



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 23, 2020 – 08:04 am BST

PDB ID : 1FQV  
Title : Insights into scf ubiquitin ligases from the structure of the skp1-skp2 complex  
Authors : Schulman, B.A.; Carrano, A.C.; Jeffrey, P.D.; Bowen, Z.; Kinnucan, E.R.;  
Finnin, M.S.; Elledge, S.J.; Harper, J.W.; Pagano, M.; Pavletich, N.P.  
Deposited on : 2000-09-06  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

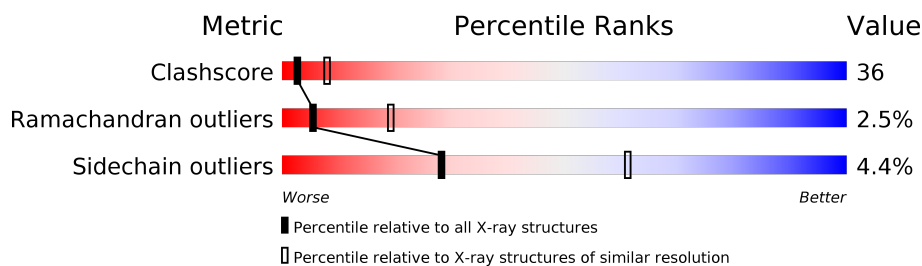
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	336	
1	C	336	
1	E	336	
1	G	336	
1	I	336	
1	K	336	
1	M	336	
1	O	336	

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Mol	Chain	Length	Quality of chain
2	B	149	
2	D	149	
2	F	149	
2	H	149	
2	J	149	
2	L	149	
2	N	149	
2	P	149	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 29256 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 SKP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	C	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	E	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	G	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	I	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	K	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	M	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			
1	O	325	Total	C	N	O	S	4	0	0
			2563	1630	441	476	16			

- Molecule 2 is a protein called SKP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	D	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	F	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	H	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	J	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	L	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			
2	P	137	Total	C	N	O	S	0	0	0
			1094	697	178	213	6			

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	GLY	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	PRO	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	ASP	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	ASN	DELETION	UNP P63208
B	?	-	LYS	DELETION	UNP P63208
B	?	-	GLU	DELETION	UNP P63208
B	?	-	LYS	DELETION	UNP P63208
B	?	-	ARG	DELETION	UNP P63208
B	?	-	THR	DELETION	UNP P63208
B	78	GLY	-	SEE REMARK 999	UNP P63208
B	79	GLY	-	SEE REMARK 999	UNP P63208
B	80	SER	-	SEE REMARK 999	UNP P63208
B	81	GLY	-	SEE REMARK 999	UNP P63208
B	82	THR	-	SEE REMARK 999	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	GLY	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	PRO	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	ASP	DELETION	UNP P63208
D	?	-	ASP	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	ASN	DELETION	UNP P63208
D	?	-	LYS	DELETION	UNP P63208
D	?	-	GLU	DELETION	UNP P63208
D	?	-	LYS	DELETION	UNP P63208
D	?	-	ARG	DELETION	UNP P63208
D	?	-	THR	DELETION	UNP P63208
D	78	GLY	-	SEE REMARK 999	UNP P63208
