wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:56 pm BST

PDB ID	:	6H0F
Title	:	Structure of DDB1-CRBN-pomalidomide complex bound to IKZF1(ZF2)
Authors	:	Petzold, G.; Bunker, R.D.; Thoma, N.H.
Deposited on	:	2018-07-09
Resolution	:	3.25 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 following versions of software and data (see references (i)) were used in the production of this report:

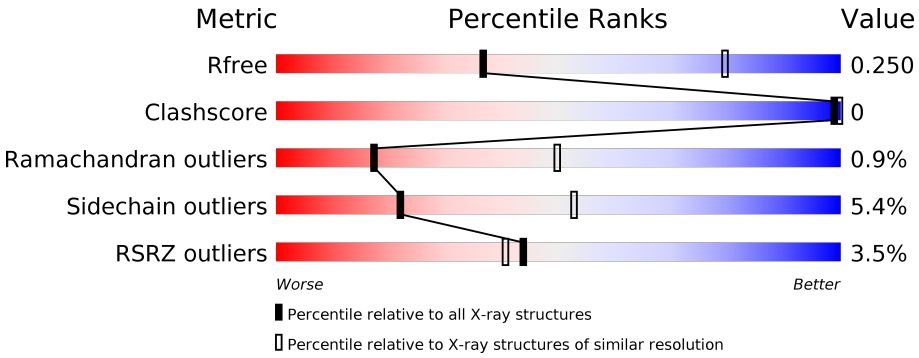
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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 >=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	856	92%
1	D	856	6% 92%
1	G	856	3% 91% 5%
1	J	856	4% 92% 6%
2	B	426	4% 79% 8% 12%
2	E	426	4% 81% 7% 12%

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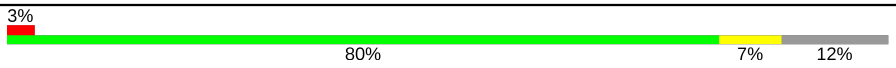
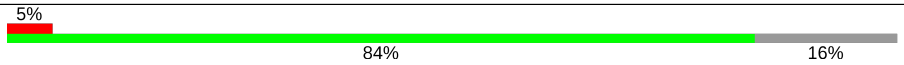
Mol	Chain	Length	Quality of chain
2	H	426	
2	K	426	
3	C	38	
3	F	38	
3	I	38	
3	L	38	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 77598 atoms, of which 38594 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 DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	826	Total	C	H	N	O	S	6417	0	0
			12887	4099	6417	1093	1242	36			
1	D	821	Total	C	H	N	O	S	6381	0	0
			12814	4078	6381	1087	1232	36			
1	G	826	Total	C	H	N	O	S	6418	0	0
			12888	4099	6418	1093	1242	36			
1	J	843	Total	C	H	N	O	S	6526	0	0
			13119	4174	6526	1116	1267	36			

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			
2	E	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			
2	H	374	Total	C	H	N	O	S	2959	0	0
			5937	1899	2959	509	546	24			
2	K	374	Total	C	H	N	O	S	2967	2	0
			5955	1905	2967	512	547	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	initiating methionine	UNP Q96SW2
B	18	ASP	-	expression tag	UNP Q96SW2
B	19	TRP	-	expression tag	UNP Q96SW2
B	20	SER	-	expression tag	UNP Q96SW2
B	21	HIS	-	expression tag	UNP Q96SW2
B	22	PRO	-	expression tag	UNP Q96SW2
B	23	GLN	-	expression tag	UNP Q96SW2
B	24	PHE	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	GLU	-	expression tag	UNP Q96SW2
B	26	LYS	-	expression tag	UNP Q96SW2
B	27	SER	-	expression tag	UNP Q96SW2
B	28	ALA	-	expression tag	UNP Q96SW2
B	29	VAL	-	expression tag	UNP Q96SW2
B	30	ASP	-	expression tag	UNP Q96SW2
B	31	GLU	-	expression tag	UNP Q96SW2
B	32	ASN	-	expression tag	UNP Q96SW2
B	33	LEU	-	expression tag	UNP Q96SW2
B	34	TYR	-	expression tag	UNP Q96SW2
B	35	PHE	-	expression tag	UNP Q96SW2
B	37	GLY	ASP	conflict	UNP Q96SW2
B	38	GLY	SER	conflict	UNP Q96SW2
B	39	GLY	LYS	conflict	UNP Q96SW2
B	40	ARG	GLU	conflict	UNP Q96SW2
E	17	MET	-	initiating methionine	UNP Q96SW2
E	18	ASP	-	expression tag	UNP Q96SW2
E	19	TRP	-	expression tag	UNP Q96SW2
E	20	SER	-	expression tag	UNP Q96SW2
E	21	HIS	-	expression tag	UNP Q96SW2
E	22	PRO	-	expression tag	UNP Q96SW2
E	23	GLN	-	expression tag	UNP Q96SW2
E	24	PHE	-	expression tag	UNP Q96SW2
E	25	GLU	-	expression tag	UNP Q96SW2
E	26	LYS	-	expression tag	UNP Q96SW2
E	27	SER	-	expression tag	UNP Q96SW2
E	28	ALA	-	expression tag	UNP Q96SW2
E	29	VAL	-	expression tag	UNP Q96SW2
E	30	ASP	-	expression tag	UNP Q96SW2
E	31	GLU	-	expression tag	UNP Q96SW2
E	32	ASN	-	expression tag	UNP Q96SW2
E	33	LEU	-	expression tag	UNP Q96SW2
E	34	TYR	-	expression tag	UNP Q96SW2
E	35	PHE	-	expression tag	UNP Q96SW2
E	37	GLY	ASP	conflict	UNP Q96SW2
E	38	GLY	SER	conflict	UNP Q96SW2
E	39	GLY	LYS	conflict	UNP Q96SW2
E	40	ARG	GLU	conflict	UNP Q96SW2
H	17	MET	-	initiating methionine	UNP Q96SW2
H	18	ASP	-	expression tag	UNP Q96SW2
H	19	TRP	-	expression tag	UNP Q96SW2
H	20	SER	-	expression tag	UNP Q96SW2

