Full wwPDB X-ray Structure Validation Report ⓘ

Feb 21, 2022 – 06:29 pm GMT

PDB ID	:	7QQ6
Title	:	GCN2 (EIF2ALPHA KINASE 4, E2AK4) IN COMPLEX WITH COMPOUND 1 (dovitinib)
Authors	:	Maia de Oliveira, T.
Deposited on	:	2022-01-06
Resolution	:	2.80 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

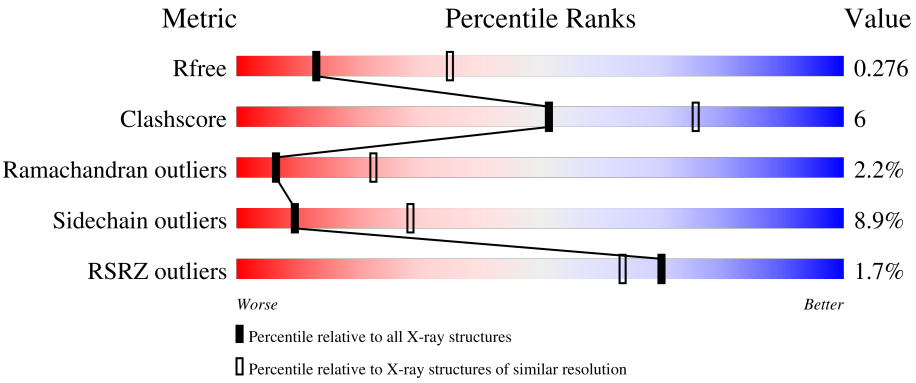
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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 <=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	320	66% 17% • 16%
1	B	320	67% 18% • 14%
1	C	320	62% 19% • 17%
1	D	320	67% 14% • 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8692 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 eIF-2-alpha kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2124	1365	363	388	8			
1	B	275	Total	C	N	O	S	0	0	0
			2188	1405	376	398	9			
1	C	267	Total	C	N	O	S	0	0	0
			2133	1364	368	393	8			
1	D	260	Total	C	N	O	S	0	0	0
			2086	1341	361	376	8			

There are 516 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	575	GLY	-	expression tag	UNP Q9P2K8
A	576	SER	-	expression tag	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	THR	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	LEU	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	LYS	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ARG	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	ARG	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	GLN	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	THR	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	LEU	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	VAL	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ILE	deletion	UNP Q9P2K8
A	?	-	LEU	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	VAL	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	TRP	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	THR	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ARG	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	ARG	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	THR	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	HIS	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	VAL	deletion	UNP Q9P2K8
A	?	-	PHE	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLN	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	PHE	deletion	UNP Q9P2K8
A	?	-	LEU	deletion	UNP Q9P2K8
A	?	-	PRO	deletion	UNP Q9P2K8
A	?	-	ALA	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ILE	deletion	UNP Q9P2K8
A	?	-	ILE	deletion	UNP Q9P2K8
A	?	-	PHE	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	ASN	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ASN	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	LYS	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLN	deletion	UNP Q9P2K8
A	?	-	ASN	deletion	UNP Q9P2K8
A	?	-	GLN	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	ASP	deletion	UNP Q9P2K8
A	?	-	CYS	deletion	UNP Q9P2K8
A	?	-	ASN	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	LYS	deletion	UNP Q9P2K8
A	?	-	ASN	deletion	UNP Q9P2K8
A	?	-	GLY	deletion	UNP Q9P2K8
A	?	-	CYS	deletion	UNP Q9P2K8
A	?	-	HIS	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	?	-	SER	deletion	UNP Q9P2K8
A	?	-	GLU	deletion	UNP Q9P2K8
A	848	ASN	ASP	engineered mutation	UNP Q9P2K8
B	575	GLY	-	expression tag	UNP Q9P2K8
B	576	SER	-	expression tag	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	THR	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	LEU	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	LYS	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ARG	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	ARG	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	GLN	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	THR	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	LEU	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	VAL	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ILE	deletion	UNP Q9P2K8
B	?	-	LEU	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	VAL	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	TRP	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	THR	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ARG	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	ARG	deletion	UNP Q9P2K8
B	?	-	PHE	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	THR	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	HIS	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	VAL	deletion	UNP Q9P2K8
B	?	-	PHE	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLN	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	PHE	deletion	UNP Q9P2K8
B	?	-	LEU	deletion	UNP Q9P2K8
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ILE	deletion	UNP Q9P2K8
B	?	-	ILE	deletion	UNP Q9P2K8
B	?	-	PHE	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ASN	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ASN	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	LYS	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLN	deletion	UNP Q9P2K8
B	?	-	ASN	deletion	UNP Q9P2K8
B	?	-	GLN	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	CYS	deletion	UNP Q9P2K8
B	?	-	ASN	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	LYS	deletion	UNP Q9P2K8
B	?	-	ASN	deletion	UNP Q9P2K8
B	?	-	GLY	deletion	UNP Q9P2K8
B	?	-	CYS	deletion	UNP Q9P2K8
B	?	-	HIS	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	?	-	SER	deletion	UNP Q9P2K8
B	?	-	GLU	deletion	UNP Q9P2K8
B	848	ASN	ASP	engineered mutation	UNP Q9P2K8
C	575	GLY	-	expression tag	UNP Q9P2K8
C	576	SER	-	expression tag	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	THR	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	LYS	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ARG	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	ARG	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	GLN	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	THR	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	LEU	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	VAL	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ILE	deletion	UNP Q9P2K8
C	?	-	LEU	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	VAL	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	TRP	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	THR	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	ARG	deletion	UNP Q9P2K8
C	?	-	PHE	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	THR	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	HIS	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	VAL	deletion	UNP Q9P2K8
C	?	-	PHE	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLN	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	PHE	deletion	UNP Q9P2K8
C	?	-	LEU	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
C	?	-	ALA	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	deletion	UNP Q9P2K8
C	?	-	ILE	deletion	UNP Q9P2K8
C	?	-	PHE	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	ASN	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ASN	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	LYS	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLN	deletion	UNP Q9P2K8
C	?	-	ASN	deletion	UNP Q9P2K8
C	?	-	GLN	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
C	?	-	CYS	deletion	UNP Q9P2K8
C	?	-	ASN	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	LYS	deletion	UNP Q9P2K8
C	?	-	ASN	deletion	UNP Q9P2K8
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	CYS	deletion	UNP Q9P2K8
C	?	-	HIS	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
C	848	ASN	ASP	engineered mutation	UNP Q9P2K8
D	575	GLY	-	expression tag	UNP Q9P2K8
D	576	SER	-	expression tag	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	THR	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	LEU	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	LYS	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	GLN	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	THR	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	LEU	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	VAL	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ILE	deletion	UNP Q9P2K8
D	?	-	LEU	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	VAL	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	TRP	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	THR	deletion	UNP Q9P2K8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	UNP Q9P2K8
D	?	-	PHE	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	THR	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	HIS	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	VAL	deletion	UNP Q9P2K8
D	?	-	PHE	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLN	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	PHE	deletion	UNP Q9P2K8
D	?	-	LEU	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8

