



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2022 – 09:30 pm BST

PDB ID : 7QWK
Title : GCN2 (EIF2ALPHA KINASE 4, E2AK4) IN COMPLEX WITH COM-
POUND 2
Authors : Maia de Oliveira, T.
Deposited on : 2022-01-25
Resolution : 2.30 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 : 2.28
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) : 2.28

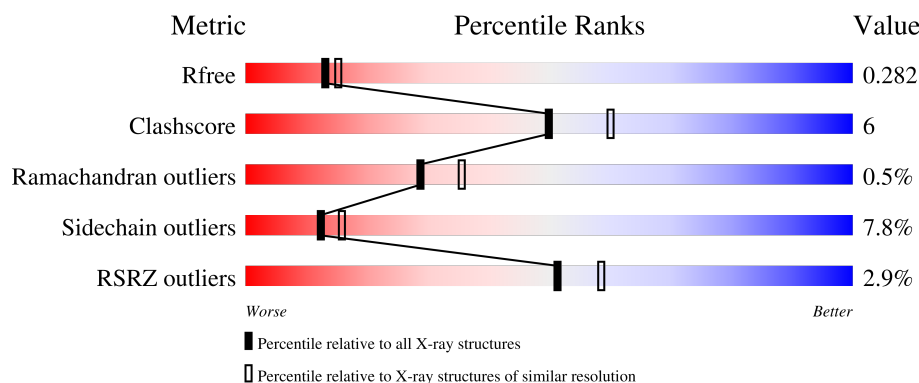
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1649	<div> <div>13% .</div> <div>85%</div> </div>
1	B	1649	<div> <div>13% .</div> <div>85%</div> </div>
1	C	1649	<div> <div>%</div> <div>12% .</div> <div>85%</div> </div>
1	D	1649	<div> <div>13% .</div> <div>85%</div> </div>
1	E	1649	<div> <div>%</div> <div>11% .</div> <div>85%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	1649	<div><div></div><div>13%<div></div></div><div>85%</div></div>
1	G	1649	<div><div></div><div>13%<div></div></div><div>84%</div></div>
1	H	1649	<div><div></div><div>13%<div></div></div><div>84%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16000 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.

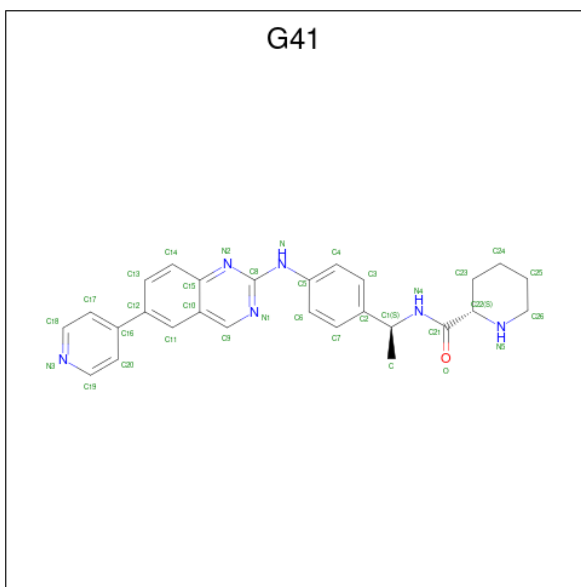
- Molecule 1 is a protein called eIF-2-alpha kinase GCN2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1865	1205	315	338	7			
1	B	249	Total	C	N	O	S	0	0	0
			1934	1248	331	348	7			
1	C	249	Total	C	N	O	S	0	0	0
			1928	1249	327	345	7			
1	D	254	Total	C	N	O	S	0	0	0
			1993	1289	337	360	7			
1	E	241	Total	C	N	O	S	0	0	0
			1897	1225	327	338	7			
1	F	254	Total	C	N	O	S	0	0	0
			1990	1285	340	357	8			
1	G	257	Total	C	N	O	S	0	0	0
			2005	1293	340	364	8			
1	H	259	Total	C	N	O	S	0	0	0
			2024	1306	343	366	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	848	ASN	ASP	conflict	UNP Q9P2K8
B	848	ASN	ASP	conflict	UNP Q9P2K8
C	848	ASN	ASP	conflict	UNP Q9P2K8
D	848	ASN	ASP	conflict	UNP Q9P2K8
E	848	ASN	ASP	conflict	UNP Q9P2K8
F	848	ASN	ASP	conflict	UNP Q9P2K8
G	848	ASN	ASP	conflict	UNP Q9P2K8
H	848	ASN	ASP	conflict	UNP Q9P2K8

- Molecule 2 is (2 {S})- {N}-[(1 {S})-1-[4-[(6-pyridin-4-ylquinazolin-2-yl)amino]phenyl]ethyl]piperidine-2-carboxamide (three-letter code: G41) (formula: C₂₇H₂₈N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			34	27	6	1		
2	B	1	Total	C	N	O	0	0
			34	27	6	1		
2	C	1	Total	C	N	O	0	0
			34	27	6	1		
2	D	1	Total	C	N	O	0	0
			34	27	6	1		
2	E	1	Total	C	N	O	0	0
			34	27	6	1		
2	F	1	Total	C	N	O	0	0
			34	27	6	1		
2	G	1	Total	C	N	O	0	0
			34	27	6	1		
2	H	1	Total	C	N	O	0	0
			34	27	6	1		

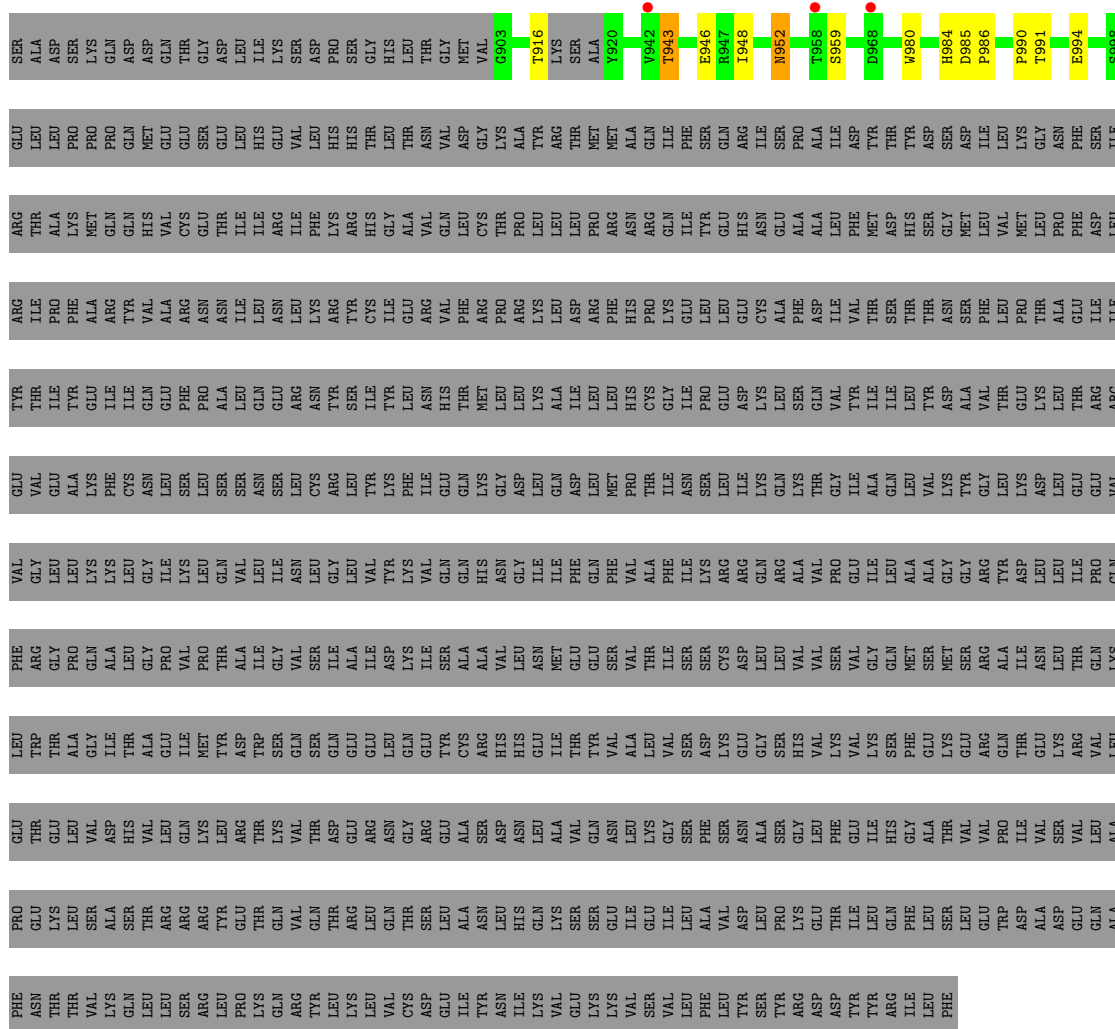
- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	O	S	0	0
			4	2	1	1		
3	H	1	Total	C	O	S	0	0
			4	2	1	1		

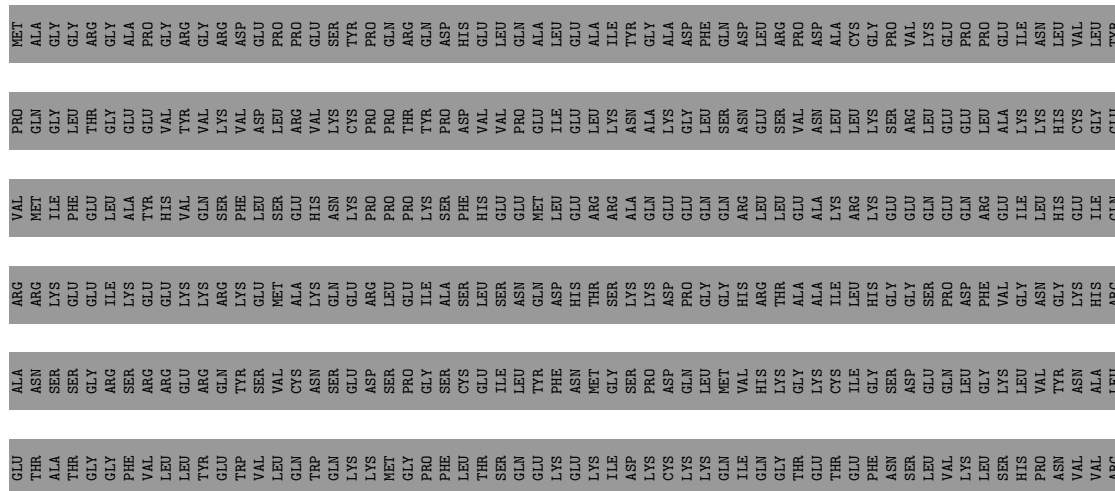
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	17	Total	O	0	0
			17	17		
4	C	4	Total	O	0	0
			4	4		
4	D	8	Total	O	0	0
			8	8		
4	E	8	Total	O	0	0
			8	8		
4	F	14	Total	O	0	0
			14	14		
4	G	9	Total	O	0	0
			9	9		
4	H	16	Total	O	0	0
			16	16		



