



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 2, 2024 – 08:46 PM EST

PDB ID : 9FMR
Title : Structure of DDB1/Cdk12/Cyclin K with molecular glue SR-4835
Authors : Anand, K.; Schmitz, M.; Geyer, M.
Deposited on : 2024-06-07
Resolution : 3.90 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

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>.

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)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

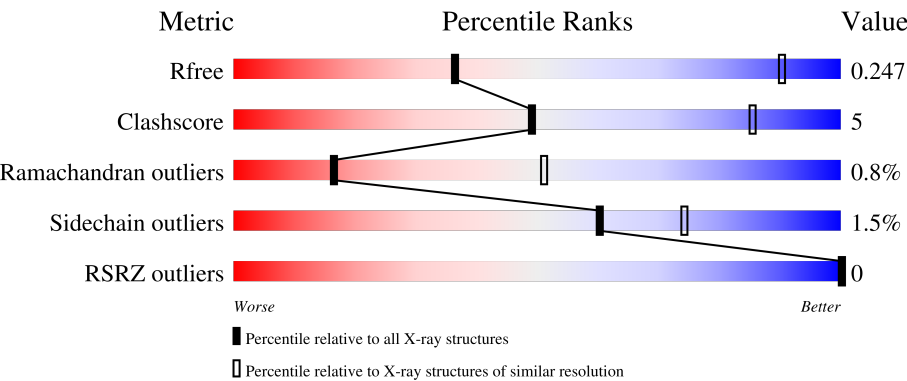
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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	1157 (4.10-3.70)
Clashscore	180529	1219 (4.10-3.70)
Ramachandran outliers	177936	1177 (4.10-3.70)
Sidechain outliers	177891	1169 (4.10-3.70)
RSRZ outliers	164620	1157 (4.10-3.70)

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 ≥ 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	864	<div><div>83%</div><div>12%</div><div></div></div>
1	D	864	<div><div>80%</div><div>16%</div><div></div></div>
1	G	864	<div><div>79%</div><div>17%</div><div></div></div>
2	B	351	<div><div>76%</div><div>17%</div><div>5%</div></div>
2	E	351	<div><div>75%</div><div>17%</div><div>6%</div></div>
2	H	351	<div><div>80%</div><div>13%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
3	C	268	<div><div></div><div>85%</div><div><div></div><div>7%</div><div>7%</div></div></div>
3	F	268	<div><div></div><div>78%</div><div><div></div><div>13%</div><div>7%</div></div></div>
3	I	268	<div><div></div><div>84%</div><div><div></div><div>9%</div><div>7%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33885 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	827	Total	C	N	O	S	0	0	0
			6495	4111	1095	1253	36			
1	D	826	Total	C	N	O	S	36	0	0
			6487	4105	1094	1252	36			
1	G	826	Total	C	N	O	S	0	0	0
			6486	4106	1093	1251	36			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP Q16531
A	-26	GLY	-	expression tag	UNP Q16531
A	-25	SER	-	expression tag	UNP Q16531
A	-24	SER	-	expression tag	UNP Q16531
A	-23	HIS	-	expression tag	UNP Q16531
A	-22	HIS	-	expression tag	UNP Q16531
A	-21	HIS	-	expression tag	UNP Q16531
A	-20	HIS	-	expression tag	UNP Q16531
A	-19	HIS	-	expression tag	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	SER	-	expression tag	UNP Q16531
A	-16	ALA	-	expression tag	UNP Q16531
A	-15	ALA	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	ILE	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	MET	-	expression tag	UNP Q16531
A	-10	VAL	-	expression tag	UNP Q16531
A	-9	ASP	-	expression tag	UNP Q16531
A	-8	ALA	-	expression tag	UNP Q16531
A	-7	TYR	-	expression tag	UNP Q16531
A	-6	LYS	-	expression tag	UNP Q16531
A	-5	PRO	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	THR	-	expression tag	UNP Q16531
A	-3	LYS	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
A	392	ASN	-	linker	UNP Q16531
A	393	GLY	-	linker	UNP Q16531
A	394	ILE	-	linker	UNP Q16531
A	699	GLY	-	linker	UNP Q16531
A	700	GLY	-	linker	UNP Q16531
A	701	ASN	-	linker	UNP Q16531
A	702	GLY	-	linker	UNP Q16531
A	703	ASN	-	linker	UNP Q16531
A	704	SER	-	linker	UNP Q16531
A	705	GLY	-	linker	UNP Q16531
A	706	GLU	-	linker	UNP Q16531
A	707	ILE	-	linker	UNP Q16531
D	-27	MET	-	initiating methionine	UNP Q16531
D	-26	GLY	-	expression tag	UNP Q16531
D	-25	SER	-	expression tag	UNP Q16531
D	-24	SER	-	expression tag	UNP Q16531
D	-23	HIS	-	expression tag	UNP Q16531
D	-22	HIS	-	expression tag	UNP Q16531
D	-21	HIS	-	expression tag	UNP Q16531
D	-20	HIS	-	expression tag	UNP Q16531
D	-19	HIS	-	expression tag	UNP Q16531
D	-18	HIS	-	expression tag	UNP Q16531
D	-17	SER	-	expression tag	UNP Q16531
D	-16	ALA	-	expression tag	UNP Q16531
D	-15	ALA	-	expression tag	UNP Q16531
D	-14	HIS	-	expression tag	UNP Q16531
D	-13	ILE	-	expression tag	UNP Q16531
D	-12	VAL	-	expression tag	UNP Q16531
D	-11	MET	-	expression tag	UNP Q16531
D	-10	VAL	-	expression tag	UNP Q16531
D	-9	ASP	-	expression tag	UNP Q16531
D	-8	ALA	-	expression tag	UNP Q16531
D	-7	TYR	-	expression tag	UNP Q16531
D	-6	LYS	-	expression tag	UNP Q16531
D	-5	PRO	-	expression tag	UNP Q16531
D	-4	THR	-	expression tag	UNP Q16531
D	-3	LYS	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531
D	392	ASN	-	linker	UNP Q16531
D	393	GLY	-	linker	UNP Q16531
D	698	ILE	-	linker	UNP Q16531
D	699	GLY	-	linker	UNP Q16531
D	700	GLY	-	linker	UNP Q16531
D	701	ASN	-	linker	UNP Q16531
D	702	GLY	-	linker	UNP Q16531
D	703	ASN	-	linker	UNP Q16531
D	704	SER	-	linker	UNP Q16531
D	705	GLY	-	linker	UNP Q16531
D	706	GLU	-	linker	UNP Q16531
D	707	ILE	-	linker	UNP Q16531
G	-27	MET	-	initiating methionine	UNP Q16531
G	-26	GLY	-	expression tag	UNP Q16531
G	-25	SER	-	expression tag	UNP Q16531
G	-24	SER	-	expression tag	UNP Q16531
G	-23	HIS	-	expression tag	UNP Q16531
G	-22	HIS	-	expression tag	UNP Q16531
G	-21	HIS	-	expression tag	UNP Q16531
G	-20	HIS	-	expression tag	UNP Q16531
G	-19	HIS	-	expression tag	UNP Q16531
G	-18	HIS	-	expression tag	UNP Q16531
G	-17	SER	-	expression tag	UNP Q16531
G	-16	ALA	-	expression tag	UNP Q16531
G	-15	ALA	-	expression tag	UNP Q16531
G	-14	HIS	-	expression tag	UNP Q16531
G	-13	ILE	-	expression tag	UNP Q16531
G	-12	VAL	-	expression tag	UNP Q16531
G	-11	MET	-	expression tag	UNP Q16531
G	-10	VAL	-	expression tag	UNP Q16531
G	-9	ASP	-	expression tag	UNP Q16531
G	-8	ALA	-	expression tag	UNP Q16531
G	-7	TYR	-	expression tag	UNP Q16531
G	-6	LYS	-	expression tag	UNP Q16531
G	-5	PRO	-	expression tag	UNP Q16531
G	-4	THR	-	expression tag	UNP Q16531
G	-3	LYS	-	expression tag	UNP Q16531
G	-2	GLY	-	expression tag	UNP Q16531
G	-1	GLY	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	ARG	-	expression tag	UNP Q16531
G	392	ASN	-	linker	UNP Q16531
G	393	GLY	-	linker	UNP Q16531
G	394	ILE	-	linker	UNP Q16531
G	699	GLY	-	linker	UNP Q16531
G	700	GLY	-	linker	UNP Q16531
G	701	ASN	-	linker	UNP Q16531
G	702	GLY	-	linker	UNP Q16531
G	703	ASN	-	linker	UNP Q16531
G	704	SER	-	linker	UNP Q16531
G	705	GLY	-	linker	UNP Q16531
G	706	GLU	-	linker	UNP Q16531
G	707	ILE	-	linker	UNP Q16531