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Chain	Residue	Modelled	Actual	Comment	Reference
H	21	HIS	-	expression tag	UNP Q96SW2
H	22	PRO	-	expression tag	UNP Q96SW2
H	23	GLN	-	expression tag	UNP Q96SW2
H	24	PHE	-	expression tag	UNP Q96SW2
H	25	GLU	-	expression tag	UNP Q96SW2
H	26	LYS	-	expression tag	UNP Q96SW2
H	27	SER	-	expression tag	UNP Q96SW2
H	28	ALA	-	expression tag	UNP Q96SW2
H	29	VAL	-	expression tag	UNP Q96SW2
H	30	ASP	-	expression tag	UNP Q96SW2
H	31	GLU	-	expression tag	UNP Q96SW2
H	32	ASN	-	expression tag	UNP Q96SW2
H	33	LEU	-	expression tag	UNP Q96SW2
H	34	TYR	-	expression tag	UNP Q96SW2
H	35	PHE	-	expression tag	UNP Q96SW2
H	37	GLY	ASP	conflict	UNP Q96SW2
H	38	GLY	SER	conflict	UNP Q96SW2
H	39	GLY	LYS	conflict	UNP Q96SW2
H	40	ARG	GLU	conflict	UNP Q96SW2
K	17	MET	-	initiating methionine	UNP Q96SW2
K	18	ASP	-	expression tag	UNP Q96SW2
K	19	TRP	-	expression tag	UNP Q96SW2
K	20	SER	-	expression tag	UNP Q96SW2
K	21	HIS	-	expression tag	UNP Q96SW2
K	22	PRO	-	expression tag	UNP Q96SW2
K	23	GLN	-	expression tag	UNP Q96SW2
K	24	PHE	-	expression tag	UNP Q96SW2
K	25	GLU	-	expression tag	UNP Q96SW2
K	26	LYS	-	expression tag	UNP Q96SW2
K	27	SER	-	expression tag	UNP Q96SW2
K	28	ALA	-	expression tag	UNP Q96SW2
K	29	VAL	-	expression tag	UNP Q96SW2
K	30	ASP	-	expression tag	UNP Q96SW2
K	31	GLU	-	expression tag	UNP Q96SW2
K	32	ASN	-	expression tag	UNP Q96SW2
K	33	LEU	-	expression tag	UNP Q96SW2
K	34	TYR	-	expression tag	UNP Q96SW2
K	35	PHE	-	expression tag	UNP Q96SW2
K	37	GLY	ASP	conflict	UNP Q96SW2
K	38	GLY	SER	conflict	UNP Q96SW2
K	39	GLY	LYS	conflict	UNP Q96SW2
K	40	ARG	GLU	conflict	UNP Q96SW2

- Molecule 3 is a protein called DNA-binding protein Ikaros.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	F	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	I	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			
3	L	32	Total	C	H	N	O	S	237	0	0
			481	148	237	52	42	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	137	GLY	-	expression tag	UNP Q13422
C	138	GLY	-	expression tag	UNP Q13422
C	139	GLY	-	expression tag	UNP Q13422
C	140	ARG	-	expression tag	UNP Q13422
F	137	GLY	-	expression tag	UNP Q13422
F	138	GLY	-	expression tag	UNP Q13422
F	139	GLY	-	expression tag	UNP Q13422
F	140	ARG	-	expression tag	UNP Q13422
I	137	GLY	-	expression tag	UNP Q13422
I	138	GLY	-	expression tag	UNP Q13422
I	139	GLY	-	expression tag	UNP Q13422
I	140	ARG	-	expression tag	UNP Q13422
L	137	GLY	-	expression tag	UNP Q13422
L	138	GLY	-	expression tag	UNP Q13422
L	139	GLY	-	expression tag	UNP Q13422
L	140	ARG	-	expression tag	UNP Q13422

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	K	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		
4	H	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	I	1	Total	Zn	0	0
			1	1		

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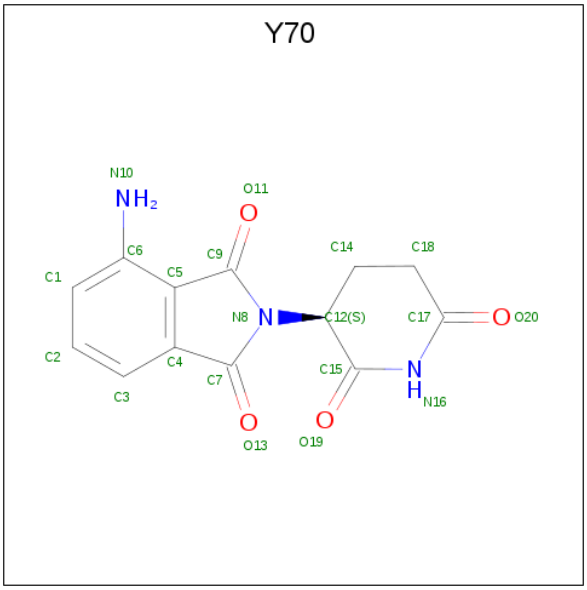
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

- Molecule 5 is S-Pomalidomide (three-letter code: Y70) (formula: $C_{13}H_{11}N_3O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C H N O 31 13 11 3 4	11	0
5	E	1	Total C H N O 31 13 11 3 4	11	0
5	H	1	Total C H N O 31 13 11 3 4	11	0
5	K	1	Total C H N O 31 13 11 3 4	11	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	8	Total O 8 8	0	0
6	B	3	Total O 3 3	0	0

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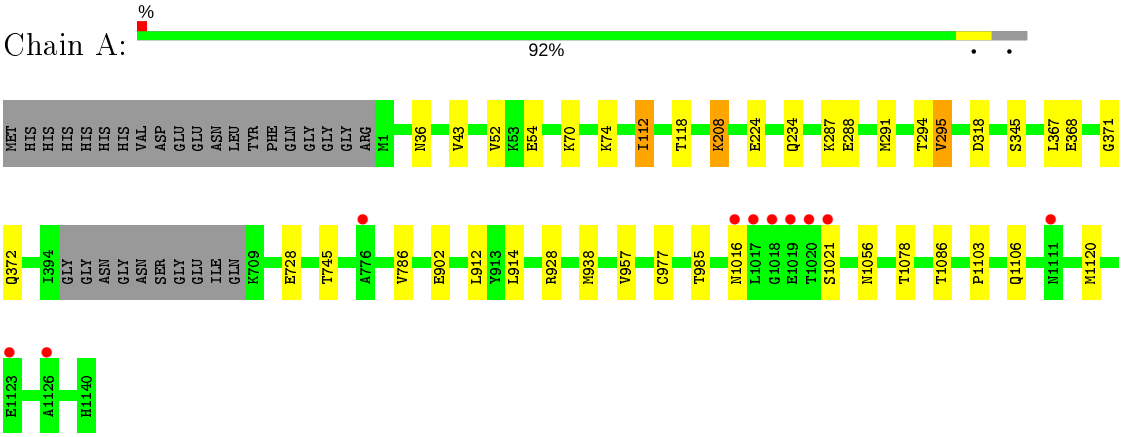
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total O 3 3	0	0
6	E	4	Total O 4 4	0	0
6	G	3	Total O 3 3	0	0
6	H	5	Total O 5 5	0	0
6	J	6	Total O 6 6	0	0

3 Residue-property plots (i)

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 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.