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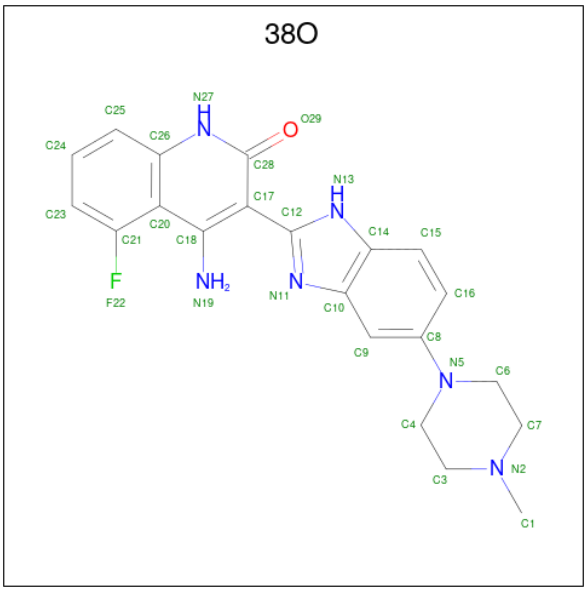
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ILE	deletion	UNP Q9P2K8
D	?	-	ILE	deletion	UNP Q9P2K8
D	?	-	PHE	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	ASN	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ASN	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	LYS	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLN	deletion	UNP Q9P2K8
D	?	-	ASN	deletion	UNP Q9P2K8
D	?	-	GLN	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8
D	?	-	CYS	deletion	UNP Q9P2K8
D	?	-	ASN	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	LYS	deletion	UNP Q9P2K8
D	?	-	ASN	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	CYS	deletion	UNP Q9P2K8
D	?	-	HIS	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	848	ASN	ASP	engineered mutation	UNP Q9P2K8

- Molecule 2 is 4-amino-5-fluoro-3-[5-(4-methylpiperazin-1-yl)-1H-benzimidazol-2-yl]quinolin-2(1H)-one (three-letter code: 38O) (formula: $C_{21}H_{21}FN_6O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F N O 29 21 1 6 1	0	0
2	B	1	Total C F N O 29 21 1 6 1	0	0
2	C	1	Total C F N O 29 21 1 6 1	0	0
2	D	1	Total C F N O 29 21 1 6 1	0	0

- Molecule 3 is water.

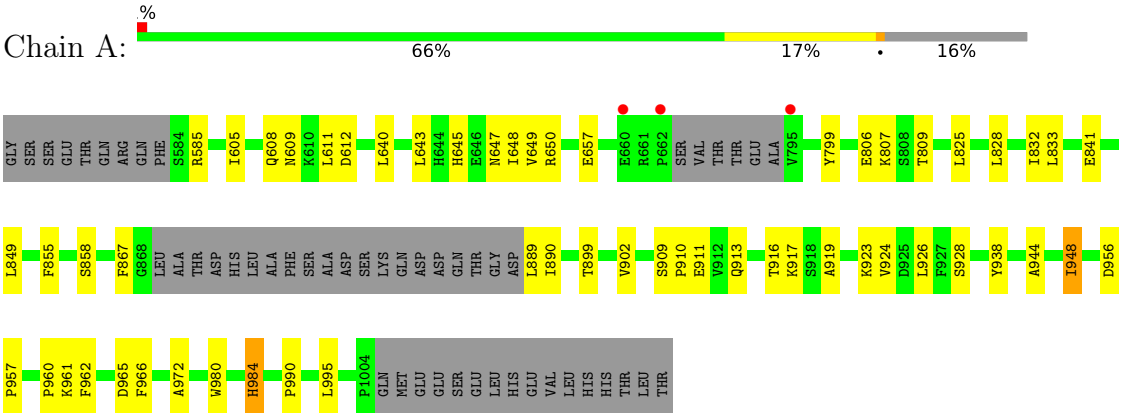
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	13	Total O 13 13	0	0
3	C	8	Total O 8 8	0	0
3	D	6	Total O 6 6	0	0

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.

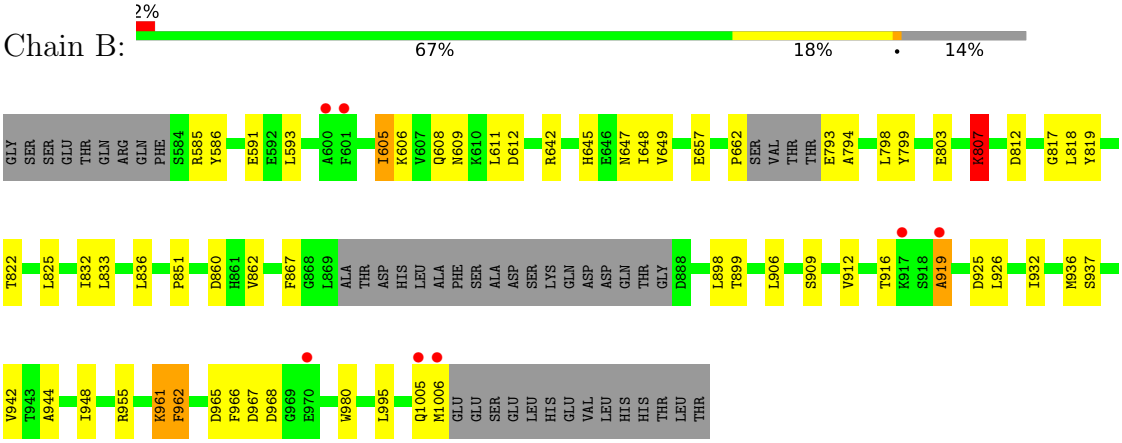
• Molecule 1: eIF-2-alpha kinase GCN2

Chain A:



