



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2024 – 06:10 PM JST

PDB ID : 8ITV  
Title : KL2.1 in complex with CRM1-Ran-RanBP1  
Authors : Sun, Q.; Jian, L.  
Deposited on : 2023-03-23  
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

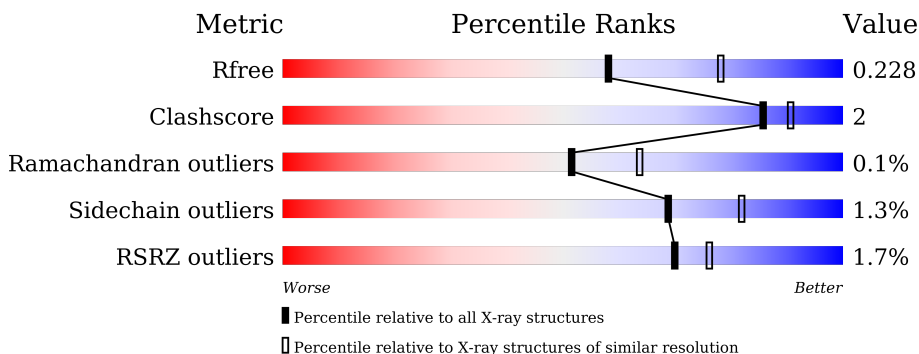
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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 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	216	 3% 88% 7%
2	B	140	 4% 86% 14%
3	C	1003	 % 93% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
6	DMS	A	303	-	-	-	X
7	GOL	C	1115	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 11602 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 GTP-binding nuclear protein Ran.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1671	1078	286	301	6	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	LEU	GLN	engineered mutation	UNP P62826
A	182	ALA	LEU	engineered mutation	UNP P62826

- Molecule 2 is a protein called YRB1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	992	628	174	186	4	0	0	0

- Molecule 3 is a protein called CRM1 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	995	8064	5182	1328	1512	42	0	3	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP A0A6A5PZI8
C	-1	GLY	-	expression tag	UNP A0A6A5PZI8
C	0	SER	-	expression tag	UNP A0A6A5PZI8
C	27	GLU	SER	engineered mutation	UNP A0A6A5PZI8
C	49	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	51	VAL	ALA	engineered mutation	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLN	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	ALA	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	PRO	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	TYR	deletion	UNP A0A6A5PZI8
C	?	-	MET	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LEU	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ASN	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8

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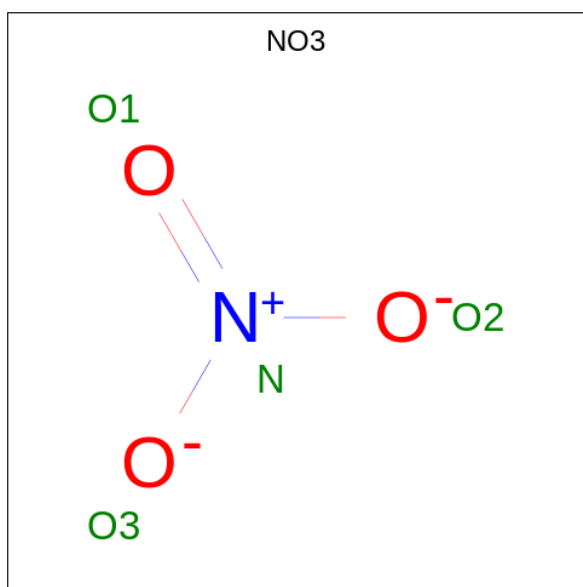
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	GLY	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	ILE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	ARG	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	PHE	deletion	UNP A0A6A5PZI8
C	?	-	VAL	deletion	UNP A0A6A5PZI8
C	?	-	LYS	deletion	UNP A0A6A5PZI8
C	?	-	GLU	deletion	UNP A0A6A5PZI8
C	?	-	SER	deletion	UNP A0A6A5PZI8
C	?	-	ASP	deletion	UNP A0A6A5PZI8
C	?	-	THR	deletion	UNP A0A6A5PZI8
C	537	GLY	ASP	engineered mutation	UNP A0A6A5PZI8
C	539	CYS	THR	engineered mutation	UNP A0A6A5PZI8
C	540	GLU	VAL	engineered mutation	UNP A0A6A5PZI8
C	541	GLN	LYS	engineered mutation	UNP A0A6A5PZI8
C	553	ARG	SER	engineered mutation	UNP A0A6A5PZI8
C	561	GLU	GLN	engineered mutation	UNP A0A6A5PZI8
C	741	THR	ALA	engineered mutation	UNP A0A6A5PZI8
C	1022	CYS	TYR	engineered mutation	UNP A0A6A5PZI8

