Full wwPDB X-ray Structure Validation Report ⓘ

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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

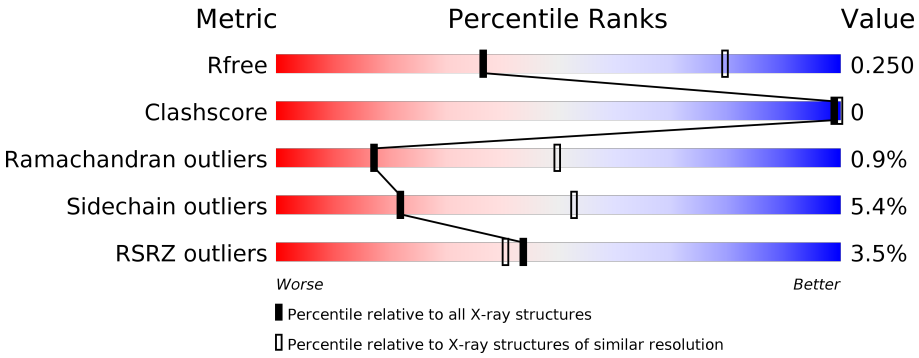
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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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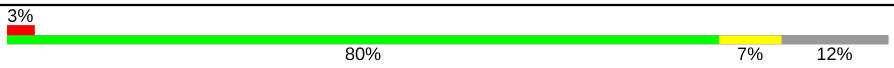
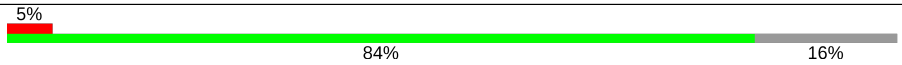
Mol	Chain	Length	Quality of chain
2	H	426	
2	K	426	
3	C	38	
3	F	38	
3	I	38	
3	L	38	

2 Entry composition

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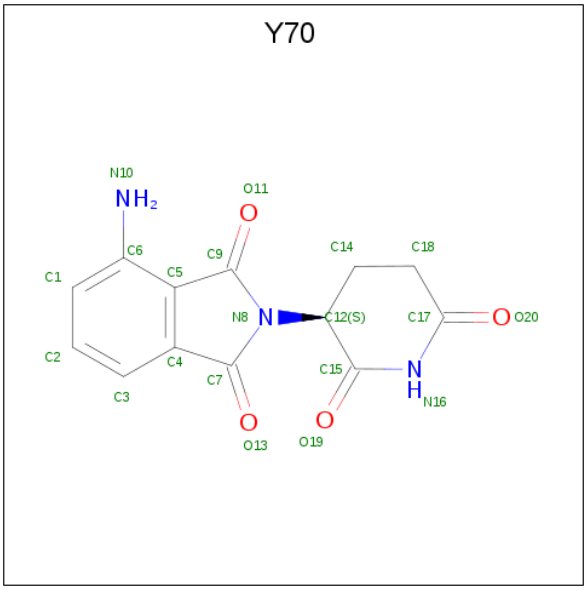
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Zn 1 1	0	0
4	L	1	Total Zn 1 1	0	0
4	F	1	Total Zn 1 1	0	0