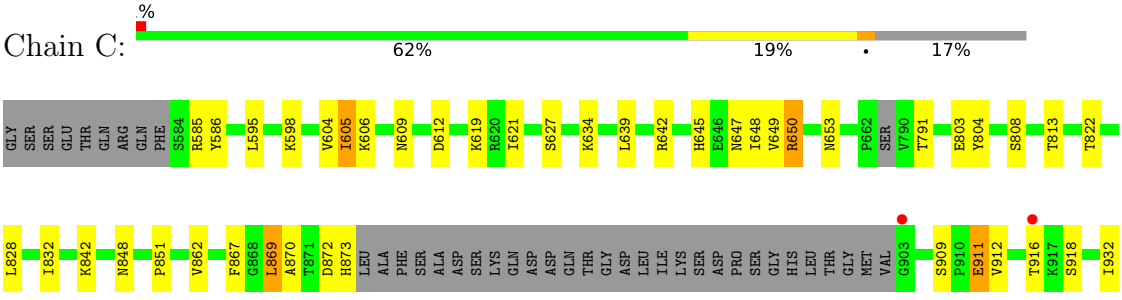
• Molecule 1: eIF-2-alpha kinase GCN2

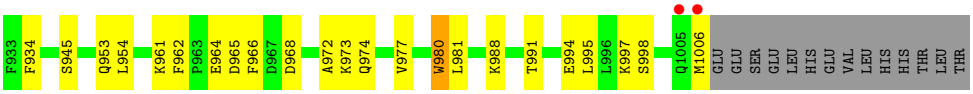
Chain B:



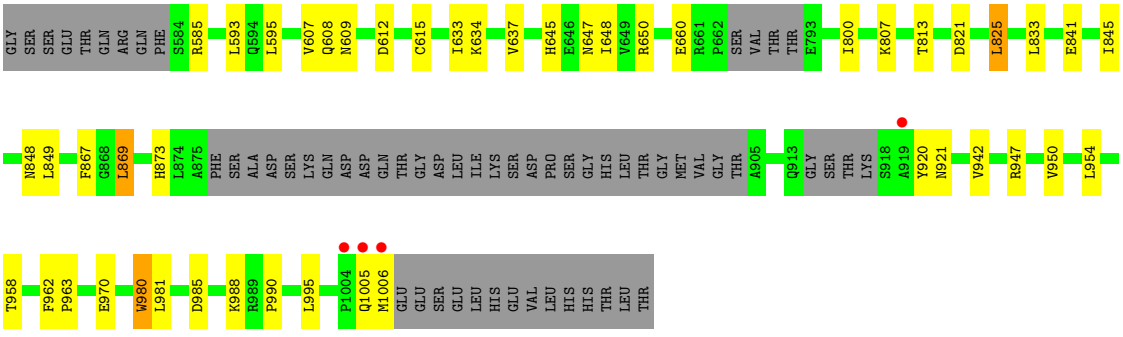
• Molecule 1: eIF-2-alpha kinase GCN2

Chain C:





• Molecule 1: eIF-2-alpha kinase GCN2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.42Å 162.60Å 123.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 – 2.80 24.64 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (24.64-2.80) 99.7 (24.64-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 2.80Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.211 , 0.258 0.224 , 0.276	Depositor DCC
R_{free} test set	1946 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	92.5	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.062 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8692	wwPDB-VP
Average B, all atoms (Å^2)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 38O

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	0.51	0/2175	0.76	0/2950
1	B	0.50	0/2240	0.74	0/3034
1	C	0.50	0/2183	0.75	0/2960
1	D	0.54	0/2136	0.76	0/2893
All	All	0.51	0/8734	0.75	0/11837

