



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:43 AM UTC

PDB ID : 7QQ6 / pdb_00007qq6
Title : GCN2 (EIF2ALPHA KINASE 4, E2AK4) IN COMPLEX WITH COM-
POUND 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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

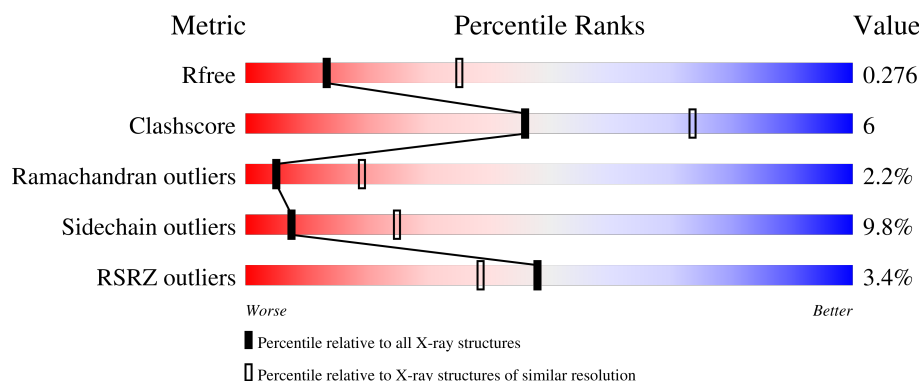
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

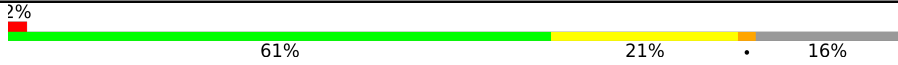
The reported resolution of this entry is 2.80 Å.

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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. 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	320	
1	B	320	
1	C	320	
1	D	320	

2 Entry composition

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	?	-	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	?	-	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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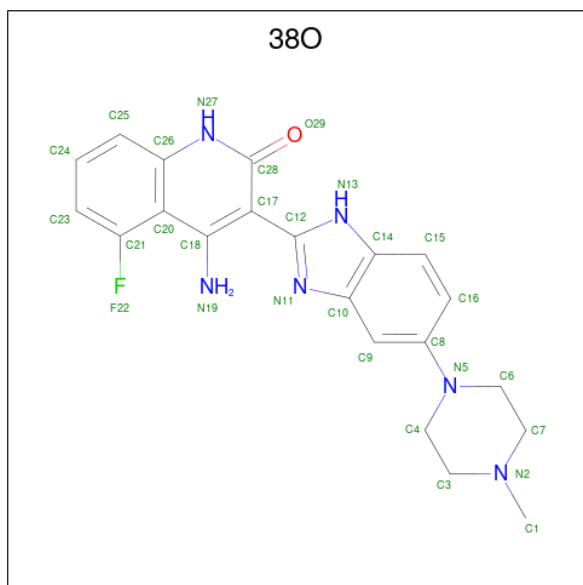
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	GLU	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	SER	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	ARG	deletion	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	?	-	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 (CCD ID: 38O) (formula: C₂₁H₂₁FN₆O) (labeled as "Ligand of Interest" by depositor).



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

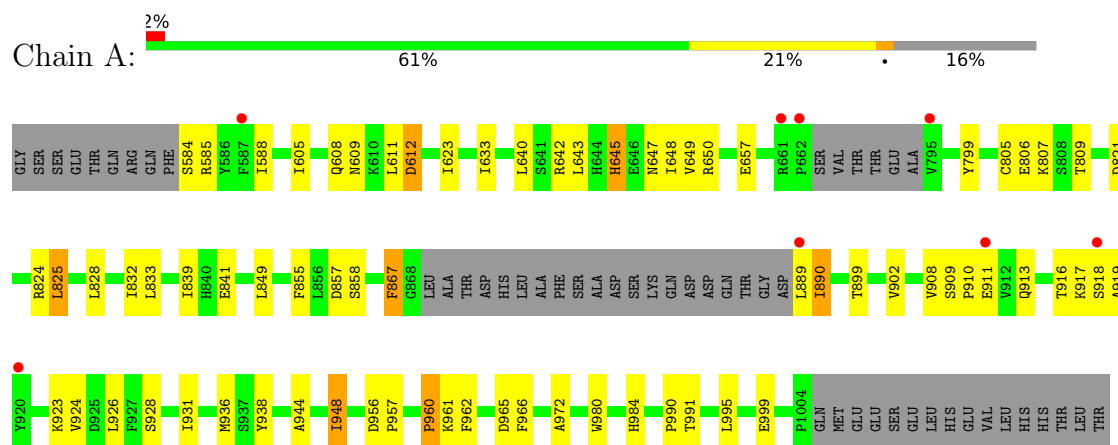
- Molecule 3 is water.