- Molecule 1: eIF-2-alpha kinase GCN2

Chain B: 13% 85%





Chain C: 12% 85%

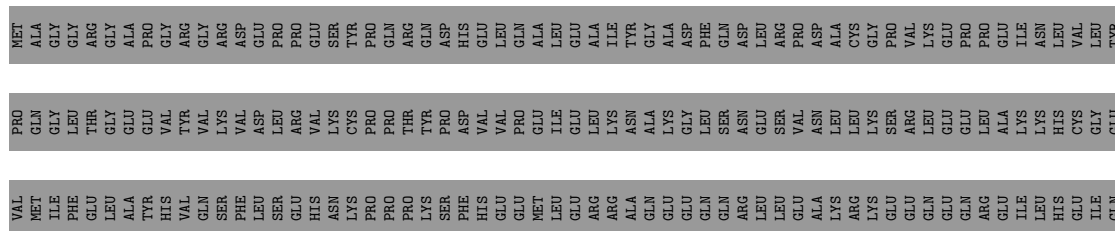


TYR ARG ILE LEU PHE	LEU	ILE	LYS	GLY	ILE	ALA	ILE	GLN	ILE	THR
	GLN	HIS	SER	GLN	LEU	GLN	LEU	LEU	ILE	SER
	PHE	GLY	PHE	MET	ALA	VAL	LEU	LEU	ILE	THR
	LEU	ALA	GLU	SER	GLY	LYS	LYS	ASP	TYR	ASN
	LEU	VAL	GLU	SER	GLY	TYR	GLY	ALA	SER	PHE
	GLU	PRO	ARG	ARG	ARG	GLY	LEU	VAL	THR	LEU
	TRP	PRO	GLN	ALA	TYR	GLN	LEU	THR	PRO	LEU
	ASP	ILE	THR	ILE	ASP	LYS	GLU	GLU	THR	THR
	ALA	VAL	GLU	ASN	LEU	ASP	LEU	LEU	LYS	ALA
	ASP	SER	LYS	LEU	LEU	LEU	GLU	THR	GLU	GLU
GLU	VAL	ARG	THR	ILE	PRO	GLU	ARG	ILE	ILE	
GLN	LEU	VAL	GLN	PRO	GLN	LYS	LYS	THR	TYR	
ALA	ALA	LEU	LYS	ILE	ALA	VAL	PHE	GLY	GLU	
ASN	PRO	GLU	LEU	PHE	VAL	VAL	GLY	VAL	ILE	
THR	GLY	THR	TRP	ARG	GLY	LEU	GLY	LEU	THR	
THR	LYS	GLU	THR	THR	PRO	LEU	ALA	TYR	GLU	
THR	LEU	LEU	ALA	GLY	GLN	LYS	LYS	ALA	GLU	
VAL	SER	VAL	GLY	ILE	VAL	LEU	LEU	ARG	ILE	
LYS	ALA	ASP	ILE	ALA	ASP	LYS	PHE	ARG	ILE	
GLN	THR	HIS	THR	LEU	LEU	LEU	CYS	THR	TYR	
LEU	ARG	THR	ALA	GLY	ILE	GLY	ASN	SER	GLY	
SER	ARG	LEU	ILE	PRO	VAL	LYS	SER	LEU	PHE	
ARG	ARG	LYS	MET	PRO	LEU	LEU	LEU	LEU	PRO	
LEU	TYR	LEU	THR	THR	GLN	VAL	ASN	GLN	ALA	
PRO	GLU	GLU	ASP	ASP	ALA	VAL	SER	SER	SER	
LYS	THR	THR	TRP	TRP	ILE	ILE	LEU	ASN	GLN	
GLN	GLN	LYS	SER	GLY	ILE	ILE	SER	SER	GLU	
ARG	VAL	VAL	GLN	VAL	ASN	ASN	LEU	LEU	ARG	
TYR	GLN	THR	THR	SER	SER	LEU	CYS	ASN	ASN	
LEU	THR	LEU	GLN	GLN	ILE	VAL	ARG	GLY	TYR	
LYS	ARG	GLU	GLU	ALA	LEU	GLY	GLU	GLN	HIS	
LEU	LEU	LEU	GLU	ILE	VAL	VAL	TYR	GLN	THR	
VAL	GLN	ASN	GLY	ASP	TYR	LYS	LYS	LYS	TYR	
CYS	THR	GLY	GLN	LEU	ASP	LYS	PHE	LEU	LEU	
ASP	SER	SER	GLU	GLU	ILE	VAL	ILE	LEU	ASN	
GLU	LEU	ASN	ASN	HIS	VAL	GLY	GLY	ASP	ILE	
ILE	HIS	ASN	HIS	HIS	VAL	ASN	GLY	MET	LEU	
LYS	GLN	LEU	GLU	GLU	ASN	ILE	ILE	PRO	THR	
VAL	LYS	ALA	ILE	MET	ILE	ILE	GLN	THR	CYS	
GLU	SER	VAL	THR	GLU	PHE	PHE	ASN	ILE	GLY	
LYS	SER	ASN	TYR	GLN	GLN	GLN	SER	SER	PRO	
VAL	GLY	ASN	VAL	SER	VAL	VAL	ARG	LEU	GLU	
SER	GLU	LEU	ALA	VAL	VAL	ARG	ILE	ILE	ASP	
THR	GLU	THR	LEU	THR	ALA	ARG	LYS	LYS	LEU	
LEU	ILE	GLY	VAL	ILE	PHE	GLN	THR	THR	GLY	
PHE	ALA	PHE	ASP	SER	LYS	ARG	SER	GLY	THR	
LEU	VAL	SER	LYS	CYS	ASP	ARG	ILE	ILE	VAL	
ASP	ASP	ASN	GLU	ASP	THR	THR	THR	GLY	GLY	
TYR	THR	THR	PHE	VAL	VAL	GLN	PRO	PRO	THR	
THR	ILE	GLU	THR	VAL	VAL	GLN	GLN	GLN	THR	
THR	THR	THR	THR	VAL	VAL	GLN	GLN	GLN	THR	
THR	THR	THR	THR	VAL	VAL	GLN	GLN	GLN	THR	

- Molecule 1: eIF-2-alpha kinase GCN2

Chain D: 13% . 85%

PRO	GLN	TRP	VAL	VAL	TTR	GLU	ALA	ARG	VAL	PRO	MET
GLN	TRP	TRP	VAL	VAL	ALA	THR	ASN	ARG	MET	GLN	ALA
PRO	PRO	GLY	HIS	ALA	ALA	ALA	LYS	LYS	ILE	GLY	GLY
LYS	LEU	LEU	VAL	VAL	ASN	THR	SER	GLU	GLU	THR	GLY
MET	GLY	GLY	VAL	VAL	LEU	GLY	GLY	ILE	LEU	GLY	GLY
PRO	LEU	LEU	SER	LEU	GLY	PHE	SER	LYS	ALA	GLU	PRO
LEU	LEU	LEU	ALA	VAL	LYS	VAL	ARG	GLU	TTR	GLU	ALA
VAL	LEU	LEU	SER	GLN	GLY	THR	ASN	GLU	VAL	GLU	PRO
GLU	LEU	LEU	SER	ASN	ASP	LEU	ARG	GLU	VAL	GLY	GLY
GLN	SER	SER	VAL	VAL	ASP	THR	GLN	LYS	VAL	TYR	ARG
PRO	LEU	LEU	SER	LEU	ILE	TRP	TTR	LYS	PHE	VAL	ASP
GLU	GLN	GLN	VAL	VAL	ILE	TRP	TTR	LYS	PHE	VAL	ASP
ASP	GLY	GLY	ASP	ASP	VAL	VAL	SER	GLU	LEU	ASP	GLU
SER	GLN	GLN	ALA	ALA	VAL	LEU	VAL	MET	SER	LEU	GLU
ASP	GLY	GLY	GLY	GLY	ASP	GLN	CYS	ALA	GLU	ARG	PRO
GLY	GLY	CYS	GLY	THR	ILE	TRP	ASN	LYS	HIS	VAL	VAL
GLN	GLY	THR	THR	THR	LEU	GLN	SER	GLN	ASN	LYS	SER
ASP	GLY	VAL	VAL	VAL	VAL	LYS	GLU	GLU	LYS	CYS	THR
TYR	LYS	LYS	LYS	LYS	GLU	LYS	ASP	ARG	PRO	PRO	GLN
PRO	VAL	PRO	ILE	ILE	HIS	THR	SER	LEU	LEU	PRO	GLN
VAL	VAL	VAL	THR	THR	ILE	GLY	PRO	GLU	THR	THR	ARG
THR	THR	THR	ASP	ASP	SER	PRO	GLY	ILE	LYS	GLN	GLN
VAL	ILE	ILE	TYR	SER	GLY	PHE	SER	ALA	PRO	PRO	ASP
ILE	PRO	PRO	SER	SER	VAL	LEU	CYS	SER	PHE	ASP	HIS
PRO	SER	SER	ASP	SER	ILE	THR	GLU	LEU	VAL	VAL	GLY
PRO	ASN	LEU	LEU	LEU	LYS	GLN	LEU	ASN	GLU	PRO	LEU
ASN	LEU	LEU	LEU	ALA	ALA	GLU	ILE	GLN	GLU	GLN	ALA
ARG	PRO	ALA	ARG	ARG	ALA	LYS	PHE	ASP	LEU	ILE	LEU
LEU	ASP	ASP	ALA	ALA	HIS	LYS	ASN	GLU	GLU	GLU	GLU
PRO	SER	PHE	ASP	ASP	LEU	GLY	GLU	HIS	ASN	GLU	ALA
ASN	ALA	GLN	ILE	ILE	HIS	LYS	MET	THR	ARG	LEU	LEU
ALA	ASP	ASP	CYS	CYS	SER	ASP	GLY	LYS	ALA	LYS	ALA
PHE	PHE	PHE	LYS	LYS	GLY	LYS	PRO	LYS	GLN	ALA	GLY
SER	PHE	LEU	GLU	ASP	PRO	CYS	ASP	ASP	GLU	LYS	ALA
GLU	LYS	LYS	VAL	VAL	ILE	LYS	GLN	PRO	GLU	GLY	PHE
THR	THR	CYS	PHE	THR	VAL	LYS	MET	GLY	GLN	SER	GLN
GLN	VAL	VAL	GLU	GLU	HIS	ILE	VAL	HIS	ARG	ASN	LEU
ARG	CYS	CYS	GLN	GLN	GLN	GLY	HIS	ARG	LEU	GLU	ASP
GLN	LEU	LEU	THR	THR	LEU	GLY	LYS	THR	LEU	SER	ARG
F583	ASP	ASP	VAL	VAL	ARG	THR	GLY	ALA	LEU	VAL	PRO
I588	LYS	ASP	VAL	ARG	ARG	GLU	LYS	ALA	GLU	ASN	ASP
K598	ARG	PHE	PHE	THR	TTR	THR	ILE	ILE	LYS	LEU	ALA
V604	TRP	ASP	ASP	ASP	ALA	PHE	GLY	HIS	LYS	LYS	GLY
N609	SER	PRO	ALA	LEU	SER	VAL	GLU	PRO	GLU	LEU	VAL
M609	GLN	GLN	THR	THR	GLY	LYS	LEU	ASP	GLN	LEU	PRO
D612	LEU	LEU	LYS	LYS	ASP	SER	LYS	VAL	ARG	ALA	GLU
L639	HIS	THR	GLY	GLY	TTR	THR	THR	GLY	ILE	LYS	ILE
H645	SER	LYS	LYS	VAL	SER	PRO	VAL	ASN	GLY	GLY	HIS
E646	PHE	LYS	LYS	ASN	HIS	VAL	TTR	LYS	GLY	TYR	CYS
M647	ILE	GLY	GLY	GLY	VAL	VAL	ASN	LYS	GLY	GLY	VAL
E648	ASN	GLY	GLY	GLY	ARG	ARG	THR	HIS	ILE	GLY	THR