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

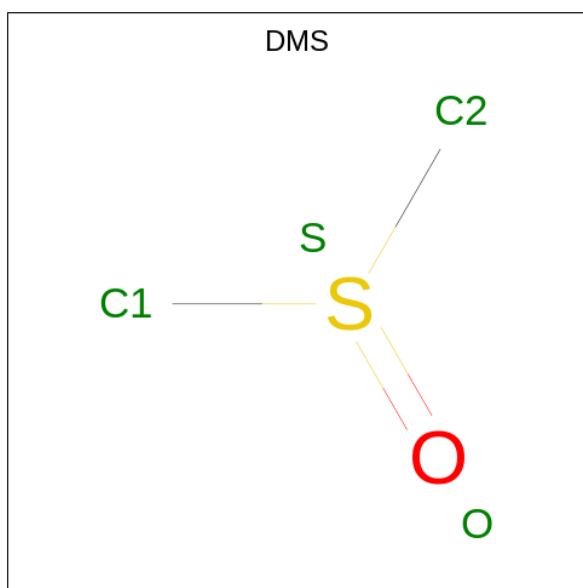
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	A	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		
5	C	1	Total	N	O	0	0
			4	1	3		

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	A	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		
6	C	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





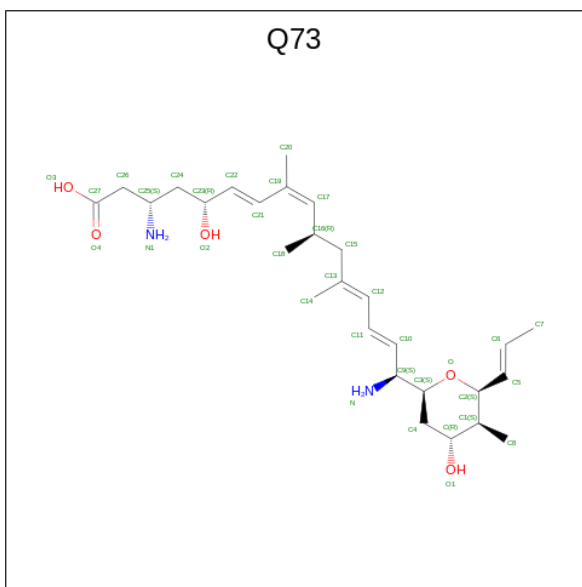
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 11 is (3 {S},5 {R},6 {E},8 {Z},10 {R},12 {E},14 {E},16 {S})-3,16-bis(azanyl)-8,10,12-trimethyl-16-[(2 {S},4 {R},5 {S},6 {S})-5-methyl-4-oxidanyl-6-[( {E})-prop-1-enyl]oxan-2-yl]-5-oxidanyl-hexadeca-6,8,12,14-tetraenoic acid (three-letter code: Q73) (formula: C<sub>28</sub>H<sub>46</sub>N<sub>2</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	N	O	0	0
			35	28	2	5		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	132	Total	O	0	0
			132	132		
12	B	36	Total	O	0	0
			36	36		
12	C	512	Total	O	0	0
			512	512		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.01Å 106.01Å 305.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.44 – 2.30 47.40 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.44-2.30) 99.6 (47.40-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.8.0403	Depositor
R, $R_{free}$	0.186 , 0.224 0.191 , 0.228	Depositor DCC
$R_{free}$ test set	3949 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtrriage
Anisotropy	0.094	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11602	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, ACT, Q73, NO3, CL, GOL, MG, GTP