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

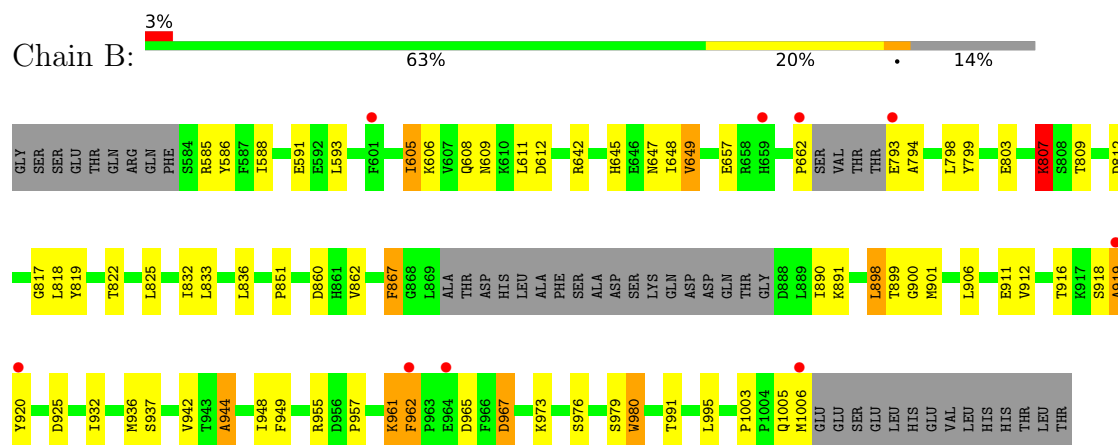
3 Residue-property plots [i](#)

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.