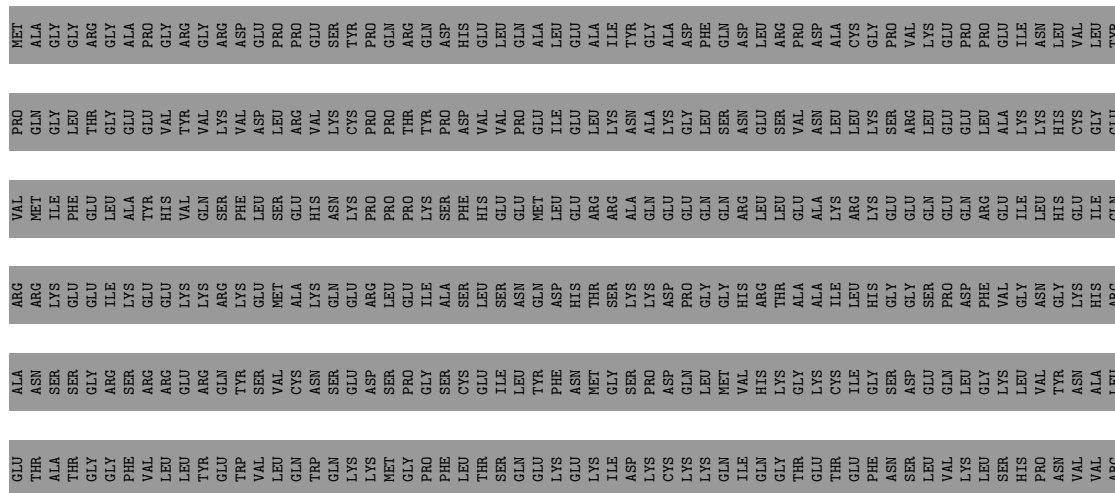


[illegible]

- Molecule 1: eIF-2-alpha kinase GCN2

Chain F:  13% 85%

[illegible]





ASP	ALA	ASP	GLU	GLN	ALA	PHE	ASN	ASN	THR	THR	VAL	LYS	GLN	LEU	LEU	SER	ARG	LEU	PRO	LYS	GLN	ARG	TYR	LEU	LYS	ASP	GLU	ILE	TYR	ASN	ILE	LYS	VAL	CYS	CYS	ASP	GLU	ILE	TYR	ASN	ILE	LYS	VAL	PHE	LEU	LEU	LEU	TYR	SER	TYR	ARG	ASP	ASP	TYR	TYR	ARG	ILE	LEU
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- Molecule 1: eIF-2-alpha kinase GCN2

Chain H:  13% . 84%

NET	ALA	GLY	GLY	GLY	ALA	PRO	GLY	ARG	GLY	ARG	ARG	GLU	ASP	PRO	PRO	GLU	SER	TYR	PRO	PRO	GLN	ARG	GLN	ASP	HIS	GLU	LEU	LEU	GLN	ALA	LEU	GLU	ALA	ILE	TYR	GLY	GLY	ALA	ASP	PHE	GLN	GLN	ASP	LEU	LEU	ARG	PRO	ASP	ALA	CYS	GLY	PRO	PRO	VAL	VAL	LYS	PRO	GLU	PRO	GLU	GLU	ASN	LEU	VAL	LEU	LEU
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PRO GLN GLY LEU THR GLY GLU VAL TYR VAL VAL VAL VAL ASP LEU ARG VAL VAL VAL CYS CYS PRO PRO THR TYR PRO ASP VAL VAL VAL PRO GLU ILE GLU LEU LEU LEU ASN ALA ALA LYS LEU SER SER ASN GLU GLY SER SER ASN LEU LEU LEU LEU ALA LYS LYS SER ARG LEU LEU GLU LEU LEU ALA LYS HIS CYS GLY

VAL	PHE	LEU	ALA	TYS	HIS	VAL	GLN	SER	PHE	LEU	SER	GLU	HIS	ASN	LYS	PRO	PRO	PRO	LYS	SER	PHE	HIS	GLU	GLU	MET	LEU	GLU	ARG	ARG	ALA	GLN	GLN	GLU	GLU	GLN	GLN	ARG	LEU	LEU	GLU	GLU	ALA	LYS	ARG	LYS	ILE	HIS	GLU	ILE
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ARG	ARG	LYS	GLU	GLU	LYS	GLU	GLU	LYS	ARG	LYS	GLU	MET	ALA	ALA	GLN	GLU	ARG	LEU	LEU	GLU	ILE	ALA	SER	LEU	SER	ASN	ASN	GLN	ASP	HIS	THR	SER	LYS	LYS	ASP	PRO	GLY	GLY	HIS	ARG	THR	THR	ALA	ALA	ILE	LEU	HIS	GLY	GLY	SER	PRO	ASP	PHE	VAL	GLY	ASN	GLY	LYS	HIS
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ALA	ASN	ASN	SER	SER	GLY	ARG	SER	ARG	ARG	GLU	ARG	GLN	TYR	SER	VAL	CYS	ASN	SER	GLU	ASP	ASP	PRO	PRO	GLY	SER	CYS	GLU	ILE	TYR	PHE	ASN	MET	GLY	SER	PRO	ASP	GLN	LEU	MET	VAL	HIS	LYS	GLY	LYS	CYS	ILE	GLY	SER	ASP	GLU	LEU	GLY	LYS	VAL	TYR	ASN	ALA
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GLU	THR	ALA	THR	GLY	GLY	PHE	VAL	LEU	LEU	TYR	GLU	TRP	VAL	LEU	GLN	TRP	GLN	LYS	LYS	MET	GLY	PRO	PHE	LEU	THR	SER	GLN	GLY	LYS	GLU	GLU	LYS	ILE	ILE	GLN	GLN	CYS	LYS	LYS	GLN	ILE	GLY	THR	THR	GLU	GLU	PHE	ASN	SER	SER	LEU	VAL	LYS	LEU	SER	HIS	PRO	ASN	VAL	VAL
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TYR	LEU	ALA	MET	ASN	LEU	LYS	GLU	GLN	ASP	ASP	ASP	SER	ILE	VAL	VAL	ASP	ILE	LEU	VAL	GLU	HIS	ILE	SER	GLY	VAL	SER	LEU	ALA	ALA	HIS	LEU	HIS	HIS	SER	SER	GLY	PRO	ILE	PRO	VAL	GLN	LEU	LEU	ARG	ARG	TYR	THR	ALA	GLN	LEU	LEU	LEU	HIS	SER	SER	GLY	ASP	TYR	ASN
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VAL	VAL	HIS	LVS	LVS	LEU	SER	ALA	SER	ASN	VAL	VAL	ASP	ALA	GLU	GLY	THR	VAL	LVS	ILE	THR	ASP	Tyr	SER	ILE	SER	LVS	ARG	LEU	ALA	ASP	CYS	LVS	GLU	ASP	VAL	PHE	GLU	GLN	THR	ARG	VAL	ARG	PHE	SER	ASN	ASP	ASN	ALA	LEU	PRO	Tyr	LVS	THR	GLY	LVS	GLY
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VAL	TRP	ARG	LEU	GLY	LEU	LEU	LEU	LEU	SER	SER	SER	GLN	GLY	GLN	GLU	CYS	GLY	GLY	GLY	TYR	PRO	PRO	VAL	THR	THR	ILE	PRO	SER	SER	ASP	LEU	LEU	LYS	LYS	CYS	VAL	GLU	ARG	TRP	SER	SER	PRO	GLN	GLN	LEU	LEU	LYS	HIS	SER	SER	PHE	ILE
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PRO	GLN	PRO	LYS	MET	PRO	LEU	VAL	GLU	GLN	SER	PRO	GLU	ASP	SER	GLU	GLY	GLN	ASP	TYR	VAL	GLU	THR	VAL	ILE	PRO	SER	ASN	ARG	LEU	PRO	SER	ALA	PHE	PHE	SER	GLU	THR	GLN	ARG	GLN	PHE	SE84	R585	L593	A600	G608	N609	D612	K619	R620	R621	R640
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H645	H646	N647	I648	I649	R650	Y651	Y652	N653	H659	GLU	ARG	PRO	ALA	GLY	PRO	GLY	THR	PRO	PRO	ASP	SER	GLY	PRO	LEU	ALA	LYS	ASP	ASP	ARG	ALA	ALA	ALA	ARG	GLY	GLN	PRO	ALA	SER	SER	ASP	THR	ASP	GLY	LEU	ASP	SER	SER	VAL	GLU	ALA	ALA	PRO	PRO	PRO	PRO	ILE	LEU	SER
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SER	VAL	GLU	TRP	SER	SER	THR	SER	GLY	GLU	ARG	SER	SER	ALA	ALA	ARG	PHE	PRO	THR	GLY	PRO	GLY	SER	SER	ASP	ASP	GLU	ASP	ASP	ASP	GLU	GLU	HIS	GLY	GLY	VAL	PHE	SER	SER	SER	PHE	LEU	PRO	ALA	SER	ASP	SER	SER	GLU	GLU	ASP	ASN	GLU	ASP	GLU
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[illegible]

ALA	ASP	SER	GLN	ASP	ASP	GLN	THR	GLY	ASP	LEU	ILE	LYS	SER	D883	L898	G903	L906	S909	V912	GLY	GLY	SER	THR	N921	D925	S928	M936	A944	I948	D956	PRO	THR	SER	P960	S967	ASP	GLY	GLU	H971	S979	L995
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E999	P1003	M1006	GLU GLU SER GLU LEU HIS GLU VAL LEU HIS HIS THR LEU THR ASN VAL ASP GLY LYS ALA TYR ARG THR MET MET ALA ILE GLN PHE SER SER GLN ARG ILE SER PRO ALA ILE ILE ASP TYR THR TYR ASP SER ASP ILE LEU LYS GLY ASN PHE SER ILE ARG THR
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lys met gln gln his his val val cys glj thr ile ile ile arg arg phe phe lys arg his gly ala ala val val gln gln cys thr pro pro leu leu leu leu pro pro arg asn arg arg gln ile ile tyr thr glu his asn glu ala ala leu leu phe phe met met asp asp his ser gly phe phe asp asp leu leu val val met met leu leu pro pro pro phe phe arg arg ile

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.80Å 77.80Å 101.69Å 89.86° 90.05° 68.58°	Depositor
Resolution (Å)	42.00 – 2.30 39.43 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (42.00-2.30) 95.8 (39.43-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.29Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.214 , 0.243 0.225 , 0.282	Depositor DCC
R_{free} test set	4728 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.448 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16000	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8623e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DMS, G41