D	79	GLY	-	SEE REMARK 999	UNP P63208
D	80	SER	-	SEE REMARK 999	UNP P63208
D	81	GLY	-	SEE REMARK 999	UNP P63208
D	82	THR	-	SEE REMARK 999	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	GLY	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	PRO	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	ASP	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	ASN	DELETION	UNP P63208
F	?	-	LYS	DELETION	UNP P63208
F	?	-	GLU	DELETION	UNP P63208
F	?	-	LYS	DELETION	UNP P63208
F	?	-	ARG	DELETION	UNP P63208
F	?	-	THR	DELETION	UNP P63208
F	78	GLY	-	SEE REMARK 999	UNP P63208
F	79	GLY	-	SEE REMARK 999	UNP P63208
F	80	SER	-	SEE REMARK 999	UNP P63208
F	81	GLY	-	SEE REMARK 999	UNP P63208
F	82	THR	-	SEE REMARK 999	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	GLY	DELETION	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	PRO	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	ASP	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	ASN	DELETION	UNP P63208
H	?	-	LYS	DELETION	UNP P63208
H	?	-	GLU	DELETION	UNP P63208
H	?	-	LYS	DELETION	UNP P63208
H	?	-	ARG	DELETION	UNP P63208
H	?	-	THR	DELETION	UNP P63208
H	78	GLY	-	SEE REMARK 999	UNP P63208
H	79	GLY	-	SEE REMARK 999	UNP P63208
H	80	SER	-	SEE REMARK 999	UNP P63208
H	81	GLY	-	SEE REMARK 999	UNP P63208
H	82	THR	-	SEE REMARK 999	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	GLY	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	PRO	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	ASP	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	ASN	DELETION	UNP P63208
J	?	-	LYS	DELETION	UNP P63208
J	?	-	GLU	DELETION	UNP P63208
J	?	-	LYS	DELETION	UNP P63208
J	?	-	ARG	DELETION	UNP P63208
J	?	-	THR	DELETION	UNP P63208
J	78	GLY	-	SEE REMARK 999	UNP P63208
J	79	GLY	-	SEE REMARK 999	UNP P63208
J	80	SER	-	SEE REMARK 999	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
J	81	GLY	-	SEE REMARK 999	UNP P63208
J	82	THR	-	SEE REMARK 999	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	GLY	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	PRO	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	ASP	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	ASN	DELETION	UNP P63208
L	?	-	LYS	DELETION	UNP P63208
L	?	-	GLU	DELETION	UNP P63208
L	?	-	LYS	DELETION	UNP P63208
L	?	-	ARG	DELETION	UNP P63208
L	?	-	THR	DELETION	UNP P63208
L	78	GLY	-	SEE REMARK 999	UNP P63208
L	79	GLY	-	SEE REMARK 999	UNP P63208
L	80	SER	-	SEE REMARK 999	UNP P63208
L	81	GLY	-	SEE REMARK 999	UNP P63208
L	82	THR	-	SEE REMARK 999	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	GLY	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	PRO	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	ASP	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208
N	?	-	ASN	DELETION	UNP P63208
N	?	-	LYS	DELETION	UNP P63208
N	?	-	GLU	DELETION	UNP P63208

