



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 12:23 PM EDT

PDB ID : 4GMX  
Title : Crystal structure of KPT185 in complex with CRM1-Ran-RanBP1  
Authors : Sun, Q.; Chook, Y.M.  
Deposited on : 2012-08-16  
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

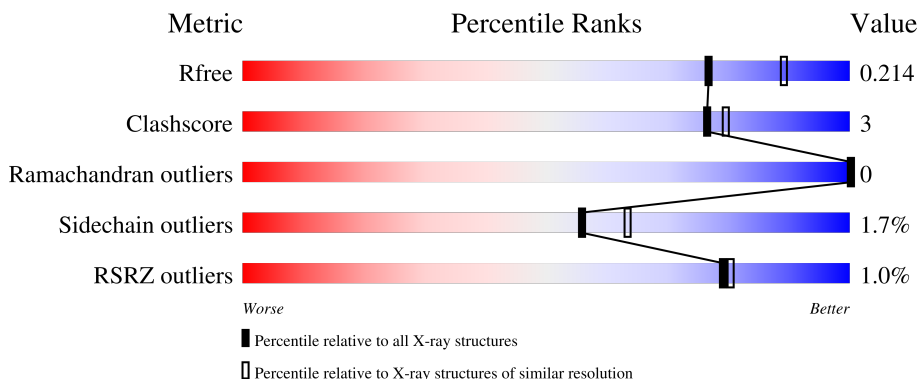
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

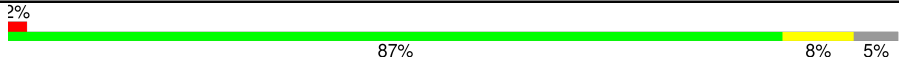
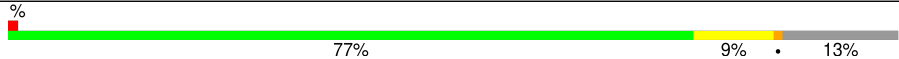

The reported resolution of this entry is 2.10 Å.

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))
$R_{free}$	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	216	
2	B	141	
3	C	1060	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12477 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
1	A	205	Total	C	N	O	S	0	3	0
			1672	1079	287	300	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	123	Total	C	N	O	S	0	3	0
			1031	652	179	195	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	61	SER	-	expression tag	UNP P41920

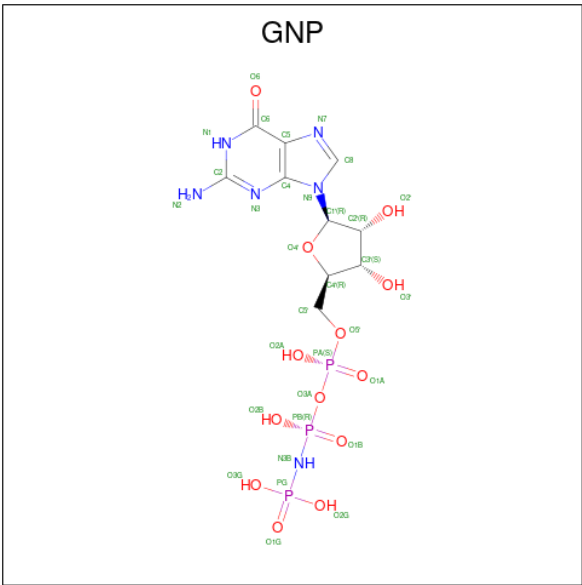
- Molecule 3 is a protein called Exportin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1015	Total	C	N	O	S	0	40	0
			8439	5437	1380	1579	43			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP P30822
C	0	ALA	-	expression tag	UNP P30822
C	539	CYS	THR	engineered mutation	UNP P30822
C	1022	CYS	TYR	conflict	UNP P30822