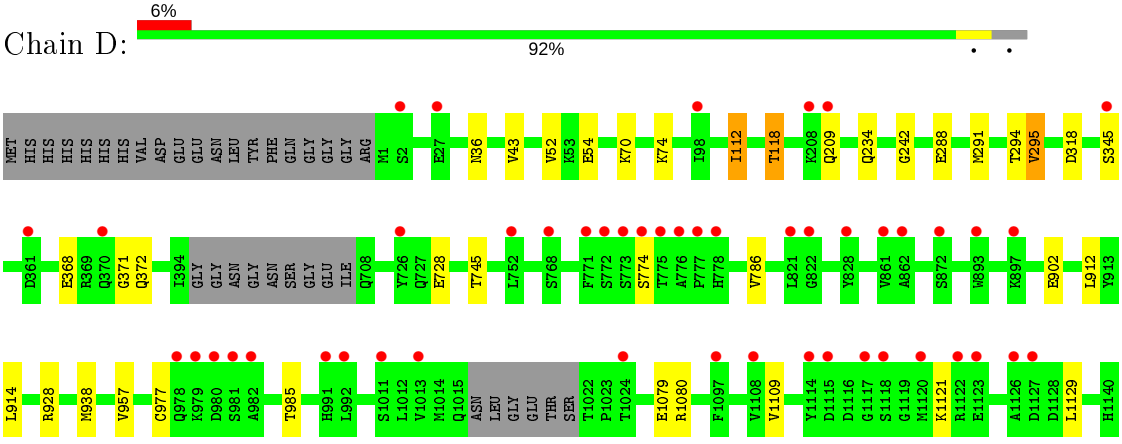
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

Chain A:



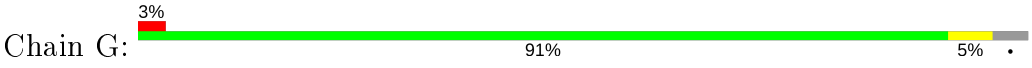
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

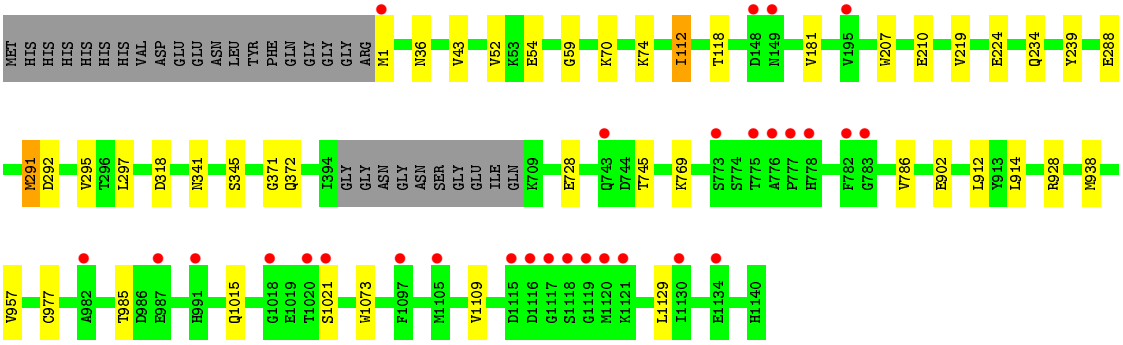
Chain D:



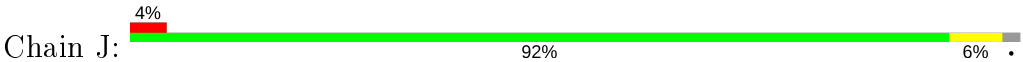
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

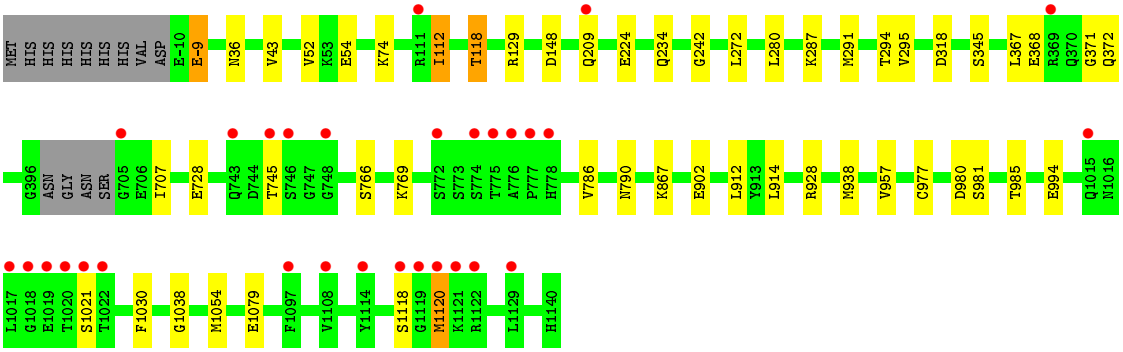
Chain G:



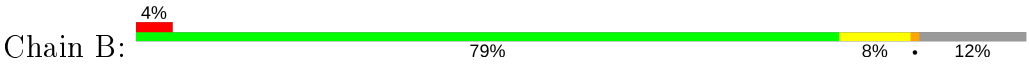


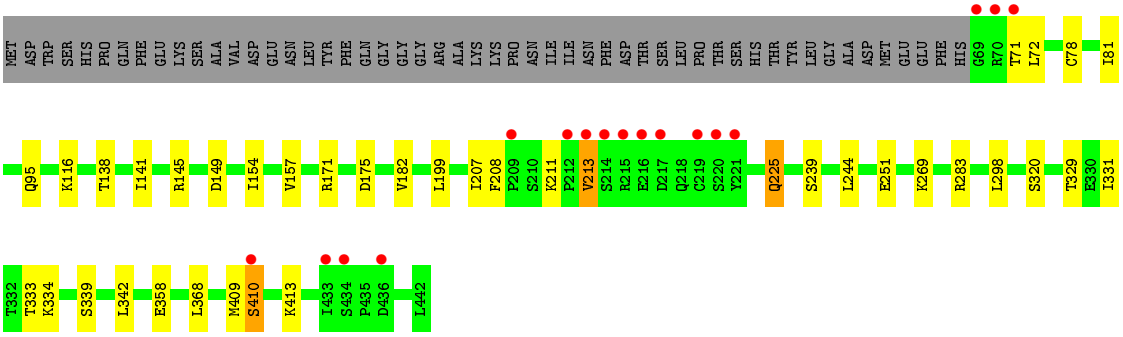
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1