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	2124	0	2052	23	0
1	B	2188	0	2147	27	0
1	C	2133	0	2073	33	0
1	D	2086	0	2028	17	0
2	A	29	0	21	0	0
2	B	29	0	21	4	0
2	C	29	0	21	1	0
2	D	29	0	21	0	0
3	A	18	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	13	0	0	0	0
3	C	8	0	0	0	0
3	D	6	0	0	0	0
All	All	8692	0	8384	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (96) 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:C:650:ARG:HH11	1:C:650:ARG:HG2	1.32	0.92
1:A:645:HIS:HB3	1:A:648:ILE:HG12	1.55	0.89
1:C:645:HIS:HB3	1:C:648:ILE:HG12	1.64	0.80
1:B:645:HIS:HB3	1:B:648:ILE:HG12	1.62	0.79
1:B:645:HIS:HD2	1:B:647:ASN:H	1.31	0.76
1:A:645:HIS:HD2	1:A:647:ASN:H	1.33	0.76
1:A:944:ALA:O	1:A:948:ILE:HG12	1.90	0.71
1:B:812:ASP:CG	2:B:1701:38O:H10	2.12	0.69
1:A:645:HIS:CD2	1:A:647:ASN:H	2.11	0.69
1:C:609:ASN:HD22	1:C:612:ASP:H	1.41	0.68
1:C:650:ARG:HG2	1:C:650:ARG:NH1	2.09	0.68
2:B:1701:38O:H4	2:B:1701:38O:H14	1.78	0.65
1:D:609:ASN:HD22	1:D:612:ASP:H	1.43	0.65
1:A:650:ARG:NH2	1:D:650:ARG:HB3	2.12	0.64
1:B:944:ALA:O	1:B:948:ILE:HG12	1.98	0.63
1:C:595:LEU:HD21	1:C:598:LYS:HB2	1.82	0.62
1:C:645:HIS:CD2	1:C:647:ASN:H	2.18	0.62
1:C:645:HIS:HD2	1:C:647:ASN:H	1.48	0.61
1:D:645:HIS:HB3	1:D:648:ILE:HG12	1.83	0.61
1:A:609:ASN:HD22	1:A:612:ASP:H	1.50	0.60
1:C:980:TRP:HZ3	1:C:988:LYS:O	1.86	0.58
1:D:821:ASP:O	1:D:825:LEU:HB2	2.03	0.58
1:A:923:LYS:HA	1:A:926:LEU:HD12	1.86	0.58
1:B:609:ASN:HD22	1:B:612:ASP:H	1.50	0.58
1:B:916:THR:HG23	1:B:919:ALA:HB3	1.87	0.56
1:B:609:ASN:HB3	1:B:612:ASP:OD1	2.06	0.55
1:A:890:ILE:HD13	1:A:948:ILE:HG21	1.88	0.55
1:D:593:LEU:HD11	1:D:608:GLN:HB2	1.88	0.55
1:C:828:LEU:O	1:C:832:ILE:HG13	2.07	0.55
1:D:607:VAL:O	1:D:615:CYS:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:645:HIS:HD2	1:D:647:ASN:H	1.54	0.54
1:B:818:LEU:HD23	1:B:936:MET:HG2	1.89	0.54
1:C:595:LEU:HD12	1:C:605:ILE:HG23	1.89	0.54
1:B:657:GLU:HB2	1:B:799:TYR:HE1	1.73	0.53
1:C:848:ASN:HB2	1:C:869:LEU:HD11	1.90	0.53
1:B:662:PRO:HG3	1:B:793:GLU:HA	1.90	0.53
1:C:851:PRO:HD3	1:C:932:ILE:HG12	1.91	0.52
1:B:825:LEU:HD11	1:B:937:SER:HA	1.90	0.52
1:B:585:ARG:HD2	1:C:585:ARG:HD2	1.91	0.52
1:A:609:ASN:HB3	1:A:612:ASP:OD1	2.10	0.52
1:A:640:LEU:HA	1:A:643:LEU:HD12	1.92	0.52
1:A:833:LEU:HD11	1:A:995:LEU:HD23	1.92	0.51
1:B:812:ASP:OD2	2:B:1701:38O:H1	2.11	0.51
1:C:586:TYR:OH	1:C:605:ILE:HG13	2.11	0.51
1:D:980:TRP:CE3	1:D:990:PRO:HD3	2.45	0.50
1:C:977:VAL:HG13	1:C:995:LEU:HD11	1.94	0.50
1:A:910:PRO:HA	1:A:913:GLN:HE21	1.77	0.50
1:A:980:TRP:CD1	1:A:990:PRO:HD3	2.46	0.50
1:B:645:HIS:CD2	1:B:647:ASN:H	2.20	0.50
1:B:812:ASP:OD2	2:B:1701:38O:H10	2.11	0.49
1:C:909:SER:HB2	1:C:912:VAL:HG23	1.94	0.49
1:D:981:LEU:HD21	1:D:995:LEU:HD22	1.94	0.48
1:B:833:LEU:HD11	1:B:995:LEU:HD23	1.96	0.48
1:C:808:SER:OG	2:C:1701:38O:H7	2.13	0.48
1:C:980:TRP:CZ3	1:C:988:LYS:O	2.67	0.47
1:C:981:LEU:HD21	1:C:995:LEU:HD22	1.96	0.47
1:B:961:LYS:O	1:B:962:PHE:HB2	2.15	0.47
1:D:833:LEU:HD11	1:D:995:LEU:HD23	1.97	0.47
1:C:619:LYS:HG2	1:C:621:ILE:HD11	1.97	0.47
1:C:828:LEU:HD22	1:C:862:VAL:HG23	1.97	0.47
1:A:611:LEU:HD12	1:D:634:LYS:HE2	1.97	0.45
1:A:828:LEU:O	1:A:832:ILE:HG13	2.16	0.45
1:C:911:GLU:HB3	1:C:918:SER:HB2	1.97	0.45
1:D:950:VAL:HG13	1:D:963:PRO:HG3	1.98	0.45
1:B:593:LEU:HD12	1:B:606:LYS:HE2	1.99	0.45
1:B:611:LEU:HD12	1:C:634:LYS:HE2	1.99	0.45
1:A:957:PRO:HB3	1:A:984:HIS:CD2	2.52	0.44
1:C:973:LYS:O	1:C:977:VAL:HG23	2.16	0.44
1:C:639:LEU:HB2	1:C:867:PHE:HE2	1.81	0.44
1:C:649:VAL:HG13	1:C:803:GLU:HG2	2.00	0.44
1:D:645:HIS:CD2	1:D:647:ASN:H	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:968:ASP:O	1:C:972:ALA:HB2	2.18	0.43
1:B:836:LEU:HD11	1:B:925:ASP:HB3	2.01	0.43
1:C:645:HIS:HB3	1:C:648:ILE:CG1	2.42	0.43
1:C:991:THR:H	1:C:994:GLU:HB3	1.83	0.43
1:A:960:PRO:HB2	3:A:1813:HOH:O	2.18	0.43
1:A:909:SER:HB2	1:A:924:VAL:HG13	2.02	0.42
1:B:906:LEU:O	1:B:955:ARG:HD2	2.18	0.42
1:B:912:VAL:HA	1:B:919:ALA:HB1	2.02	0.42
1:B:898:LEU:HD13	1:B:948:ILE:HB	2.01	0.42
1:C:604:VAL:HG22	1:C:619:LYS:HG3	2.01	0.42
1:D:833:LEU:HD21	1:D:995:LEU:HD23	2.01	0.42
1:B:851:PRO:HD3	1:B:932:ILE:HG12	2.02	0.42
1:C:609:ASN:ND2	1:C:612:ASP:H	2.11	0.41
1:D:633:ILE:O	1:D:637:VAL:HG23	2.21	0.41
1:B:832:ILE:HG12	1:B:862:VAL:HG11	2.03	0.41
1:A:657:GLU:HB2	1:A:799:TYR:HE1	1.85	0.41
1:D:985:ASP:HB3	1:D:988:LYS:HG2	2.02	0.41
1:A:809:THR:HG22	1:A:855:PHE:CD1	2.55	0.41
1:C:934:PHE:CG	1:C:954:LEU:HD21	2.56	0.41
1:A:938:TYR:HD1	1:A:966:PHE:HD1	1.67	0.40
1:B:807:LYS:HE2	1:B:860:ASP:HB2	2.03	0.40
1:C:606:LYS:HD2	1:C:804:TYR:CZ	2.56	0.40
1:A:585:ARG:HD2	1:D:585:ARG:HD2	2.04	0.40
1:A:902:VAL:HG23	1:A:948:ILE:HD12	2.02	0.40
1:B:586:TYR:OH	1:B:605:ILE:HG13	2.22	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	263/320 (82%)	240 (91%)	19 (7%)	4 (2%)	10 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	269/320 (84%)	237 (88%)	24 (9%)	8 (3%)	4	15
1	C	261/320 (82%)	229 (88%)	27 (10%)	5 (2%)	8	26
1	D	252/320 (79%)	229 (91%)	17 (7%)	6 (2%)	6	20
All	All	1045/1280 (82%)	935 (90%)	87 (8%)	23 (2%)	6	22