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Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	LYS	DELETION	UNP P63208
N	?	-	ARG	DELETION	UNP P63208
N	?	-	THR	DELETION	UNP P63208
N	78	GLY	-	SEE REMARK 999	UNP P63208
N	79	GLY	-	SEE REMARK 999	UNP P63208
N	80	SER	-	SEE REMARK 999	UNP P63208
N	81	GLY	-	SEE REMARK 999	UNP P63208
N	82	THR	-	SEE REMARK 999	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	GLY	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	PRO	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	ASP	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	ASN	DELETION	UNP P63208
P	?	-	LYS	DELETION	UNP P63208
P	?	-	GLU	DELETION	UNP P63208
P	?	-	LYS	DELETION	UNP P63208
P	?	-	ARG	DELETION	UNP P63208
P	?	-	THR	DELETION	UNP P63208
P	78	GLY	-	SEE REMARK 999	UNP P63208
P	79	GLY	-	SEE REMARK 999	UNP P63208
P	80	SER	-	SEE REMARK 999	UNP P63208
P	81	GLY	-	SEE REMARK 999	UNP P63208
P	82	THR	-	SEE REMARK 999	UNP P63208

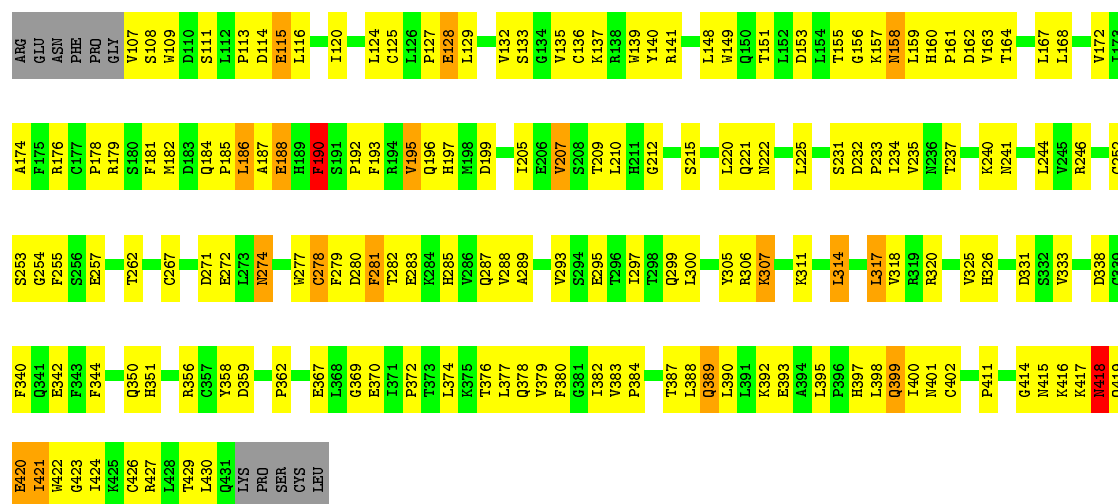
### 3 Residue-property plots

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

Note EDS was not executed.

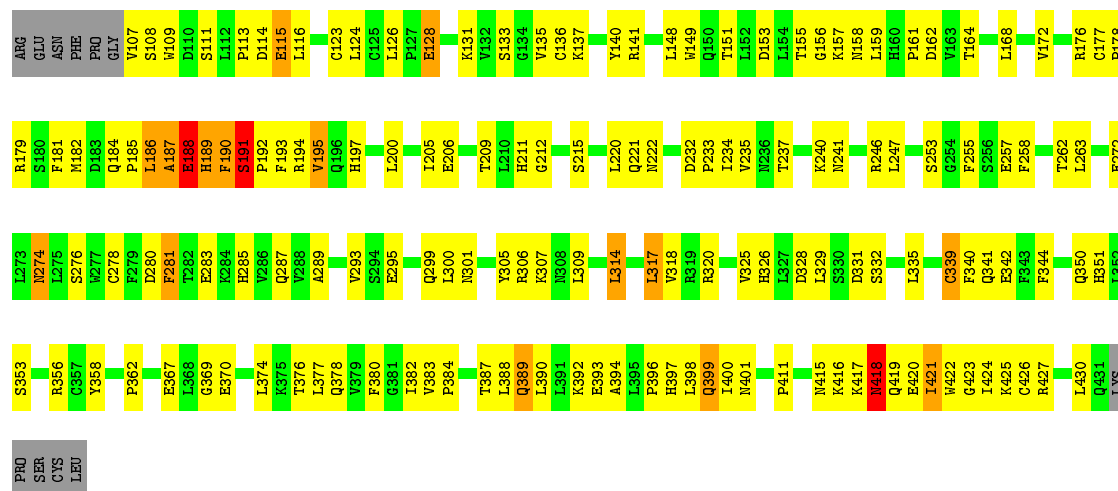
#### • Molecule 1: SKP2

Chain A: 

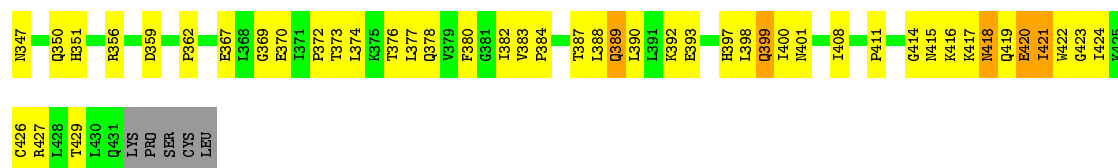


#### • Molecule 1: SKP2

Chain C: 