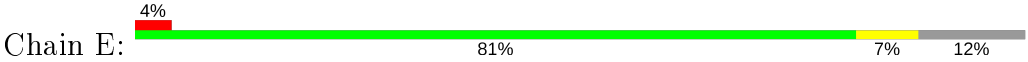


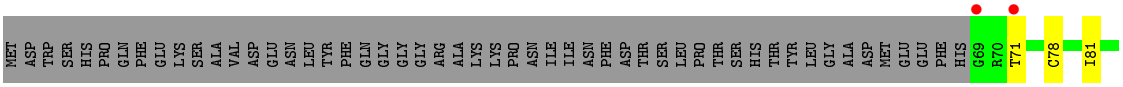
• Molecule 2: Protein cereblon

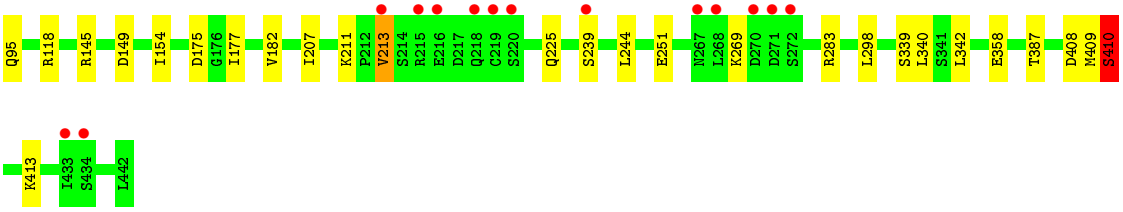




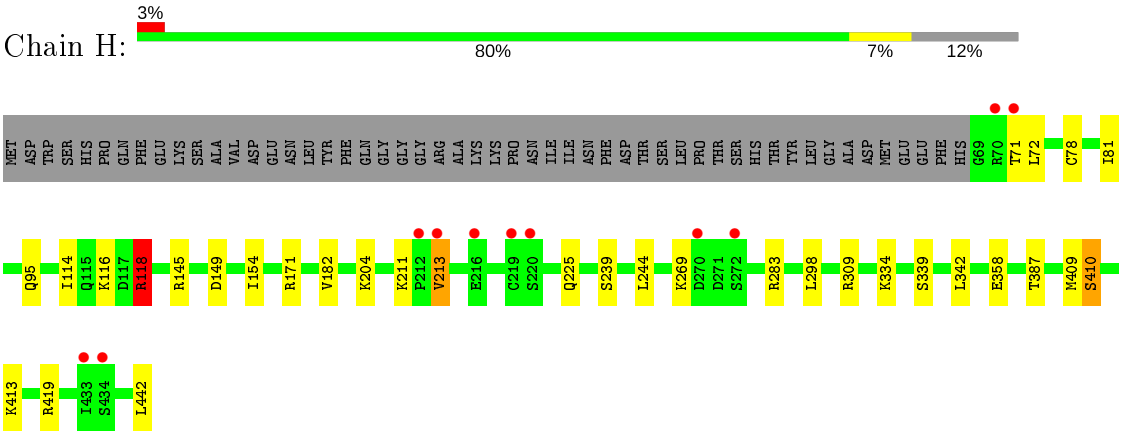
• Molecule 2: Protein cereblon



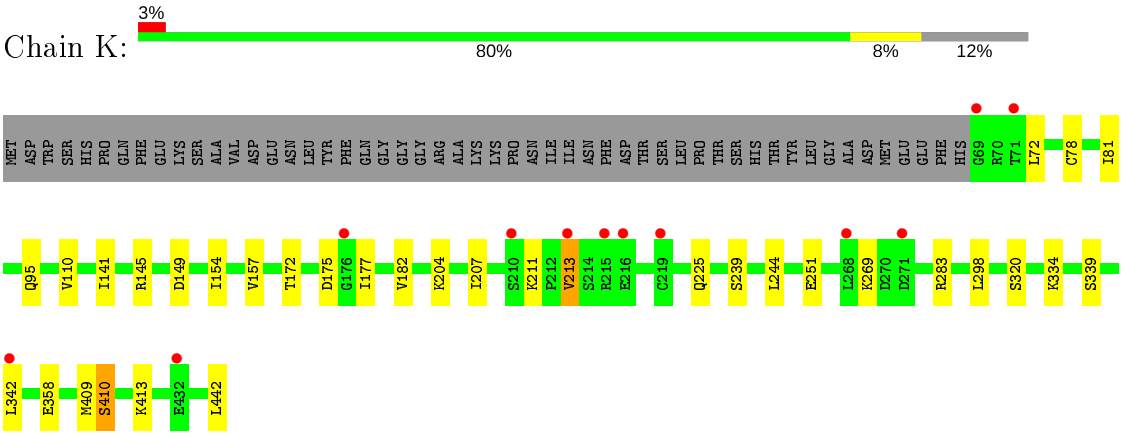




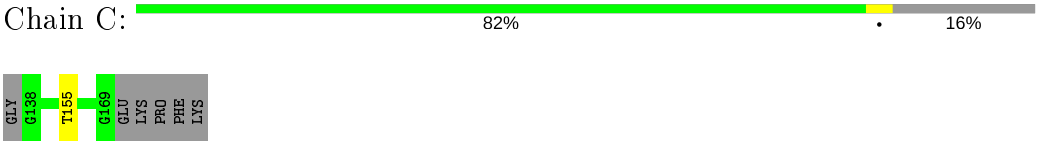
- Molecule 2: Protein cereblon



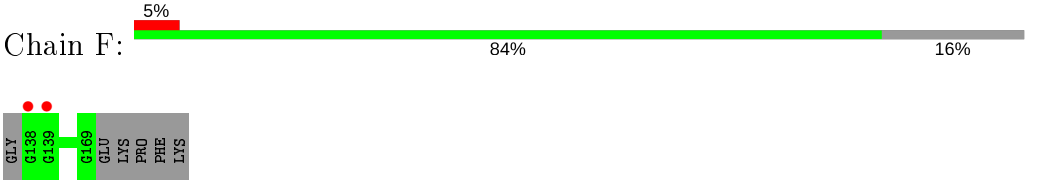
- Molecule 2: Protein cereblon



- Molecule 3: DNA-binding protein Ikaros

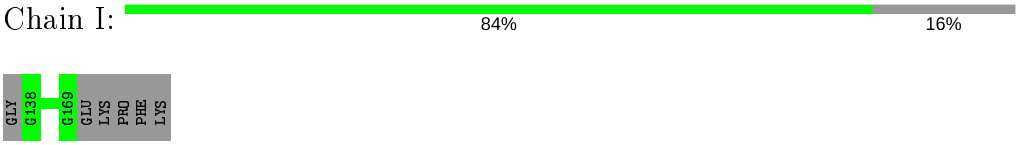


- Molecule 3: DNA-binding protein Ikaros



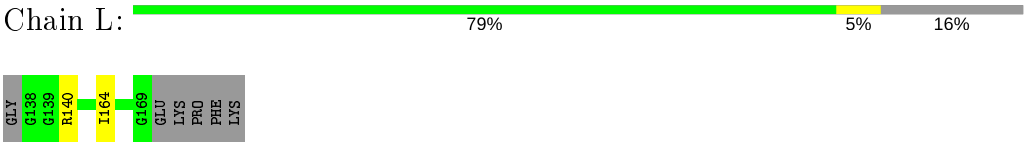
• Molecule 3: DNA-binding protein Ikaros

Chain I:



• Molecule 3: DNA-binding protein Ikaros

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	161.45Å 177.86Å 242.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.85 – 3.25 39.85 – 3.15	Depositor EDS
% Data completeness (in resolution range)	93.2 (39.85-3.25) 86.7 (39.85-3.15)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.212 , 0.234 0.225 , 0.250	Depositor DCC
R_{free} test set	5190 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	76.2	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 75.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	77598	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, Y70

