wwPDB X-ray Structure Validation Summary Report (i)

Jul 6, 2023 – 05:34 pm BST

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

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

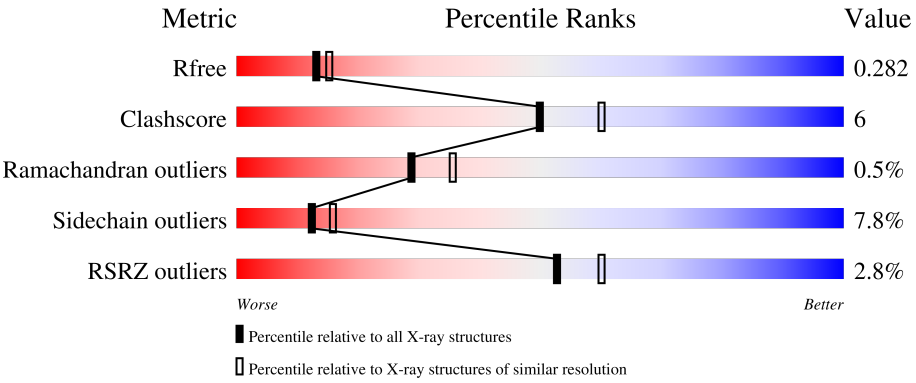
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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 <=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	318	2% 65% 11% • 23%
1	B	318	2% 65% 12% • 22%
1	C	318	3% 64% 13% • 22%
1	D	318	2% 68% 11% • 20%
1	E	318	4% 57% 18% • 24%

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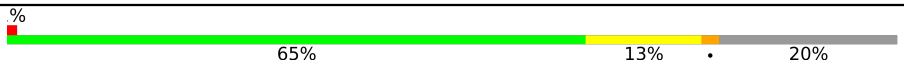
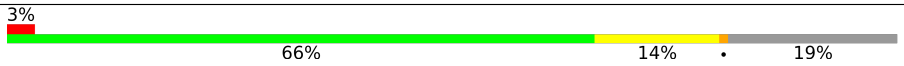
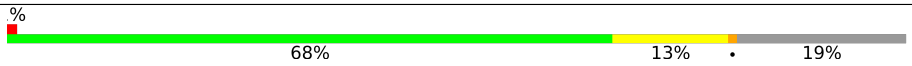
Mol	Chain	Length	Quality of chain
1	F	318	
1	G	318	
1	H	318	

2 Entry composition (i)

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 1016 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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	?	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q9P2K8
B	?	-	LEU	deletion	UNP Q9P2K8
B	?	-	ALA	deletion	UNP Q9P2K8
B	?	-	LYS	deletion	UNP Q9P2K8
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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	deletion	UNP Q9P2K8
B	?	-	ILE	deletion	UNP Q9P2K8
B	?	-	ILE	deletion	UNP Q9P2K8
B	?	-	PHE	deletion	UNP Q9P2K8
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	?	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	PRO	deletion	UNP Q9P2K8
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLY	deletion	UNP Q9P2K8
C	?	-	GLU	deletion	UNP Q9P2K8
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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP Q9P2K8
C	?	-	ASP	deletion	UNP Q9P2K8
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	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ALA	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	GLY	deletion	UNP Q9P2K8
D	?	-	THR	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	PRO	deletion	UNP Q9P2K8
D	?	-	ASP	deletion	UNP Q9P2K8

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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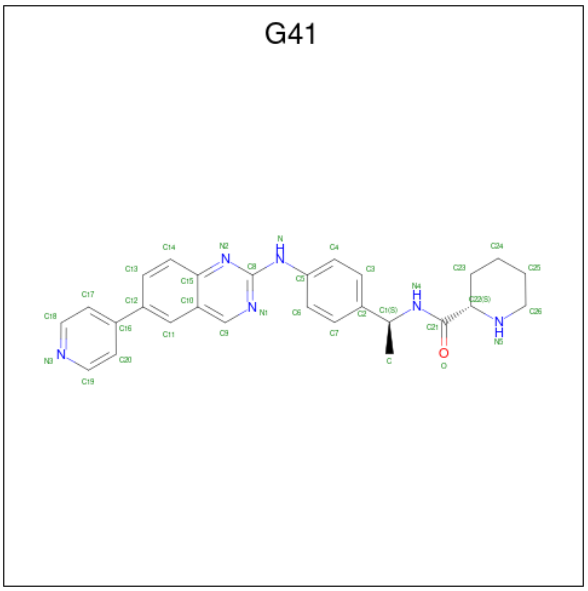
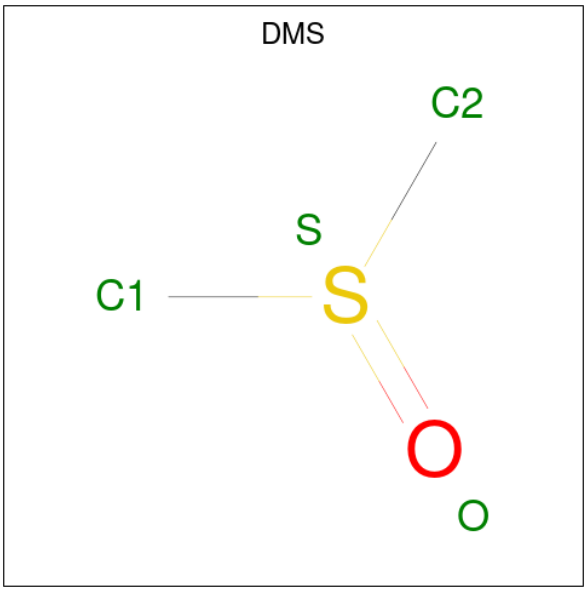
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ALA	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	ILE	deletion	UNP Q9P2K8
H	?	-	ILE	deletion	UNP Q9P2K8
H	?	-	PHE	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	ASN	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	ASN	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	LYS	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	GLN	deletion	UNP Q9P2K8
H	?	-	ASN	deletion	UNP Q9P2K8
H	?	-	GLN	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	ASP	deletion	UNP Q9P2K8
H	?	-	CYS	deletion	UNP Q9P2K8
H	?	-	ASN	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	LYS	deletion	UNP Q9P2K8
H	?	-	ASN	deletion	UNP Q9P2K8
H	?	-	GLY	deletion	UNP Q9P2K8
H	?	-	CYS	deletion	UNP Q9P2K8
H	?	-	HIS	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	?	-	SER	deletion	UNP Q9P2K8
H	?	-	GLU	deletion	UNP Q9P2K8
H	848	ASN	ASP	engineered mutation	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: $C_{27}H_{28}N_6O$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 4 is water.