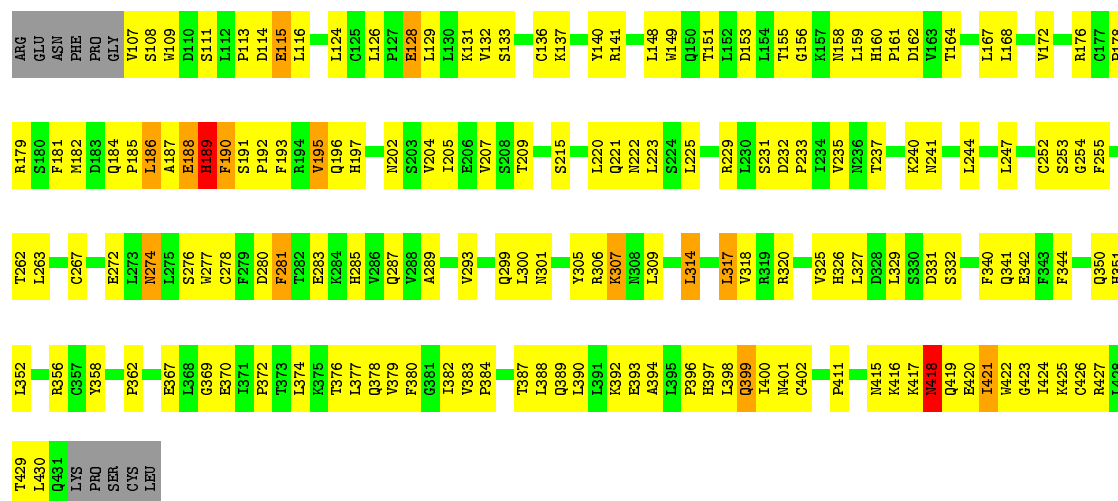






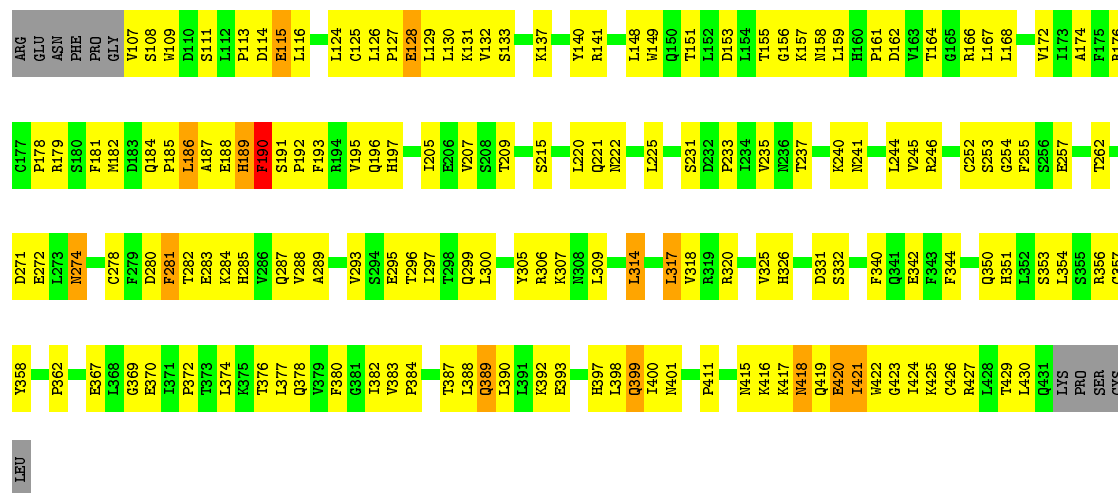
• Molecule 1: SKP2

Chain K: 49% 44%



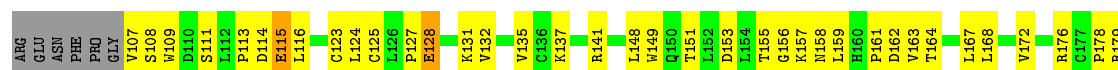
• Molecule 1: SKP2

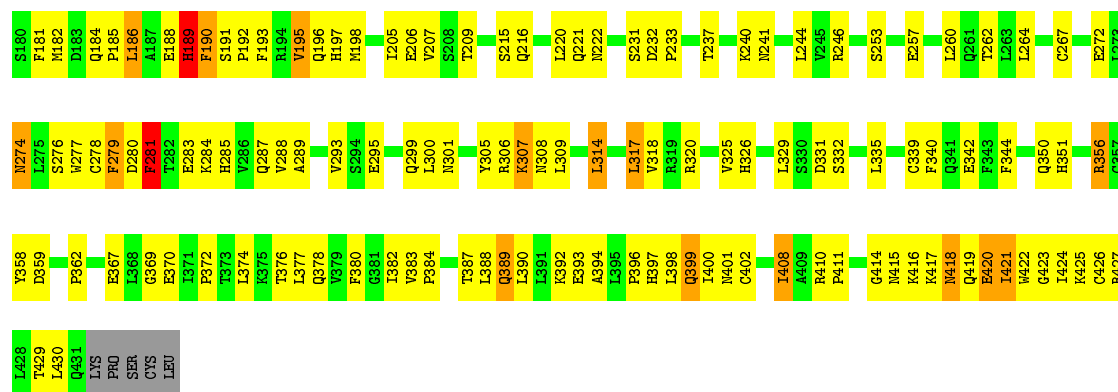
Chain M: 49% 43%



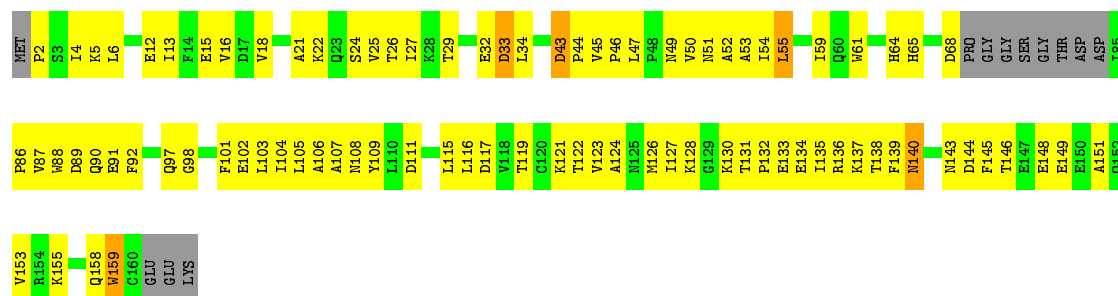
• Molecule 1: SKP2

Chain O: 48% 43% 5%

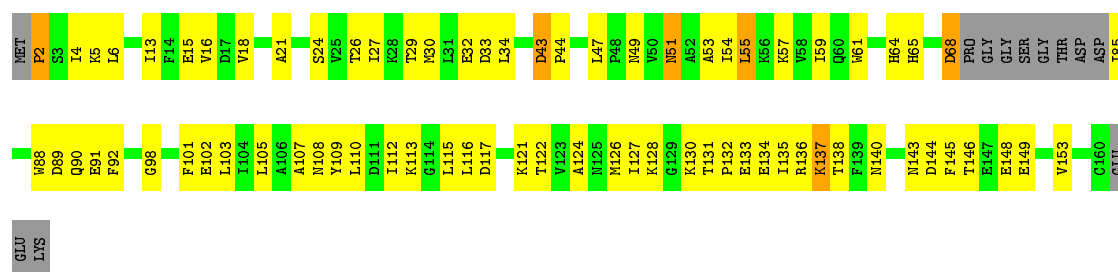




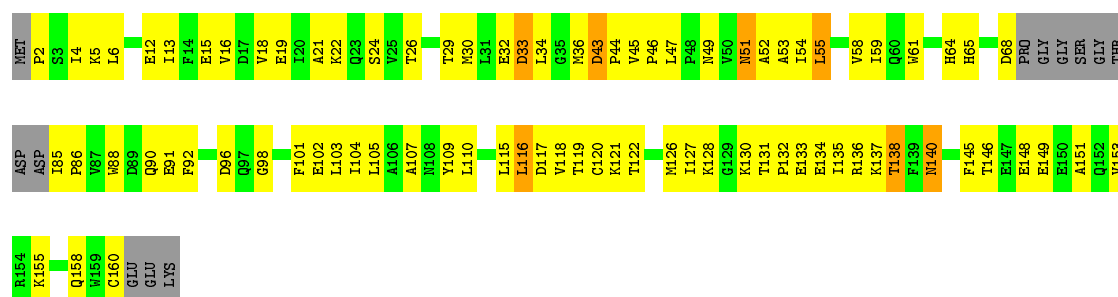
• Molecule 2: SKP1



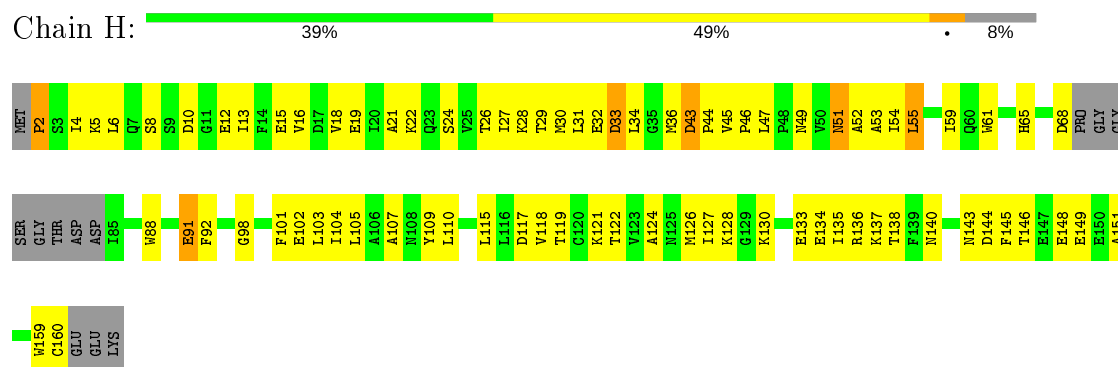
• Molecule 2: SKP1



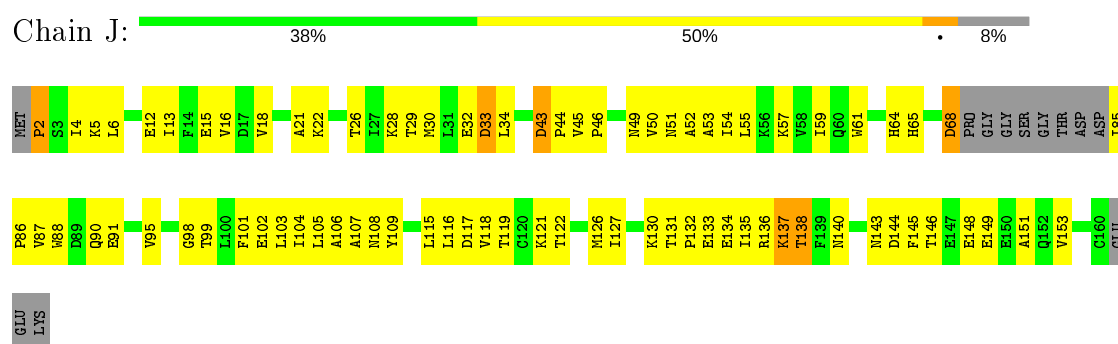
• Molecule 2: SKP1



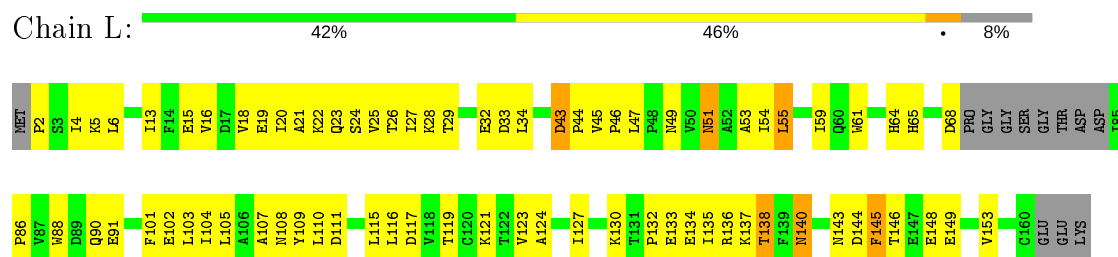
- Molecule 2: SKP1



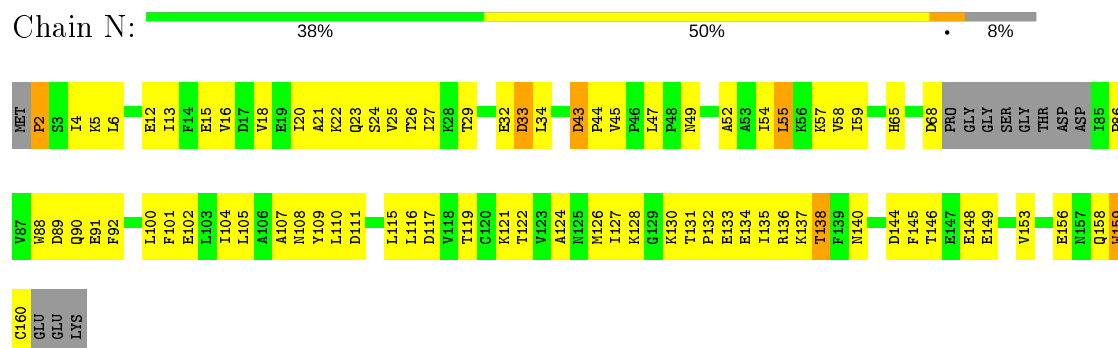
- Molecule 2: SKP1