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	0.36	0/6587	0.59	0/8909
1	D	0.35	0/6549	0.58	0/8856
1	G	0.36	0/6587	0.58	0/8909
1	J	0.36	0/6712	0.60	1/9075 (0.0%)
2	B	0.42	1/3063 (0.0%)	0.57	0/4157
2	E	0.39	0/3064	0.58	0/4160
2	H	0.39	0/3047	0.60	4/4137 (0.1%)
2	K	0.39	0/3064	0.58	0/4160
3	C	0.39	0/248	0.55	0/328
3	F	0.39	0/248	0.54	0/328
3	I	0.41	0/248	0.53	0/328
3	L	0.40	0/248	0.58	0/328
All	All	0.37	1/39665 (0.0%)	0.58	5/53675 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	225	GLN	C-N	8.09	1.52	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	-9	GLU	N-CA-CB	6.47	122.24	110.60
2	H	309	ARG	CD-NE-CZ	6.40	132.56	123.60
2	H	309	ARG	CG-CD-NE	-5.21	100.87	111.80
2	H	118	ARG	CG-CD-NE	5.18	122.69	111.80
2	H	118	ARG	CD-NE-CZ	5.17	130.83	123.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6470	6417	6421	7	0
1	D	6433	6381	6384	5	0
1	G	6470	6418	6421	6	0
1	J	6593	6526	6528	6	0
2	B	2988	2967	2960	9	0
2	E	2988	2967	2961	5	0
2	H	2978	2959	2959	2	0
2	K	2988	2967	2961	5	0
3	C	244	237	237	0	0
3	F	244	237	237	0	0
3	I	244	237	237	0	0
3	L	244	237	237	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	1	0	0	0	0
5	B	20	11	11	0	0
5	E	20	11	11	0	0
5	H	20	11	11	0	0
5	K	20	11	11	0	0
6	A	8	0	0	0	0
6	B	3	0	0	0	0
6	C	3	0	0	0	0
6	E	4	0	0	0	0
6	G	3	0	0	0	0
6	H	5	0	0	0	0
6	J	6	0	0	0	0
All	All	39004	38594	38587	33	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 0.

The worst 5 of 33 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)
2:B:207:ILE:C	2:B:208:PHE:N	2.27	0.88
1:A:1103:PRO:HG3	1:D:774:SER:HA	1.71	0.72
1:G:43:VAL:HG23	1:G:52:VAL:HG21	1.77	0.66
1:A:43:VAL:HG23	1:A:52:VAL:HG21	1.77	0.66
1:D:43:VAL:HG23	1:D:52:VAL:HG21	1.77	0.66

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	822/856 (96%)	762 (93%)	52 (6%)	8 (1%)	15	47
1	D	815/856 (95%)	757 (93%)	51 (6%)	7 (1%)	17	50
1	G	822/856 (96%)	769 (94%)	47 (6%)	6 (1%)	22	56
1	J	839/856 (98%)	775 (92%)	52 (6%)	12 (1%)	11	40
2	B	372/426 (87%)	354 (95%)	15 (4%)	3 (1%)	19	52
2	E	374/426 (88%)	354 (95%)	17 (4%)	3 (1%)	19	52
2	H	372/426 (87%)	355 (95%)	14 (4%)	3 (1%)	19	52
2	K	374/426 (88%)	356 (95%)	15 (4%)	3 (1%)	19	52
3	C	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	F	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	I	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
3	L	30/38 (79%)	27 (90%)	3 (10%)	0	100	100
All	All	4910/5280 (93%)	4593 (94%)	272 (6%)	45 (1%)	17	50

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	209	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	71	THR
2	H	116	LYS
1	J	291	MET
1	A	291	MET

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	713/744 (96%)	683 (96%)	30 (4%)	30 59
1	D	708/744 (95%)	682 (96%)	26 (4%)	34 62
1	G	713/744 (96%)	684 (96%)	29 (4%)	30 60
1	J	723/744 (97%)	688 (95%)	35 (5%)	25 56
2	B	332/385 (86%)	305 (92%)	27 (8%)	11 36
2	E	332/385 (86%)	306 (92%)	26 (8%)	12 38
2	H	330/385 (86%)	300 (91%)	30 (9%)	9 31
2	K	332/385 (86%)	305 (92%)	27 (8%)	11 36
3	C	25/30 (83%)	24 (96%)	1 (4%)	31 61
3	F	25/30 (83%)	25 (100%)	0	100 100
3	I	25/30 (83%)	25 (100%)	0	100 100
3	L	25/30 (83%)	23 (92%)	2 (8%)	12 37
All	All	4283/4636 (92%)	4050 (95%)	233 (5%)	22 53

5 of 233 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	358	GLU
1	G	786	VAL
2	K	213	VAL
2	E	410	SER
1	G	224	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	209	GLN
1	A	1056	ASN
1	G	4	ASN
1	G	1056	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
5	Y70	H	502	-	22,22,22	0.27	0	31,33,33	0.75	2 (6%)
5	Y70	E	502	-	22,22,22	0.26	0	31,33,33	0.73	2 (6%)
5	Y70	K	502	-	22,22,22	0.29	0	31,33,33	0.75	2 (6%)
5	Y70	B	502	-	22,22,22	0.29	0	31,33,33	0.74	2 (6%)

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
5	Y70	H	502	-	-	0/4/33/33	0/3/3/3
5	Y70	E	502	-	-	0/4/33/33	0/3/3/3
5	Y70	K	502	-	-	0/4/33/33	0/3/3/3
5	Y70	B	502	-	-	0/4/33/33	0/3/3/3

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})
5	K	502	Y70	C14-C12-N8	-2.80	107.07	113.85
5	E	502	Y70	C14-C12-N8	-2.79	107.10	113.85
5	H	502	Y70	C14-C12-N8	-2.73	107.22	113.85
5	B	502	Y70	C14-C12-N8	-2.71	107.28	113.85
5	K	502	Y70	C15-C12-N8	2.25	111.13	109.08

There are no chirality outliers.

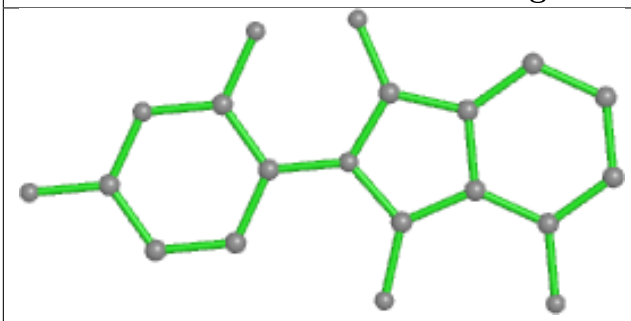
There are no torsion outliers.

There are no ring outliers.

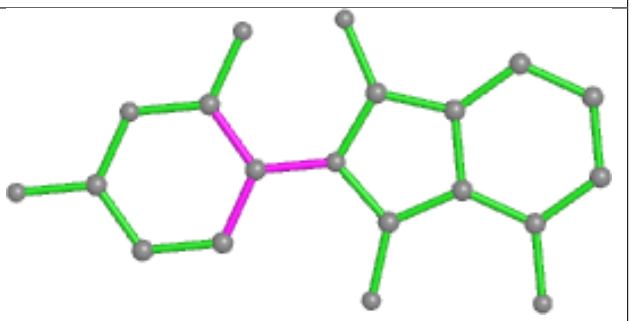
No monomer is involved in short contacts.

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.