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	0/1909	0.70	0/2598
1	B	0.53	0/1979	0.68	0/2686
1	C	0.51	0/1976	0.70	0/2686
1	D	0.53	0/2041	0.69	0/2770
1	E	0.52	0/1942	0.70	0/2632
1	F	0.54	0/2035	0.73	0/2759
1	G	0.52	0/2049	0.69	0/2779
1	H	0.52	0/2071	0.70	0/2809
All	All	0.52	0/16002	0.70	0/21719

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 [i](#)

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	1865	0	1731	17	0
1	B	1934	0	1820	20	0
1	C	1928	0	1815	18	0
1	D	1993	0	1896	18	0
1	E	1897	0	1823	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1990	0	1912	24	0
1	G	2005	0	1919	22	0
1	H	2024	0	1934	25	0
2	A	34	0	0	1	0
2	B	34	0	0	1	0
2	C	34	0	0	1	0
2	D	34	0	0	1	0
2	E	34	0	0	2	0
2	F	34	0	0	5	0
2	G	34	0	0	2	0
2	H	34	0	0	6	0
3	H	8	0	12	2	0
4	A	8	0	0	0	0
4	B	17	0	0	1	0
4	C	4	0	0	0	0
4	D	8	0	0	0	0
4	E	8	0	0	0	0
4	F	14	0	0	0	0
4	G	9	0	0	1	0
4	H	16	0	0	1	0
All	All	16000	0	14862	177	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 (177) 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:845:ILE:HD11	1:C:922:GLN:HA	1.51	0.91
1:F:636:GLU:HG2	1:F:868:GLY:HA2	1.59	0.83
1:D:609:ASN:HD22	1:D:612:ASP:H	1.25	0.83
1:G:866:ASP:HB2	1:G:870:ALA:HA	1.58	0.83
1:G:609:ASN:HD22	1:G:612:ASP:H	1.28	0.81
1:H:645:HIS:HD2	1:H:647:ASN:H	1.30	0.80
1:B:853:ASN:ND2	1:B:867:PHE:H	1.82	0.76
1:D:853:ASN:ND2	1:D:867:PHE:H	1.84	0.76
1:F:855:PHE:CE2	2:F:1701:G41:C14	2.70	0.75
1:B:853:ASN:HD22	1:B:867:PHE:H	1.33	0.74
1:E:920:TYR:HB3	1:E:924:VAL:HG21	1.70	0.74
1:D:639:LEU:HD12	1:D:875:ALA:HB1	1.69	0.73
1:C:609:ASN:HD22	1:C:612:ASP:H	1.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:VAL:HG23	1:A:803:GLU:HG2	1.72	0.72
1:H:609:ASN:HD22	1:H:612:ASP:H	1.37	0.70
1:F:645:HIS:HD2	1:F:647:ASN:H	1.39	0.70
1:B:609:ASN:HD22	1:B:612:ASP:H	1.39	0.70
1:H:645:HIS:CD2	1:H:647:ASN:H	2.09	0.70
1:B:604:VAL:HG23	1:B:869:LEU:HD21	1.75	0.69
1:A:609:ASN:HD22	1:A:612:ASP:H	1.39	0.68
1:C:845:ILE:HD11	1:C:922:GLN:CA	2.23	0.68
1:F:609:ASN:HD22	1:F:612:ASP:H	1.39	0.68
1:E:609:ASN:HD22	1:E:612:ASP:H	1.40	0.67
1:D:645:HIS:HD2	1:D:647:ASN:H	1.41	0.66
1:B:645:HIS:HD2	1:B:647:ASN:H	1.43	0.66
1:D:795:VAL:HG11	1:F:1005:GLN:HB3	1.77	0.66
1:D:853:ASN:HD22	1:D:867:PHE:H	1.42	0.66
1:H:960:PRO:HG2	1:H:979:SER:HA	1.79	0.65
1:E:649:VAL:HG23	1:E:803:GLU:HG2	1.79	0.65
1:B:645:HIS:CD2	1:B:647:ASN:H	2.15	0.64
1:D:609:ASN:ND2	1:D:612:ASP:H	1.95	0.64
1:F:645:HIS:CD2	1:F:647:ASN:H	2.16	0.64
1:D:645:HIS:CD2	1:D:647:ASN:H	2.16	0.63
1:F:855:PHE:CZ	2:F:1701:G41:C13	2.82	0.63
1:E:609:ASN:HB3	1:E:612:ASP:OD1	1.99	0.63
1:G:859:ASP:HB3	1:G:861:HIS:HD2	1.64	0.63
1:H:619:LYS:HE2	1:H:621:ILE:HD11	1.81	0.62
1:G:609:ASN:ND2	1:G:612:ASP:H	1.96	0.61
1:E:593:LEU:HD11	1:E:608:GLN:HB2	1.83	0.61
1:D:604:VAL:HG23	1:D:869:LEU:HD21	1.83	0.61
1:C:816:GLN:HB3	1:H:806:GLU:HG2	1.82	0.60
1:F:648:ILE:HG22	1:F:866:ASP:OD2	2.01	0.60
1:G:846:HIS:O	1:G:847:ARG:HB2	2.00	0.60
1:A:645:HIS:HD2	1:A:647:ASN:H	1.49	0.60
1:G:609:ASN:HB3	1:G:612:ASP:OD1	2.01	0.60
1:F:855:PHE:CE2	2:F:1701:G41:C15	2.85	0.59
1:E:645:HIS:HB3	1:E:648:ILE:HG12	1.85	0.59
1:G:650:ARG:HG2	1:G:652:TYR:CE1	2.38	0.59
1:C:645:HIS:HD2	1:C:647:ASN:H	1.49	0.59
1:B:909:SER:HB2	1:B:924:VAL:HG13	1.85	0.58
1:E:609:ASN:ND2	1:E:612:ASP:H	2.02	0.58
1:F:960:PRO:HG2	1:F:979:SER:HA	1.86	0.57
1:C:931:ILE:HG12	1:C:982:LEU:HD21	1.86	0.57
1:G:645:HIS:HD2	1:G:647:ASN:H	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:GLN:O	1:C:633:ILE:HG12	2.05	0.56
1:D:650:ARG:HG2	1:D:652:TYR:CE1	2.41	0.56
1:D:909:SER:HB2	1:D:924:VAL:HG13	1.87	0.56
1:H:855:PHE:CE1	2:H:1701:G41:C14	2.89	0.55
1:C:645:HIS:CD2	1:C:647:ASN:H	2.24	0.55
1:G:645:HIS:CD2	1:G:647:ASN:H	2.24	0.55
1:B:845:ILE:HD11	1:B:922:GLN:HG2	1.88	0.55
1:H:648:ILE:HG23	1:H:866:ASP:OD2	2.06	0.55
1:D:583:PHE:N	1:D:588:ILE:HD11	2.22	0.55
1:B:645:HIS:HB3	1:B:648:ILE:HG12	1.88	0.54
1:F:855:PHE:CZ	2:F:1701:G41:C14	2.90	0.54
1:G:944:ALA:O	1:G:948:ILE:HG12	2.09	0.53
1:F:944:ALA:O	1:F:948:ILE:HG12	2.10	0.52
1:G:920:TYR:HB3	1:G:924:VAL:HG21	1.90	0.52
1:B:816:GLN:HG3	1:E:806:GLU:HG3	1.92	0.52
1:C:649:VAL:HG12	1:C:864:ILE:O	2.09	0.52
1:E:591:GLU:HG3	1:E:610:LYS:HE2	1.92	0.52
1:B:619:LYS:HE2	1:B:621:ILE:HD11	1.91	0.51
2:E:1701:G41:N2	2:E:1701:G41:C4	2.73	0.51
1:H:593:LEU:HD11	1:H:608:GLN:HB2	1.92	0.51
1:G:853:ASN:ND2	1:G:866:ASP:O	2.43	0.51
1:E:844:MET:HA	1:E:914:GLY:HA3	1.93	0.50
2:F:1701:G41:C4	2:F:1701:G41:N2	2.75	0.50
1:C:826:TRP:CZ2	1:C:974:GLN:HG3	2.47	0.49
1:C:853:ASN:ND2	1:C:867:PHE:H	2.09	0.49
1:B:824:ARG:HD2	1:E:807:LYS:HD3	1.93	0.49
2:B:1701:G41:C4	2:B:1701:G41:N2	2.76	0.49
1:E:650:ARG:HG2	1:E:652:TYR:CE1	2.47	0.49
2:G:1701:G41:C4	2:G:1701:G41:N2	2.75	0.49
1:D:920:TYR:C	1:D:922:GLN:H	2.16	0.49
1:H:855:PHE:CZ	2:H:1701:G41:C13	2.96	0.49
1:H:650:ARG:HG2	1:H:652:TYR:CE1	2.48	0.49
1:H:903:GLY:HA2	1:H:906:LEU:HD12	1.95	0.48
1:H:855:PHE:CE1	2:H:1701:G41:C15	2.96	0.48
1:A:828:LEU:HD22	1:A:862:VAL:HG23	1.96	0.48
1:C:609:ASN:ND2	1:C:612:ASP:H	2.10	0.48
1:A:584:SER:O	1:A:588:ILE:HG12	2.13	0.48
1:H:831:GLU:HB3	1:H:862:VAL:HB	1.94	0.48
1:A:645:HIS:CD2	1:A:647:ASN:H	2.29	0.48
1:E:980:TRP:CZ2	1:E:990:PRO:HB3	2.48	0.48
1:G:602:GLY:HA3	1:G:621:ILE:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:898:LEU:O	1:H:903:GLY:HA3	2.14	0.48
4:B:1803:HOH:O	1:F:650:ARG:HD2	2.14	0.48
1:G:866:ASP:O	1:G:867:PHE:CB	2.61	0.47
1:H:609:ASN:ND2	1:H:612:ASP:H	2.08	0.47
1:E:645:HIS:CD2	1:E:647:ASN:H	2.31	0.47
1:E:853:ASN:ND2	1:E:867:PHE:H	2.12	0.47
1:A:813:THR:HG22	1:A:818:LEU:HB2	1.96	0.47
2:D:1701:G41:N2	2:D:1701:G41:C4	2.75	0.47
1:E:645:HIS:HD2	1:E:647:ASN:H	1.61	0.47
1:C:650:ARG:HG2	1:C:652:TYR:CE1	2.50	0.47
1:E:931:ILE:HG23	1:E:951:LEU:HD22	1.97	0.47
1:B:649:VAL:HG13	1:B:803:GLU:HG2	1.97	0.47
1:D:639:LEU:CD1	1:D:875:ALA:HB1	2.40	0.47
1:F:825:LEU:CD2	1:F:936:MET:HB3	2.45	0.47
1:D:650:ARG:HD2	4:H:1805:HOH:O	2.15	0.46
1:A:943:THR:HG22	1:A:946:GLU:H	1.80	0.46
1:B:980:TRP:CD1	1:B:990:PRO:HD3	2.50	0.46
1:F:650:ARG:HG2	1:F:652:TYR:CE1	2.50	0.46
1:H:833:LEU:HD11	1:H:995:LEU:HG	1.97	0.46
1:B:846:HIS:O	1:B:874:LEU:O	2.34	0.46
2:H:1701:G41:N2	2:H:1701:G41:C4	2.78	0.46
1:A:612:ASP:OD1	1:A:614:CYS:HB2	2.15	0.46
1:F:845:ILE:HG12	1:F:871:THR:CG2	2.46	0.46
1:A:629:GLN:O	1:A:633:ILE:HG12	2.16	0.46
1:E:866:ASP:O	2:E:1701:G41:C17	2.64	0.46
1:G:649:VAL:HG12	1:G:864:ILE:O	2.16	0.46
1:D:980:TRP:CD1	1:D:990:PRO:HD3	2.51	0.46
1:E:826:TRP:CZ2	1:E:974:GLN:HG3	2.51	0.46
1:G:950:VAL:HG13	1:G:963:PRO:HG3	1.98	0.46
1:C:944:ALA:O	1:C:948:ILE:HG12	2.16	0.46
1:H:836:LEU:HD11	1:H:925:ASP:HB3	1.98	0.45
1:A:654:ALA:HA	1:A:799:TYR:O	2.17	0.45
1:H:944:ALA:O	1:H:948:ILE:HG12	2.16	0.45
1:G:906:LEU:HD13	1:G:951:LEU:HD12	1.98	0.45
1:B:950:VAL:HG13	1:B:963:PRO:HG3	1.97	0.45
1:F:833:LEU:HD11	1:F:995:LEU:HG	1.98	0.45
1:E:648:ILE:HD12	1:E:839:ILE:HD11	1.98	0.45
1:F:828:LEU:HD22	1:F:856:LEU:HD21	1.98	0.44
1:H:855:PHE:CZ	2:H:1701:G41:C14	3.00	0.44
1:B:650:ARG:HG2	1:B:652:TYR:CE1	2.52	0.44
1:E:847:ARG:HH11	1:E:918:SER:HB2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:867:PHE:HA	2:G:1701:G41:C13	2.47	0.44
1:A:948:ILE:O	1:A:952:ASN:HB2	2.18	0.44
2:A:1701:G41:N2	2:A:1701:G41:C4	2.79	0.44
1:F:902:VAL:HG12	1:F:948:ILE:HD12	1.99	0.44
2:C:1701:G41:C4	2:C:1701:G41:N2	2.79	0.44
1:C:595:LEU:HD21	1:C:598:LYS:HB2	2.00	0.44
1:E:845:ILE:HD13	1:E:847:ARG:HG3	2.00	0.44
1:F:976:SER:O	1:F:980:TRP:HB2	2.18	0.44
1:H:852:VAL:HG22	3:H:1702:DMS:H21	2.00	0.43
1:A:650:ARG:HG2	1:A:652:TYR:CE1	2.53	0.43
1:B:609:ASN:ND2	1:B:612:ASP:H	2.13	0.43
1:D:985:ASP:HB2	1:G:876:PHE:O	2.18	0.43
1:E:829:PHE:HE2	1:E:1001:LEU:HD11	1.83	0.43
1:E:846:HIS:O	1:E:847:ARG:HB2	2.17	0.42
1:F:903:GLY:HA2	1:F:906:LEU:HD12	2.01	0.42
1:H:812:ASP:OD1	2:H:1701:G41:N5	2.52	0.42
1:B:583:PHE:HB3	1:B:588:ILE:HD11	2.01	0.42
1:H:850:LYS:HD2	3:H:1702:DMS:H21	2.00	0.42
1:D:654:ALA:HA	1:D:799:TYR:O	2.18	0.42
1:E:639:LEU:HD21	1:E:915:SER:HB2	2.00	0.42
1:F:845:ILE:HG12	1:F:871:THR:HG21	2.02	0.42
1:C:980:TRP:CZ2	1:C:990:PRO:HB3	2.54	0.42
1:G:645:HIS:HB3	1:G:648:ILE:HG12	2.02	0.42
1:E:973:LYS:O	1:E:977:VAL:HG23	2.19	0.42
1:C:654:ALA:HA	1:C:799:TYR:O	2.20	0.42
1:C:645:HIS:HB3	1:C:648:ILE:HG12	2.02	0.42
1:B:931:ILE:HG23	1:B:951:LEU:HD22	2.02	0.41
1:E:819:TYR:CD1	1:E:939:HIS:HA	2.55	0.41
1:H:833:LEU:HD21	1:H:995:LEU:HD23	2.02	0.41
1:A:985:ASP:HA	1:A:986:PRO:HD2	1.76	0.41
1:E:614:CYS:HB3	1:E:616:TYR:CE2	2.56	0.41
1:G:650:ARG:HD2	4:G:1803:HOH:O	2.19	0.41
1:A:649:VAL:HG12	1:A:864:ILE:O	2.20	0.41
1:A:991:THR:OG1	1:A:994:GLU:HB2	2.21	0.41
1:E:859:ASP:HB3	1:E:861:HIS:HD2	1.85	0.41
1:G:991:THR:OG1	1:G:994:GLU:HB2	2.21	0.40
1:H:825:LEU:HD23	1:H:936:MET:HB3	2.03	0.40
1:A:980:TRP:CZ2	1:A:990:PRO:HB3	2.57	0.40
1:E:856:LEU:HD23	1:E:856:LEU:HA	1.91	0.40
1:F:847:ARG:HD3	1:F:869:LEU:CB	2.51	0.40
1:F:899:THR:CB	1:F:948:ILE:HD11	2.51	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	237/1649 (14%)	220 (93%)	16 (7%)	1 (0%)	34	42
1	B	241/1649 (15%)	230 (95%)	11 (5%)	0	100	100
1	C	241/1649 (15%)	227 (94%)	14 (6%)	0	100	100
1	D	246/1649 (15%)	234 (95%)	10 (4%)	2 (1%)	19	23
1	E	233/1649 (14%)	223 (96%)	8 (3%)	2 (1%)	17	20
1	F	244/1649 (15%)	228 (93%)	13 (5%)	3 (1%)	13	14
1	G	245/1649 (15%)	227 (93%)	17 (7%)	1 (0%)	34	42
1	H	247/1649 (15%)	237 (96%)	10 (4%)	0	100	100
All	All	1934/13192 (15%)	1826 (94%)	99 (5%)	9 (0%)	29	35