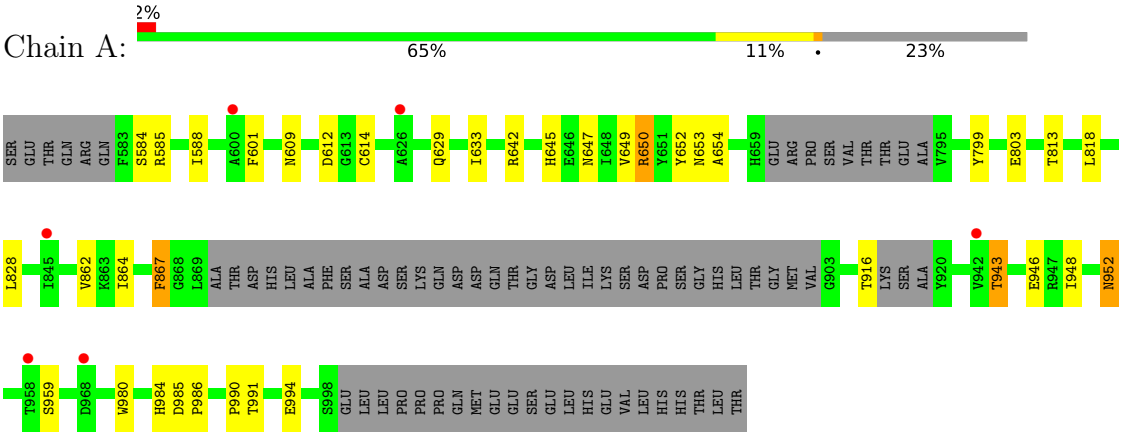
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	8	Total O 8 8	0	0
4	B	17	Total O 17 17	0	0
4	C	4	Total O 4 4	0	0
4	D	8	Total O 8 8	0	0
4	E	8	Total O 8 8	0	0
4	F	14	Total O 14 14	0	0
4	G	9	Total O 9 9	0	0
4	H	16	Total O 16 16	0	0

3 Residue-property plots (i)

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

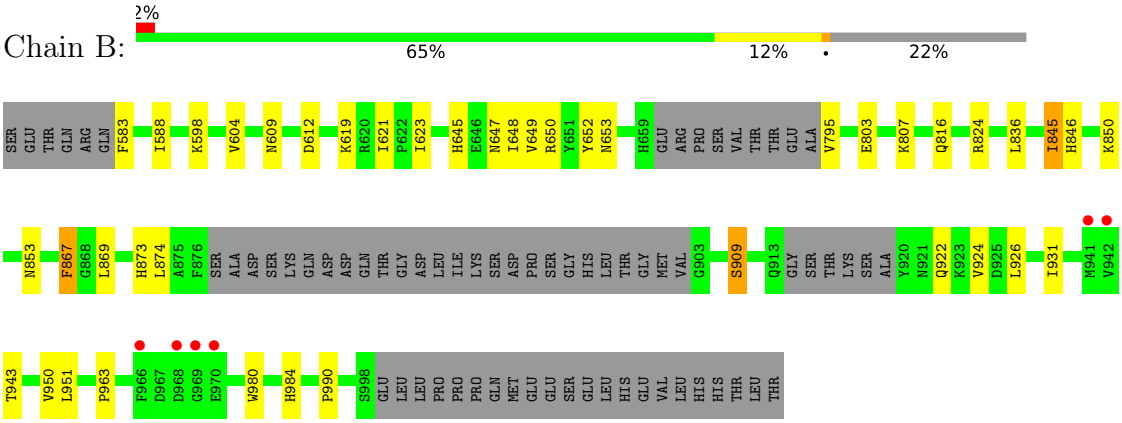
• Molecule 1: eIF-2-alpha kinase GCN2

Chain A:



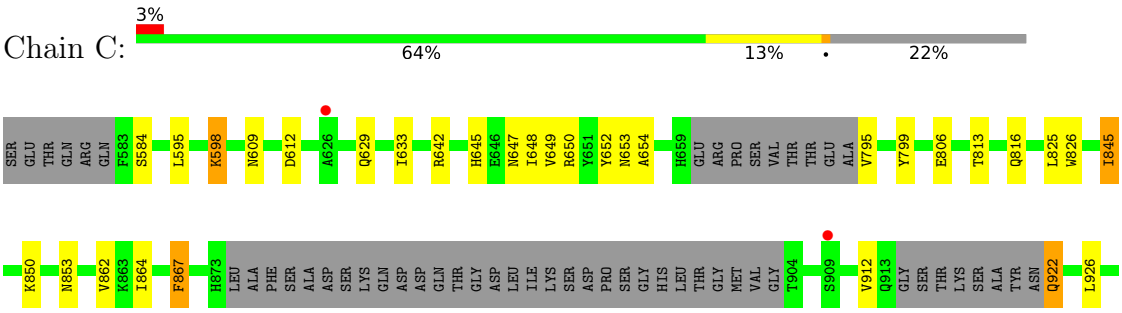
• Molecule 1: eIF-2-alpha kinase GCN2

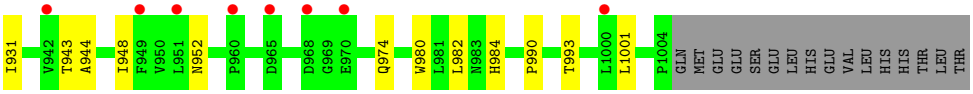
Chain B:



• Molecule 1: eIF-2-alpha kinase GCN2

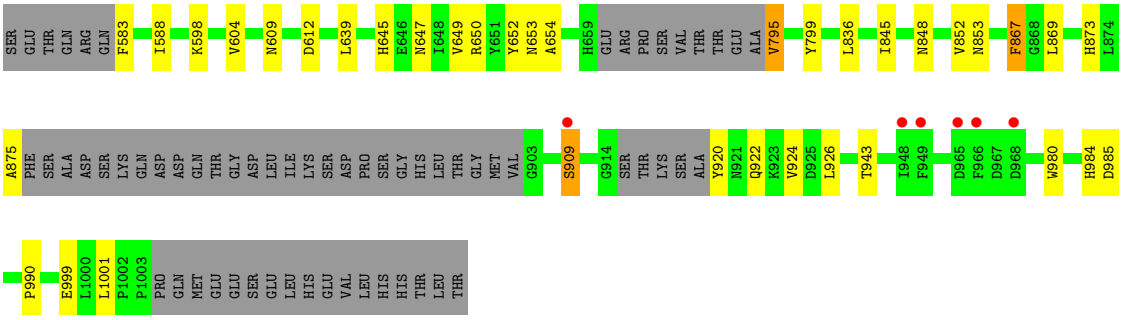
Chain C:





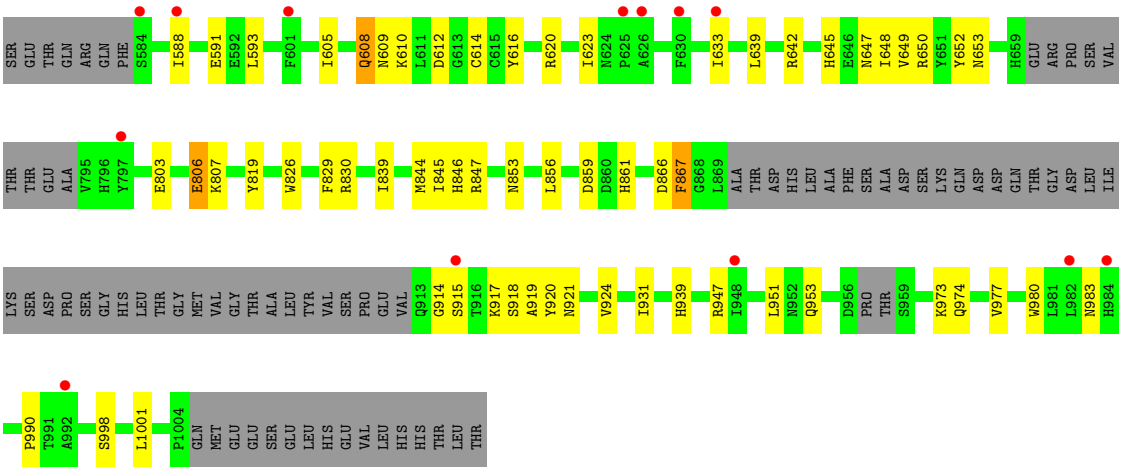
• Molecule 1: eIF-2-alpha kinase GCN2

Chain D:



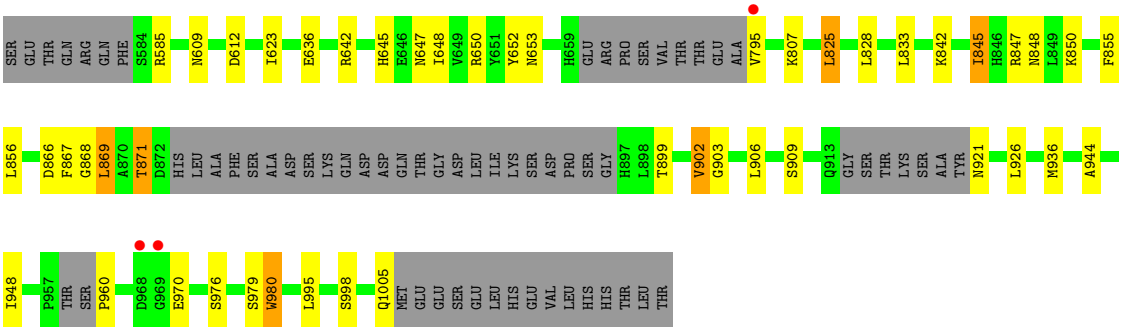
• Molecule 1: eIF-2-alpha kinase GCN2

Chain E:



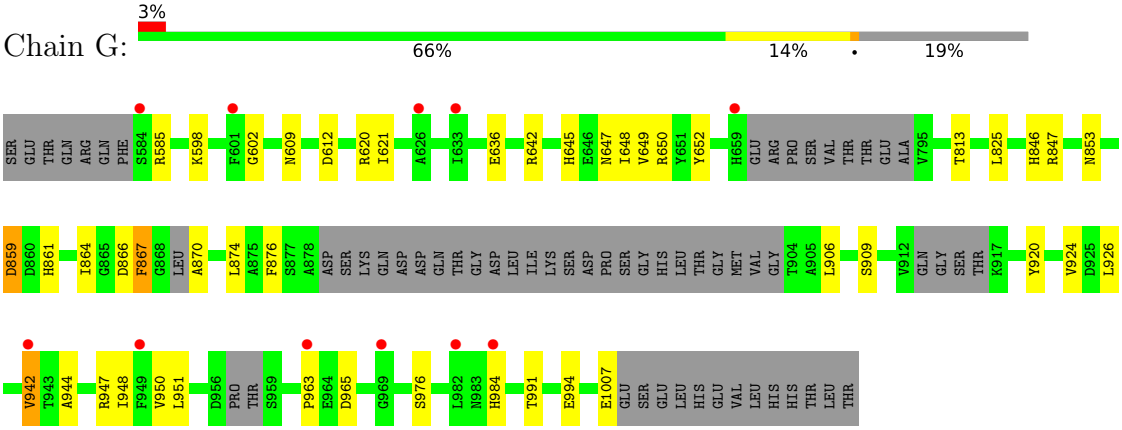
• Molecule 1: eIF-2-alpha kinase GCN2

Chain F:



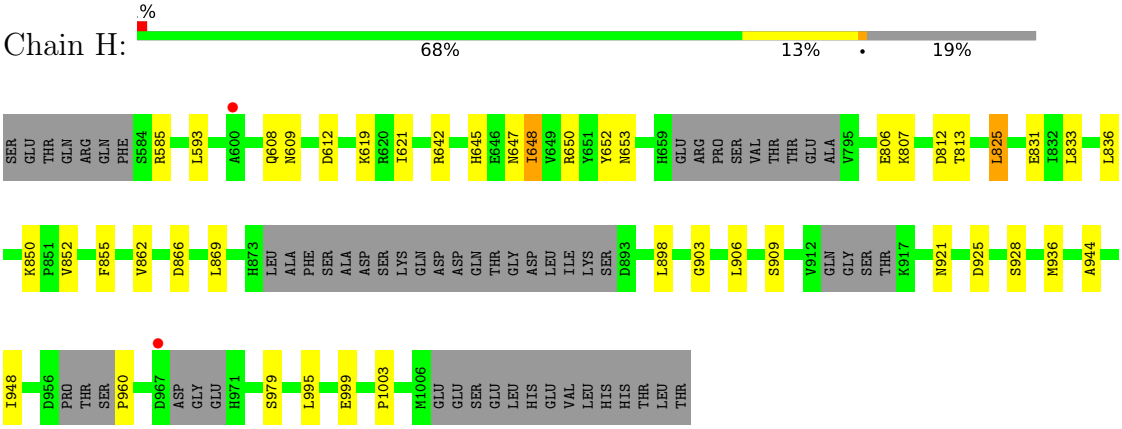
• Molecule 1: eIF-2-alpha kinase GCN2

Chain G:



• Molecule 1: eIF-2-alpha kinase GCN2

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.37 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G41, DMS

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

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.

The worst 5 of 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

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	237/318 (74%)	220 (93%)	16 (7%)	1 (0%)	34 42
1	B	241/318 (76%)	230 (95%)	11 (5%)	0	100 100
1	C	241/318 (76%)	227 (94%)	14 (6%)	0	100 100
1	D	246/318 (77%)	234 (95%)	10 (4%)	2 (1%)	19 23
1	E	233/318 (73%)	223 (96%)	8 (3%)	2 (1%)	17 20
1	F	244/318 (77%)	228 (93%)	13 (5%)	3 (1%)	13 14
1	G	245/318 (77%)	227 (93%)	17 (7%)	1 (0%)	34 42
1	H	247/318 (78%)	237 (96%)	10 (4%)	0	100 100
All	All	1934/2544 (76%)	1826 (94%)	99 (5%)	9 (0%)	29 35

5 of 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

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	184/285 (65%)	173 (94%)	11 (6%)	19 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	194/285 (68%)	180 (93%)	14 (7%)	14 18
1	C	194/285 (68%)	174 (90%)	20 (10%)	7 8
1	D	204/285 (72%)	190 (93%)	14 (7%)	15 20
1	E	195/285 (68%)	179 (92%)	16 (8%)	11 14
1	F	205/285 (72%)	187 (91%)	18 (9%)	10 12
1	G	206/285 (72%)	188 (91%)	18 (9%)	10 12
1	H	210/285 (74%)	197 (94%)	13 (6%)	18 25
All	All	1592/2280 (70%)	1468 (92%)	124 (8%)	12 16

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	999	GLU
1	G	1007	GLU
1	E	947	ARG
1	G	984	HIS
1	H	869	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	861	HIS
1	H	609	ASN
1	H	921	ASN
1	C	922	GLN
1	C	853	ASN

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	B	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
2	G41	H	1701	-	38,38,38	0.11	0	48,52,52	0.39	1 (2%)
2	G41	C	1701	-	38,38,38	0.11	0	48,52,52	0.40	1 (2%)
2	G41	F	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	E	1701	-	38,38,38	0.11	0	48,52,52	0.38	1 (2%)
3	DMS	H	1702	-	3,3,3	0.39	0	3,3,3	0.38	0
3	DMS	H	1703	-	3,3,3	0.35	0	3,3,3	0.80	0
2	G41	A	1701	-	38,38,38	0.12	0	48,52,52	0.40	1 (2%)
2	G41	D	1701	-	38,38,38	0.11	0	48,52,52	0.38	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	B	1701	-	-	0/20/28/28	0/5/5/5
2	G41	H	1701	-	-	0/20/28/28	0/5/5/5
2	G41	C	1701	-	-	1/20/28/28	0/5/5/5
2	G41	F	1701	-	-	0/20/28/28	0/5/5/5
2	G41	G	1701	-	-	6/20/28/28	0/5/5/5
2	G41	E	1701	-	-	6/20/28/28	0/5/5/5
2	G41	A	1701	-	-	2/20/28/28	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G41	D	1701	-	-	0/20/28/28	0/5/5/5

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

There are no chirality outliers.