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	0.30	0/1712	0.59	0/2321
2	B	0.27	0/1009	0.58	0/1347
3	C	0.28	0/8220	0.56	3/11139 (0.0%)
All	All	0.29	0/10941	0.56	3/14807 (0.0%)

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
3	C	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	414	PRO	CA-N-CD	-6.29	102.69	111.50
3	C	414	PRO	N-CA-CB	6.06	110.58	103.30
3	C	414	PRO	N-CD-CG	5.05	110.78	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	428	ARG	Sidechain
3	C	493	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	1671	0	1671	8	0
2	B	992	0	992	0	0
3	C	8064	0	8147	40	0
4	A	1	0	0	0	0
5	A	12	0	0	0	0
5	C	44	0	0	0	0
6	A	8	0	12	0	0
6	C	28	0	42	0	0
7	A	6	0	8	0	0
7	C	24	0	32	1	0
8	A	32	0	12	1	0
9	C	1	0	0	0	0
10	C	4	0	3	1	0
11	C	35	0	0	1	0
12	A	132	0	0	2	0
12	B	36	0	0	0	0
12	C	512	0	0	11	0
All	All	11602	0	10919	49	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 2.

The worst 5 of 49 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)
3:C:204:GLY:HA2	3:C:210:ILE:HD11	1.51	0.93
3:C:197[A]:CYS:SG	12:C:1273:HOH:O	2.36	0.82
3:C:503:HIS:O	3:C:507:THR:HG23	1.80	0.81
3:C:553:ARG:HG3	3:C:594:MET:HG2	1.62	0.81
3:C:556:MET:HE3	3:C:594:MET:CG	2.32	0.59

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	207/216 (96%)	201 (97%)	6 (3%)	0	100	100
2	B	119/140 (85%)	116 (98%)	3 (2%)	0	100	100
3	C	996/1003 (99%)	976 (98%)	19 (2%)	1 (0%)	51	64
All	All	1322/1359 (97%)	1293 (98%)	28 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	205	SER

### 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	180/184 (98%)	175 (97%)	5 (3%)	43	60
2	B	103/121 (85%)	102 (99%)	1 (1%)	76	87
3	C	913/915 (100%)	903 (99%)	10 (1%)	73	86
All	All	1196/1220 (98%)	1180 (99%)	16 (1%)	69	82

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	981	VAL
3	C	778	ARG

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Mol	Chain	Res	Type
3	C	278	PHE
3	C	666	SER
3	C	133	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	541	GLN
3	C	547	ASN
3	C	569	HIS
3	C	896	ASN
3	C	1010	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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