- Molecule 2 is a protein called Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	335	Total	C	N	O	P	S	0	0	0
			2733	1751	464	500	1	17			
2	E	330	Total	C	N	O	P	S	0	0	0
			2684	1719	453	494	1	17			
2	H	332	Total	C	N	O	P	S	11	0	0
			2704	1733	456	497	1	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	713	GLY	-	expression tag	UNP Q9NYV4
E	713	GLY	-	expression tag	UNP Q9NYV4
H	713	GLY	-	expression tag	UNP Q9NYV4

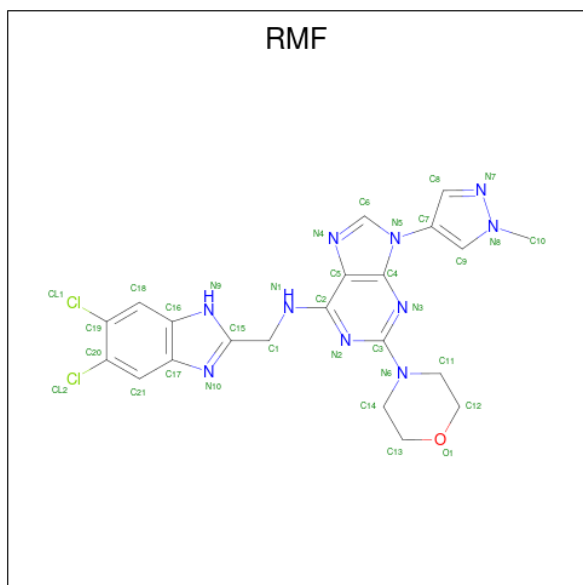
- Molecule 3 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S		0	0	0
			2063	1341	346	363	13				
3	F	248	Total	C	N	O	S		0	0	0
			2063	1341	346	363	13				
3	I	248	Total	C	N	O	S		0	0	0
			2063	1341	346	363	13				

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	expression tag	UNP O75909
F	0	GLY	-	expression tag	UNP O75909
I	0	GLY	-	expression tag	UNP O75909

- Molecule 4 is {N}-[[5,6-bis(chloranyl)-1 {H}-benzimidazol-2-yl]methyl]-9-(1-methylpyrazol-4-yl)-2-morpholin-4-yl-purin-6-amine (three-letter code: RMF) (formula: C₂₁H₂₀Cl₂N₁₀O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			34	21	2	10	1		
4	E	1	Total	C	Cl	N	O	0	0
			34	21	2	10	1		
4	H	1	Total	C	Cl	N	O	0	0
			34	21	2	10	1		