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

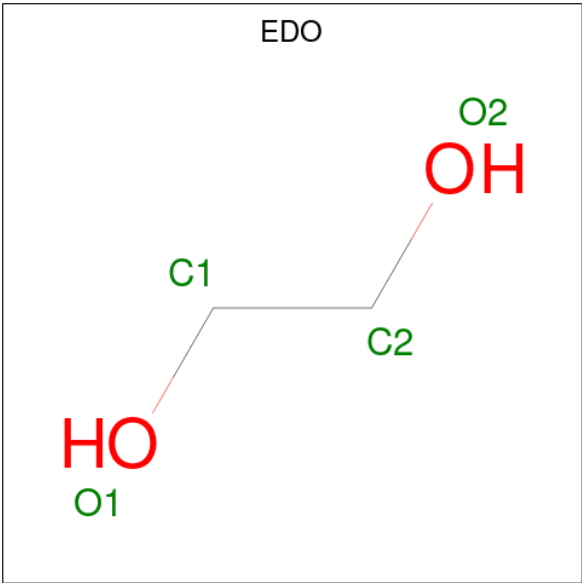


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

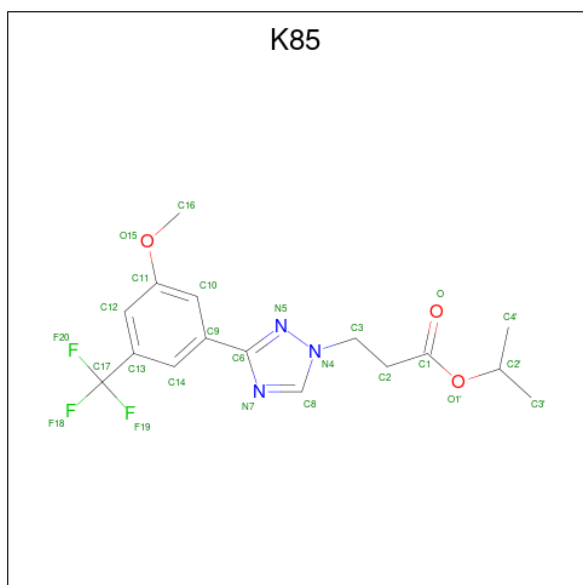
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 7 is propan-2-yl 3-{3-[3-methoxy-5-(trifluoromethyl)phenyl]-1H-1,2,4-triazol-1-yl} propanoate (three-letter code: K85) (formula: C<sub>16</sub>H<sub>18</sub>F<sub>3</sub>N<sub>3</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	F	N	O	0	0
			25	16	3	3	3		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	3	Total	Cl	0	0
			3	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	205	Total	O	0	0
			205	205		
10	B	65	Total	O	0	0
			65	65		

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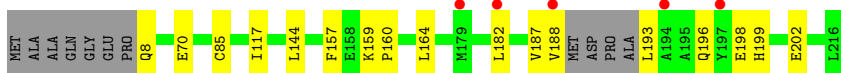
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	960	Total 960	O 960	0	0

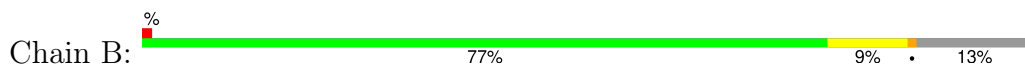
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

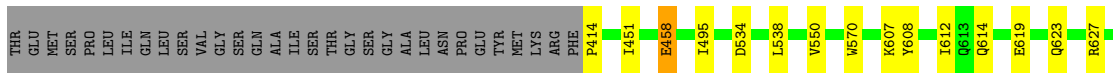
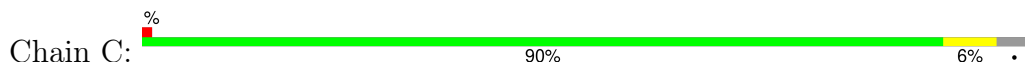
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: Ran-specific GTPase-activating protein 1



- Molecule 3: Exportin-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.49Å 106.49Å 306.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.10) 96.1 (50.00-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.148 , 0.197 0.177 , 0.214	Depositor DCC
$R_{free}$ test set	5003 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 53.2	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	0.97	EDS
Total number of atoms	12477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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: K85, MG, GNP, EDO, GOL, CL

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	0.45	0/1714	0.56	0/2319
2	B	0.41	0/1050	0.55	0/1399
3	C	0.50	1/8685 (0.0%)	0.50	0/11761
All	All	0.49	1/11449 (0.0%)	0.52	0/15479