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	848	ASN
1	E	917	LYS
1	F	902	VAL
1	F	970	GLU
1	A	867	PHE
1	D	873	HIS
1	E	919	ALA
1	G	942	VAL
1	F	869	LEU

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	184/1464 (13%)	173 (94%)	11 (6%)	19	26
1	B	194/1464 (13%)	180 (93%)	14 (7%)	14	18
1	C	194/1464 (13%)	174 (90%)	20 (10%)	7	8
1	D	204/1464 (14%)	190 (93%)	14 (7%)	15	20
1	E	195/1464 (13%)	179 (92%)	16 (8%)	11	14
1	F	205/1464 (14%)	187 (91%)	18 (9%)	10	12
1	G	206/1464 (14%)	188 (91%)	18 (9%)	10	12
1	H	210/1464 (14%)	197 (94%)	13 (6%)	18	25
All	All	1592/11712 (14%)	1468 (92%)	124 (8%)	12	16

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	ARG
1	A	601	PHE
1	A	642	ARG
1	A	650	ARG
1	A	653	ASN
1	A	867	PHE
1	A	916	THR
1	A	943	THR
1	A	952	ASN
1	A	959	SER
1	A	984	HIS
1	B	598	LYS
1	B	623	ILE
1	B	653	ASN
1	B	795	VAL
1	B	807	LYS
1	B	836	LEU
1	B	845	ILE
1	B	850	LYS
1	B	867	PHE
1	B	873	HIS
1	B	909	SER
1	B	926	LEU

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Mol	Chain	Res	Type
1	B	943	THR
1	B	984	HIS
1	C	584	SER
1	C	598	LYS
1	C	642	ARG
1	C	653	ASN
1	C	795	VAL
1	C	806	GLU
1	C	813	THR
1	C	825	LEU
1	C	845	ILE
1	C	850	LYS
1	C	862	VAL
1	C	867	PHE
1	C	912	VAL
1	C	922	GLN
1	C	926	LEU
1	C	943	THR
1	C	952	ASN
1	C	984	HIS
1	C	993	THR
1	C	1001	LEU
1	D	598	LYS
1	D	649	VAL
1	D	653	ASN
1	D	795	VAL
1	D	836	LEU
1	D	845	ILE
1	D	852	VAL
1	D	867	PHE
1	D	909	SER
1	D	926	LEU
1	D	943	THR
1	D	984	HIS
1	D	999	GLU
1	D	1001	LEU
1	E	588	ILE
1	E	605	ILE
1	E	608	GLN
1	E	620	ARG
1	E	623	ILE
1	E	633	ILE

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Mol	Chain	Res	Type
1	E	642	ARG
1	E	653	ASN
1	E	806	GLU
1	E	830	ARG
1	E	867	PHE
1	E	921	ASN
1	E	947	ARG
1	E	953	GLN
1	E	983	ASN
1	E	998	SER
1	F	585	ARG
1	F	623	ILE
1	F	642	ARG
1	F	653	ASN
1	F	795	VAL
1	F	807	LYS
1	F	825	LEU
1	F	842	LYS
1	F	845	ILE
1	F	848	ASN
1	F	850	LYS
1	F	867	PHE
1	F	871	THR
1	F	909	SER
1	F	921	ASN
1	F	926	LEU
1	F	980	TRP
1	F	998	SER
1	G	585	ARG
1	G	598	LYS
1	G	620	ARG
1	G	636	GLU
1	G	642	ARG
1	G	813	THR
1	G	825	LEU
1	G	859	ASP
1	G	867	PHE
1	G	874	LEU
1	G	909	SER
1	G	926	LEU
1	G	942	VAL
1	G	947	ARG

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Mol	Chain	Res	Type
1	G	965	ASP
1	G	976	SER
1	G	984	HIS
1	G	1007	GLU
1	H	585	ARG
1	H	642	ARG
1	H	648	ILE
1	H	653	ASN
1	H	807	LYS
1	H	813	THR
1	H	825	LEU
1	H	869	LEU
1	H	909	SER
1	H	921	ASN
1	H	928	SER
1	H	999	GLU
1	H	1003	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	609	ASN
1	A	645	HIS
1	A	848	ASN
1	A	853	ASN
1	A	984	HIS
1	B	609	ASN
1	B	624	ASN
1	B	645	HIS
1	B	853	ASN
1	C	609	ASN
1	C	645	HIS
1	C	853	ASN
1	C	922	GLN
1	D	609	ASN
1	D	645	HIS
1	D	853	ASN
1	E	609	ASN
1	E	645	HIS
1	E	853	ASN
1	E	861	HIS
1	E	921	ASN

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Mol	Chain	Res	Type
1	F	609	ASN
1	F	645	HIS
1	F	848	ASN
1	F	853	ASN
1	G	609	ASN
1	G	645	HIS
1	G	853	ASN
1	G	861	HIS
1	H	609	ASN
1	H	645	HIS
1	H	853	ASN
1	H	921	ASN
1	H	974	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	G41	D	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DMS	H	1703	-	3,3,3	0.35	0	3,3,3	0.80	0
2	G41	F	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
2	G41	B	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
2	G41	E	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
2	G41	G	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
2	G41	C	1701	-	38,38,38	0.11	0	48,52,52	0.40	1 (2%)
3	DMS	H	1702	-	3,3,3	0.39	0	3,3,3	0.38	0
2	G41	A	1701	-	38,38,38	0.12	0	48,52,52	0.40	1 (2%)
2	G41	H	1701	-	38,38,38	0.11	0	48,52,52	0.39	1 (2%)

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	G41	D	1701	-	-	0/20/28/28	0/5/5/5
2	G41	F	1701	-	-	0/20/28/28	0/5/5/5
2	G41	B	1701	-	-	0/20/28/28	0/5/5/5
2	G41	E	1701	-	-	6/20/28/28	0/5/5/5
2	G41	G	1701	-	-	6/20/28/28	0/5/5/5
2	G41	C	1701	-	-	1/20/28/28	0/5/5/5
2	G41	A	1701	-	-	2/20/28/28	0/5/5/5
2	G41	H	1701	-	-	0/20/28/28	0/5/5/5

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1701	G41	C11-C10-C9	2.28	127.85	121.75
2	G	1701	G41	C11-C10-C9	2.28	127.85	121.75
2	E	1701	G41	C11-C10-C9	2.27	127.83	121.75
2	A	1701	G41	C11-C10-C9	2.27	127.82	121.75
2	D	1701	G41	C11-C10-C9	2.27	127.82	121.75
2	F	1701	G41	C11-C10-C9	2.26	127.79	121.75
2	H	1701	G41	C11-C10-C9	2.26	127.78	121.75
2	B	1701	G41	C11-C10-C9	2.24	127.75	121.75

There are no chirality outliers.