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	919	ALA
1	A	961	LYS
1	A	972	ALA
1	C	870	ALA
1	D	869	LEU
1	B	807	LYS
1	B	819	TYR
1	C	872	ASP
1	D	660	GLU
1	A	962	PHE
1	B	794	ALA
1	B	961	LYS
1	B	919	ALA
1	C	627	SER
1	C	962	PHE
1	D	867	PHE
1	D	920	TYR
1	D	954	LEU
1	B	817	GLY
1	B	967	ASP
1	C	961	LYS
1	B	962	PHE
1	D	962	PHE

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	224/286 (78%)	204 (91%)	20 (9%)	9 28
1	B	235/286 (82%)	215 (92%)	20 (8%)	10 31
1	C	228/286 (80%)	206 (90%)	22 (10%)	8 24
1	D	221/286 (77%)	202 (91%)	19 (9%)	10 30
All	All	908/1144 (79%)	827 (91%)	81 (9%)	9 28

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	605	ILE
1	A	608	GLN
1	A	649	VAL
1	A	806	GLU
1	A	807	LYS
1	A	825	LEU
1	A	841	GLU
1	A	849	LEU
1	A	858	SER
1	A	867	PHE
1	A	889	LEU
1	A	899	THR
1	A	911	GLU
1	A	916	THR
1	A	917	LYS
1	A	928	SER
1	A	948	ILE
1	A	956	ASP
1	A	965	ASP
1	A	984	HIS
1	B	591	GLU
1	B	605	ILE
1	B	608	GLN
1	B	642	ARG
1	B	649	VAL
1	B	798	LEU
1	B	803	GLU
1	B	807	LYS
1	B	822	THR
1	B	867	PHE
1	B	899	THR
1	B	909	SER
1	B	926	LEU

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Mol	Chain	Res	Type
1	B	942	VAL
1	B	965	ASP
1	B	966	PHE
1	B	968	ASP
1	B	980	TRP
1	B	1005	GLN
1	B	1006	MET
1	C	605	ILE
1	C	642	ARG
1	C	650	ARG
1	C	653	ASN
1	C	791	THR
1	C	813	THR
1	C	822	THR
1	C	842	LYS
1	C	869	LEU
1	C	873	HIS
1	C	911	GLU
1	C	916	THR
1	C	945	SER
1	C	953	GLN
1	C	964	GLU
1	C	965	ASP
1	C	966	PHE
1	C	974	GLN
1	C	980	TRP
1	C	997	LYS
1	C	998	SER
1	C	1006	MET
1	D	595	LEU
1	D	800	ILE
1	D	807	LYS
1	D	813	THR
1	D	825	LEU
1	D	841	GLU
1	D	845	ILE
1	D	848	ASN
1	D	849	LEU
1	D	869	LEU
1	D	873	HIS
1	D	921	ASN
1	D	942	VAL

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Mol	Chain	Res	Type
1	D	947	ARG
1	D	958	THR
1	D	970	GLU
1	D	980	TRP
1	D	1005	GLN
1	D	1006	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	ASN
1	A	645	HIS
1	A	913	GLN
1	A	984	HIS
1	B	609	ASN
1	B	645	HIS
1	C	594	GLN
1	C	609	ASN
1	C	645	HIS
1	D	609	ASN
1	D	645	HIS
1	D	659	HIS
1	D	848	ASN
1	D	921	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 (i)

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	$\#\|Z\| > 2$
2	38O	A	1701	-	32,33,33	1.10	3 (9%)	33,49,49	2.07	3 (9%)
2	38O	B	1701	-	32,33,33	1.10	3 (9%)	33,49,49	2.05	3 (9%)
2	38O	C	1701	-	32,33,33	1.10	3 (9%)	33,49,49	2.05	3 (9%)
2	38O	D	1701	-	32,33,33	1.10	3 (9%)	33,49,49	2.05	3 (9%)

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	38O	A	1701	-	-	0/8/18/18	0/5/5/5
2	38O	B	1701	-	-	2/8/18/18	0/5/5/5
2	38O	C	1701	-	-	4/8/18/18	0/5/5/5
2	38O	D	1701	-	-	4/8/18/18	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1701	38O	C26-N27	2.69	1.39	1.35
2	D	1701	38O	C26-N27	2.67	1.39	1.35
2	A	1701	38O	C26-N27	2.67	1.39	1.35
2	C	1701	38O	C26-N27	2.66	1.39	1.35
2	C	1701	38O	C21-C20	-2.57	1.39	1.42
2	B	1701	38O	C21-C20	-2.55	1.39	1.42
2	D	1701	38O	C21-C20	-2.54	1.39	1.42
2	A	1701	38O	C21-C20	-2.49	1.39	1.42
2	B	1701	38O	C12-N13	-2.39	1.32	1.35
2	D	1701	38O	C12-N13	-2.38	1.32	1.35
2	A	1701	38O	C12-N13	-2.37	1.32	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1701	38O	C12-N13	-2.36	1.32	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1701	38O	C17-C28-N27	-9.13	115.99	124.09
2	C	1701	38O	C17-C28-N27	-9.08	116.03	124.09
2	B	1701	38O	C17-C28-N27	-9.05	116.06	124.09
2	D	1701	38O	C17-C28-N27	-9.03	116.08	124.09
2	D	1701	38O	C26-N27-C28	5.74	124.71	116.83
2	C	1701	38O	C26-N27-C28	5.73	124.70	116.83
2	A	1701	38O	C26-N27-C28	5.73	124.70	116.83
2	B	1701	38O	C26-N27-C28	5.69	124.64	116.83
2	B	1701	38O	C8-C9-C10	-2.89	118.99	121.02
2	D	1701	38O	C8-C9-C10	-2.85	119.02	121.02
2	A	1701	38O	C8-C9-C10	-2.81	119.05	121.02
2	C	1701	38O	C8-C9-C10	-2.81	119.05	121.02