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	376	GLU	C-N	26.84	1.85	1.34

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	1672	0	1679	6	0
2	B	1031	0	1031	8	0
3	C	8439	0	8592	49	0
4	A	32	0	13	0	0
5	A	1	0	0	0	0
6	A	4	0	6	0	0
6	C	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	25	0	16	0	0
8	C	36	0	48	0	0
9	C	3	0	0	0	0
10	A	205	0	0	1	0
10	B	65	0	0	0	0
10	C	960	0	0	4	0
All	All	12477	0	11391	63	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 (63) 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:376:GLU:C	3:C:414:PRO:N	1.85	1.28
3:C:627[B]:ARG:HG2	3:C:627[B]:ARG:HH11	1.04	1.07
3:C:627[B]:ARG:HG2	3:C:627[B]:ARG:NH1	1.84	0.90
3:C:627[B]:ARG:HH11	3:C:627[B]:ARG:CG	1.88	0.86
3:C:244:THR:HG22	3:C:285:GLN:OE1	1.87	0.75
3:C:458[A]:GLU:OE2	3:C:458[A]:GLU:HA	1.88	0.73
3:C:967:TYR:CZ	3:C:1019:THR:HG21	2.28	0.68
3:C:696:VAL:HG21	3:C:755[B]:LYS:HE3	1.81	0.63
3:C:328:ALA:HB3	10:C:1788:HOH:O	1.98	0.62
3:C:247:ASP:OD2	3:C:247:ASP:N	2.28	0.60
3:C:495:ILE:HD11	3:C:534:ASP:CG	2.22	0.59
1:A:193:LEU:HB3	1:A:196:GLN:HG2	1.85	0.58
3:C:967:TYR:CZ	3:C:1019:THR:CG2	2.86	0.58
2:B:168[B]:GLU:HA	2:B:168[B]:GLU:OE1	2.07	0.55
1:A:187:VAL:HG12	1:A:188:VAL:N	2.23	0.54
3:C:674:MET:O	3:C:678:THR:HG23	2.09	0.53
3:C:607:LYS:HG3	3:C:654:GLU:CG	2.38	0.53
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.90	0.52
3:C:119:ASP:OD2	3:C:154:ASN:ND2	2.43	0.51
3:C:627[B]:ARG:NH1	3:C:627[B]:ARG:CG	2.54	0.51
2:B:90:ARG:NH2	2:B:129:ASP:OD2	2.43	0.51
3:C:967:TYR:CE2	3:C:1019:THR:CG2	2.94	0.51
3:C:376:GLU:C	3:C:414:PRO:CA	2.76	0.51
3:C:607:LYS:HG3	3:C:654:GLU:HG3	1.94	0.50
3:C:755[B]:LYS:HA	3:C:755[B]:LYS:NZ	2.28	0.48
3:C:608:TYR:CE2	3:C:612:ILE:HD13	2.47	0.48
3:C:339:LEU:HA	3:C:342[B]:ASN:ND2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:293[B]:VAL:HG12	3:C:346:TYR:CE2	2.48	0.48
3:C:250:ALA:HB3	10:C:1764:HOH:O	2.14	0.48
2:B:78:THR:HG23	2:B:81:GLU:OE2	2.15	0.47
3:C:679:ILE:HD13	3:C:699:ILE:CG1	2.45	0.47
2:B:188:LYS:NZ	2:B:192:GLU:OE1	2.46	0.46
1:A:188:VAL:HG12	10:A:592:HOH:O	2.15	0.46
3:C:451:ILE:HG13	3:C:550:VAL:HG23	1.97	0.46
3:C:273:ARG:HA	3:C:273:ARG:HD3	1.66	0.45
3:C:699:ILE:HG21	3:C:731:LEU:HD21	1.98	0.45
3:C:696:VAL:HG11	3:C:755[B]:LYS:HZ1	1.82	0.45
3:C:967:TYR:CE2	3:C:1019:THR:HG21	2.51	0.45
3:C:238:LEU:O	3:C:252:THR:HG21	2.17	0.45
3:C:703[B]:ILE:HD13	3:C:766:ILE:HG13	1.99	0.44
3:C:141:LEU:C	3:C:141:LEU:HD23	2.37	0.44
1:A:85:CYS:HB2	1:A:164:LEU:HD22	2.00	0.44
3:C:204:GLY:HA3	3:C:210:ILE:HD11	2.00	0.44
2:B:85:VAL:HG22	2:B:114:LEU:CD2	2.47	0.44
3:C:240:THR:O	3:C:244:THR:HG23	2.17	0.43
2:B:197:ILE:O	2:B:200[A]:LYS:HG3	2.18	0.43
3:C:679:ILE:HD13	3:C:699:ILE:HG13	2.01	0.43
3:C:691:LEU:HG	3:C:738:MET:SD	2.59	0.42
3:C:325:ARG:NH2	10:C:1790:HOH:O	2.53	0.42
3:C:534:ASP:O	3:C:538:LEU:HD23	2.20	0.42
3:C:111[A]:GLN:HA	3:C:111[A]:GLN:OE1	2.19	0.42
3:C:864:LYS:NZ	3:C:868[A]:GLU:OE2	2.51	0.41
3:C:570:TRP:CE2	3:C:614:GLN:HG3	2.55	0.41
3:C:293[A]:VAL:HG23	10:C:1321:HOH:O	2.20	0.41
3:C:6:ASP:OD2	3:C:9:ASN:ND2	2.54	0.41
1:A:159:LYS:HB2	1:A:160:PRO:HD3	2.03	0.41
3:C:607:LYS:HD2	3:C:650:ILE:HG22	2.02	0.41
3:C:696:VAL:HG21	3:C:755[B]:LYS:CE	2.50	0.41
3:C:981:VAL:HG13	3:C:982:PRO:HD2	2.02	0.40
3:C:190:PHE:CZ	3:C:224:ILE:HG21	2.56	0.40
3:C:619:GLU:OE2	3:C:623[A]:GLN:NE2	2.54	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	204/216 (94%)	199 (98%)	5 (2%)	0	100	100
2	B	123/141 (87%)	118 (96%)	5 (4%)	0	100	100
3	C	1051/1060 (99%)	1033 (98%)	18 (2%)	0	100	100
All	All	1378/1417 (97%)	1350 (98%)	28 (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	181/185 (98%)	174 (96%)	7 (4%)	27	29
2	B	108/122 (88%)	102 (94%)	6 (6%)	17	16
3	C	966/964 (100%)	956 (99%)	10 (1%)	73	79
All	All	1255/1271 (99%)	1232 (98%)	23 (2%)	56	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	70	GLU
1	A	157	PHE
1	A	182	LEU
1	A	198	GLU