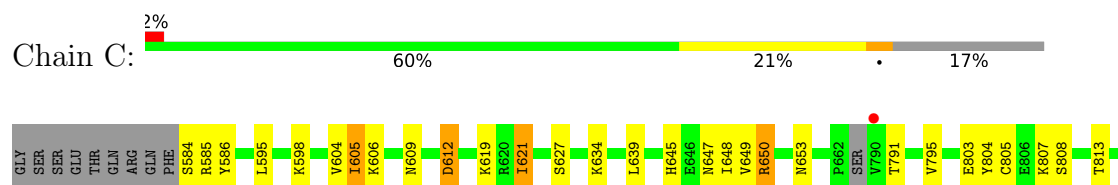
• Molecule 1: eIF-2-alpha kinase GCN2

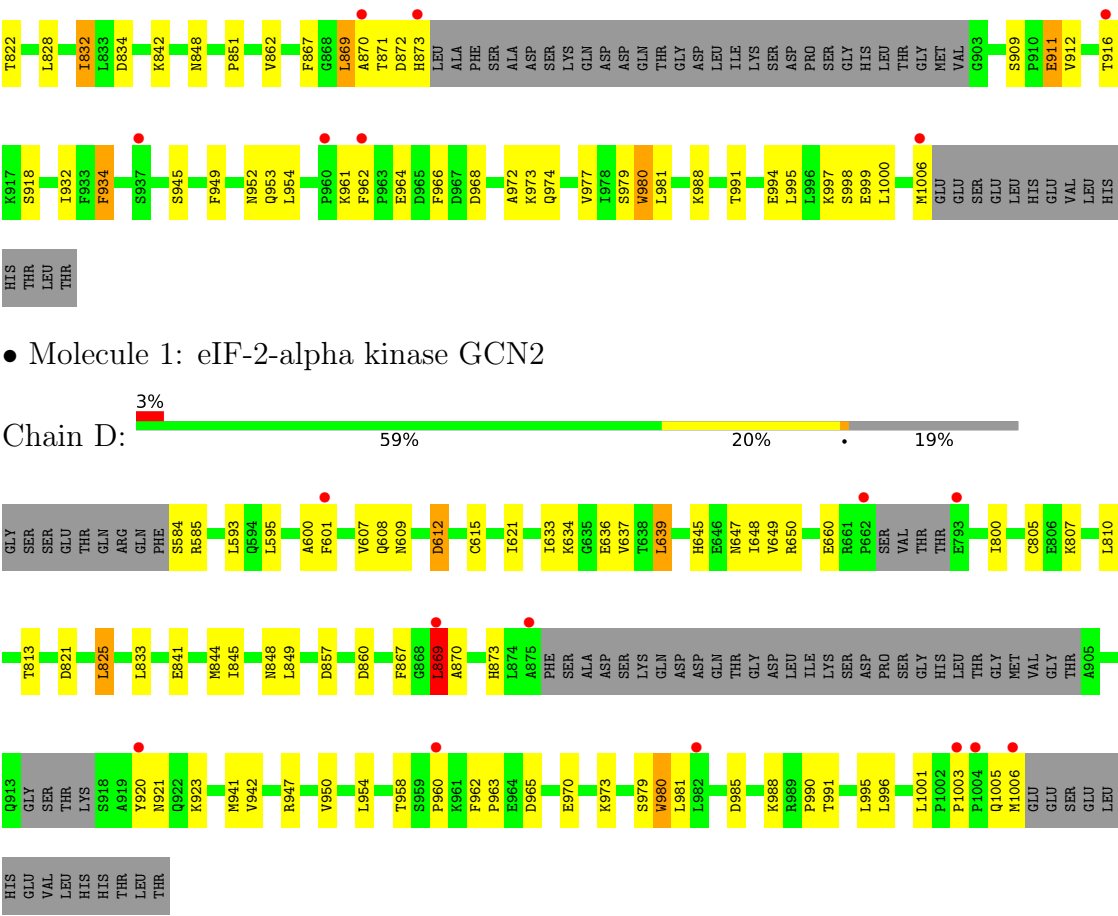


• Molecule 1: eIF-2-alpha kinase GCN2



• Molecule 1: eIF-2-alpha kinase GCN2





● Molecule 1: eIF-2-alpha kinase GCN2

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 75.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.89	0/2175	1.48	24/2950 (0.8%)
1	B	0.89	0/2240	1.48	24/3034 (0.8%)
1	C	0.89	2/2183 (0.1%)	1.48	19/2960 (0.6%)
1	D	0.95	2/2136 (0.1%)	1.53	34/2893 (1.2%)
All	All	0.90	4/8734 (0.0%)	1.49	101/11837 (0.9%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	869	LEU	CA-C	7.91	1.63	1.52
1	C	621	ILE	CA-CB	6.36	1.59	1.54
1	C	871	THR	CA-C	5.38	1.59	1.52
1	D	621	ILE	CA-CB	5.14	1.58	1.54

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	960	PRO	CA-C-N	8.38	133.38	120.82
1	D	960	PRO	C-N-CA	8.38	133.38	120.82
1	D	805	CYS	CA-C-N	8.01	131.35	120.54
1	D	805	CYS	C-N-CA	8.01	131.35	120.54
1	C	612	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	867	PHE	CA-CB-CG	7.18	120.98	113.80
1	B	967	ASP	CA-CB-CG	7.07	119.67	112.60
1	D	601	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	980	TRP	CA-C-N	6.67	129.22	120.28
1	B	980	TRP	C-N-CA	6.67	129.22	120.28
1	B	957	PRO	CA-C-N	6.55	129.38	120.54
1	B	957	PRO	C-N-CA	6.55	129.38	120.54
1	B	900	GLY	N-CA-C	6.45	118.08	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	612	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	871	THR	CA-C-N	6.33	133.62	121.54
1	C	871	THR	C-N-CA	6.33	133.62	121.54
1	D	869	LEU	CA-C-N	6.29	133.55	121.54
1	D	869	LEU	C-N-CA	6.29	133.55	121.54
1	D	965	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	960	PRO	CA-C-N	6.21	133.41	121.54
1	A	960	PRO	C-N-CA	6.21	133.41	121.54
1	D	584	SER	CA-C-N	6.16	128.81	120.38
1	D	584	SER	C-N-CA	6.16	128.81	120.38
1	C	584	SER	CA-C-N	6.09	128.44	120.28
1	C	584	SER	C-N-CA	6.09	128.44	120.28
1	A	918	SER	CA-C-N	6.09	133.17	121.54
1	A	918	SER	C-N-CA	6.09	133.17	121.54
1	C	979	SER	CA-C-N	6.07	128.67	120.65
1	C	979	SER	C-N-CA	6.07	128.67	120.65
1	B	1003	PRO	N-CA-C	6.07	116.30	110.47
1	A	908	VAL	CA-C-N	6.03	129.25	120.51
1	A	908	VAL	C-N-CA	6.03	129.25	120.51
1	A	584	SER	CA-C-N	5.96	128.54	120.38
1	A	584	SER	C-N-CA	5.96	128.54	120.38
1	C	934	PHE	CA-C-N	5.89	128.18	120.28
1	C	934	PHE	C-N-CA	5.89	128.18	120.28
1	C	999	GLU	CA-C-N	5.88	128.15	120.28
1	C	999	GLU	C-N-CA	5.88	128.15	120.28
1	D	923	LYS	CA-C-N	5.78	127.96	120.56
1	D	923	LYS	C-N-CA	5.78	127.96	120.56
1	D	612	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	805	CYS	CA-C-N	5.65	127.78	120.44
1	C	805	CYS	C-N-CA	5.65	127.78	120.44
1	B	991	THR	N-CA-C	-5.64	102.17	110.52
1	D	600	ALA	CA-C-N	5.60	127.79	120.28
1	D	600	ALA	C-N-CA	5.60	127.79	120.28
1	A	991	THR	N-CA-C	-5.60	102.17	110.46
1	C	834	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	931	ILE	N-CA-C	-5.52	105.47	110.82
1	D	979	SER	CA-C-N	5.52	127.61	120.44
1	D	979	SER	C-N-CA	5.52	127.61	120.44
1	B	809	THR	N-CA-C	-5.50	102.33	110.46
1	D	870	ALA	CA-C-N	5.49	130.22	122.09
1	D	870	ALA	C-N-CA	5.49	130.22	122.09
1	D	857	ASP	CA-CB-CG	5.47	118.07	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	996	LEU	CA-C-N	5.47	128.06	120.29
1	D	996	LEU	C-N-CA	5.47	128.06	120.29
1	B	979	SER	CA-C-N	5.46	128.38	120.79
1	B	979	SER	C-N-CA	5.46	128.38	120.79
1	C	952	ASN	CA-C-N	5.40	127.95	120.29
1	C	952	ASN	C-N-CA	5.40	127.95	120.29
1	D	810	LEU	N-CA-C	-5.37	105.59	111.82
1	A	867	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	636	GLU	CA-C-N	5.29	127.94	120.42
1	D	636	GLU	C-N-CA	5.29	127.94	120.42
1	D	941	MET	CA-C-N	5.29	127.31	120.70
1	D	941	MET	C-N-CA	5.29	127.31	120.70
1	A	857	ASP	CA-C-N	5.26	128.06	120.38
1	A	857	ASP	C-N-CA	5.26	128.06	120.38
1	D	639	LEU	CA-C-N	5.25	127.32	120.28
1	D	639	LEU	C-N-CA	5.25	127.32	120.28
1	A	839	ILE	CA-C-N	5.23	127.71	120.29
1	A	839	ILE	C-N-CA	5.23	127.71	120.29
1	D	860	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	645	HIS	CA-C-N	5.22	128.96	120.60
1	A	645	HIS	C-N-CA	5.22	128.96	120.60
1	B	976	SER	CA-C-N	5.20	127.21	120.56
1	B	976	SER	C-N-CA	5.20	127.21	120.56
1	B	973	LYS	CA-C-N	5.16	127.50	120.54
1	B	973	LYS	C-N-CA	5.16	127.50	120.54
1	B	898	LEU	CA-C-N	5.14	130.87	122.81
1	B	898	LEU	C-N-CA	5.14	130.87	122.81
1	D	1003	PRO	N-CA-C	5.13	116.97	110.70
1	C	832	ILE	N-CA-C	-5.12	105.55	110.72
1	B	649	VAL	CA-C-N	5.09	127.99	120.82
1	B	649	VAL	C-N-CA	5.09	127.99	120.82
1	D	973	LYS	CA-C-N	5.08	127.05	120.44
1	D	973	LYS	C-N-CA	5.08	127.05	120.44
1	B	965	ASP	CA-CB-CG	5.08	117.68	112.60
1	A	805	CYS	CA-C-N	5.07	127.39	120.54
1	A	805	CYS	C-N-CA	5.07	127.39	120.54
1	D	991	THR	N-CA-C	-5.06	103.72	110.55
1	A	821	ASP	CA-C-N	5.05	127.29	120.38
1	A	821	ASP	C-N-CA	5.05	127.29	120.38
1	B	949	PHE	CA-C-N	5.04	126.91	120.56
1	B	949	PHE	C-N-CA	5.04	126.91	120.56
1	B	944	ALA	N-CA-C	-5.04	105.70	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	949	PHE	CA-C-N	5.02	127.61	120.53
1	C	949	PHE	C-N-CA	5.02	127.61	120.53
1	A	824	ARG	CA-C-N	5.01	129.16	121.19
1	A	824	ARG	C-N-CA	5.01	129.16	121.19