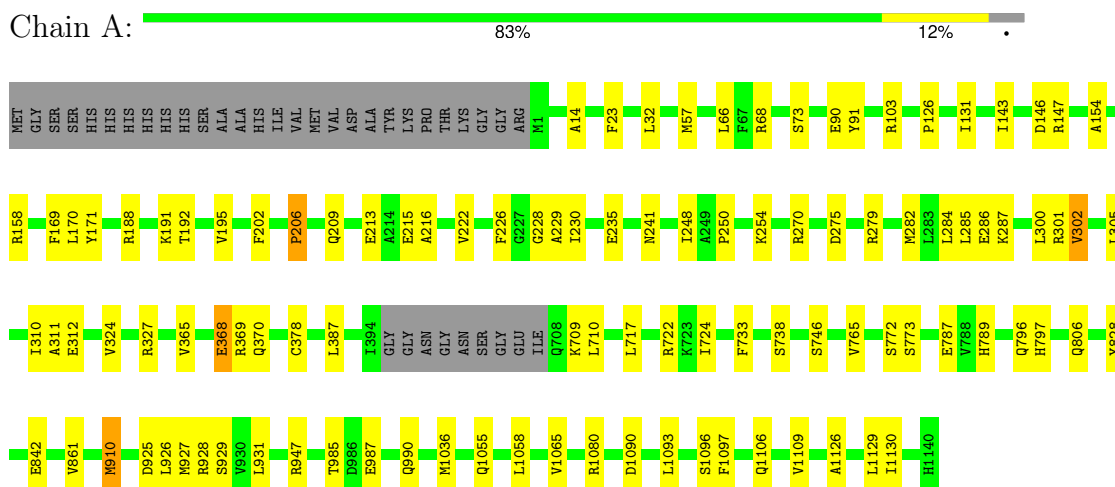
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	F	1	Total	O	0	0
			1	1		
5	I	2	Total	O	0	0
			2	2		

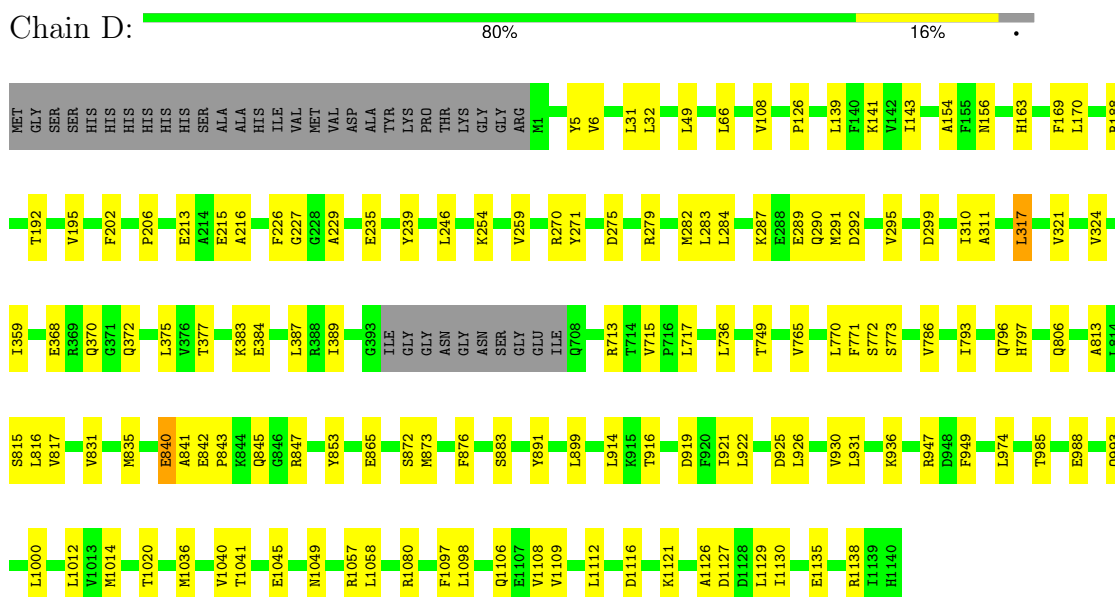
3 Residue-property plots [i](#)

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. 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. 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.

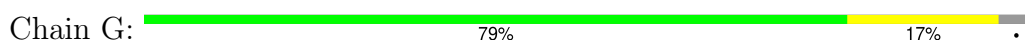
- Molecule 1: DNA damage-binding protein 1

