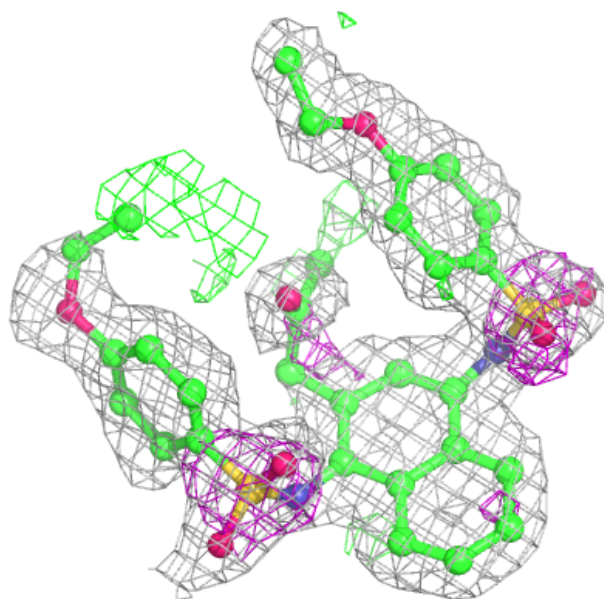
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K67	B	702	40/40	0.96	0.10	23,30,37,46	0
2	FMT	B	701	3/3	0.98	0.06	22,22,26,27	0
2	FMT	A	701	3/3	0.99	0.08	23,23,25,27	0

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.

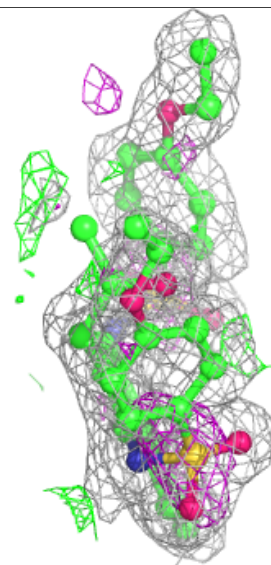
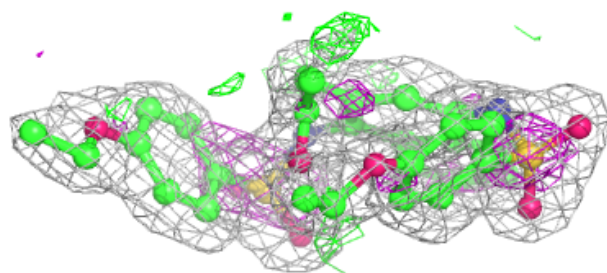
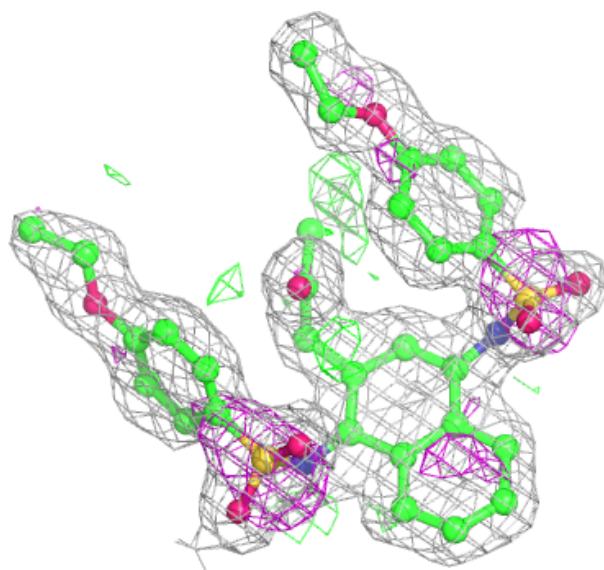
**Electron density around K67 A 702:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around K67 B 702:**

$2mF_o-DF_c$  (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.