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	24	0
1	B	2188	0	2147	28	0
1	C	2133	0	2073	33	0
1	D	2086	0	2028	18	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
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	99	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 (99) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:812:ASP:CG	2:B:1701:38O:H10	2.12	0.74
1:A:944:ALA:O	1:A:948:ILE:HG12	1.90	0.71
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:639:LEU:HD22	1:D:844:MET:HE2	2.00	0.43
1:D:645:HIS:CD2	1:D:647:ASN:H	2.34	0.43
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:A:825:LEU:HD21	1:A:936:MET:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:918:SER:C	1:B:920:TYR:H	2.28	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%)	8	28
1	B	269/320 (84%)	237 (88%)	24 (9%)	8 (3%)	3	12
1	C	261/320 (82%)	229 (88%)	27 (10%)	5 (2%)	6	22
1	D	252/320 (79%)	229 (91%)	17 (7%)	6 (2%)	4	17
All	All	1045/1280 (82%)	935 (90%)	87 (8%)	23 (2%)	5	19

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	919	ALA
1	A	961	LYS

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Mol	Chain	Res	Type
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 ⓘ

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%)	199 (89%)	25 (11%)	6	19
1	B	235/286 (82%)	215 (92%)	20 (8%)	10	31
1	C	228/286 (80%)	205 (90%)	23 (10%)	7	23
1	D	221/286 (77%)	200 (90%)	21 (10%)	8	26
All	All	908/1144 (79%)	819 (90%)	89 (10%)	7	25

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	588	ILE
1	A	605	ILE
1	A	608	GLN
1	A	623	ILE
1	A	633	ILE
1	A	642	ARG
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	890	ILE
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	999	GLU
1	B	588	ILE
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	890	ILE
1	B	891	LYS
1	B	899	THR
1	B	901	MET
1	B	911	GLU
1	B	942	VAL
1	B	980	TRP

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Mol	Chain	Res	Type
1	B	1005	GLN
1	B	1006	MET
1	C	605	ILE
1	C	650	ARG
1	C	653	ASN
1	C	791	THR
1	C	795	VAL
1	C	807	LYS
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	966	PHE
1	C	974	GLN
1	C	980	TRP
1	C	997	LYS
1	C	998	SER
1	C	1000	LEU
1	C	1006	MET
1	D	595	LEU
1	D	649	VAL
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
1	D	947	ARG
1	D	958	THR
1	D	970	GLU