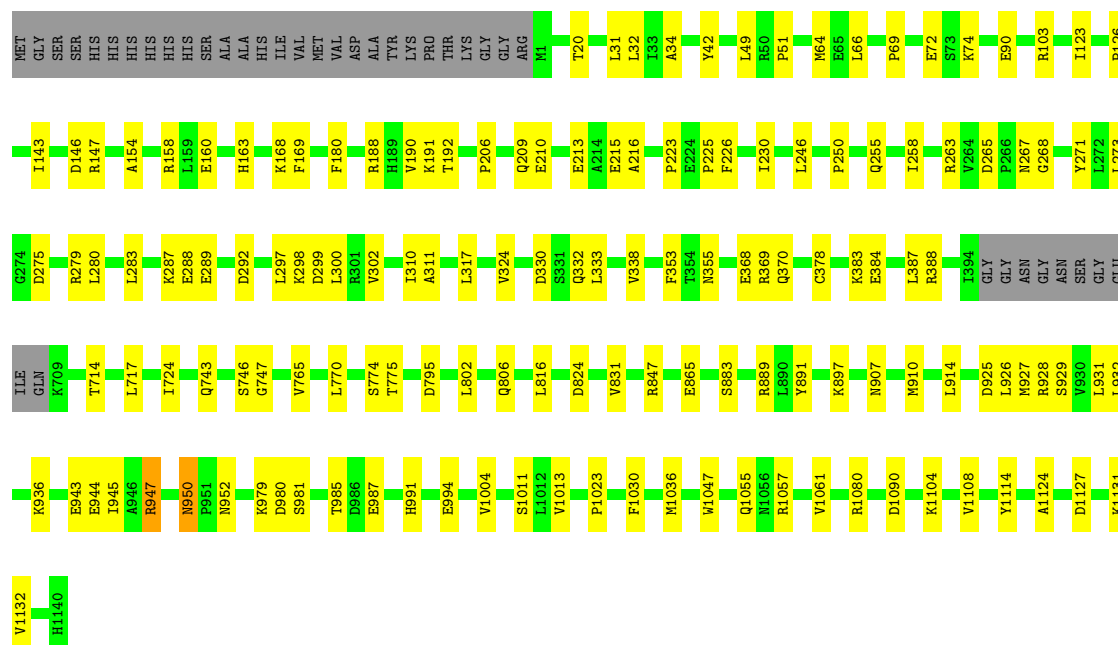


- Molecule 1: DNA damage-binding protein 1



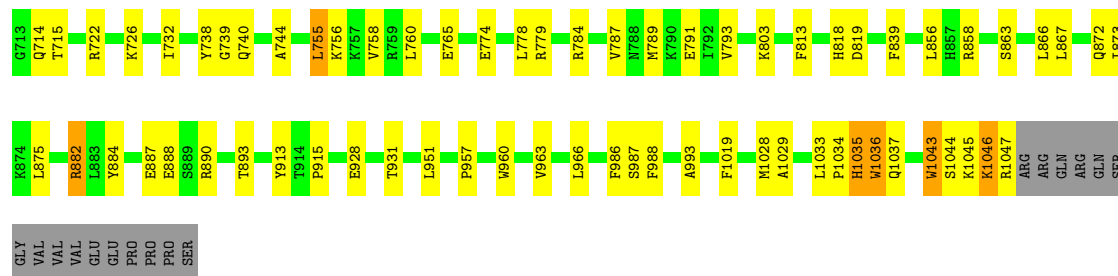
- Molecule 1: DNA damage-binding protein 1





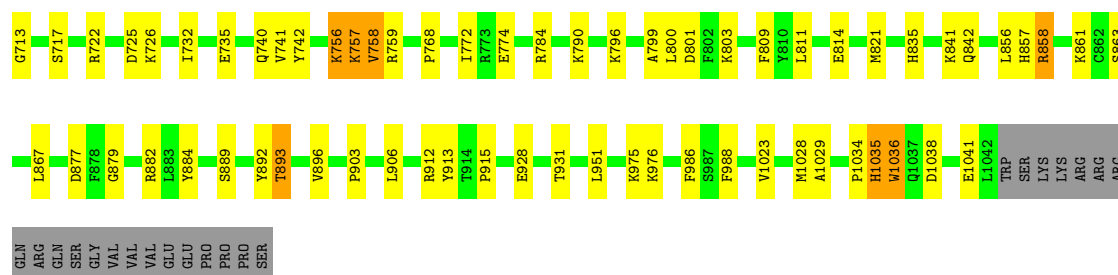
• Molecule 2: Cyclin-dependent kinase 12

Chain B: 76% 17% • 5%



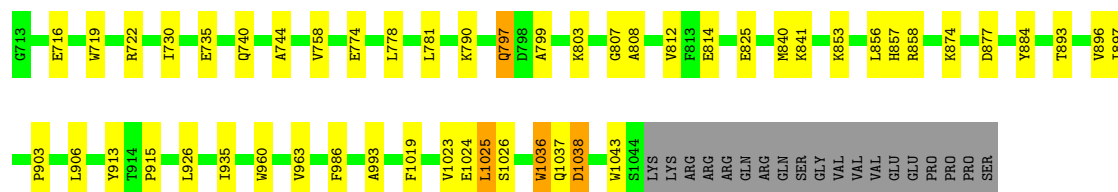
• Molecule 2: Cyclin-dependent kinase 12

Chain E: 75% 17% • 6%



• Molecule 2: Cyclin-dependent kinase 12

Chain H: 80% 13% • 5%



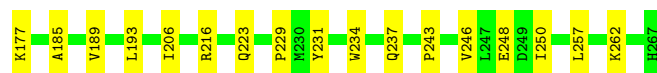
- Molecule 3: Cyclin-K

Chain C: 85% 7% • 7%



- Molecule 3: Cyclin-K

Chain F: 78% 13% • 7%



- Molecule 3: Cyclin-K

Chain I: 84% 9% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	249.52Å 249.52Å 218.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.71 – 3.90 36.71 – 3.90	Depositor EDS
% Data completeness (in resolution range)	89.1 (36.71-3.90) 78.2 (36.71-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.64 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.208 , 0.250 0.208 , 0.247	Depositor DCC
R_{free} test set	69699 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 204.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33885	wwPDB-VP
Average B, all atoms (Å ²)	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: RMF, TPO

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	0.25	0/6612	0.50	0/8942
1	D	0.25	0/6604	0.50	0/8931
1	G	0.25	0/6603	0.50	0/8930
2	B	0.25	0/2783	0.49	0/3749
2	E	0.25	0/2732	0.48	0/3682
2	H	0.29	0/2754	0.50	0/3713
3	C	0.26	0/2120	0.44	0/2868
3	F	0.24	0/2120	0.42	0/2868
3	I	0.24	0/2120	0.43	0/2868
All	All	0.25	0/34448	0.48	0/46551

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6495	0	6464	61	0
1	D	6487	0	6451	78	0
1	G	6486	0	6454	80	0
2	B	2733	0	2752	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2684	0	2698	38	0
2	H	2704	0	2713	31	0
3	C	2063	0	2048	16	0
3	F	2063	0	2048	24	0
3	I	2063	0	2048	13	0
4	B	34	0	0	0	0
4	E	34	0	0	0	0
4	H	34	0	0	2	0
5	A	2	0	0	0	0
5	F	1	0	0	1	0
5	I	2	0	0	0	0
All	All	33885	0	33676	356	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 5.

The worst 5 of 356 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:947:ARG:NH1	4:H:1101:RMF:CL1	2.51	0.81
3:C:231:TYR:HA	3:C:232:ARG:NH2	1.98	0.78
1:A:927:MET:O	1:A:929:SER:N	2.19	0.75
1:D:1109:VAL:HG11	1:D:1126:ALA:HA	1.71	0.73
1:D:317:LEU:HB2	1:D:321:VAL:HG23	1.71	0.73

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	823/864 (95%)	785 (95%)	34 (4%)	4 (0%)	25 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	822/864 (95%)	782 (95%)	34 (4%)	6 (1%)	19	54
1	G	822/864 (95%)	782 (95%)	34 (4%)	6 (1%)	19	54
2	B	332/351 (95%)	310 (93%)	16 (5%)	6 (2%)	7	35
2	E	327/351 (93%)	306 (94%)	13 (4%)	8 (2%)	5	30
2	H	329/351 (94%)	311 (94%)	15 (5%)	3 (1%)	14	48
3	C	246/268 (92%)	243 (99%)	3 (1%)	0	100	100
3	F	246/268 (92%)	243 (99%)	3 (1%)	0	100	100
3	I	246/268 (92%)	242 (98%)	4 (2%)	0	100	100
All	All	4193/4449 (94%)	4004 (96%)	156 (4%)	33 (1%)	16	51