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Mol	Chain	Res	Type
1	A	199	HIS
1	A	202	GLU
2	B	78	THR
2	B	101	LYS
2	B	157	VAL
2	B	166	GLU
2	B	200[A]	LYS
2	B	200[B]	LYS
3	C	203	GLN
3	C	247	ASP
3	C	273	ARG
3	C	291	MET
3	C	458[A]	GLU
3	C	458[B]	GLU
3	C	682	GLN
3	C	940	PHE
3	C	981	VAL
3	C	1020	LYS

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

Mol	Chain	Res	Type
1	A	62	ASN
1	A	199	HIS
3	C	9	ASN
3	C	30	GLN
3	C	56	GLN
3	C	233	ASN
3	C	434	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 [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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
8	GOL	C	1104	-	5,5,5	0.32	0	5,5,5	0.16	0
6	EDO	A	303	-	3,3,3	0.49	0	2,2,2	0.18	0
7	K85	C	1101	3	25,26,26	0.97	1 (4%)	34,37,37	4.05	5 (14%)
8	GOL	C	1103	-	5,5,5	0.36	0	5,5,5	0.16	0
8	GOL	C	1105	-	5,5,5	0.46	0	5,5,5	0.72	0
6	EDO	C	1107	-	3,3,3	0.48	0	2,2,2	0.33	0
8	GOL	C	1106	-	5,5,5	0.38	0	5,5,5	0.33	0
8	GOL	C	1102	-	5,5,5	0.36	0	5,5,5	0.26	0
8	GOL	C	1111	-	5,5,5	0.38	0	5,5,5	0.32	0
4	GNP	A	301	5	29,34,34	1.58	4 (13%)	33,54,54	1.89	7 (21%)