5 of 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

There are no ring outliers.

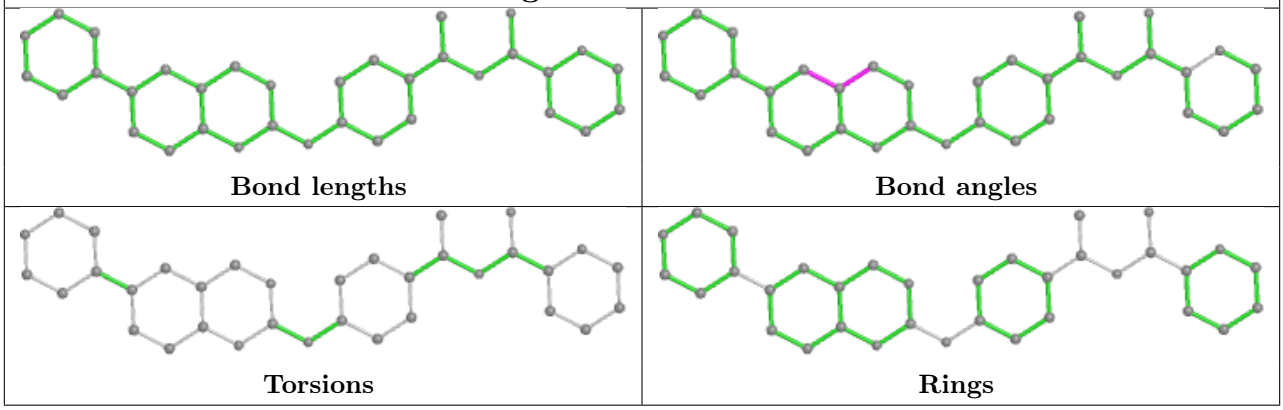
9 monomers are involved in 21 short contacts:

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

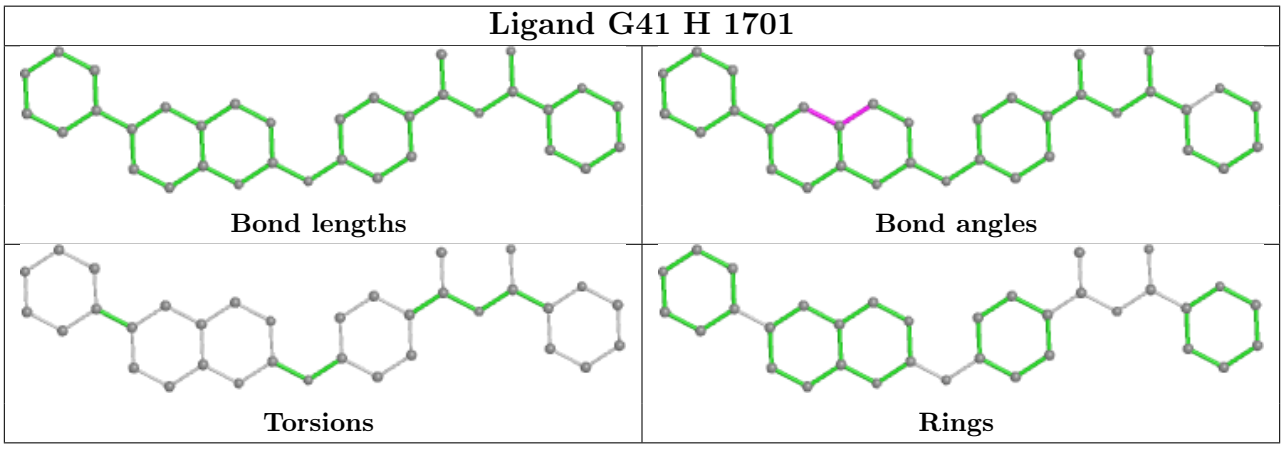
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