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	ARG
1	A	928	ARG
1	D	291	MET
1	D	1121	LYS
1	G	929	SER

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	722/749 (96%)	718 (99%)	4 (1%)	84	88
1	D	721/749 (96%)	712 (99%)	9 (1%)	67	78
1	G	721/749 (96%)	711 (99%)	10 (1%)	62	75
2	B	301/316 (95%)	288 (96%)	13 (4%)	25	49
2	E	296/316 (94%)	290 (98%)	6 (2%)	50	68
2	H	298/316 (94%)	293 (98%)	5 (2%)	56	72
3	C	223/241 (92%)	221 (99%)	2 (1%)	75	83
3	F	223/241 (92%)	218 (98%)	5 (2%)	47	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	I	223/241 (92%)	220 (99%)	3 (1%)	65 76
All	All	3728/3918 (95%)	3671 (98%)	57 (2%)	60 74

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	742	TYR
3	I	231	TYR
3	F	92	ARG
3	I	28	LYS
2	H	722	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	727	GLN
2	H	944	GLN
3	I	253	GLN
2	B	740	GLN
1	A	789	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TPO	H	893	2	8,10,11	1.12	0	10,14,16	1.97	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TPO	B	893	2	8,10,11	1.19	0	10,14,16	1.81	2 (20%)
2	TPO	E	893	2	8,10,11	1.15	0	10,14,16	2.00	2 (20%)

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	TPO	H	893	2	-	0/9/11/13	-
2	TPO	B	893	2	-	0/9/11/13	-
2	TPO	E	893	2	-	0/9/11/13	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	893	TPO	P-OG1-CB	-5.52	108.34	123.33
2	E	893	TPO	P-OG1-CB	-5.51	108.36	123.33
2	B	893	TPO	P-OG1-CB	-4.73	110.48	123.33
2	B	893	TPO	CG2-CB-CA	-2.23	108.91	113.26
2	E	893	TPO	CG2-CB-CA	-2.06	109.25	113.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	893	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
4	RMF	H	1101	-	32,39,39	2.15	7 (21%)	32,57,57	2.47	12 (37%)
4	RMF	B	1101	-	32,39,39	2.16	8 (25%)	32,57,57	2.46	12 (37%)
4	RMF	E	1101	-	32,39,39	2.10	8 (25%)	32,57,57	2.43	11 (34%)

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
4	RMF	H	1101	-	-	2/7/21/21	0/6/6/6
4	RMF	B	1101	-	-	5/7/21/21	0/6/6/6
4	RMF	E	1101	-	-	4/7/21/21	0/6/6/6

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1101	RMF	C2-N1	7.13	1.46	1.34
4	H	1101	RMF	C2-N1	7.04	1.46	1.34
4	E	1101	RMF	C2-N1	6.75	1.45	1.34
4	B	1101	RMF	C3-N6	4.97	1.46	1.35
4	H	1101	RMF	C3-N6	4.89	1.45	1.35

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1101	RMF	C8-N7-N8	5.49	109.95	104.23
4	B	1101	RMF	C8-N7-N8	5.39	109.84	104.23
4	E	1101	RMF	C12-C11-N6	5.38	120.10	109.93
4	E	1101	RMF	C8-N7-N8	5.31	109.76	104.23
4	B	1101	RMF	C12-C11-N6	5.29	119.94	109.93

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

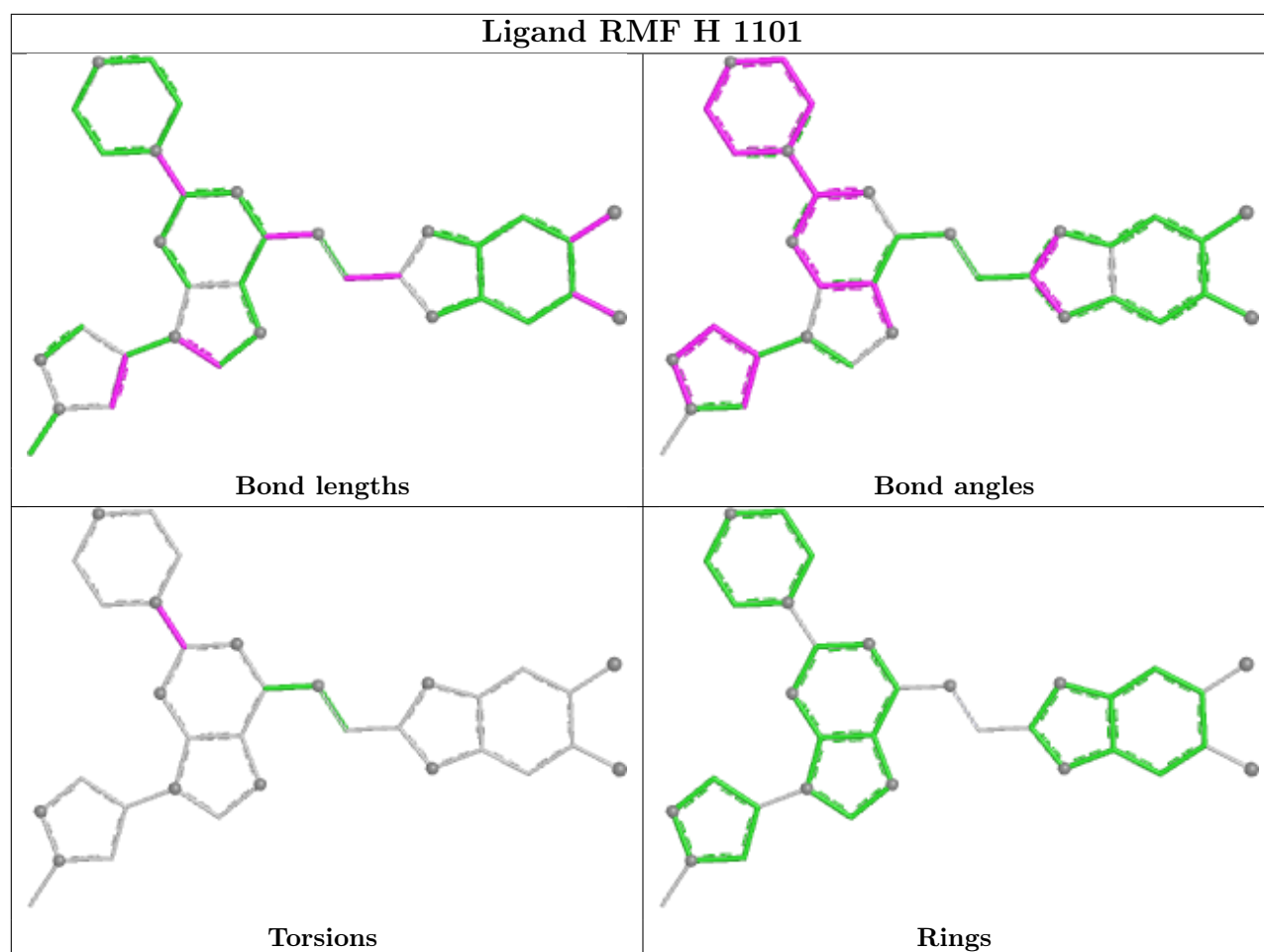
Mol	Chain	Res	Type	Atoms
4	E	1101	RMF	N2-C3-N6-C14
4	E	1101	RMF	N3-C3-N6-C14
4	B	1101	RMF	N2-C2-N1-C1
4	H	1101	RMF	N2-C3-N6-C14
4	E	1101	RMF	N2-C2-N1-C1