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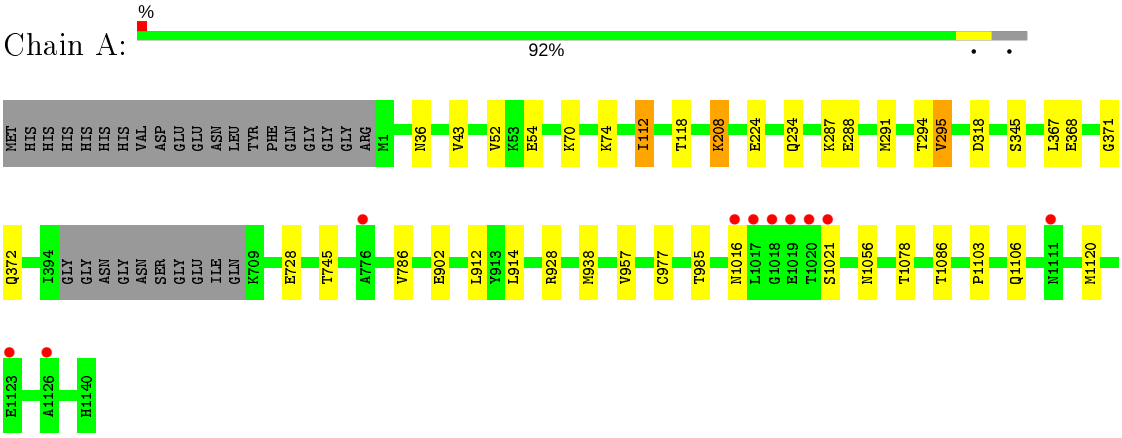
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	3	Total O 3 3	0	0
6	E	4	Total O 4 4	0	0
6	G	3	Total O 3 3	0	0
6	H	5	Total O 5 5	0	0
6	J	6	Total O 6 6	0	0

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.

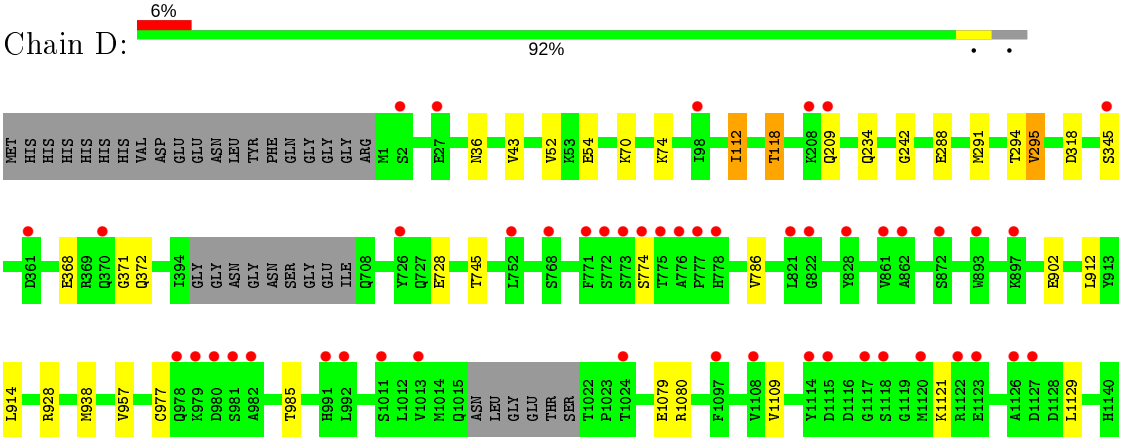
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

Chain A:



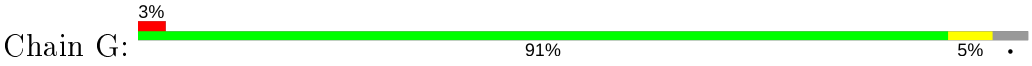
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

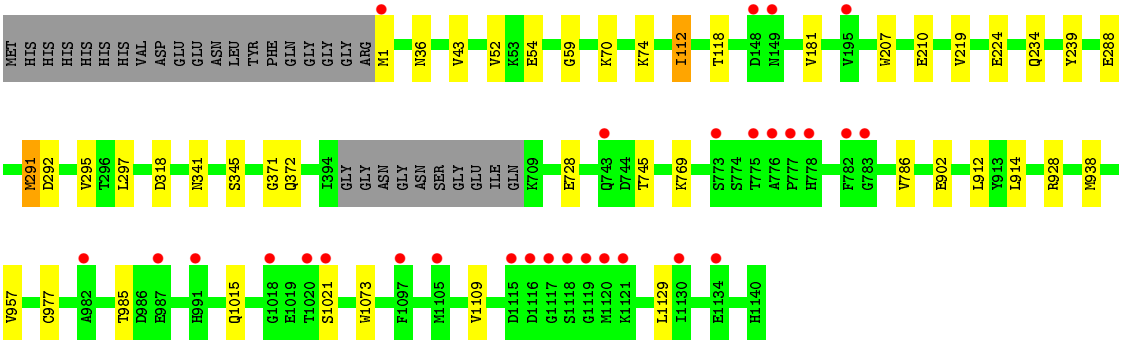
Chain D:



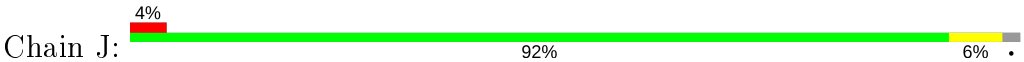
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1

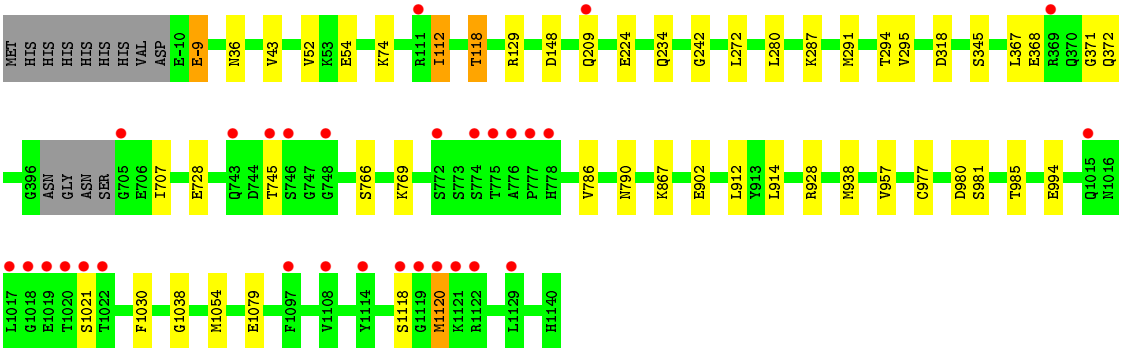
Chain G:



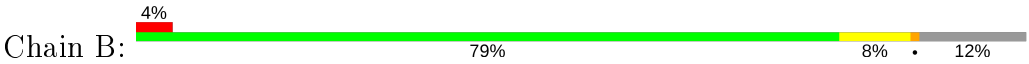


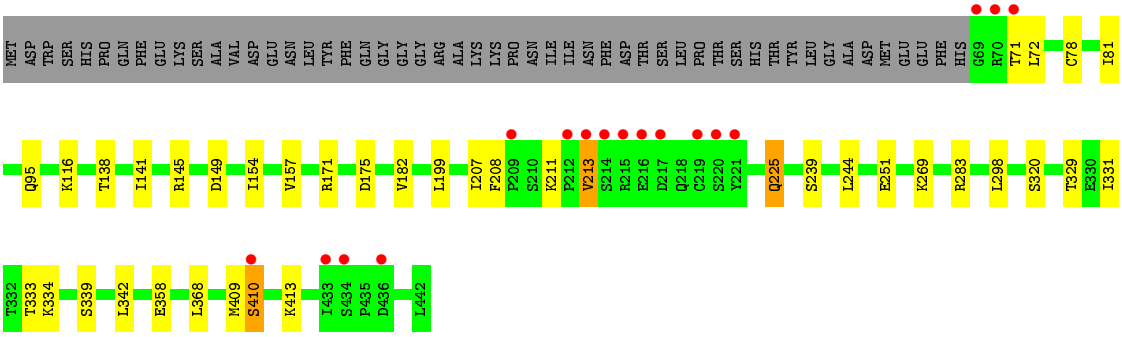
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1