Of 33 ligands modelled in this entry, 2 are monoatomic - leaving 31 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	$\# Z  > 2$
6	DMS	C	1121	-	3,3,3	0.26	0	3,3,3	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	DMS	C	1125	-	3,3,3	0.32	0	3,3,3	0.10	0
7	GOL	A	305	-	5,5,5	0.10	0	5,5,5	0.30	0
5	NO3	C	1110	-	1,3,3	0.16	0	0,3,3	-	-
6	DMS	A	307	-	3,3,3	0.26	0	3,3,3	0.28	0
5	NO3	C	1119	-	1,3,3	0.00	0	0,3,3	-	-
6	DMS	A	303	-	3,3,3	0.25	0	3,3,3	0.05	0
5	NO3	C	1101	-	1,3,3	0.28	0	0,3,3	-	-
5	NO3	C	1103	-	1,3,3	0.19	0	0,3,3	-	-
7	GOL	C	1114	-	5,5,5	0.18	0	5,5,5	0.44	0
5	NO3	A	306	-	1,3,3	0.16	0	0,3,3	-	-
5	NO3	A	304	-	1,3,3	0.22	0	0,3,3	-	-
5	NO3	C	1111	-	1,3,3	0.03	0	0,3,3	-	-
5	NO3	C	1109	-	1,3,3	0.04	0	0,3,3	-	-
8	GTP	A	308	4	26,34,34	0.95	2 (7%)	32,54,54	0.76	1 (3%)
5	NO3	C	1117	-	1,3,3	0.08	0	0,3,3	-	-
7	GOL	C	1106	-	5,5,5	0.16	0	5,5,5	0.41	0
5	NO3	C	1112	-	1,3,3	0.02	0	0,3,3	-	-
5	NO3	C	1120	-	1,3,3	0.23	0	0,3,3	-	-
5	NO3	C	1105	-	1,3,3	0.06	0	0,3,3	-	-
7	GOL	C	1115	-	5,5,5	0.13	0	5,5,5	0.36	0
6	DMS	C	1113	-	3,3,3	0.24	0	3,3,3	0.09	0
6	DMS	C	1116	-	3,3,3	0.24	0	3,3,3	0.15	0
10	ACT	C	1122	-	3,3,3	0.95	0	3,3,3	1.00	0
5	NO3	C	1108	-	1,3,3	0.09	0	0,3,3	-	-
7	GOL	C	1104	-	5,5,5	0.13	0	5,5,5	0.38	0
6	DMS	C	1107	-	3,3,3	0.30	0	3,3,3	0.07	0
6	DMS	C	1123	-	3,3,3	0.27	0	3,3,3	0.08	0
6	DMS	C	1118	-	3,3,3	0.27	0	3,3,3	0.05	0
11	Q73	C	1124	-	32,35,35	0.61	0	27,46,46	2.04	5 (18%)
5	NO3	A	302	-	1,3,3	0.51	0	0,3,3	-	-

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
8	GTP	A	308	4	-	3/18/38/38	0/3/3/3
7	GOL	C	1106	-	-	2/4/4/4	-
7	GOL	C	1115	-	-	4/4/4/4	-
7	GOL	A	305	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	C	1104	-	-	4/4/4/4	-
7	GOL	C	1114	-	-	4/4/4/4	-
11	Q73	C	1124	-	-	9/31/50/50	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	308	GTP	C5-C6	-2.51	1.42	1.47
8	A	308	GTP	C8-N7	-2.29	1.31	1.35

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	1124	Q73	C16-C17-C19	-6.49	118.77	128.47
11	C	1124	Q73	C20-C19-C21	5.83	127.26	118.08
11	C	1124	Q73	C23-C22-C21	-2.73	118.82	125.19
11	C	1124	Q73	C9-C10-C11	-2.59	119.75	123.64
8	A	308	GTP	O6-C6-C5	2.17	128.61	124.37

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1104	GOL	O1-C1-C2-C3
7	C	1104	GOL	C1-C2-C3-O3
7	C	1106	GOL	O1-C1-C2-C3
7	C	1114	GOL	C1-C2-C3-O3
7	C	1115	GOL	C1-C2-C3-O3