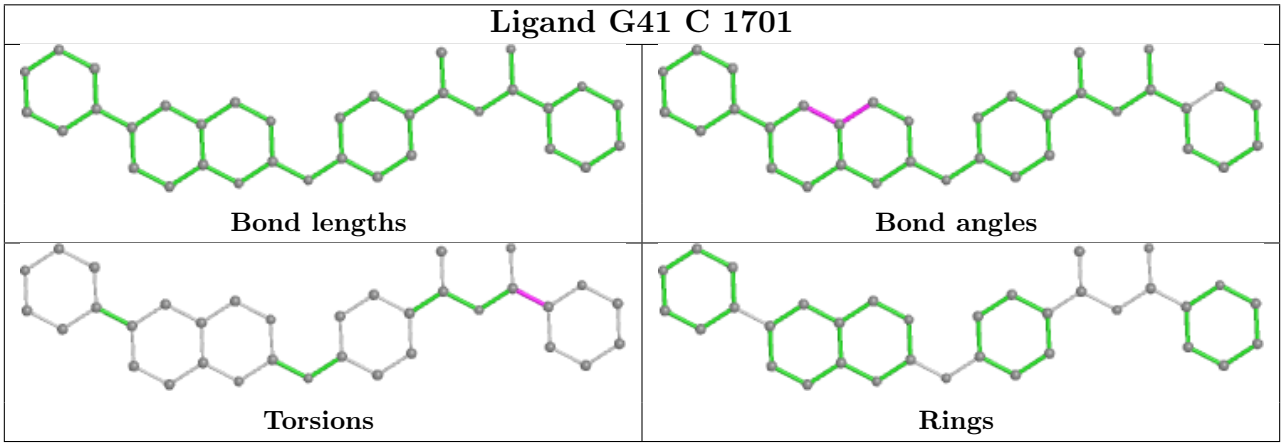
Ligand G41 B 1701



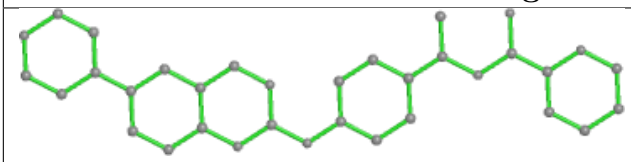
Ligand G41 H 1701



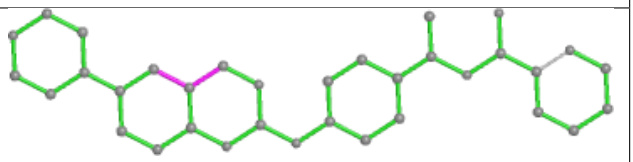
Ligand G41 C 1701



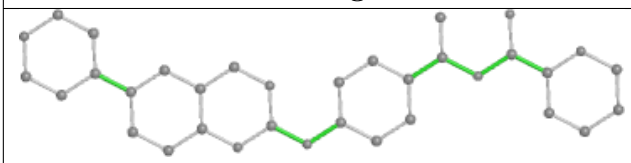
Ligand G41 F 1701



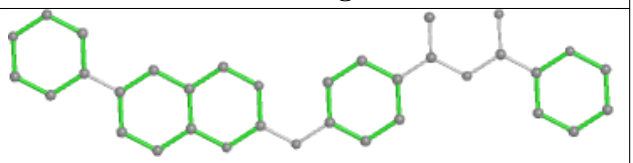
Bond lengths



Bond angles

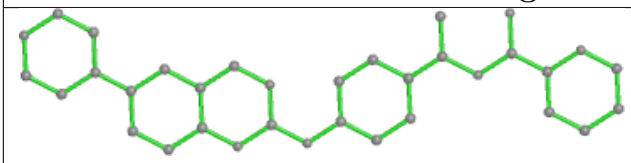


Torsions

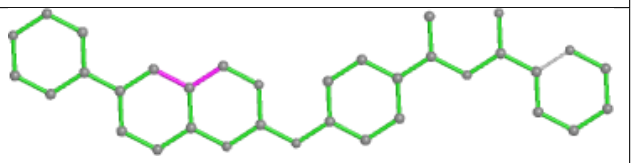


Rings

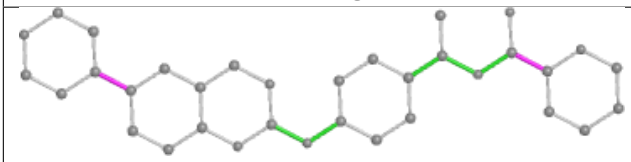
Ligand G41 G 1701



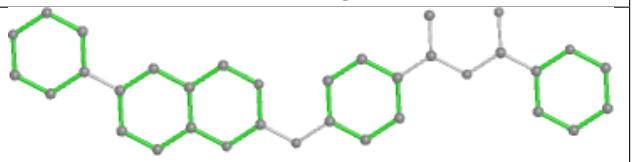
Bond lengths



Bond angles

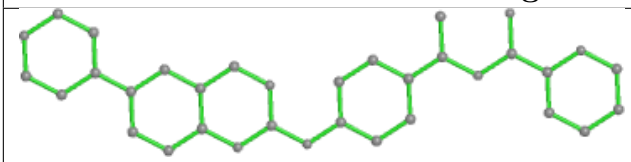


Torsions

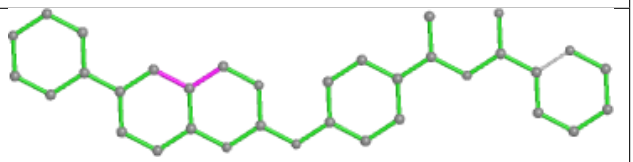


Rings

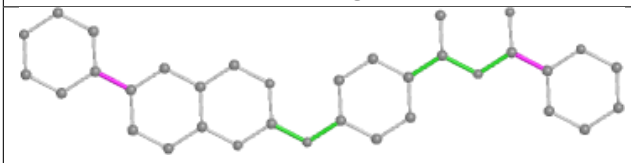
Ligand G41 E 1701



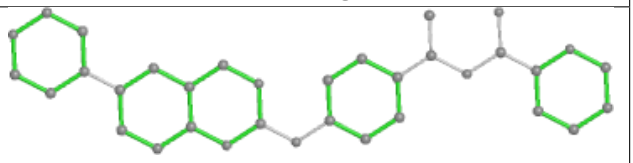
Bond lengths



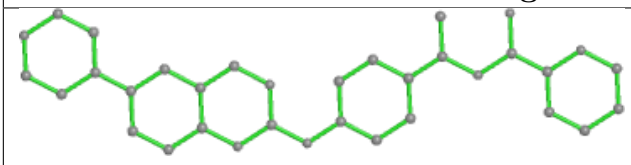
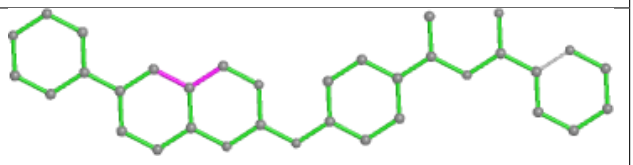
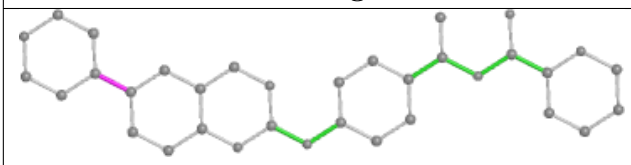
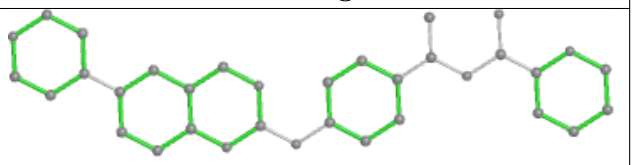
Bond angles

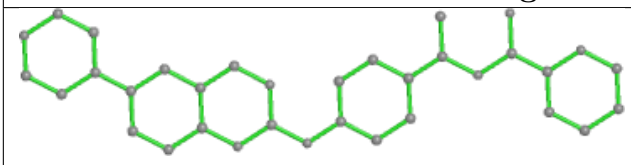
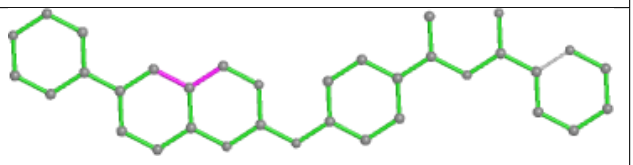
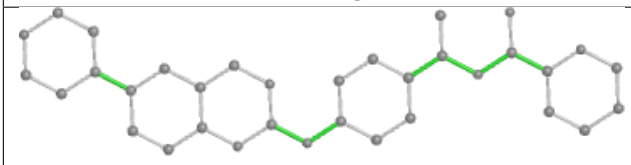
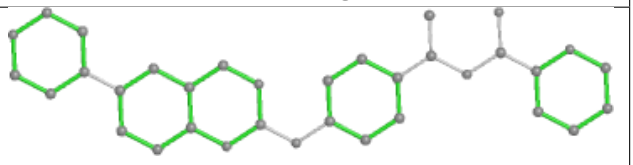


Torsions



Rings

Ligand G41 A 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand G41 D 1701	
 Bond lengths	 Bond angles
 Torsions	 Rings

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	245/318 (77%)	-0.01	6 (2%) 59 66	23, 49, 89, 102	0
1	B	249/318 (78%)	-0.08	6 (2%) 59 66	23, 45, 76, 97	0
1	C	249/318 (78%)	0.11	10 (4%) 38 45	24, 51, 96, 111	0
1	D	254/318 (79%)	-0.00	6 (2%) 59 66	23, 46, 80, 99	0
1	E	241/318 (75%)	0.07	13 (5%) 25 32	28, 51, 82, 102	0
1	F	254/318 (79%)	-0.08	3 (1%) 79 83	23, 46, 76, 100	0
1	G	257/318 (80%)	0.10	11 (4%) 35 42	29, 52, 84, 100	0
1	H	259/318 (81%)	-0.13	2 (0%) 86 89	23, 46, 74, 110	0
All	All	2008/2544 (78%)	-0.00	57 (2%) 53 60	23, 48, 84, 111	0