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Mol	Chain	Res	Type
1	D	980	TRP
1	D	1001	LEU
1	D	1005	GLN
1	D	1006	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	ASN
1	A	645	HIS
1	A	853	ASN
1	A	913	GLN
1	A	983	ASN
1	A	984	HIS
1	B	609	ASN
1	B	624	ASN
1	B	645	HIS
1	B	647	ASN
1	B	974	GLN
1	C	594	GLN
1	C	609	ASN
1	C	624	ASN
1	C	644	HIS
1	C	645	HIS
1	C	873	HIS
1	C	983	ASN
1	C	984	HIS
1	D	609	ASN
1	D	624	ASN
1	D	645	HIS
1	D	647	ASN
1	D	659	HIS
1	D	796	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 [i](#)

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](#)

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	B	1701	-	33,33,33	0.68	2 (6%)	40,49,49	1.01	4 (10%)
2	38O	A	1701	-	33,33,33	0.67	2 (6%)	40,49,49	1.02	4 (10%)
2	38O	C	1701	-	33,33,33	0.67	2 (6%)	40,49,49	1.02	4 (10%)
2	38O	D	1701	-	33,33,33	0.68	2 (6%)	40,49,49	1.00	4 (10%)

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	B	1701	-	-	2/6/18/18	0/5/5/5
2	38O	A	1701	-	-	0/6/18/18	0/5/5/5
2	38O	C	1701	-	-	4/6/18/18	0/5/5/5
2	38O	D	1701	-	-	4/6/18/18	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1701	38O	C12-N11	2.48	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1701	38O	C12-N11	2.48	1.36	1.32
2	C	1701	38O	C12-N11	2.47	1.36	1.32
2	A	1701	38O	C12-N11	2.44	1.36	1.32
2	B	1701	38O	C12-N13	-2.30	1.32	1.36
2	D	1701	38O	C12-N13	-2.30	1.32	1.36
2	A	1701	38O	C12-N13	-2.28	1.32	1.36
2	C	1701	38O	C12-N13	-2.28	1.32	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1701	38O	C10-C14-N13	3.43	109.84	105.71
2	B	1701	38O	C10-C14-N13	3.41	109.80	105.71
2	A	1701	38O	C10-C14-N13	3.41	109.80	105.71
2	D	1701	38O	C10-C14-N13	3.35	109.74	105.71
2	C	1701	38O	C14-C10-N11	-2.78	105.61	109.42
2	A	1701	38O	C14-C10-N11	-2.77	105.62	109.42
2	B	1701	38O	C14-C10-N11	-2.76	105.64	109.42
2	D	1701	38O	C14-C10-N11	-2.74	105.66	109.42
2	B	1701	38O	C15-C14-C10	-2.39	119.48	122.10
2	C	1701	38O	C15-C14-C10	-2.38	119.49	122.10
2	A	1701	38O	C15-C14-C10	-2.38	119.49	122.10
2	D	1701	38O	C15-C14-C10	-2.35	119.52	122.10
2	A	1701	38O	C10-N11-C12	2.14	106.86	104.68
2	C	1701	38O	C10-N11-C12	2.13	106.84	104.68
2	D	1701	38O	C10-N11-C12	2.12	106.83	104.68
2	B	1701	38O	C10-N11-C12	2.10	106.81	104.68

There are no chirality outliers.

All (10) torsion outliers are listed below:

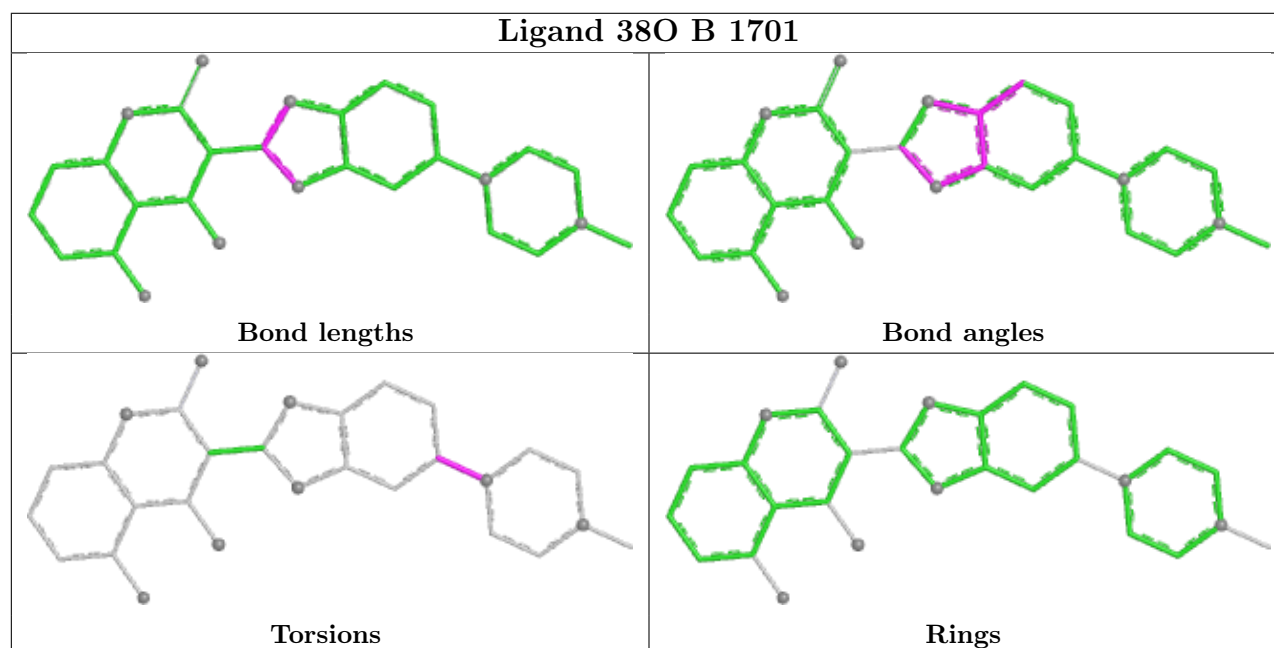
Mol	Chain	Res	Type	Atoms
2	C	1701	38O	C9-C8-N5-C4
2	C	1701	38O	C16-C8-N5-C4
2	D	1701	38O	C16-C8-N5-C6
2	D	1701	38O	C16-C8-N5-C4
2	D	1701	38O	C9-C8-N5-C6
2	D	1701	38O	C9-C8-N5-C4
2	B	1701	38O	C16-C8-N5-C6
2	B	1701	38O	C9-C8-N5-C6
2	C	1701	38O	C9-C8-N5-C6
2	C	1701	38O	C16-C8-N5-C6