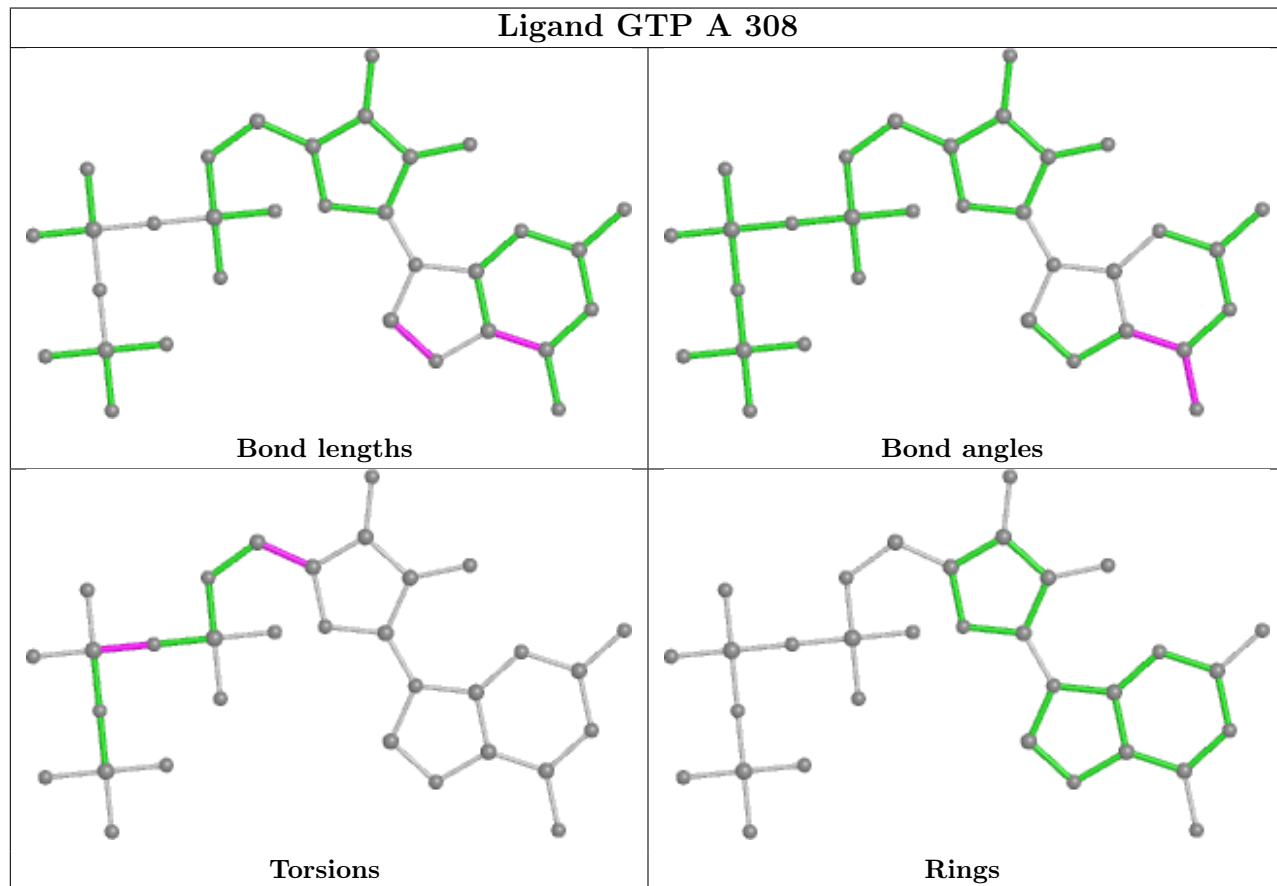
There are no ring outliers.