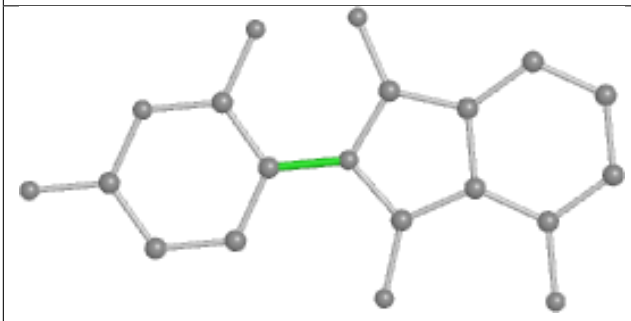
Ligand Y70 H 502



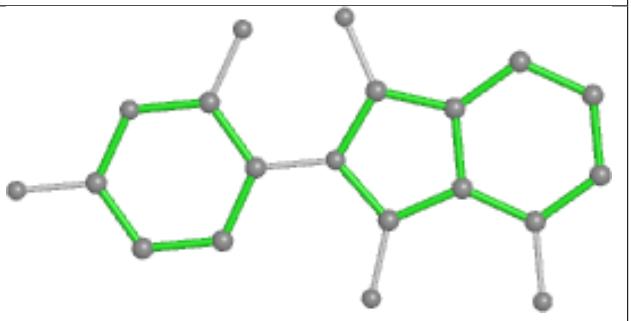
Bond lengths



Bond angles

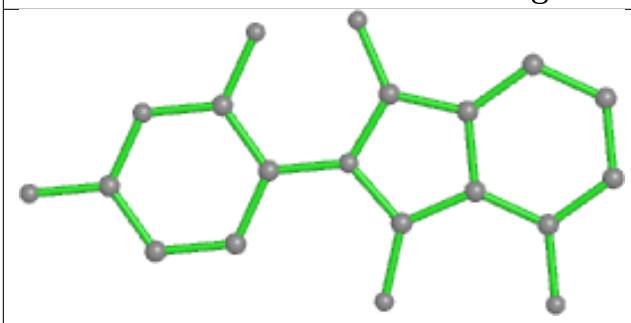


Torsions

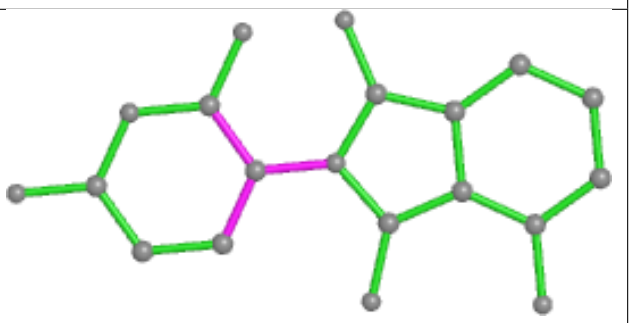


Rings

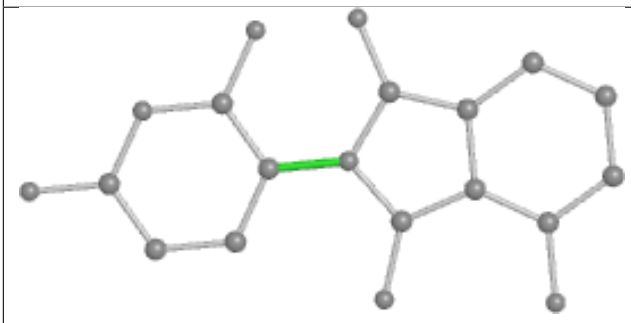
Ligand Y70 E 502



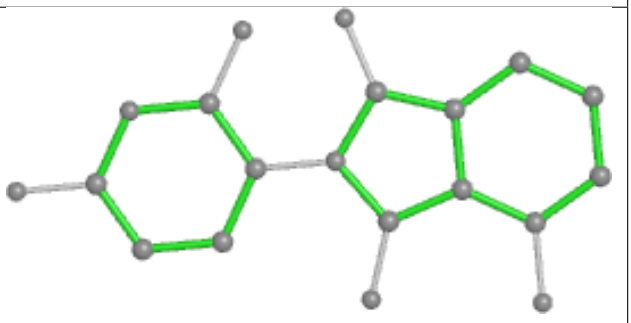
Bond lengths



Bond angles

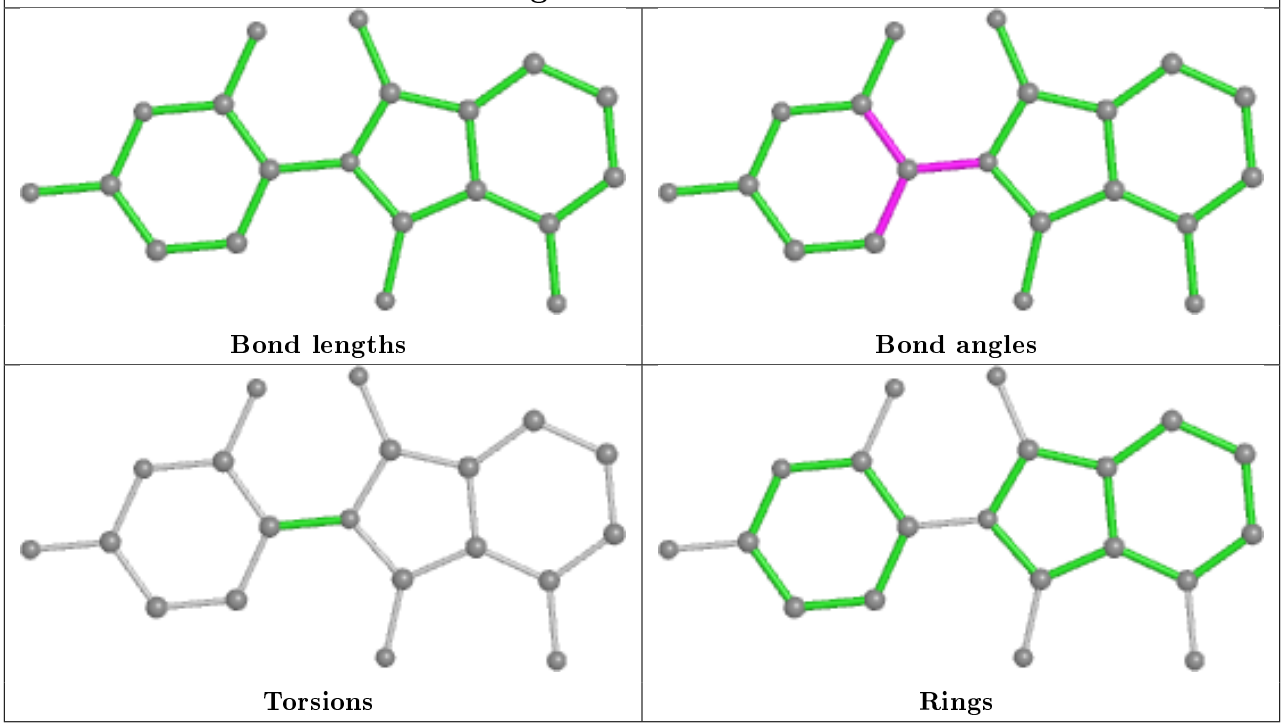


Torsions

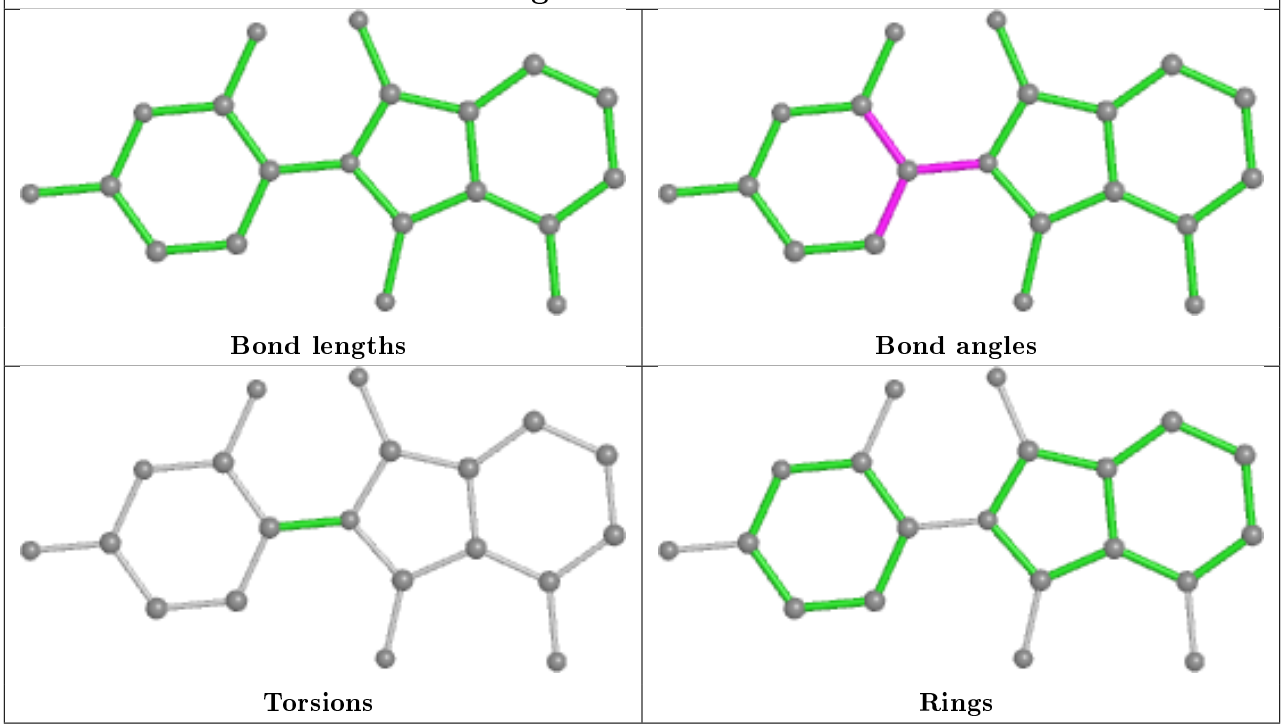


Rings

Ligand Y70 K 502



Ligand Y70 B 502



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
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	207:ILE	C	208:PHE	N	2.27

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	826/856 (96%)	-0.19	10 (1%) 79 77	26, 78, 158, 299	0
1	D	821/856 (95%)	0.23	48 (5%) 23 22	56, 124, 284, 299	0
1	G	826/856 (96%)	0.04	29 (3%) 44 40	45, 101, 242, 299	0
1	J	843/856 (98%)	-0.00	30 (3%) 42 39	37, 87, 162, 299	0
2	B	374/426 (87%)	0.01	17 (4%) 33 31	34, 69, 141, 198	0
2	E	374/426 (87%)	-0.01	16 (4%) 35 33	40, 73, 129, 174	0
2	H	374/426 (87%)	-0.05	11 (2%) 51 50	32, 76, 144, 181	0
2	K	374/426 (87%)	0.04	12 (3%) 47 45	40, 78, 143, 201	0