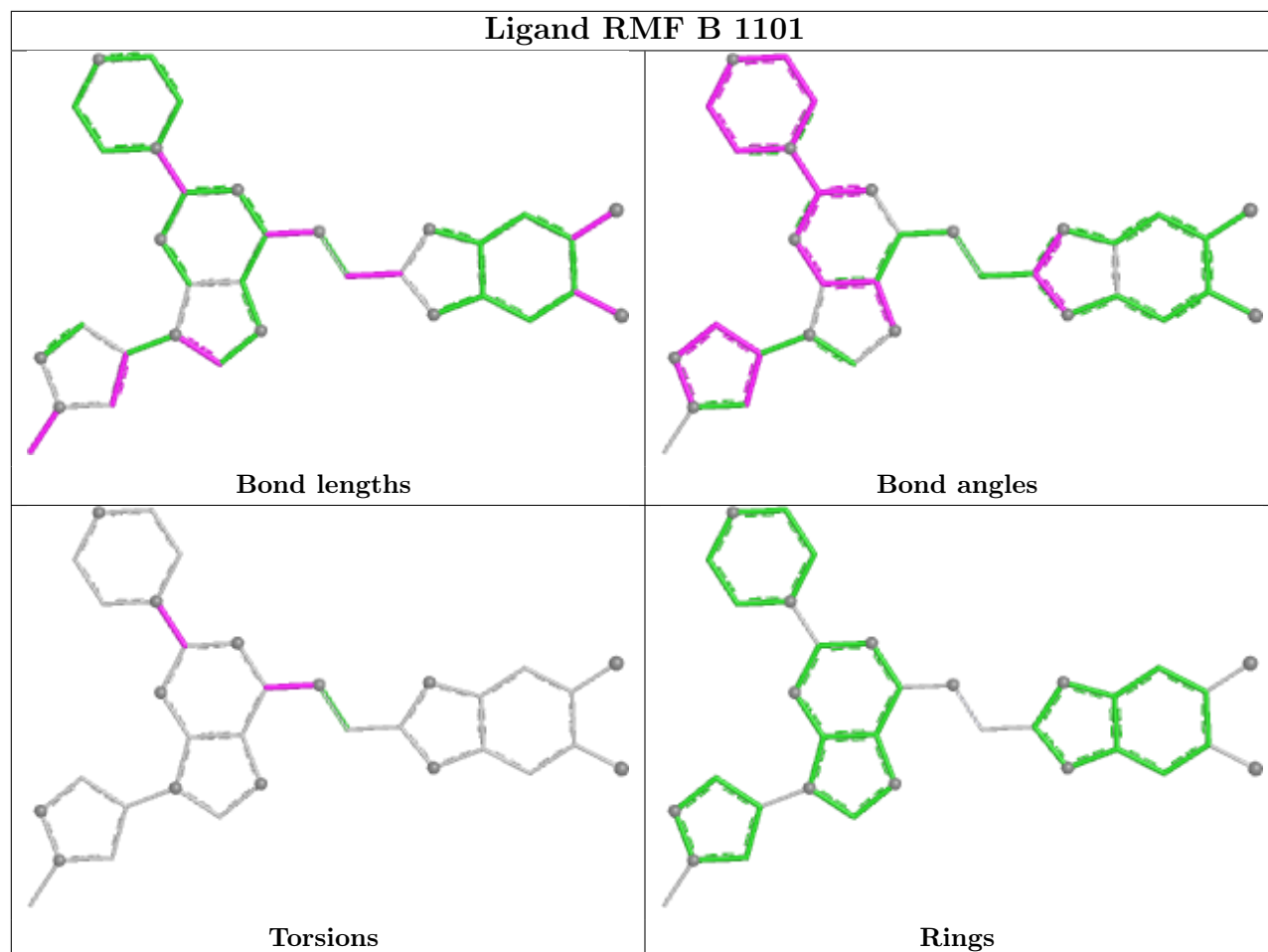
There are no ring outliers.