All (15) torsion outliers are listed below:

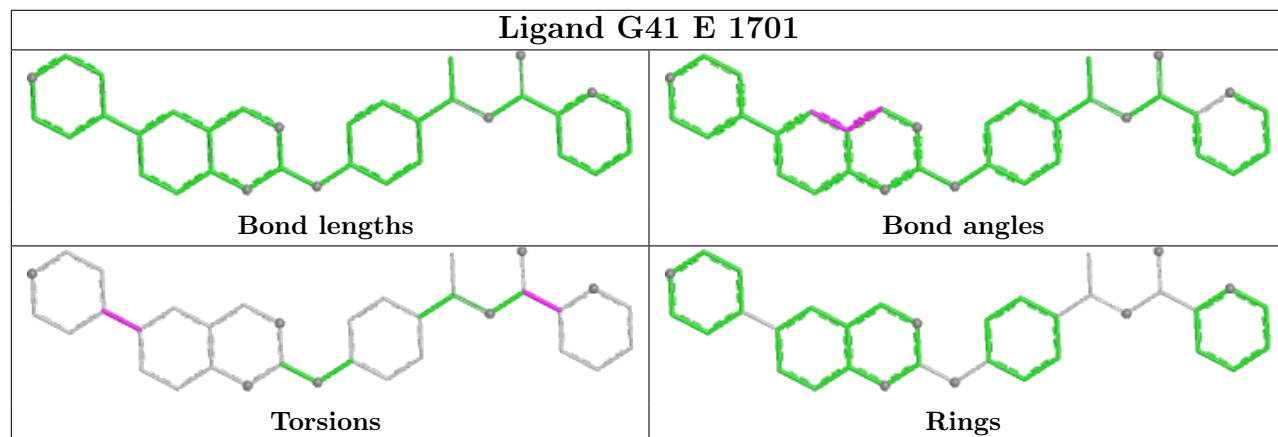
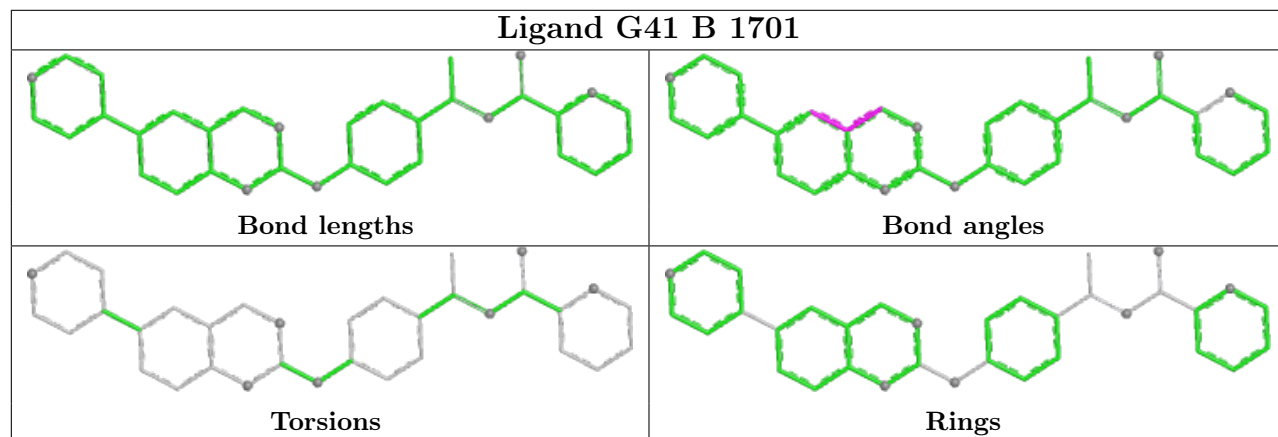
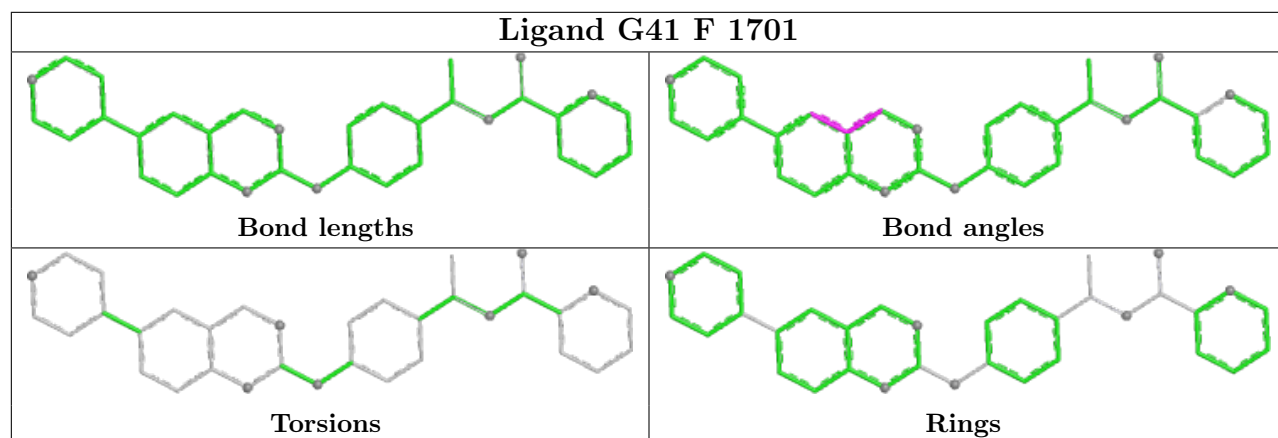
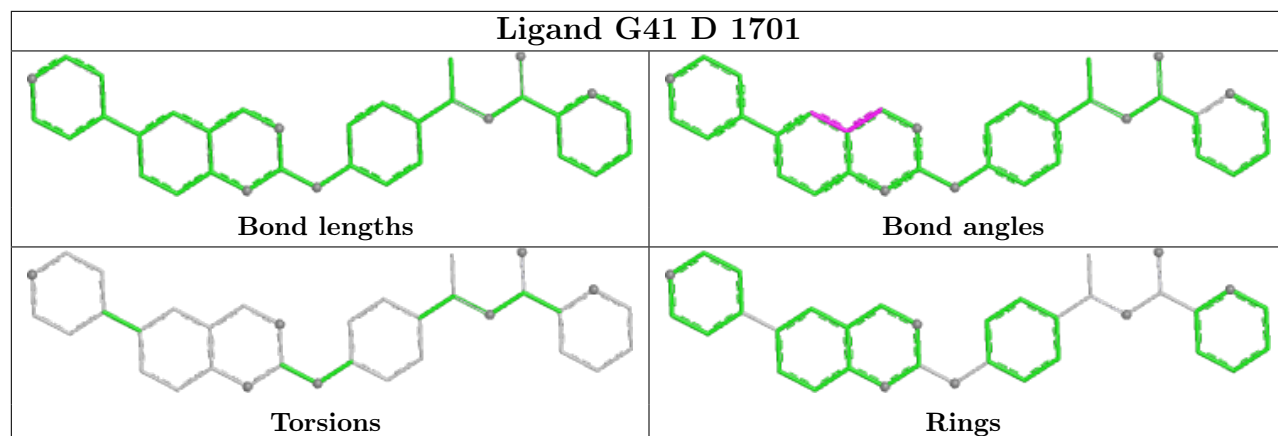
Mol	Chain	Res	Type	Atoms
2	G	1701	G41	C11-C12-C16-C20
2	G	1701	G41	C11-C12-C16-C17
2	G	1701	G41	C13-C12-C16-C20
2	G	1701	G41	C13-C12-C16-C17
2	E	1701	G41	C11-C12-C16-C20
2	E	1701	G41	C11-C12-C16-C17
2	E	1701	G41	C13-C12-C16-C20
2	E	1701	G41	C13-C12-C16-C17
2	C	1701	G41	O-C21-C22-C23
2	E	1701	G41	O-C21-C22-C23
2	E	1701	G41	N4-C21-C22-C23
2	G	1701	G41	O-C21-C22-C23
2	G	1701	G41	N4-C21-C22-C23
2	A	1701	G41	C13-C12-C16-C17
2	A	1701	G41	C13-C12-C16-C20