The worst 5 of 57 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	584	SER	7.2
1	B	966	PHE	6.0
1	G	982	LEU	5.1
1	G	584	SER	5.1
1	C	968	ASP	4.6

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

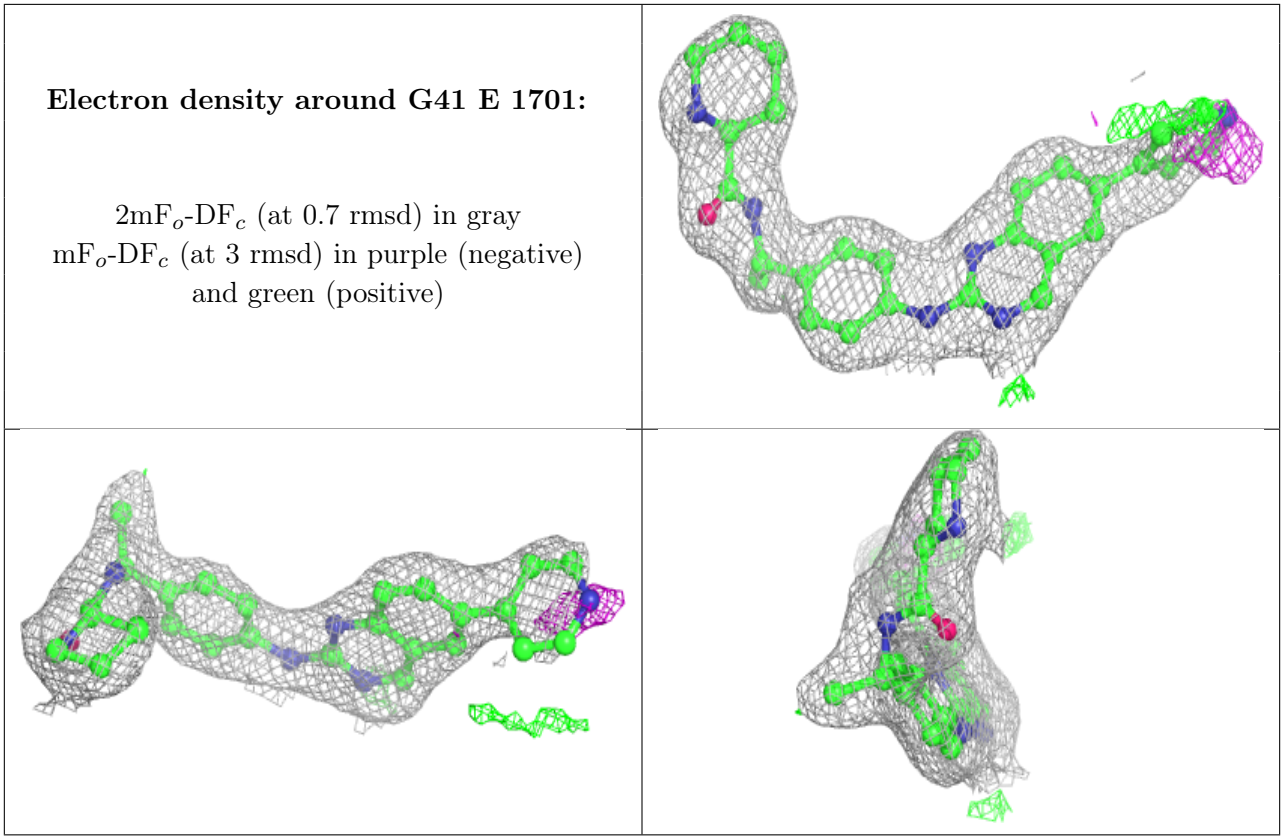
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	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	0.20	78,81,81,83	0
2	G41	B	1701	34/34	0.96	0.12	21,28,40,43	0
2	G41	C	1701	34/34	0.96	0.11	25,36,42,43	0
2	G41	A	1701	34/34	0.97	0.12	20,28,44,47	0
2	G41	D	1701	34/34	0.97	0.12	24,32,43,43	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.

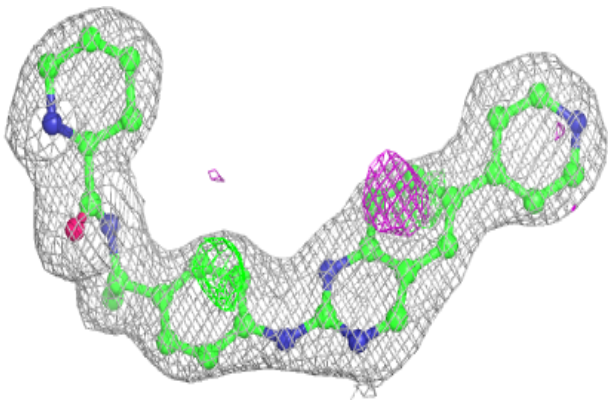
Electron density around G41 E 1701:

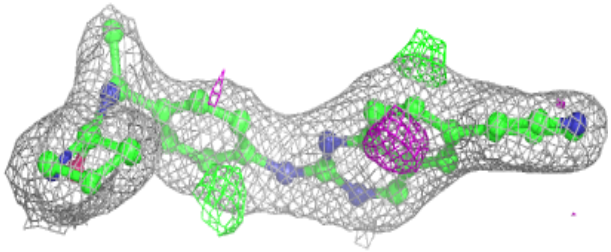
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

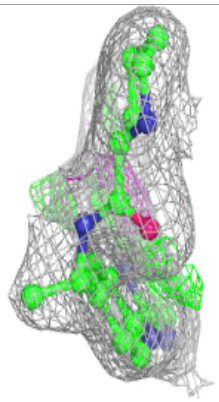


Electron density around G41 F 1701:

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

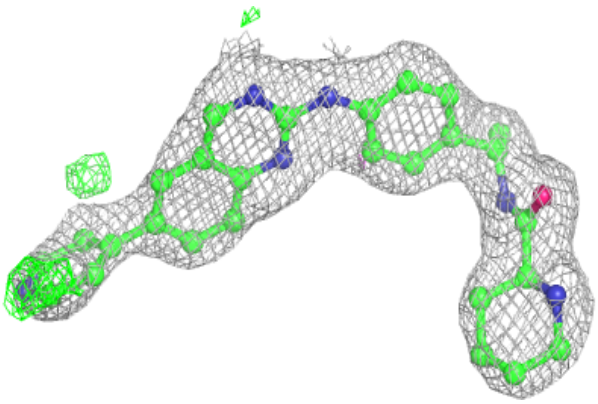


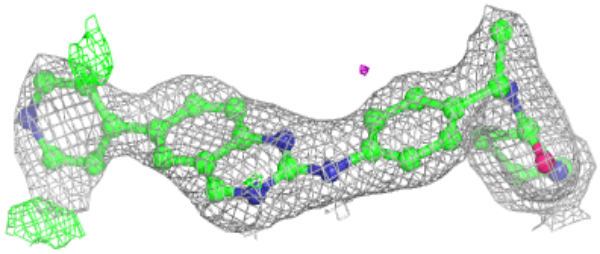


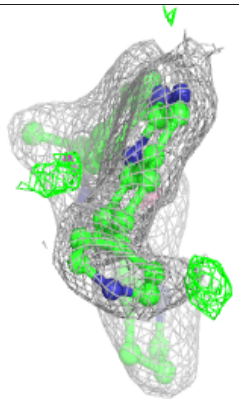


Electron density around G41 G 1701:

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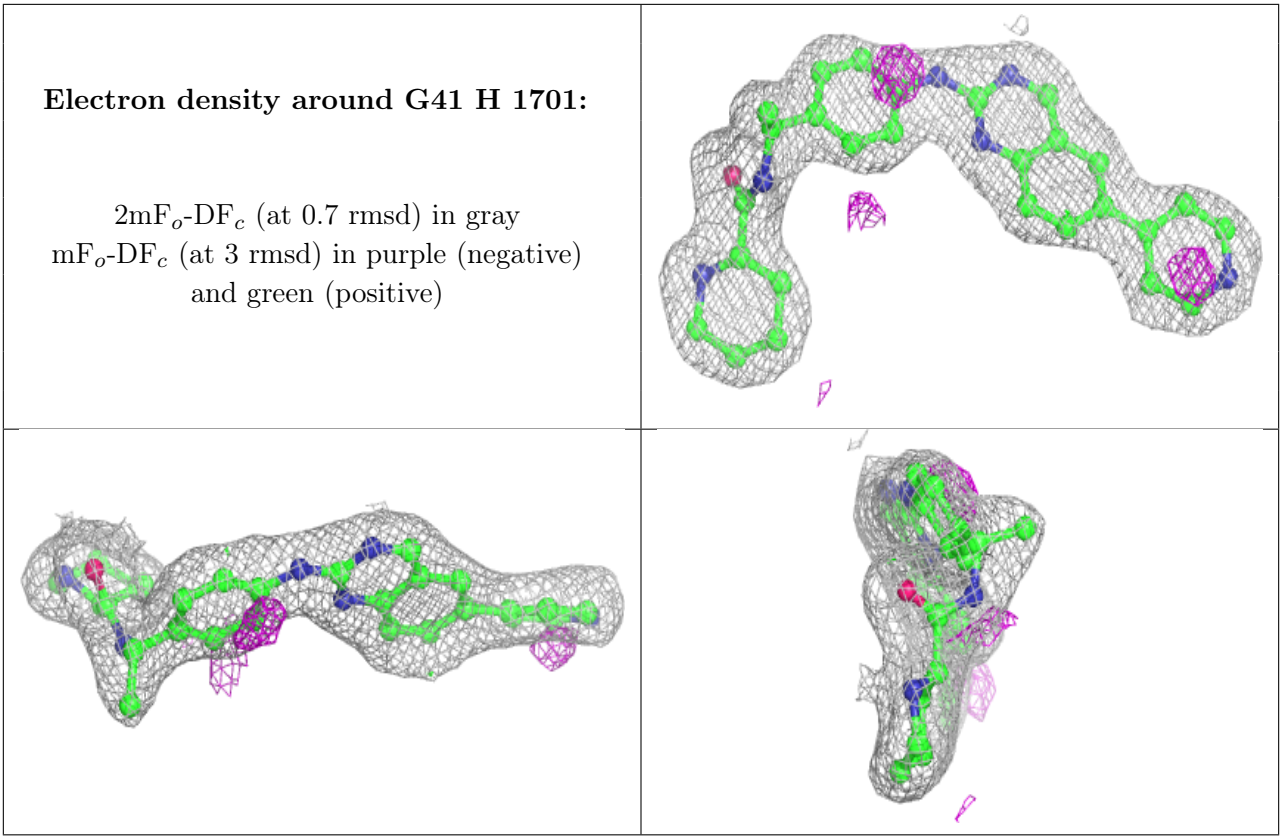
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around G41 B 1701:

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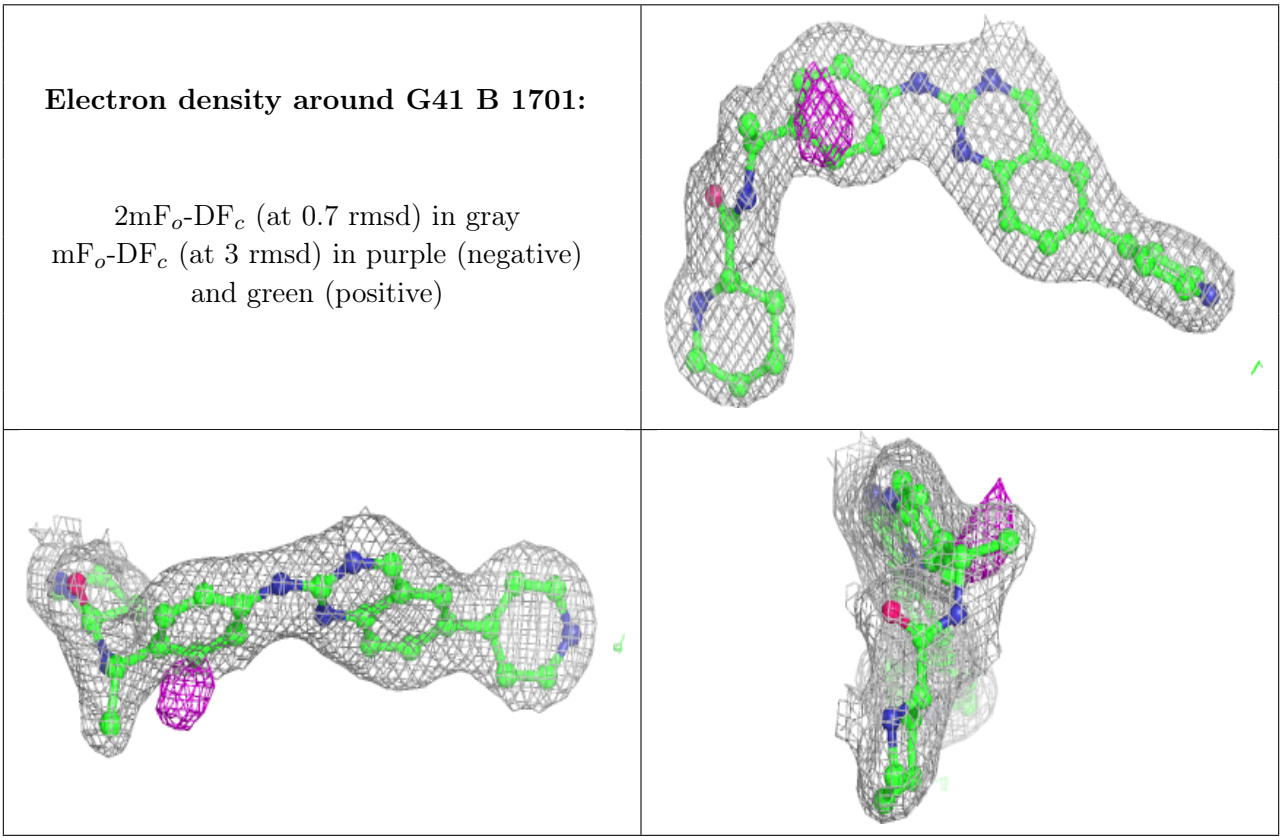
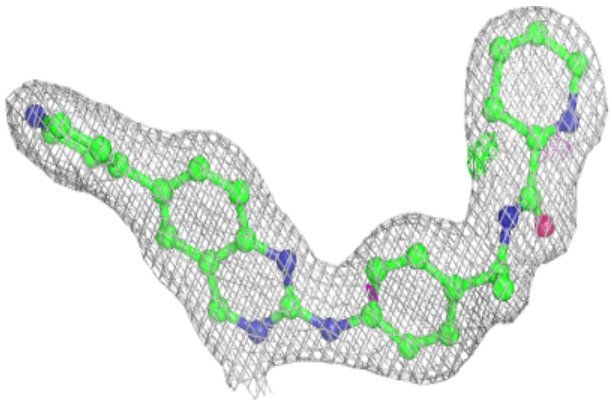
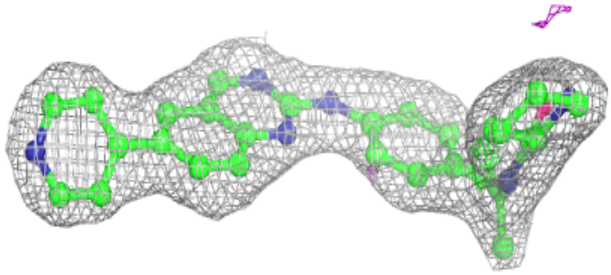
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