3	C	32/38 (84%)	-0.42	0 100 100	38, 53, 91, 96	0
3	F	32/38 (84%)	-0.03	2 (6%) 20 19	42, 64, 120, 128	0
3	I	32/38 (84%)	-0.50	0 100 100	38, 52, 92, 124	0
3	L	32/38 (84%)	-0.38	0 100 100	43, 57, 105, 108	0
All	All	4940/5280 (93%)	0.00	175 (3%) 44 40	26, 88, 189, 299	0

The worst 5 of 175 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	772	SER	10.2
1	G	1120	MET	7.4
2	B	71	THR	6.4
2	B	69	GLY	6.3
1	J	1118	SER	6.2

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

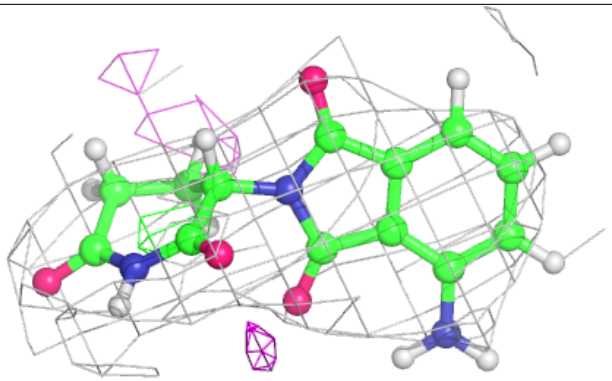
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

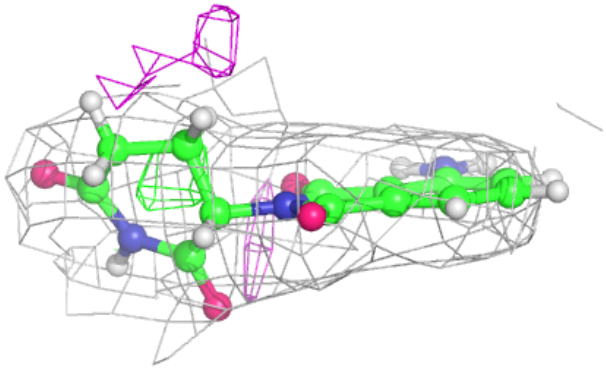
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	Y70	B	502	20/20	0.96	0.24	47,58,72,73	11
5	Y70	H	502	20/20	0.97	0.23	41,48,57,58	11
5	Y70	K	502	20/20	0.97	0.27	60,69,84,86	11
5	Y70	E	502	20/20	0.98	0.33	44,51,55,58	11
4	ZN	I	201	1/1	0.99	0.10	43,43,43,43	0
4	ZN	C	201	1/1	0.99	0.10	49,49,49,49	0
4	ZN	K	501	1/1	0.99	0.13	45,45,45,45	0
4	ZN	B	501	1/1	0.99	0.13	35,35,35,35	0
4	ZN	L	201	1/1	0.99	0.12	53,53,53,53	0
4	ZN	E	501	1/1	1.00	0.15	48,48,48,48	0
4	ZN	F	201	1/1	1.00	0.10	51,51,51,51	0
4	ZN	H	501	1/1	1.00	0.12	38,38,38,38	0