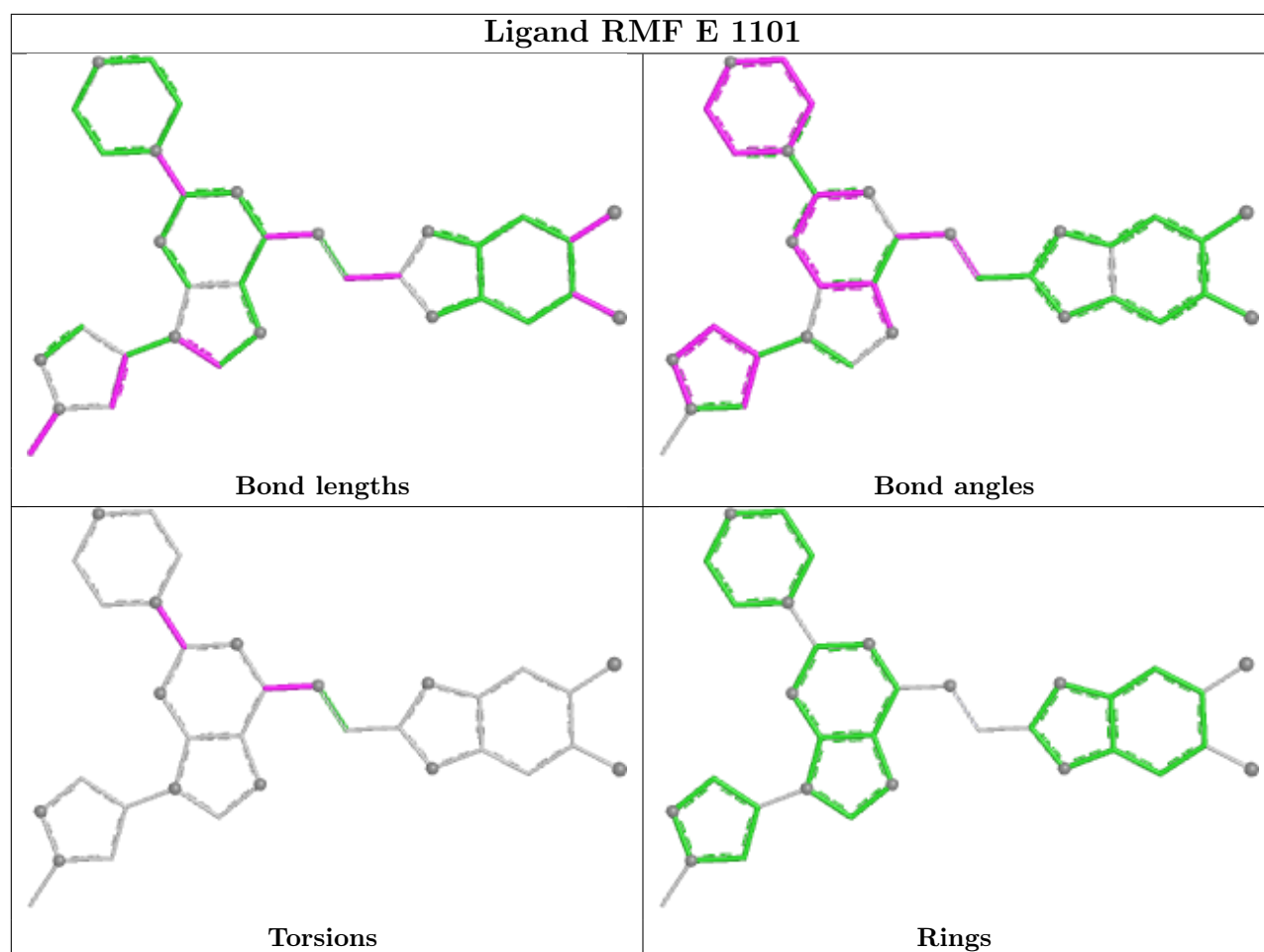
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	1101	RMF	2	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Warning: The R factor obtained from EDS is 0.264, which does not match the depositor's R factor of 0.2078. Please interpret the results in this section carefully.

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, 95th 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 ²)	Q < 0.9
1	A	827/864 (95%)	-1.05	0 100 100	183, 234, 286, 356	0
1	D	821/864 (95%)	-1.05	0 100 100	181, 245, 303, 376	0
1	G	826/864 (95%)	-0.97	0 100 100	194, 259, 319, 365	0
2	B	334/351 (95%)	-0.95	0 100 100	181, 227, 302, 351	0
2	E	329/351 (93%)	-0.93	0 100 100	199, 246, 295, 324	0
2	H	331/351 (94%)	-0.91	0 100 100	179, 228, 298, 351	0
3	C	248/268 (92%)	-1.00	0 100 100	173, 215, 259, 310	0
3	F	248/268 (92%)	-1.04	0 100 100	191, 229, 270, 314	0
3	I	248/268 (92%)	-1.07	0 100 100	179, 223, 258, 316	0
All	All	4212/4449 (94%)	-1.00	0 100 100	173, 238, 303, 376	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