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	GOL	C	1104	-	-	4/4/4/4	-
6	EDO	A	303	-	-	0/1/1/1	-
7	K85	C	1101	3	-	4/21/21/21	0/2/2/2
8	GOL	C	1103	-	-	2/4/4/4	-
8	GOL	C	1105	-	-	2/4/4/4	-
6	EDO	C	1107	-	-	0/1/1/1	-
8	GOL	C	1106	-	-	0/4/4/4	-
8	GOL	C	1102	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GOL	C	1111	-	-	3/4/4/4	-
4	GNP	A	301	5	-	3/14/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1101	K85	O1'-C1	4.11	1.45	1.34
4	A	301	GNP	PG-N3B	4.00	1.73	1.63
4	A	301	GNP	C5-C6	3.92	1.48	1.41
4	A	301	GNP	PB-N3B	3.91	1.73	1.63
4	A	301	GNP	PB-O3A	2.08	1.61	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1101	K85	C8-N7-C6	21.24	109.42	101.63
7	C	1101	K85	N5-C6-N7	-7.03	108.89	114.72
4	A	301	GNP	C2-N3-C4	4.80	120.66	115.48
4	A	301	GNP	C2-N1-C6	4.74	122.55	115.96
4	A	301	GNP	C5-C6-N1	-4.09	117.95	123.42
7	C	1101	K85	N7-C8-N4	-4.07	106.42	112.33
4	A	301	GNP	N3-C2-N1	-3.57	122.67	127.21
4	A	301	GNP	O1G-PG-N3B	-3.17	107.10	111.77
7	C	1101	K85	O1'-C1-C2	3.08	118.14	111.48
7	C	1101	K85	C3-C2-C1	-2.86	110.48	114.67
4	A	301	GNP	C4-C5-C6	-2.84	116.90	121.23
4	A	301	GNP	C4-C5-N7	-2.34	106.86	109.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	GNP	PG-N3B-PB-O1B
8	C	1102	GOL	O1-C1-C2-C3
8	C	1104	GOL	C1-C2-C3-O3
8	C	1104	GOL	O2-C2-C3-O3
8	C	1105	GOL	C1-C2-C3-O3
8	C	1111	GOL	O1-C1-C2-C3
8	C	1102	GOL	C1-C2-C3-O3
8	C	1103	GOL	O1-C1-C2-C3
8	C	1111	GOL	C1-C2-C3-O3