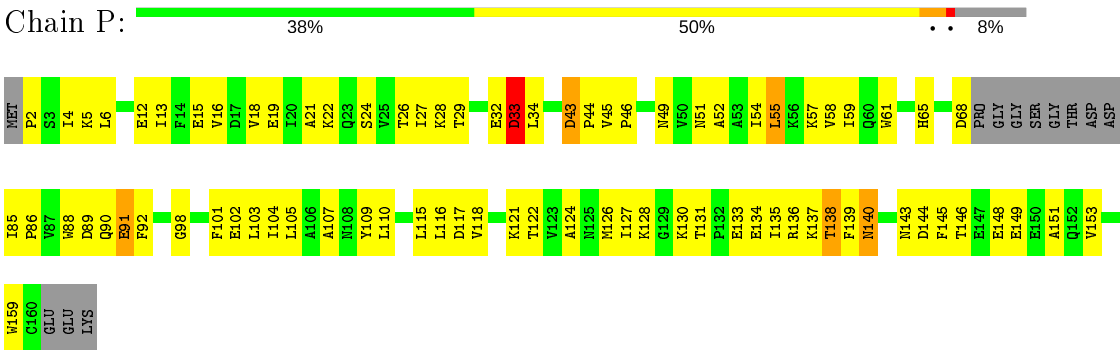
- Molecule 2: SKP1



- Molecule 2: SKP1



- Molecule 2: SKP1



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	262.70 Å   148.20 Å   133.30 Å 90.00°   120.03°   90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.275 , 0.314	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	29256	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	0.56	1/2612 (0.0%)	0.80	3/3545 (0.1%)
1	C	0.63	4/2612 (0.2%)	0.88	7/3545 (0.2%)
1	E	0.52	0/2612	0.77	1/3545 (0.0%)
1	G	0.63	2/2612 (0.1%)	1.06	7/3545 (0.2%)
1	I	0.60	2/2612 (0.1%)	1.01	6/3545 (0.2%)
1	K	0.59	1/2612 (0.0%)	1.06	7/3545 (0.2%)
1	M	0.59	3/2612 (0.1%)	0.90	4/3545 (0.1%)
1	O	0.55	1/2612 (0.0%)	1.06	8/3545 (0.2%)