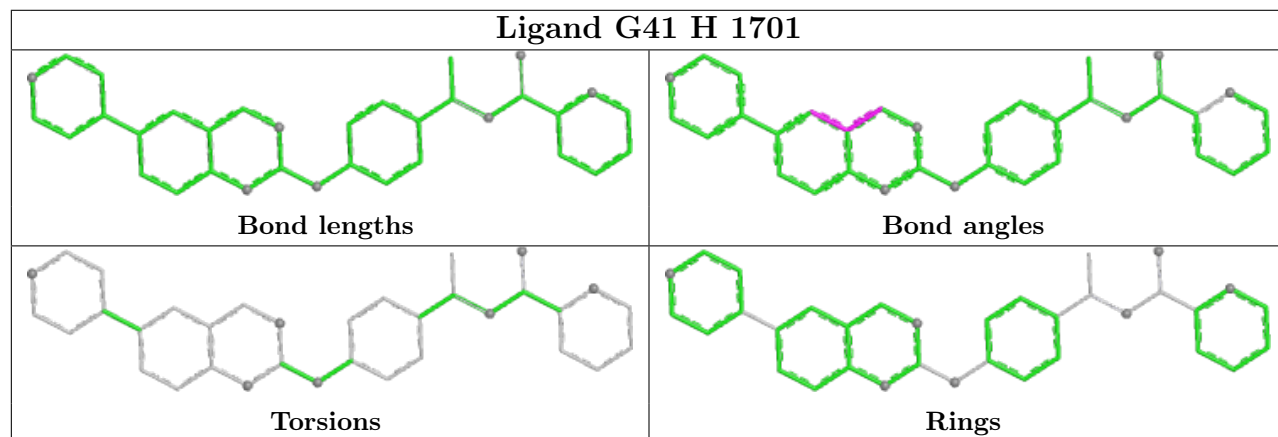
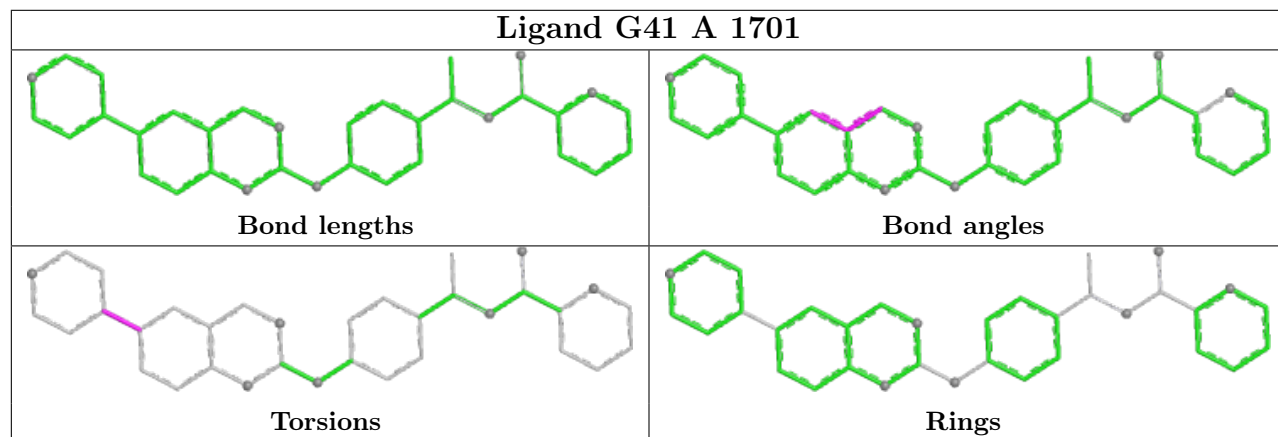
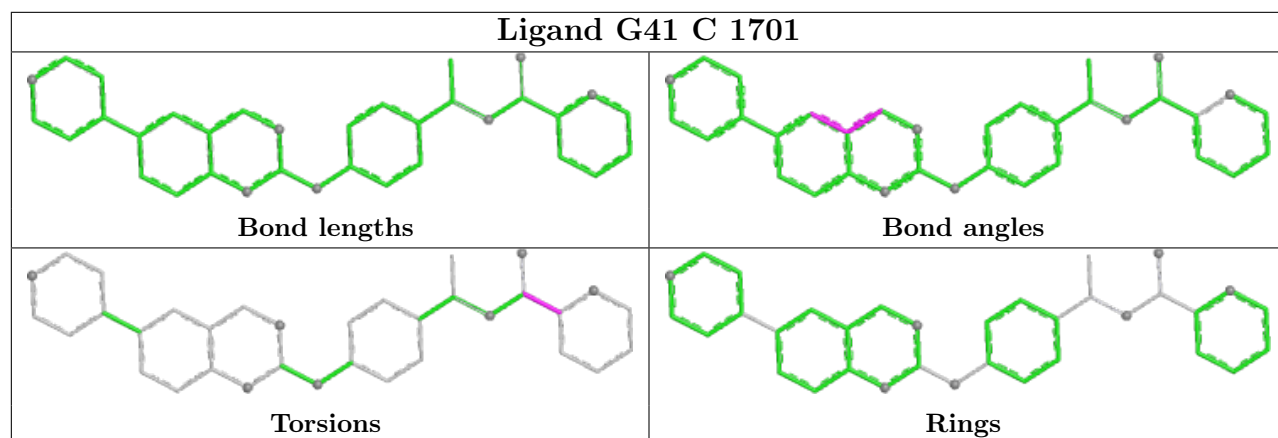
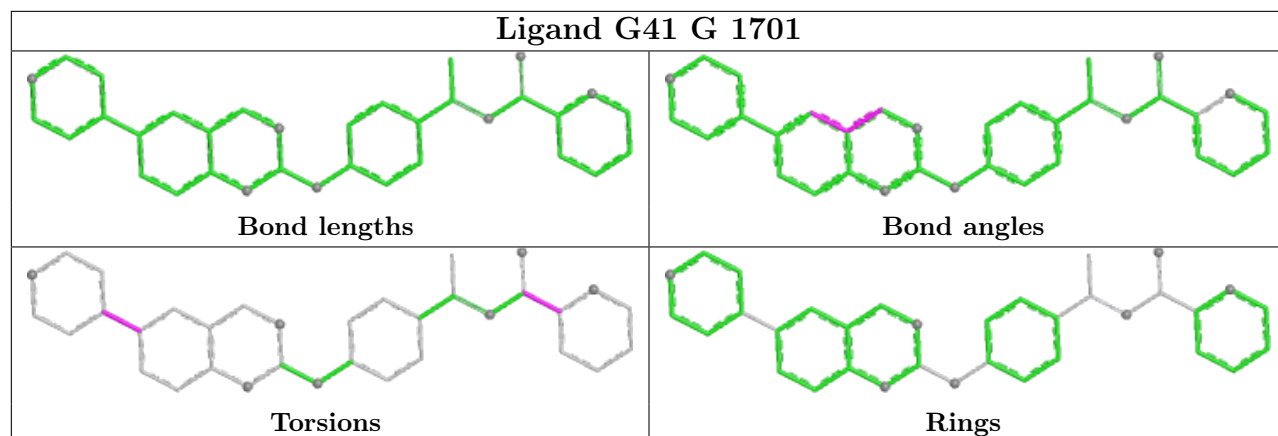
There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1701	G41	1	0
2	F	1701	G41	5	0
2	B	1701	G41	1	0
2	E	1701	G41	2	0
2	G	1701	G41	2	0
2	C	1701	G41	1	0
3	H	1702	DMS	2	0
2	A	1701	G41	1	0
2	H	1701	G41	6	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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	245/1649 (14%)	-0.00	6 (2%) 59 66	23, 49, 89, 102	0
1	B	249/1649 (15%)	-0.08	6 (2%) 59 66	23, 45, 76, 97	0
1	C	249/1649 (15%)	0.12	11 (4%) 34 41	24, 51, 96, 111	0
1	D	254/1649 (15%)	-0.00	7 (2%) 53 60	23, 46, 80, 99	0
1	E	241/1649 (14%)	0.08	13 (5%) 25 32	28, 51, 82, 102	0
1	F	254/1649 (15%)	-0.07	4 (1%) 72 77	23, 46, 76, 100	0
1	G	257/1649 (15%)	0.08	11 (4%) 35 42	29, 52, 84, 100	0
1	H	259/1649 (15%)	-0.14	1 (0%) 92 95	23, 46, 74, 110	0
All	All	2008/13192 (15%)	-0.00	59 (2%) 51 58	23, 48, 84, 111	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	584	SER	7.0
1	B	966	PHE	6.0
1	G	982	LEU	5.1
1	G	584	SER	5.1
1	C	968	ASP	4.6
1	F	795	VAL	4.6
1	B	968	ASP	4.0
1	F	968	ASP	3.7
1	C	960	PRO	3.7
1	D	968	ASP	3.5
1	G	963	PRO	3.5
1	E	601	PHE	3.4
1	G	984	HIS	3.4
1	F	969	GLY	3.4
1	A	942	VAL	3.4
1	E	982	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	626	ALA	3.4
1	C	1000	LEU	3.4
1	G	626	ALA	3.3
1	A	626	ALA	3.2
1	E	915	SER	3.2
1	E	625	PRO	3.2
1	G	601	PHE	3.2
1	D	966	PHE	3.1
1	B	942	VAL	3.0
1	E	984	HIS	3.0
1	C	949	PHE	3.0
1	D	965	ASP	3.0
1	E	992	ALA	3.0
1	E	630	PHE	3.0
1	C	970	GLU	2.9
1	B	969	GLY	2.8
1	C	942	VAL	2.7
1	G	949	PHE	2.7
1	G	942	VAL	2.6
1	A	600	ALA	2.6
1	H	600	ALA	2.6
1	E	626	ALA	2.5
1	D	949	PHE	2.5
1	G	659	HIS	2.5
1	B	970	GLU	2.5
1	E	948	ILE	2.5
1	G	633	ILE	2.5
1	D	948	ILE	2.4
1	C	965	ASP	2.4
1	D	909	SER	2.4
1	A	845	ILE	2.3
1	E	588	ILE	2.3
1	A	958	THR	2.2
1	B	941	MET	2.2
1	G	969	GLY	2.2
1	A	968	ASP	2.2
1	E	633	ILE	2.2
1	F	957	PRO	2.1
1	C	962	PHE	2.1
1	D	1000	LEU	2.1
1	C	909	SER	2.1
1	E	797	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	951	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

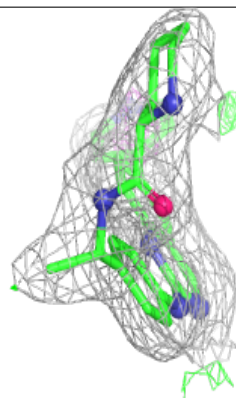
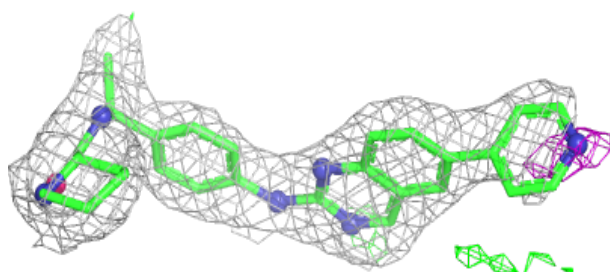
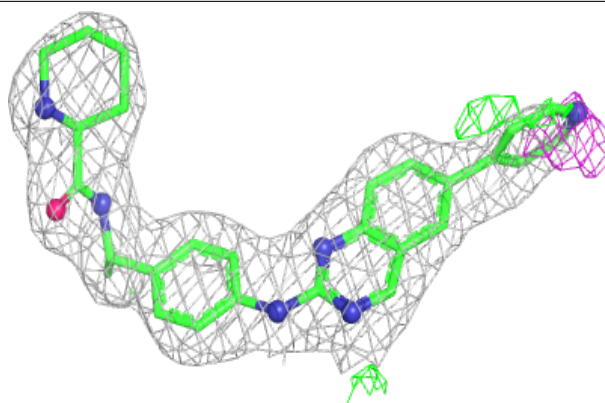
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	G41	E	1701	34/34	0.91	0.16	33,46,65,67	0
2	G41	F	1701	34/34	0.92	0.13	29,34,40,42	0
2	G41	G	1701	34/34	0.93	0.15	32,45,70,71	0
2	G41	H	1701	34/34	0.93	0.13	28,33,47,49	0
3	DMS	H	1702	4/4	0.93	0.21	76,79,80,81	0
3	DMS	H	1703	4/4	0.94	0.19	78,81,81,83	0
2	G41	C	1701	34/34	0.95	0.11	25,36,42,43	0
2	G41	B	1701	34/34	0.96	0.12	21,28,40,43	0
2	G41	D	1701	34/34	0.96	0.12	24,32,43,43	0
2	G41	A	1701	34/34	0.97	0.12	20,28,44,47	0