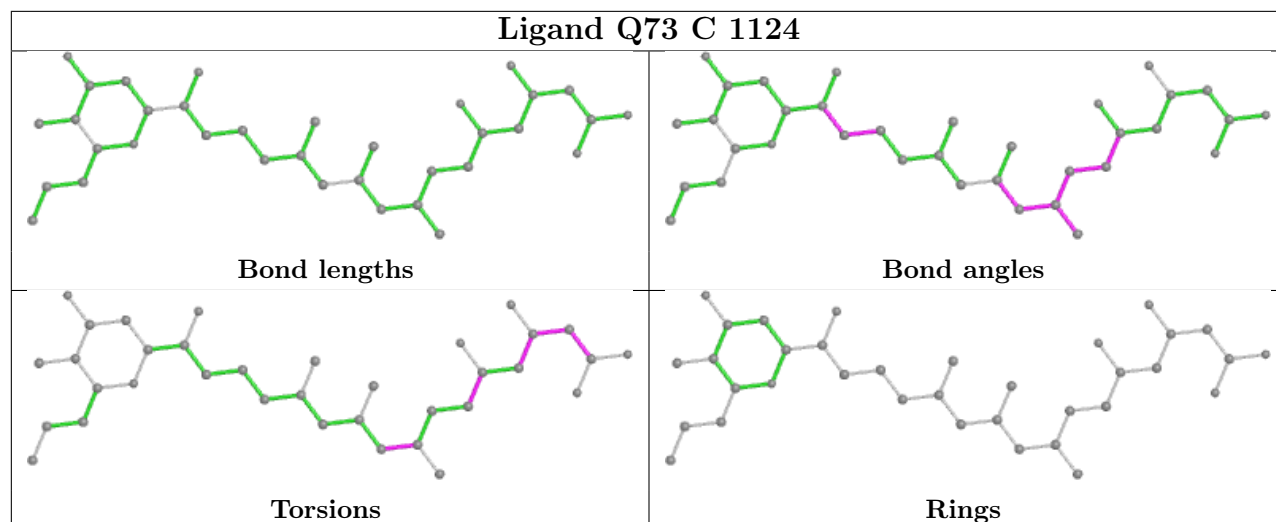
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	308	GTP	1	0
10	C	1122	ACT	1	0
7	C	1104	GOL	1	0
11	C	1124	Q73	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	208/216 (96%)	-0.13	7 (3%) 45 52	27, 39, 101, 136	0
2	B	121/140 (86%)	0.15	5 (4%) 37 44	39, 58, 93, 125	0
3	C	995/1003 (99%)	-0.34	11 (1%) 80 85	23, 41, 72, 118	0
All	All	1324/1359 (97%)	-0.26	23 (1%) 70 76	23, 42, 80, 136	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	VAL	4.0
2	B	81	GLU	4.0
3	C	979	ALA	3.7
3	C	543	ARG	3.7
2	B	80	GLU	3.3

### 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](#)

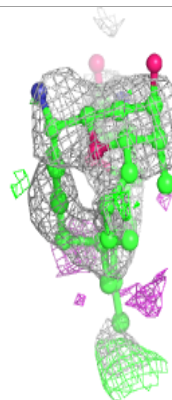
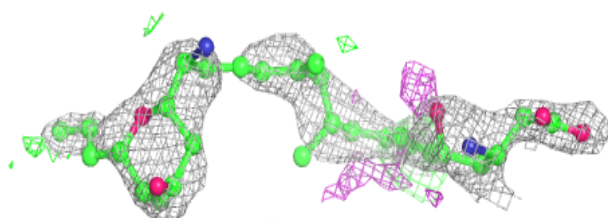
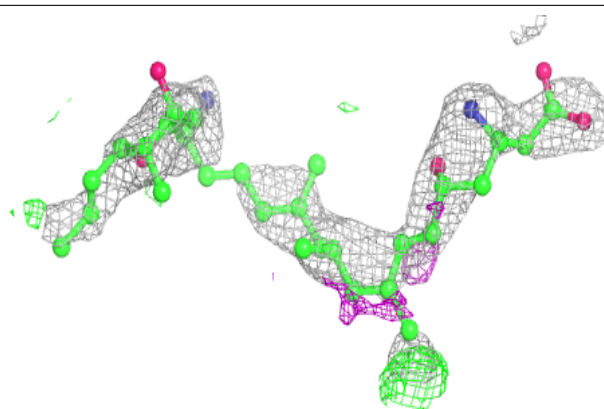
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	C	1115	6/6	-0.03	0.62	98,108,112,114	0
10	ACT	C	1122	4/4	0.52	0.24	53,54,59,65	0
7	GOL	C	1106	6/6	0.54	0.28	76,87,88,92	0
6	DMS	A	303	4/4	0.67	0.47	120,124,126,128	0
5	NO3	C	1110	4/4	0.67	0.27	68,73,80,82	0
6	DMS	C	1123	4/4	0.72	0.28	92,94,101,102	0
11	Q73	C	1124	35/35	0.75	0.35	66,85,98,98	0
7	GOL	C	1114	6/6	0.76	0.22	65,74,77,77	0
7	GOL	A	305	6/6	0.78	0.19	65,68,70,73	0
6	DMS	C	1113	4/4	0.84	0.35	113,120,122,125	0
6	DMS	C	1107	4/4	0.84	0.27	82,88,90,91	0
6	DMS	C	1116	4/4	0.85	0.33	105,106,108,112	0
6	DMS	C	1125	4/4	0.85	0.19	90,93,98,98	0
7	GOL	C	1104	6/6	0.86	0.19	53,64,66,68	0
5	NO3	C	1101	4/4	0.86	0.22	60,72,72,73	0
5	NO3	C	1119	4/4	0.87	0.20	60,63,69,76	0
5	NO3	C	1103	4/4	0.88	0.15	48,52,55,61	0
5	NO3	C	1117	4/4	0.88	0.63	73,79,83,90	0
6	DMS	C	1118	4/4	0.89	0.20	95,97,101,102	0
5	NO3	C	1112	4/4	0.89	0.18	54,62,62,63	0
5	NO3	C	1120	4/4	0.90	0.23	67,70,74,76	0
5	NO3	C	1111	4/4	0.90	0.21	58,62,67,70	0
6	DMS	A	307	4/4	0.90	0.23	75,76,77,81	0
5	NO3	C	1108	4/4	0.90	0.31	57,72,74,80	0
6	DMS	C	1121	4/4	0.91	0.55	107,111,112,113	0
5	NO3	C	1109	4/4	0.91	0.15	72,73,76,77	0
5	NO3	A	306	4/4	0.92	0.20	62,73,75,75	0
5	NO3	A	304	4/4	0.93	0.12	67,68,75,77	0
5	NO3	C	1105	4/4	0.94	0.23	74,75,78,80	0
5	NO3	A	302	4/4	0.97	0.13	35,40,41,48	0
9	CL	C	1102	1/1	0.98	0.20	56,56,56,56	0
8	GTP	A	308	32/32	0.99	0.11	28,32,35,39	0
4	MG	A	301	1/1	0.99	0.11	35,35,35,35	0