2	B	0.35	0/1111	0.61	1/1502 (0.1%)
2	D	0.42	0/1111	0.64	1/1502 (0.1%)
2	F	0.38	0/1111	0.63	1/1502 (0.1%)
2	H	0.58	0/1111	0.71	1/1502 (0.1%)
2	J	0.42	0/1111	0.66	1/1502 (0.1%)
2	L	0.44	0/1111	0.66	1/1502 (0.1%)
2	N	0.44	0/1111	0.65	1/1502 (0.1%)
2	P	0.54	0/1111	0.69	1/1502 (0.1%)
All	All	0.55	14/29784 (0.0%)	0.87	51/40376 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	186	LEU	C-N	15.94	1.70	1.34
1	I	186	LEU	C-N	12.79	1.63	1.34
1	G	189	HIS	C-N	-9.35	1.12	1.34
1	K	189	HIS	C-N	-8.94	1.13	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	190	PHE	N-CA	-7.71	1.30	1.46

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	HIS	O-C-N	23.02	159.53	122.70
1	I	189	HIS	C-N-CA	-22.18	66.25	121.70
1	K	186	LEU	O-C-N	21.78	157.54	122.70
1	G	186	LEU	O-C-N	20.23	155.06	122.70
1	O	186	LEU	O-C-N	19.63	154.11	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	189	HIS	Mainchain

## 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	2563	0	2598	214	0
1	C	2563	0	2597	206	0
1	E	2563	0	2598	217	0
1	G	2563	0	2596	217	0
1	I	2563	0	2598	188	0
1	K	2563	0	2598	217	0
1	M	2563	0	2598	194	0
1	O	2563	0	2598	221	0
2	B	1094	0	1099	87	0
2	D	1094	0	1099	75	0
2	F	1094	0	1099	84	1
2	H	1094	0	1099	71	0
2	J	1094	0	1099	75	0
2	L	1094	0	1099	84	1
2	N	1094	0	1099	77	0
2	P	1094	0	1099	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29256	0	29573	2115	1

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 36.