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1701	38O	C9-C8-N5-C4
2	C	1701	38O	C16-C8-N5-C4
2	D	1701	38O	C16-C8-N5-C6
2	D	1701	38O	C16-C8-N5-C4
2	D	1701	38O	C9-C8-N5-C6
2	D	1701	38O	C9-C8-N5-C4
2	B	1701	38O	C16-C8-N5-C6
2	B	1701	38O	C9-C8-N5-C6
2	C	1701	38O	C9-C8-N5-C6
2	C	1701	38O	C16-C8-N5-C6

There are no ring outliers.

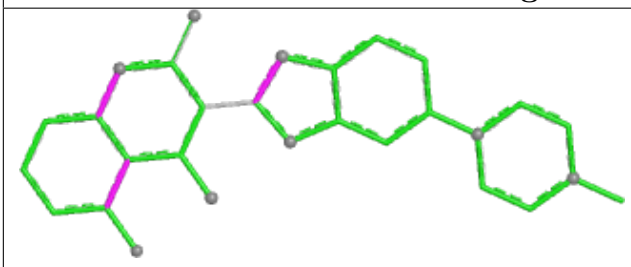
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1701	38O	4	0
2	C	1701	38O	1	0

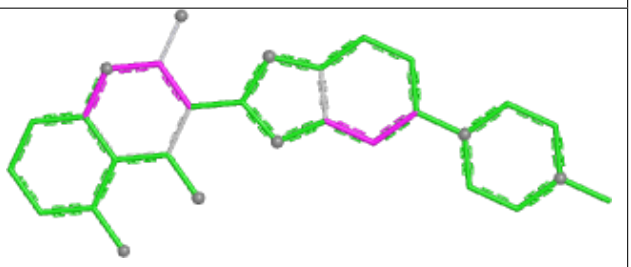
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

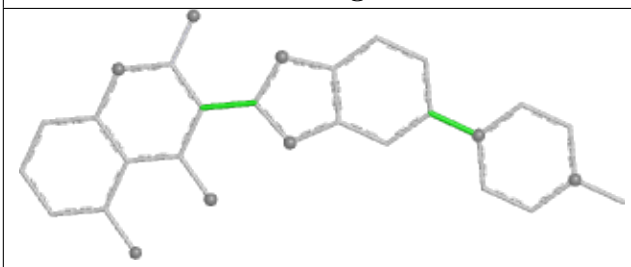
Ligand 38O A 1701



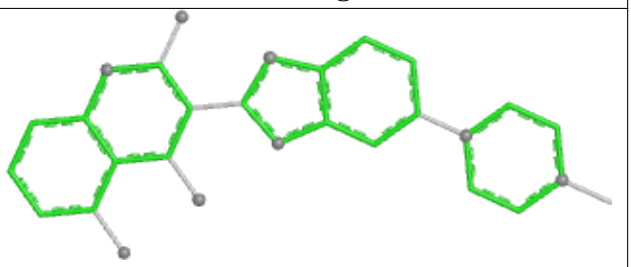
Bond lengths



Bond angles

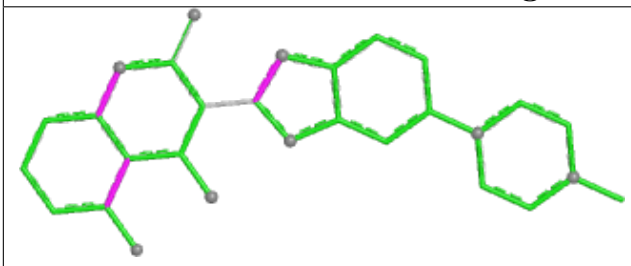


Torsions



Rings

Ligand 38O B 1701



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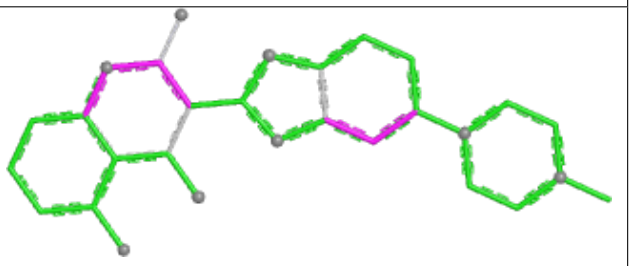
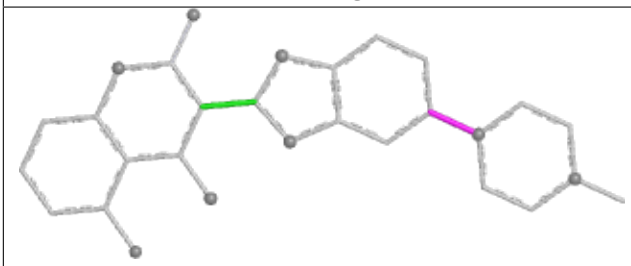
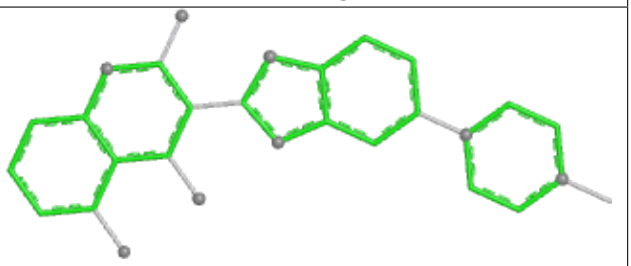