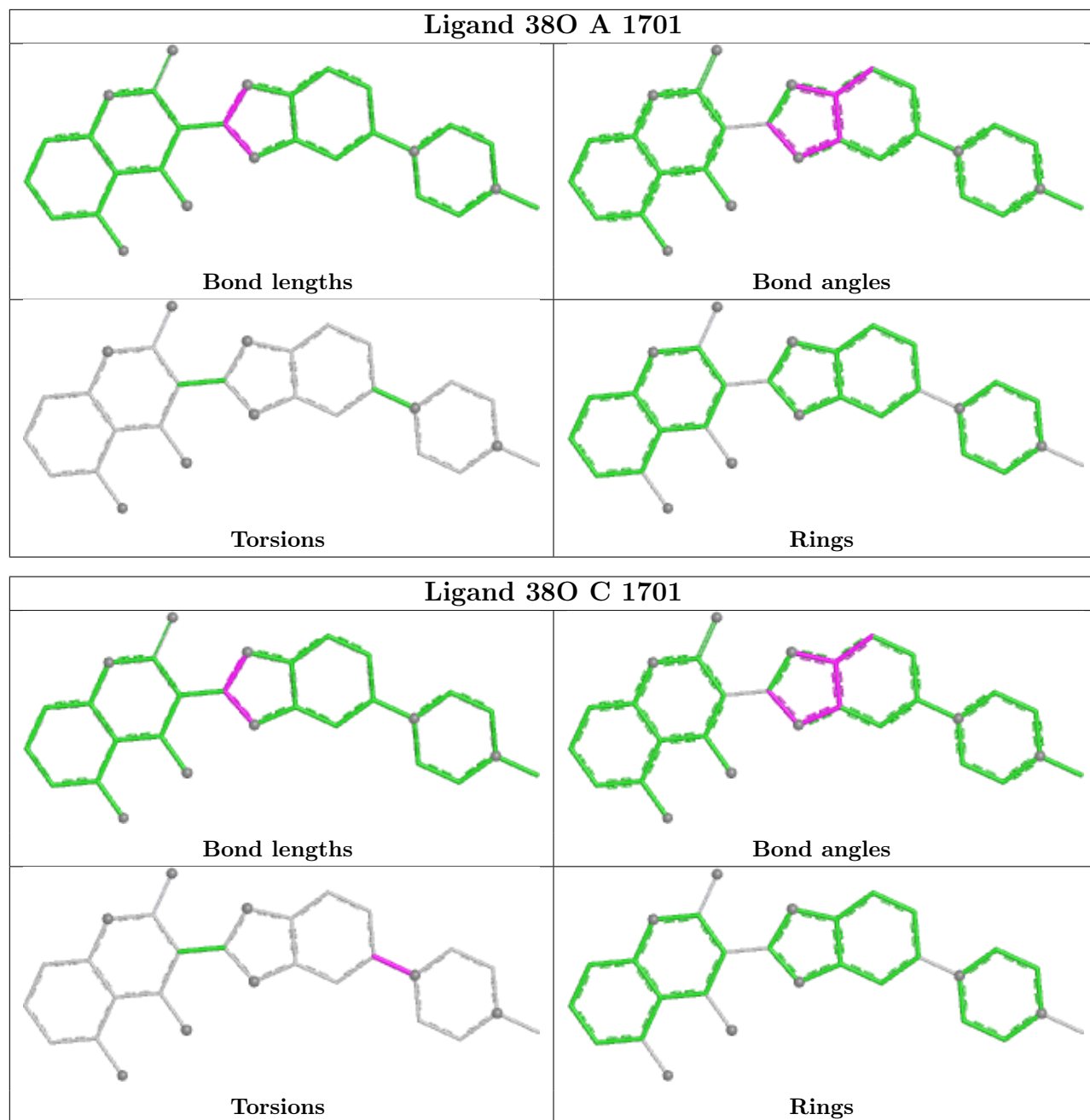
There are no ring outliers.