The worst 5 of 2115 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:LEU:C	1:G:187:ALA:N	1.70	1.40
1:M:189:HIS:O	1:M:190:PHE:O	1.58	1.17
1:K:417:LYS:CE	1:O:417:LYS:HG3	1.75	1.15
1:I:417:LYS:HG3	1:M:417:LYS:CE	1.77	1.14
2:L:43:ASP:HB2	2:L:44:PRO:HD3	1.29	1.14

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ASN:ND2	2:L:43:ASP:OD1[2_656]	1.93	0.27

## 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	323/336 (96%)	294 (91%)	21 (6%)	8 (2%)	5	19
1	C	323/336 (96%)	292 (90%)	24 (7%)	7 (2%)	6	22
1	E	323/336 (96%)	289 (90%)	27 (8%)	7 (2%)	6	22
1	G	323/336 (96%)	292 (90%)	24 (7%)	7 (2%)	6	22
1	I	323/336 (96%)	295 (91%)	21 (6%)	7 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	323/336 (96%)	291 (90%)	24 (7%)	8 (2%)	5	19
1	M	323/336 (96%)	293 (91%)	25 (8%)	5 (2%)	10	33
1	O	323/336 (96%)	294 (91%)	21 (6%)	8 (2%)	5	19
2	B	133/149 (89%)	117 (88%)	12 (9%)	4 (3%)	4	15
2	D	133/149 (89%)	118 (89%)	10 (8%)	5 (4%)	3	10
2	F	133/149 (89%)	118 (89%)	11 (8%)	4 (3%)	4	15
2	H	133/149 (89%)	118 (89%)	12 (9%)	3 (2%)	6	21
2	J	133/149 (89%)	120 (90%)	8 (6%)	5 (4%)	3	10
2	L	133/149 (89%)	119 (90%)	9 (7%)	5 (4%)	3	10
2	N	133/149 (89%)	116 (87%)	13 (10%)	4 (3%)	4	15
2	P	133/149 (89%)	117 (88%)	11 (8%)	5 (4%)	3	10
All	All	3648/3880 (94%)	3283 (90%)	273 (8%)	92 (2%)	5	19

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	PHE
1	A	306	ARG
1	C	187	ALA
1	C	306	ARG
1	C	421	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/311 (96%)	282 (94%)	17 (6%)	20	50
1	C	299/311 (96%)	286 (96%)	13 (4%)	29	62
1	E	299/311 (96%)	285 (95%)	14 (5%)	26	59
1	G	299/311 (96%)	285 (95%)	14 (5%)	26	59
1	I	299/311 (96%)	281 (94%)	18 (6%)	19	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	299/311 (96%)	287 (96%)	12 (4%)	31	65
1	M	299/311 (96%)	284 (95%)	15 (5%)	24	56
1	O	299/311 (96%)	283 (95%)	16 (5%)	22	53
2	B	124/134 (92%)	122 (98%)	2 (2%)	62	88
2	D	124/134 (92%)	120 (97%)	4 (3%)	39	73
2	F	124/134 (92%)	120 (97%)	4 (3%)	39	73
2	H	124/134 (92%)	120 (97%)	4 (3%)	39	73
2	J	124/134 (92%)	120 (97%)	4 (3%)	39	73
2	L	124/134 (92%)	121 (98%)	3 (2%)	49	81
2	N	124/134 (92%)	122 (98%)	2 (2%)	62	88
2	P	124/134 (92%)	117 (94%)	7 (6%)	21	51
All	All	3384/3560 (95%)	3235 (96%)	149 (4%)	28	61

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	420	GLU
1	I	317	LEU
1	O	359	ASP
2	H	55	LEU
1	I	207	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 154 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	7	GLN
1	I	399	GLN
1	O	350	GLN
2	H	51	ASN
1	I	211	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	2
1	K	1
1	I	1
1	C	1
1	O	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	186:LEU	C	187:ALA	N	1.70
1	I	186:LEU	C	187:ALA	N	1.63
1	C	189:HIS	C	190:PHE	N	1.19
1	O	189:HIS	C	190:PHE	N	1.17
1	K	189:HIS	C	190:PHE	N	1.13

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.