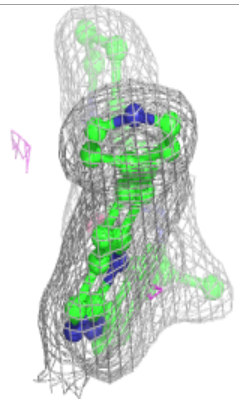


Electron density around G41 C 1701:

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

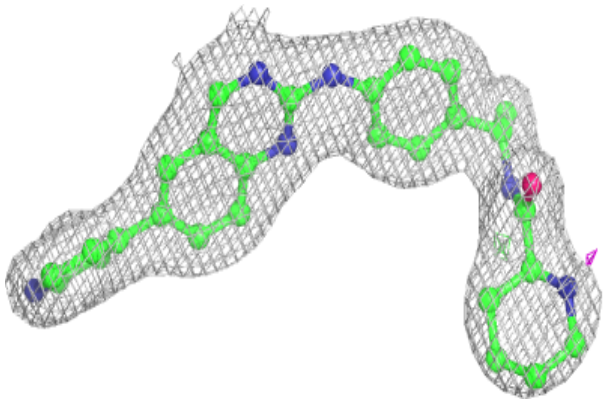


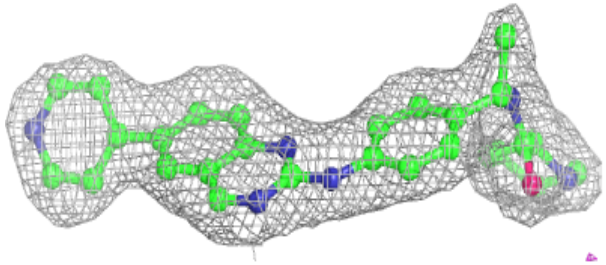


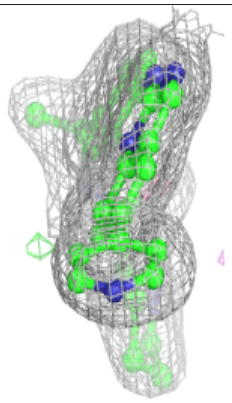


Electron density around G41 A 1701:

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

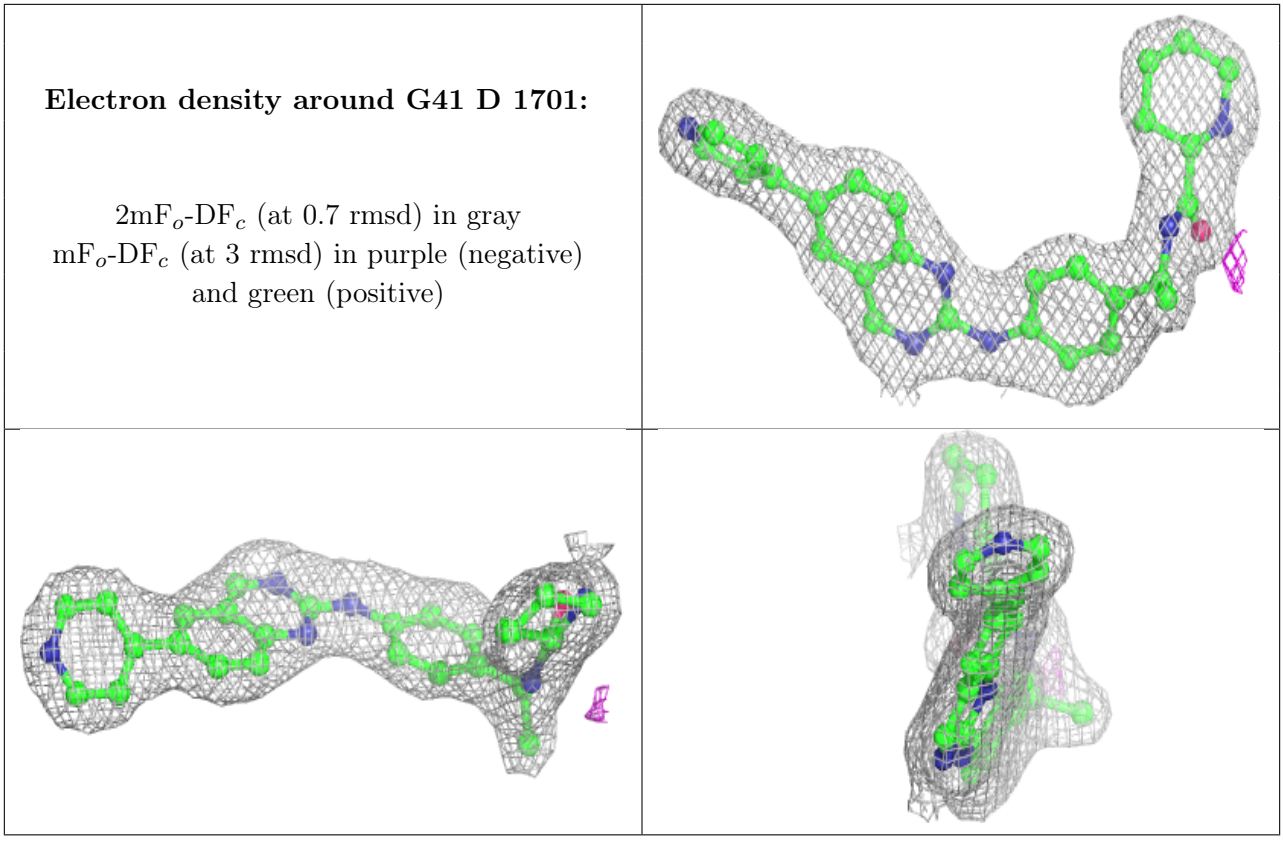






Electron density around G41 D 1701:

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



6.5 Other polymers (i)

There are no such residues in this entry.