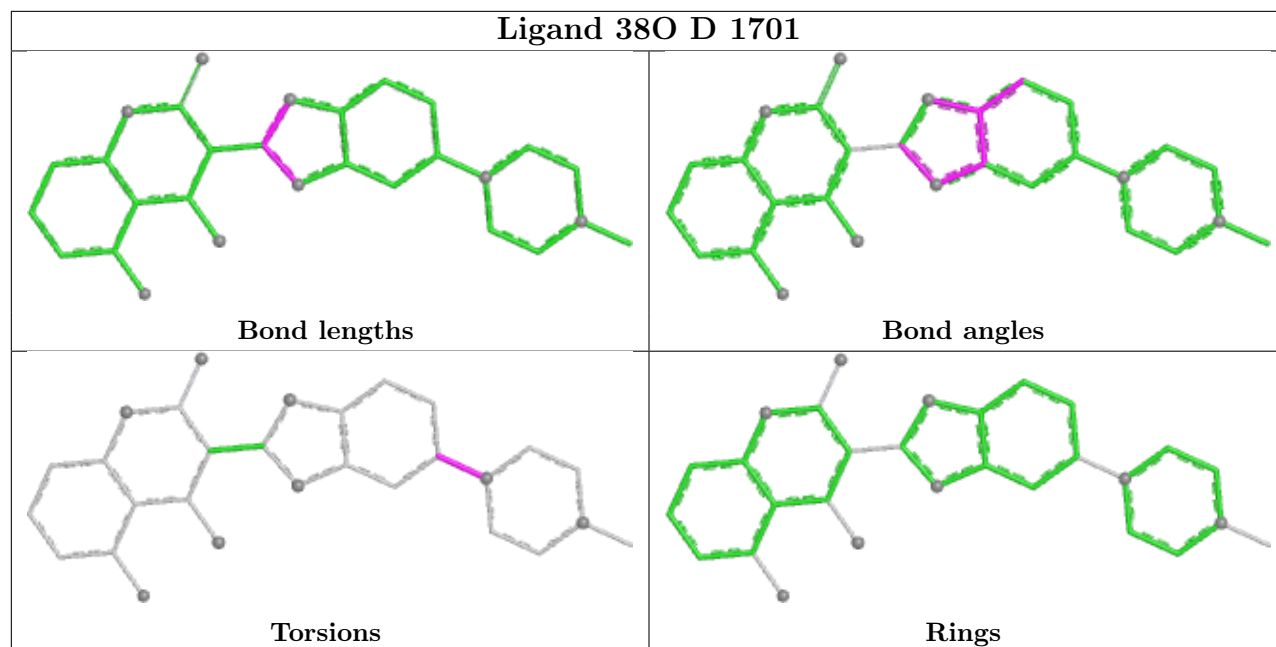
2 monomers are involved in 5 short contacts:

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 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 ⓘ

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	269/320 (84%)	0.07	8 (2%)	52	42	57, 82, 115, 145	0
1	B	275/320 (85%)	0.23	9 (3%)	49	39	62, 88, 125, 150	0
1	C	267/320 (83%)	0.23	8 (2%)	52	42	65, 89, 132, 175	0
1	D	260/320 (81%)	0.35	11 (4%)	40	32	62, 92, 139, 167	0
All	All	1071/1280 (83%)	0.22	36 (3%)	48	39	57, 88, 130, 175	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	662	PRO	3.3
1	A	918	SER	3.3
1	B	919	ALA	3.1
1	D	960	PRO	3.1
1	D	601	PHE	3.1
1	D	875	ALA	2.8
1	B	793	GLU	2.8
1	D	920	TYR	2.8
1	C	916	THR	2.8
1	D	1004	PRO	2.6
1	C	790	VAL	2.6
1	D	793	GLU	2.6
1	A	889	LEU	2.5
1	B	601	PHE	2.4
1	A	662	PRO	2.4
1	A	587	PHE	2.4
1	D	982	LEU	2.4
1	C	962	PHE	2.3
1	B	962	PHE	2.2
1	D	1006	MET	2.2
1	B	964	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1003	PRO	2.2
1	B	920	TYR	2.2
1	A	661	ARG	2.2
1	C	937	SER	2.2
1	A	795	VAL	2.2
1	A	920	TYR	2.2
1	B	659	HIS	2.1
1	C	873	HIS	2.1
1	C	1006	MET	2.1
1	B	1006	MET	2.1
1	B	662	PRO	2.0
1	C	960	PRO	2.0
1	D	869	LEU	2.0
1	C	870	ALA	2.0
1	A	911	GLU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