MODRES-RSR INFOmissingINFO

6.3 Carbohydrates ⓘ

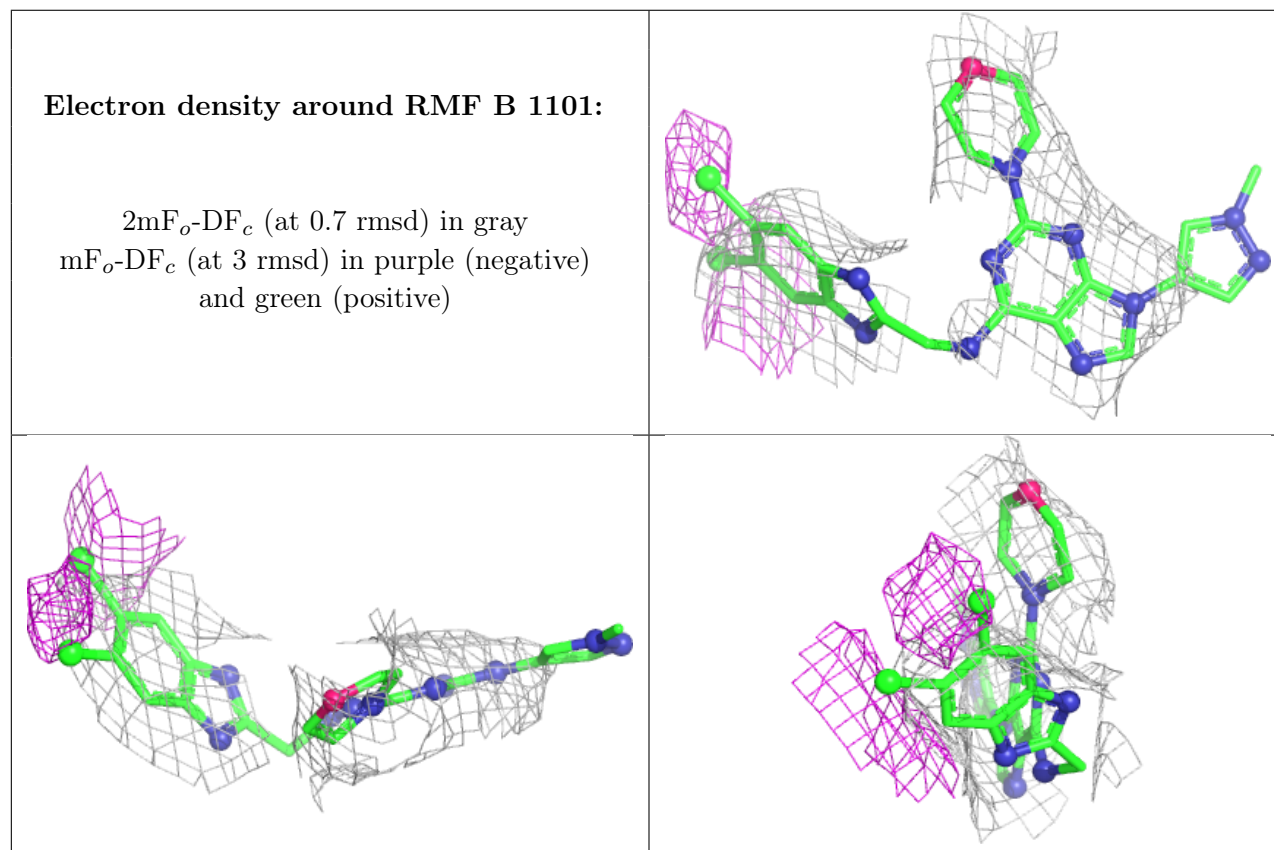
There are no monosaccharides in this entry.

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, 95th 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.

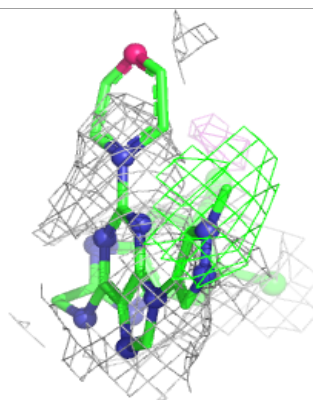
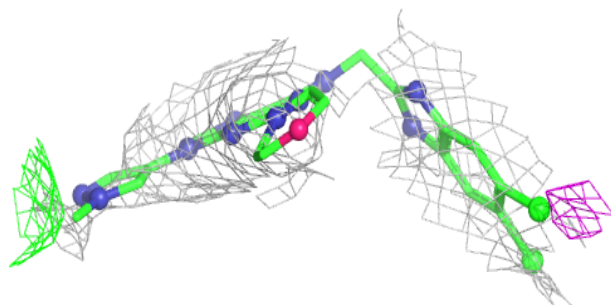
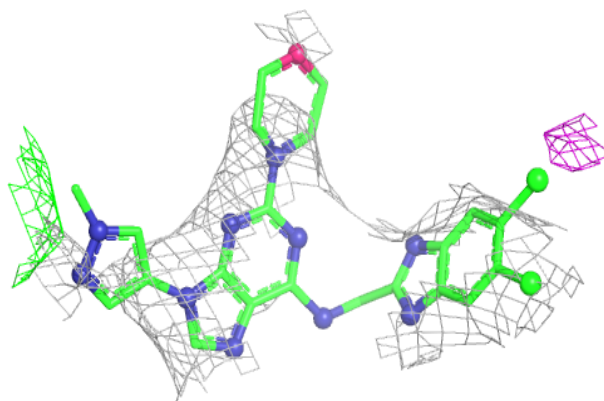
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	RMF	B	1101	34/34	0.89	0.10	202,232,250,285	0
4	RMF	H	1101	34/34	0.91	0.08	196,227,270,335	0
4	RMF	E	1101	34/34	0.92	0.07	191,213,244,247	0

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.

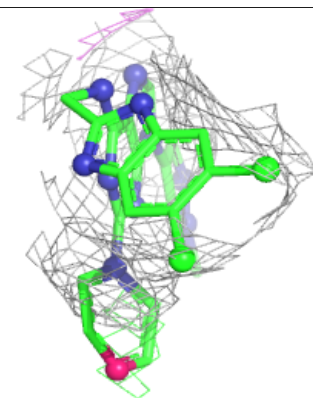
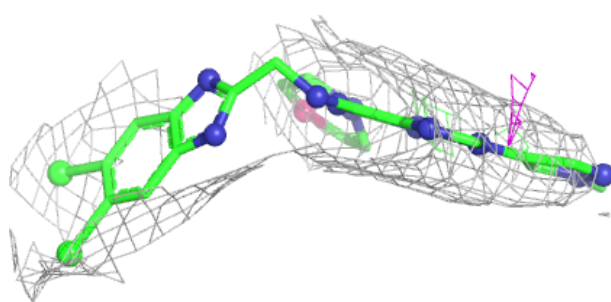
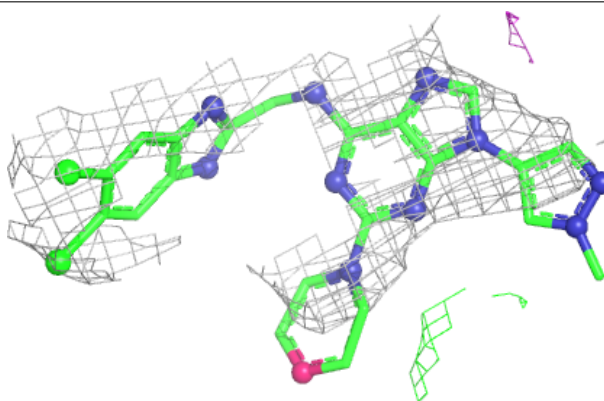


Electron density around RMF H 1101:

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

**Electron density around RMF E 1101:**

$2mF_o-DF_c$ (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.