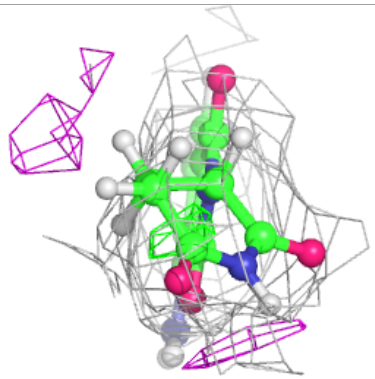
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y70 B 502:

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

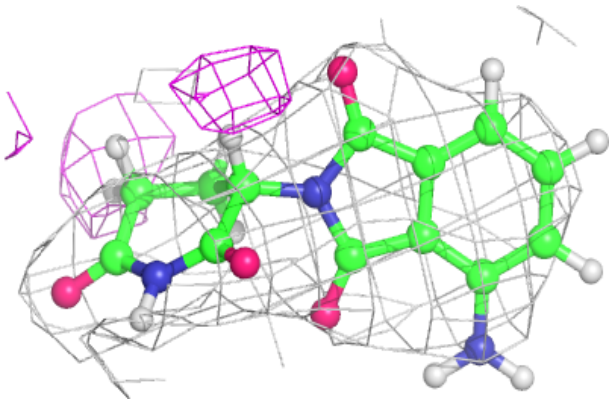


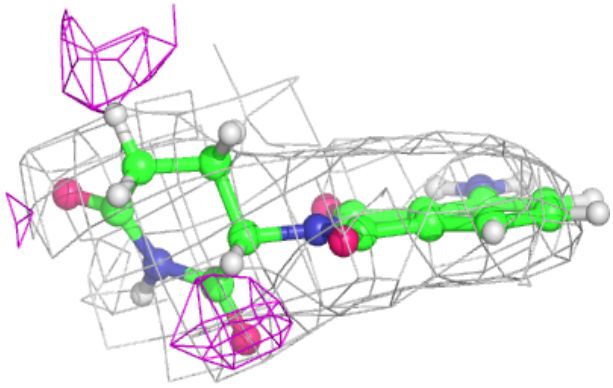


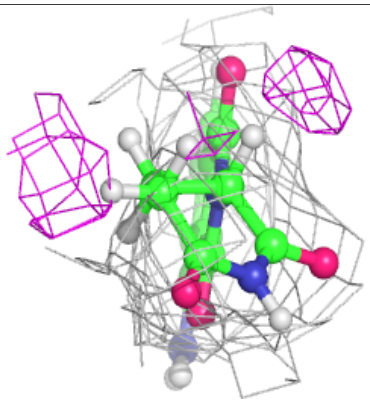


Electron density around Y70 H 502:

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

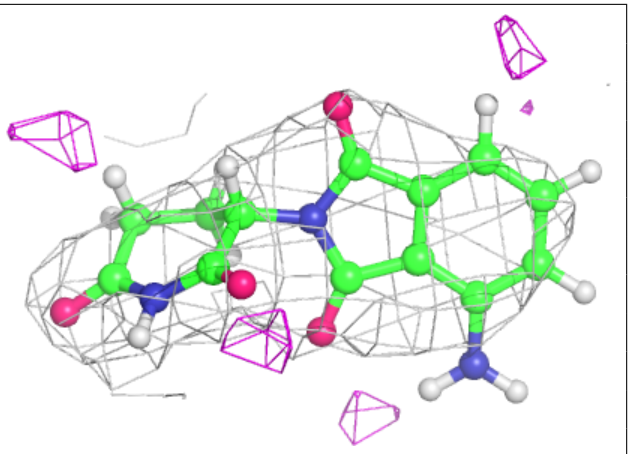


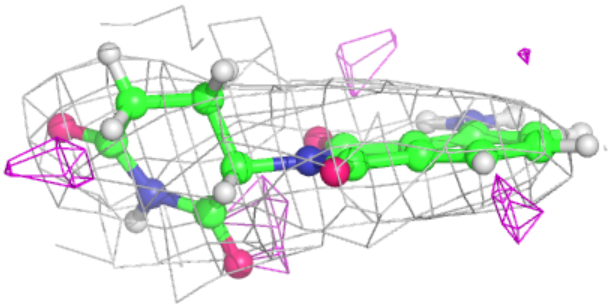


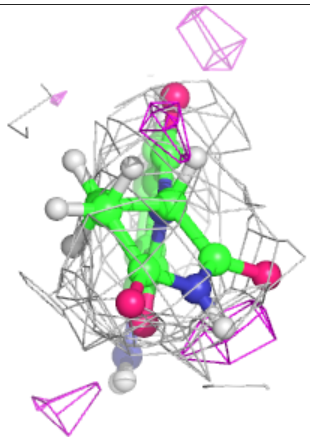


Electron density around Y70 K 502:

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

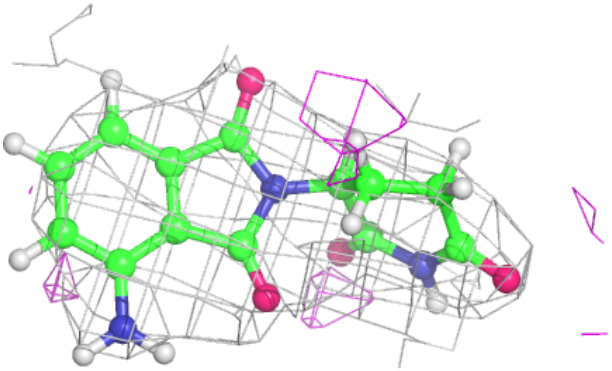


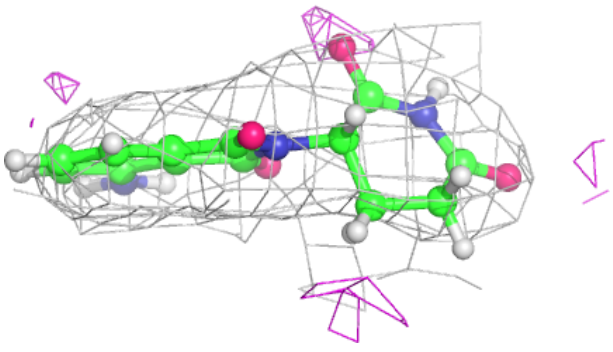


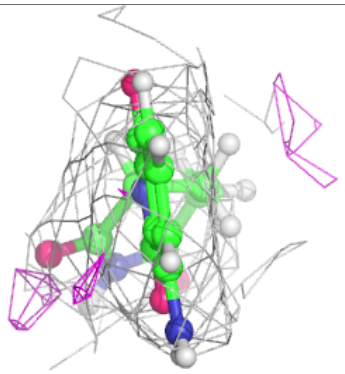


Electron density around Y70 E 502:

$2mF_o$-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.