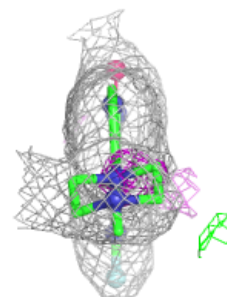
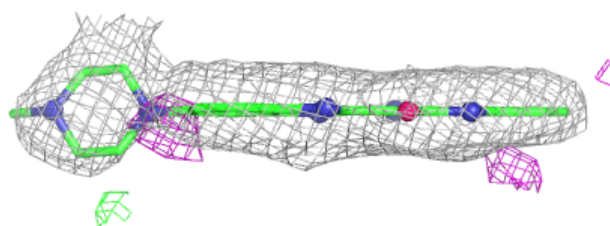
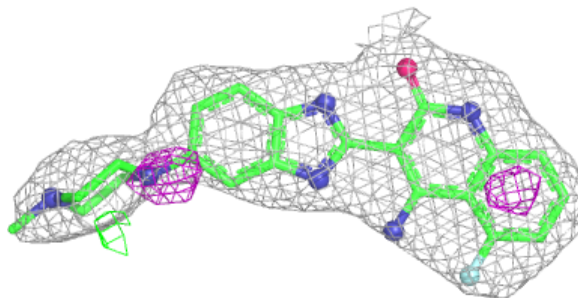
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	38O	C	1701	29/29	0.88	0.11	66,80,109,109	0
2	38O	B	1701	29/29	0.89	0.11	72,83,117,119	0
2	38O	A	1701	29/29	0.91	0.11	58,69,102,102	0
2	38O	D	1701	29/29	0.91	0.10	66,79,115,117	0

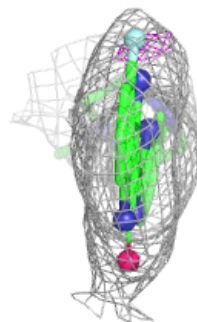
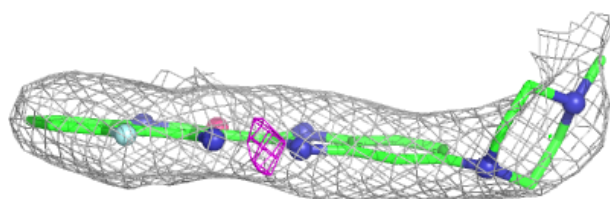
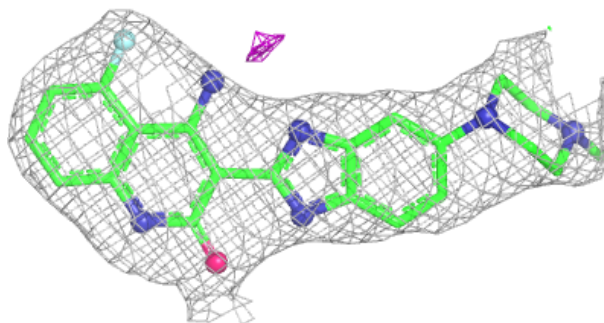
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

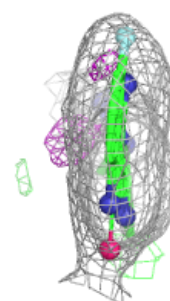
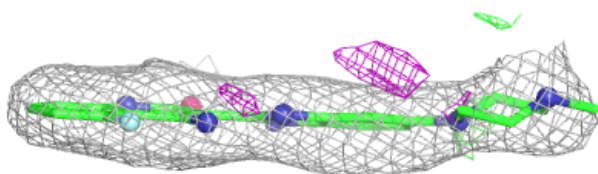
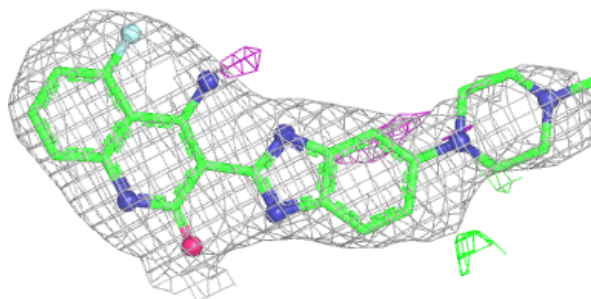
**Electron density around 38O B 1701:**

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

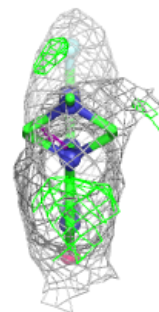
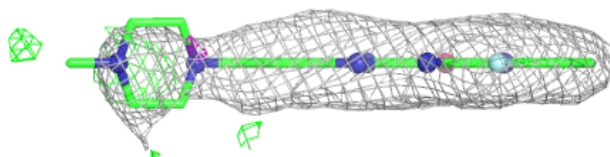
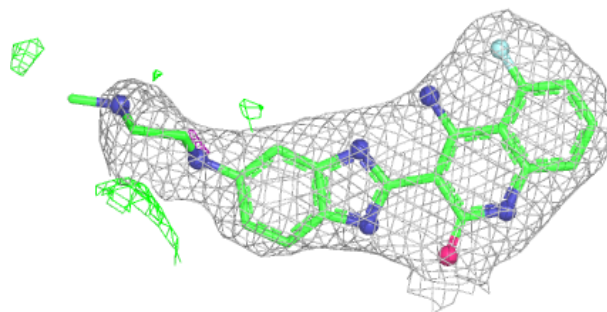


Electron density around 38O A 1701:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.