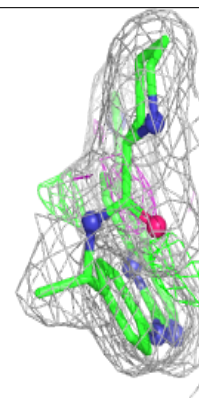
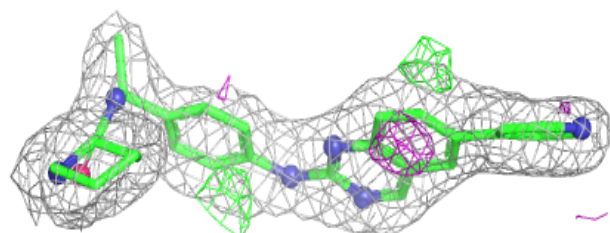
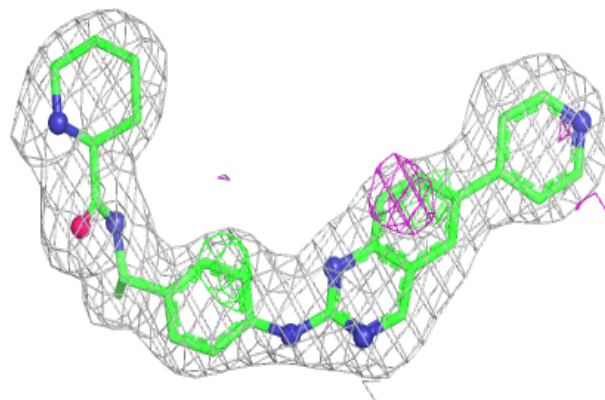
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G41 E 1701:

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

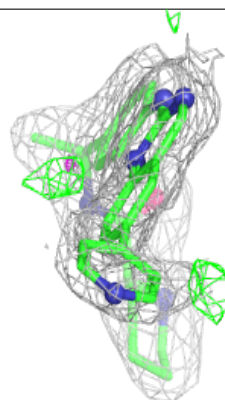
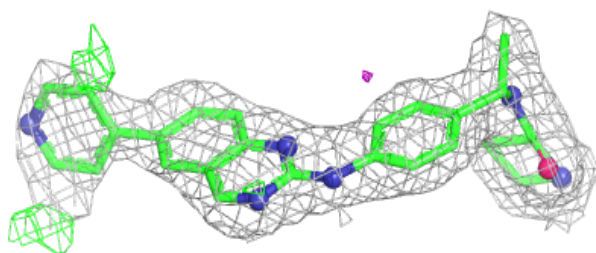
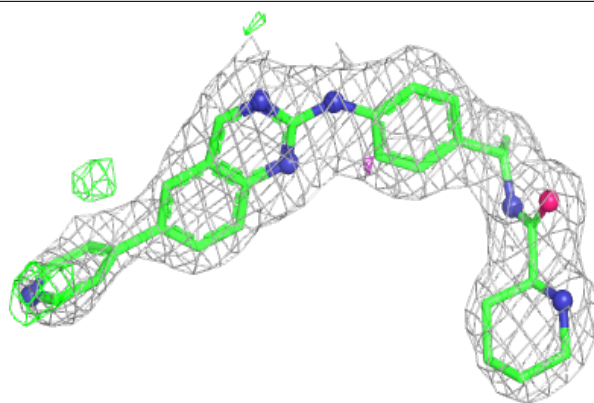
**Electron density around G41 F 1701:**

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

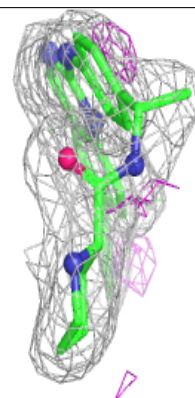
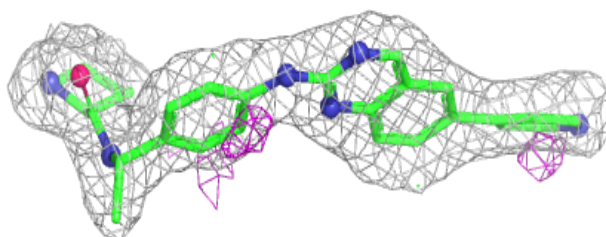
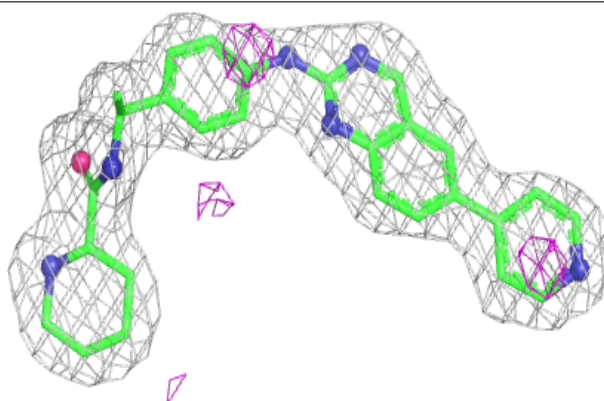


Electron density around G41 G 1701:

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

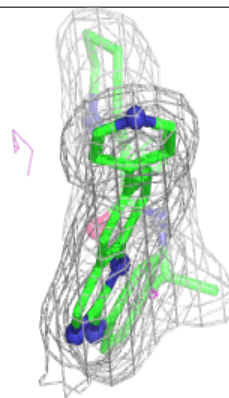
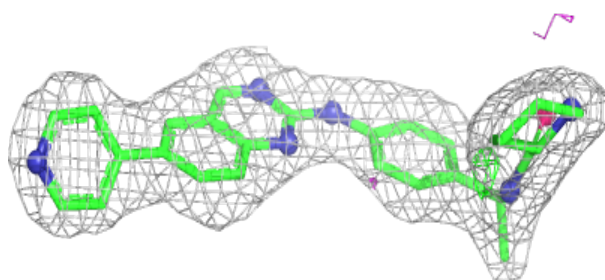
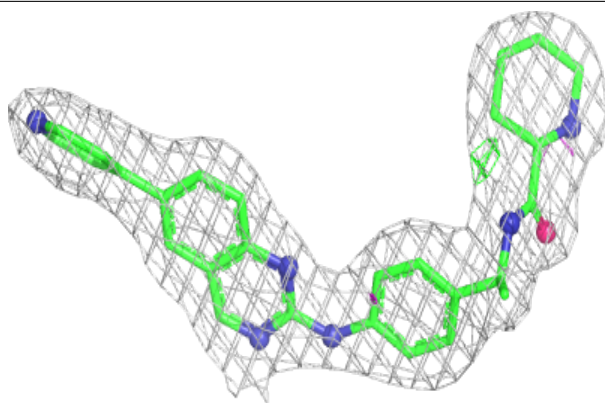
**Electron density around G41 H 1701:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

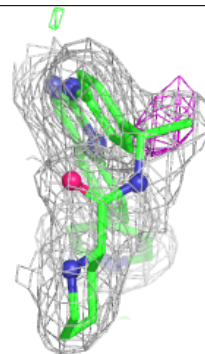
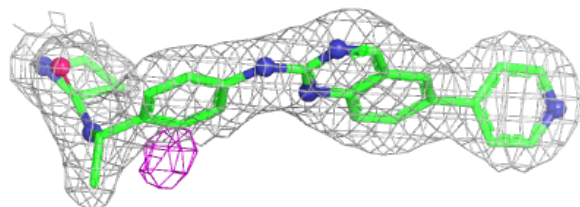
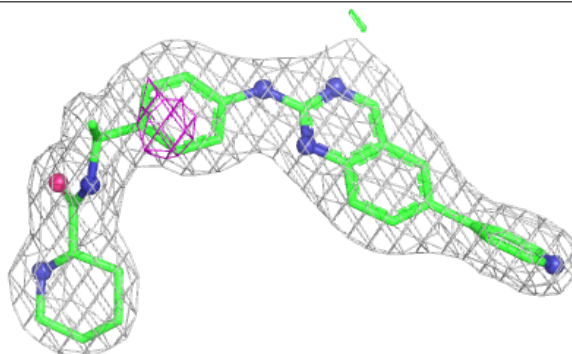


Electron density around G41 C 1701:

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

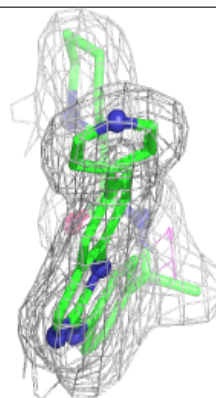
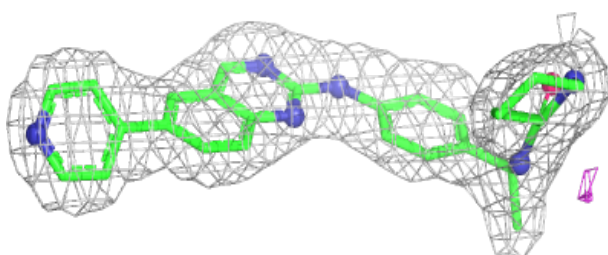
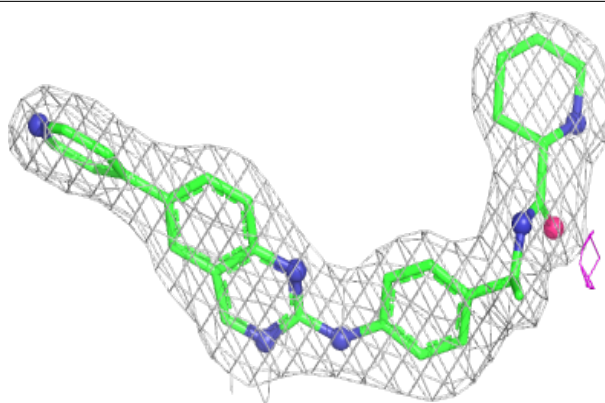
**Electron density around G41 B 1701:**

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

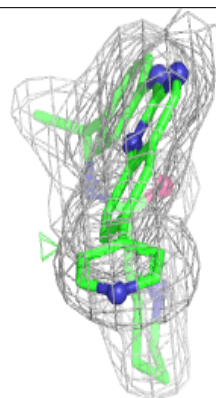
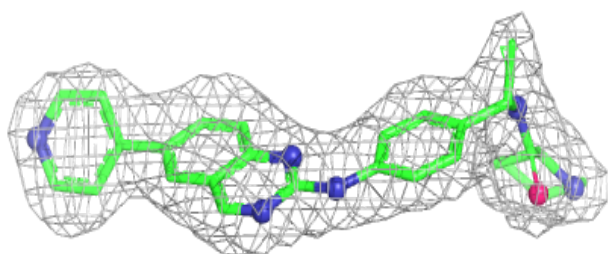
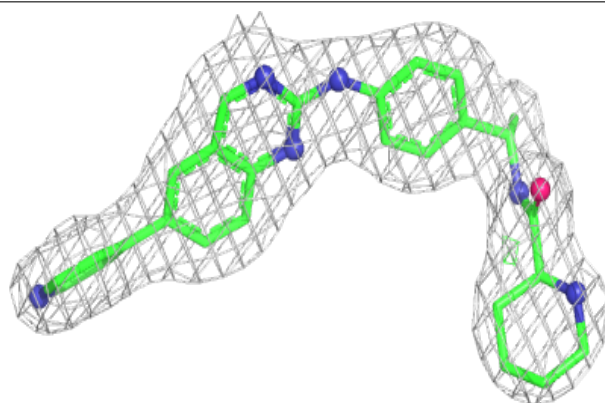


Electron density around G41 D 1701:

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

**Electron density around G41 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.