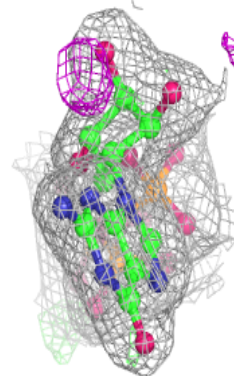
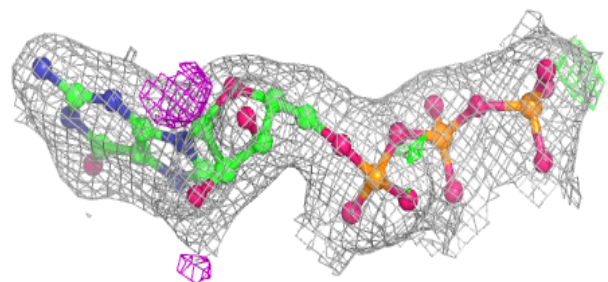
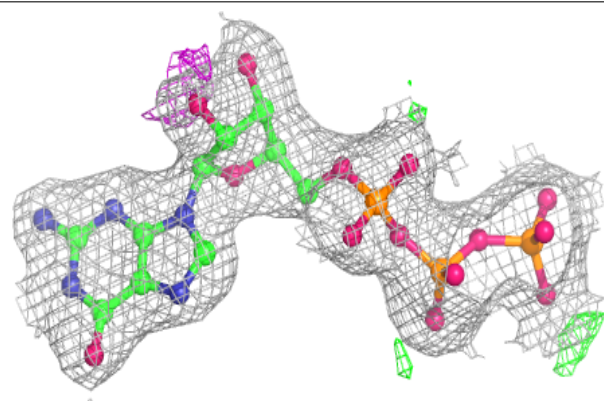
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around Q73 C 1124:**

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

**Electron density around GTP A 308:**

$2mF_o-DF_c$  (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.