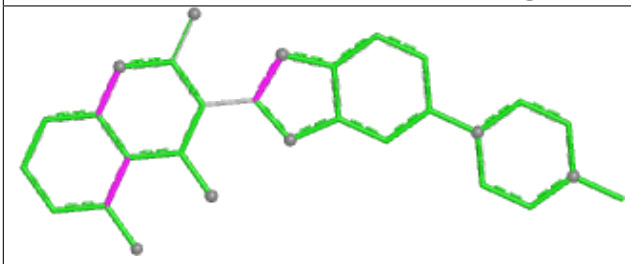
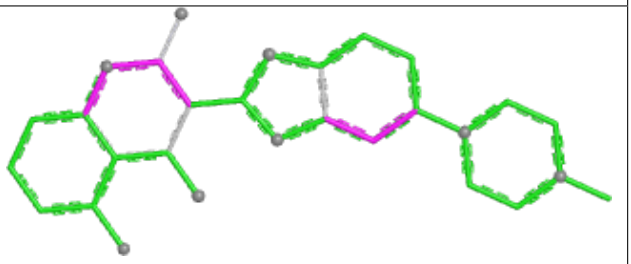
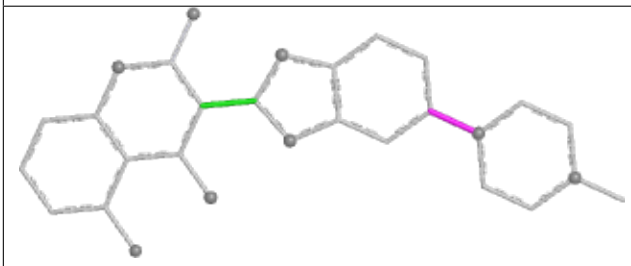
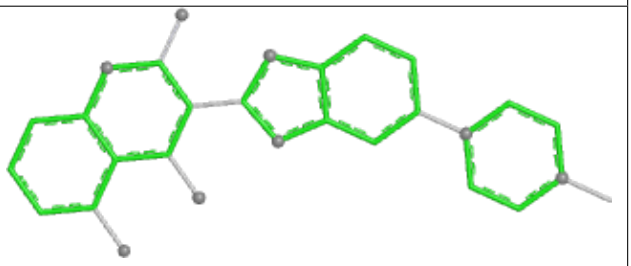
Bond angles

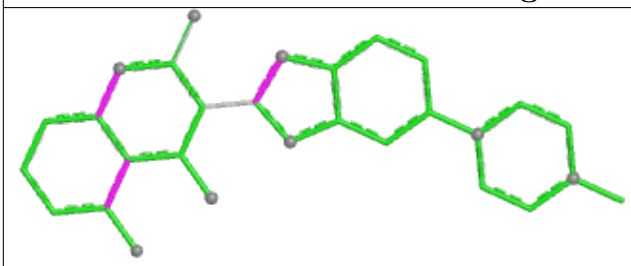
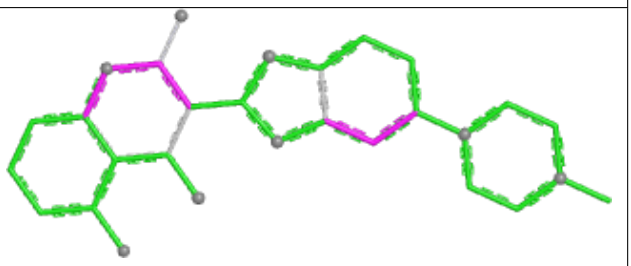
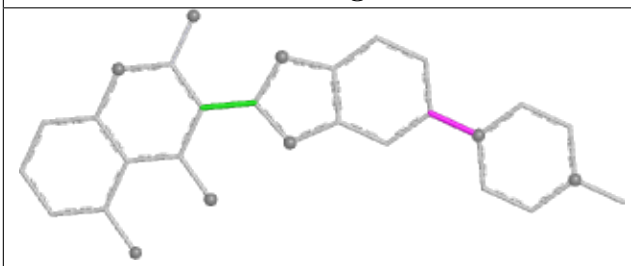
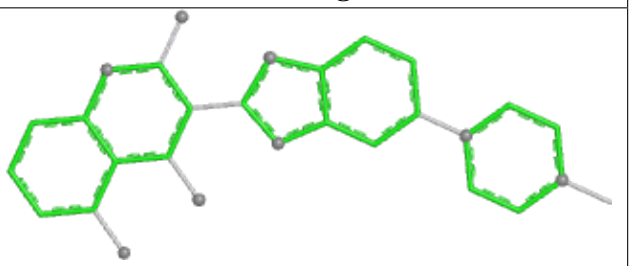


Torsions



Rings

Ligand 38O C 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 38O D 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

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^{th} 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	269/320 (84%)	-0.10	3 (1%)	80	75	57, 82, 115, 145	0
1	B	275/320 (85%)	0.07	7 (2%)	57	47	62, 88, 125, 150	0
1	C	267/320 (83%)	0.02	4 (1%)	73	68	65, 89, 132, 175	0
1	D	260/320 (81%)	0.01	4 (1%)	73	68	62, 92, 139, 167	0
All	All	1071/1280 (83%)	0.00	18 (1%)	70	63	57, 88, 130, 175	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	916	THR	7.8
1	D	1006	MET	6.9
1	C	1006	MET	6.8
1	A	662	PRO	6.7
1	C	1005	GLN	6.7
1	B	1006	MET	6.2
1	D	1005	GLN	4.6
1	B	919	ALA	4.2
1	D	919	ALA	3.8
1	A	660	GLU	3.4
1	B	600	ALA	3.2
1	B	917	LYS	3.0
1	B	1005	GLN	2.8
1	C	903	GLY	2.8
1	B	970	GLU	2.6
1	A	795	VAL	2.3
1	B	601	PHE	2.2
1	D	1004	PRO	2.1

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)

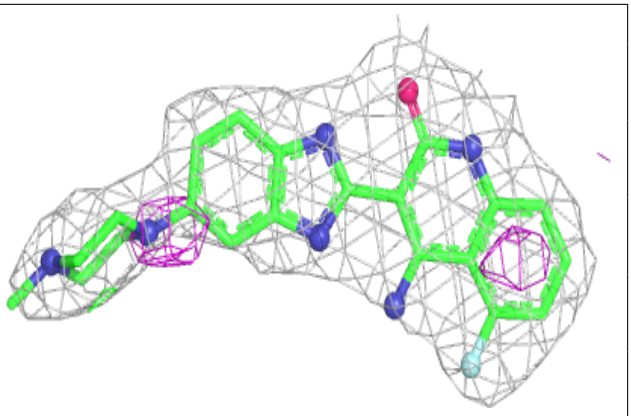
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