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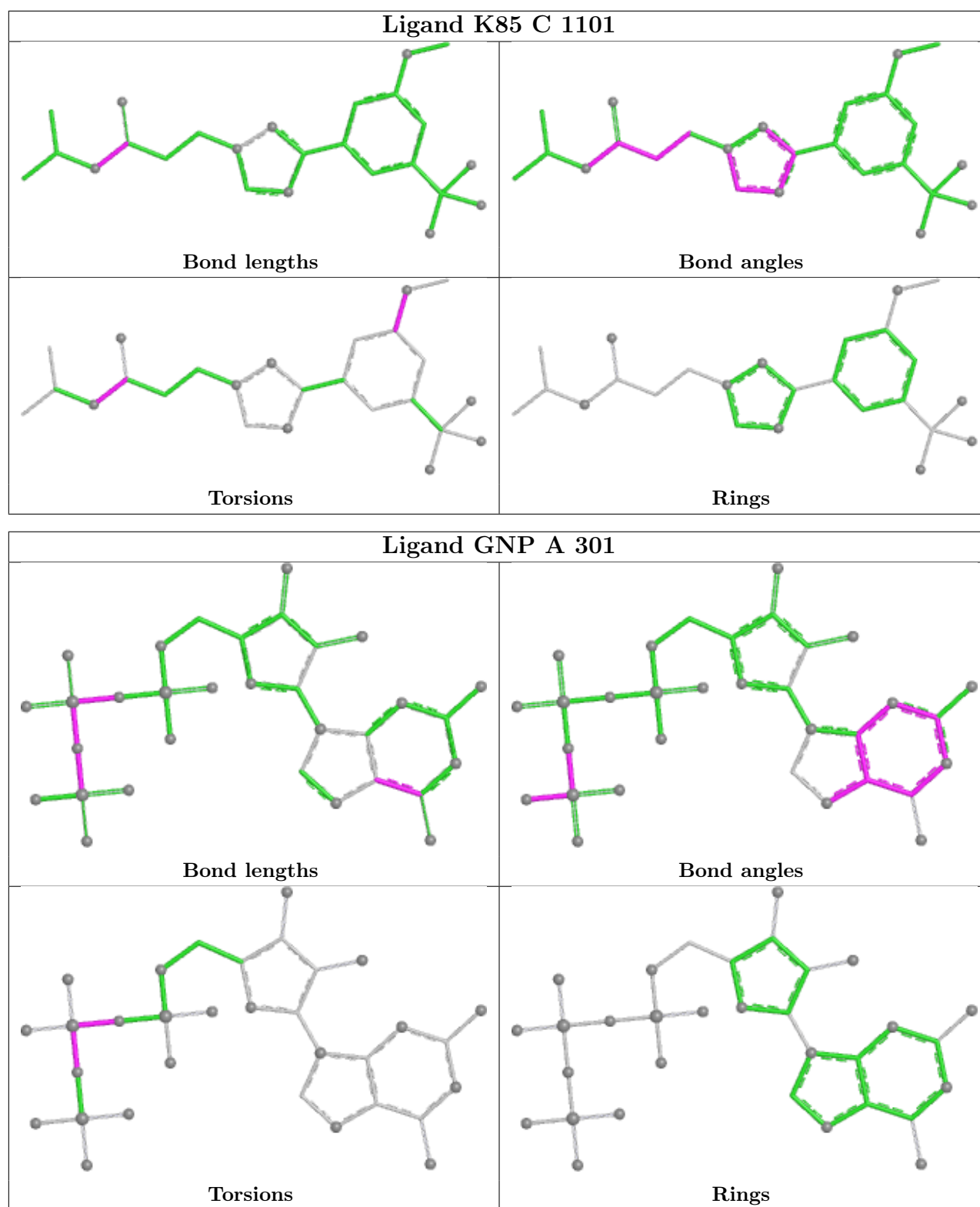
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Mol	Chain	Res	Type	Atoms
8	C	1102	GOL	O1-C1-C2-O2
8	C	1103	GOL	O1-C1-C2-O2
8	C	1105	GOL	O2-C2-C3-O3
8	C	1111	GOL	O1-C1-C2-O2
7	C	1101	K85	C10-C11-O15-C16
7	C	1101	K85	C12-C11-O15-C16
7	C	1101	K85	C2-C1-O1'-C2'
7	C	1101	K85	O-C1-O1'-C2'
8	C	1104	GOL	O1-C1-C2-O2
4	A	301	GNP	PA-O3A-PB-O2B
8	C	1104	GOL	O1-C1-C2-C3
4	A	301	GNP	PA-O3A-PB-O1B

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	205/216 (94%)	-0.35	5 (2%)	59 61	12, 30, 64, 98	3 (1%)
2	B	123/141 (87%)	-0.19	2 (1%)	70 71	16, 37, 53, 76	3 (2%)
3	C	1015/1060 (95%)	-0.44	6 (0%)	85 86	12, 33, 58, 85	40 (3%)
All	All	1343/1417 (94%)	-0.40	13 (0%)	79 80	12, 33, 58, 98	46 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	687	PRO	4.1
3	C	690	LEU	3.9
2	B	200[A]	LYS	3.8
2	B	79	MET	3.5
3	C	691	LEU	3.5
3	C	204	GLY	3.1
1	A	188	VAL	3.0
1	A	194	ALA	3.0
3	C	979	ALA	2.4
1	A	179	MET	2.3
1	A	197	TYR	2.2
1	A	182	LEU	2.1
3	C	1024	ASP	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands

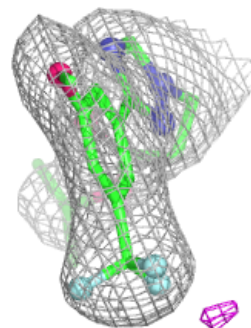
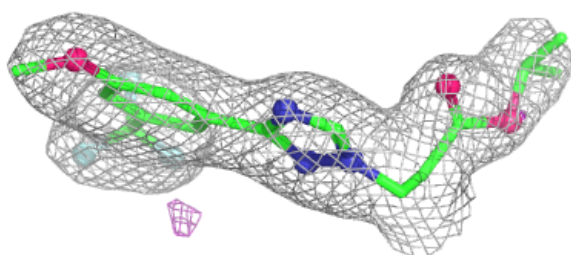
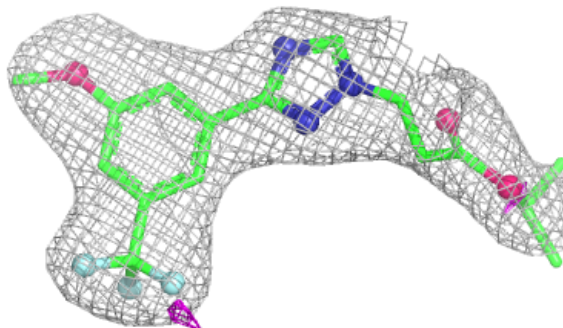
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
8	GOL	C	1105	6/6	0.82	0.15	68,75,80,81	0
8	GOL	C	1111	6/6	0.82	0.10	56,69,75,77	0
8	GOL	C	1106	6/6	0.83	0.17	58,69,75,76	0
8	GOL	C	1103	6/6	0.84	0.09	72,80,83,89	0
6	EDO	C	1107	4/4	0.87	0.18	58,59,61,70	0
6	EDO	A	303	4/4	0.89	0.21	59,65,66,69	0
8	GOL	C	1102	6/6	0.89	0.11	62,66,71,77	0
8	GOL	C	1104	6/6	0.94	0.11	59,62,63,66	0
7	K85	C	1101	25/25	0.95	0.07	37,42,57,61	0
9	CL	C	1110	1/1	0.95	0.12	89,89,89,89	0
9	CL	C	1109	1/1	0.96	0.09	66,66,66,66	0
9	CL	C	1108	1/1	0.96	0.07	71,71,71,71	0
5	MG	A	302	1/1	0.98	0.04	25,25,25,25	0
4	GNP	A	301	32/32	0.99	0.04	24,27,29,30	0

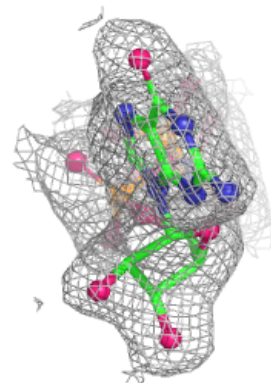
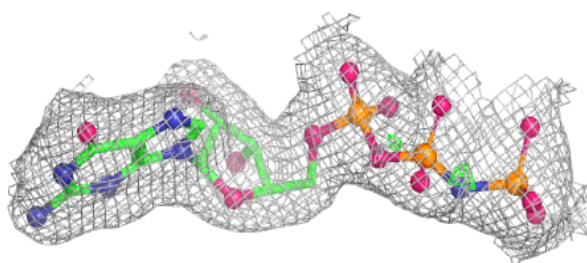
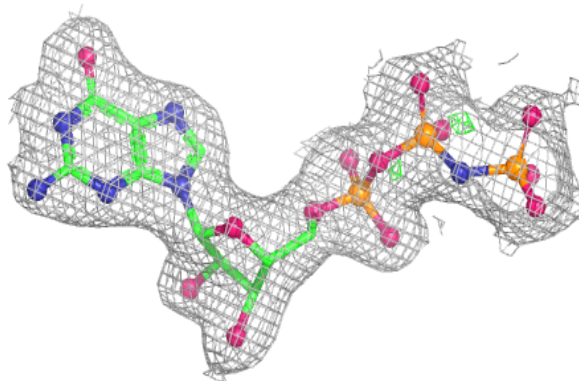
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around K85 C 1101:**

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

**Electron density around GNP A 301:**

$2mF_o-DF_c$  (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.