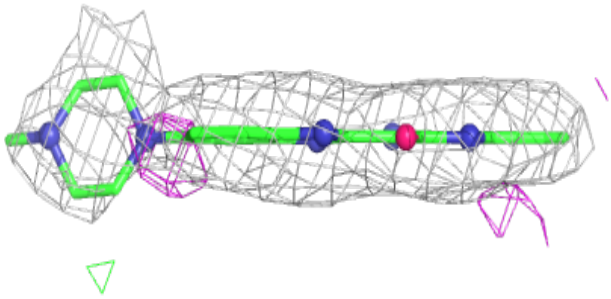
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	38O	C	1701	29/29	0.93	0.18	66,80,109,109	0
2	38O	B	1701	29/29	0.95	0.15	72,83,117,119	0
2	38O	D	1701	29/29	0.95	0.19	66,79,115,117	0
2	38O	A	1701	29/29	0.96	0.20	58,69,102,102	0

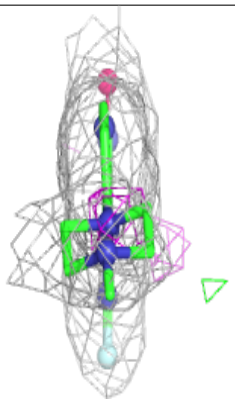
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 38O C 1701:

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

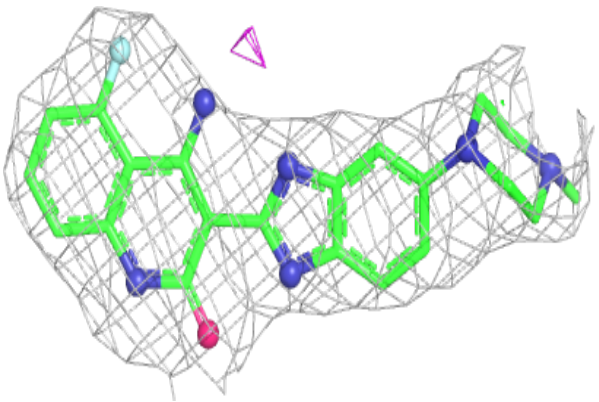


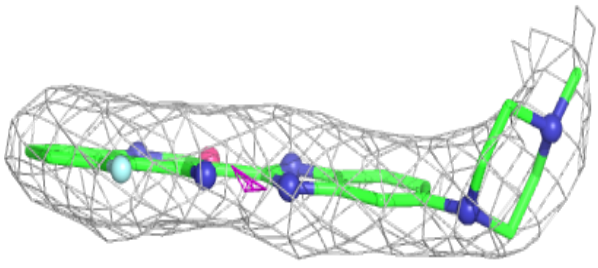


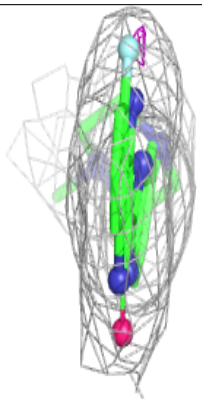


Electron density around 38O B 1701:

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

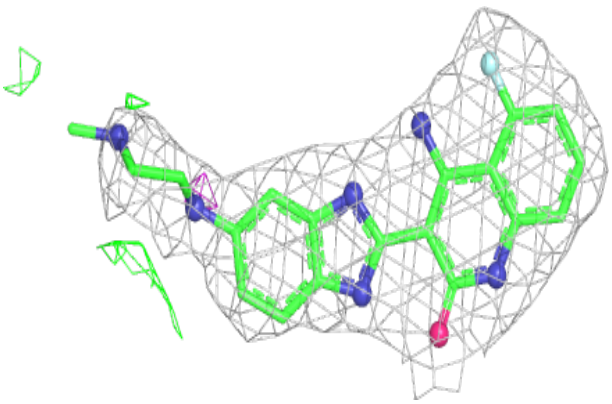


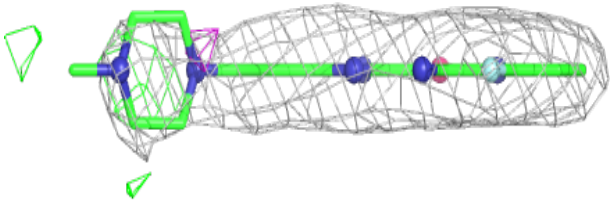


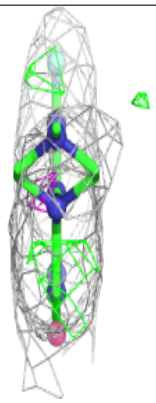


Electron density around 38O D 1701:

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

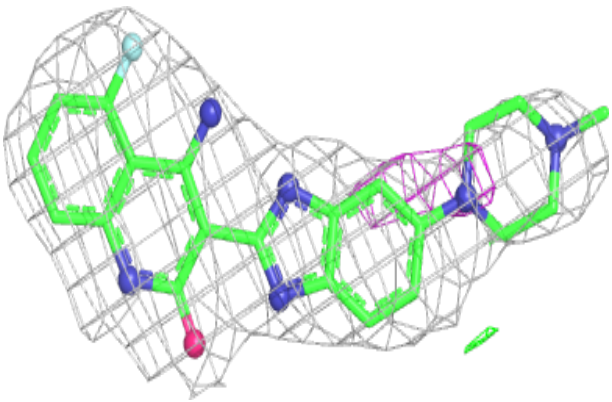


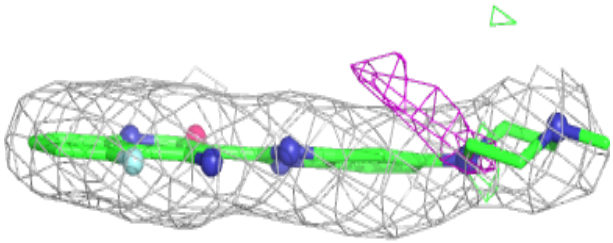


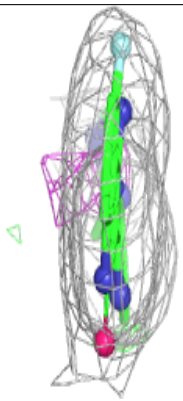


Electron density around 38O A 1701:

$2mF_o$-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.