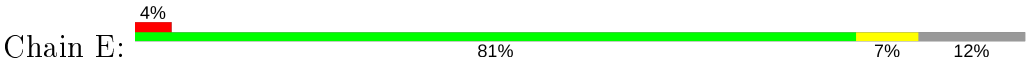


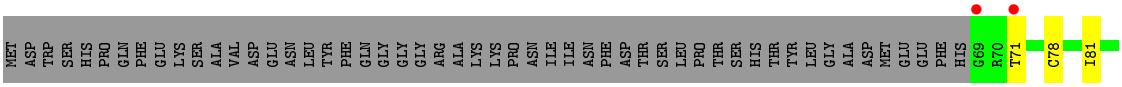
• Molecule 2: Protein cereblon

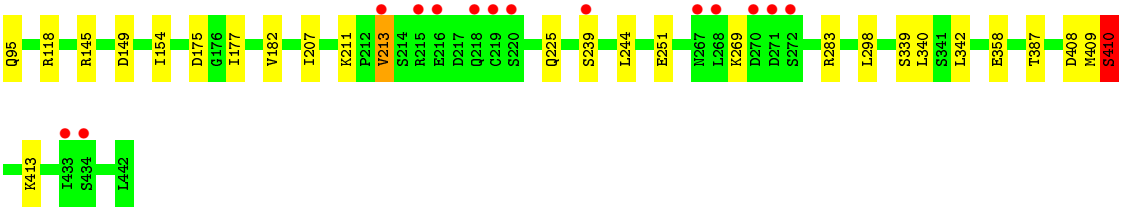




• Molecule 2: Protein cereblon

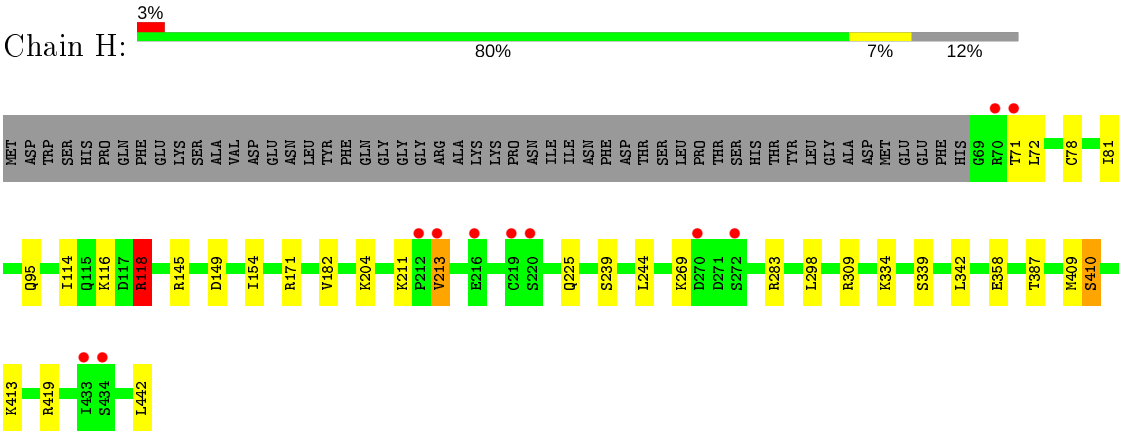






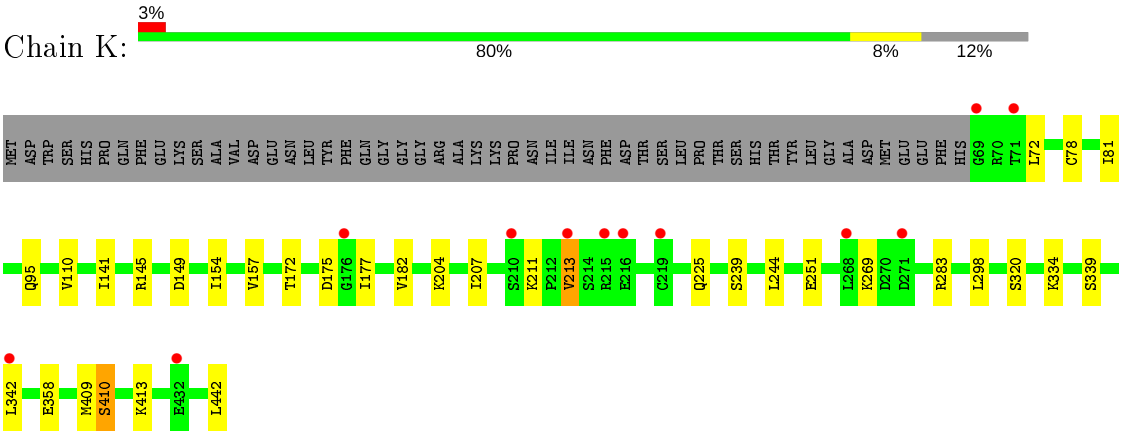
- Molecule 2: Protein cereblon

Chain H:



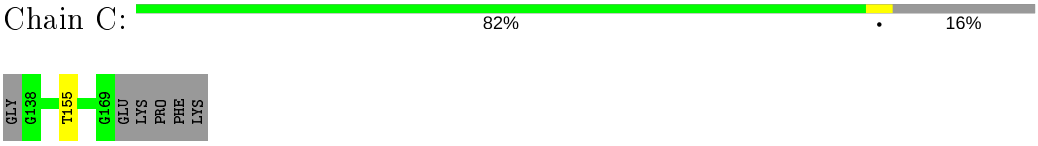
- Molecule 2: Protein cereblon

Chain K:



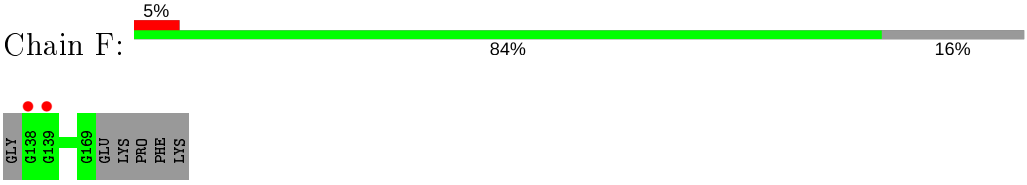
- Molecule 3: DNA-binding protein Ikaros

Chain C:



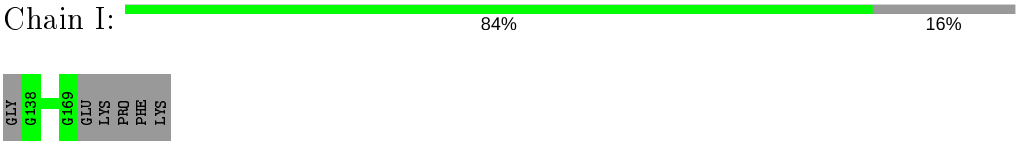
- Molecule 3: DNA-binding protein Ikaros

Chain F:



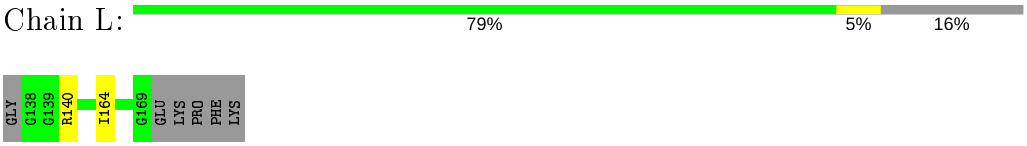
• Molecule 3: DNA-binding protein Ikaros

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.

All (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
1:J:43:VAL:HG23	1:J:52:VAL:HG21	1.77	0.66
1:J:272:LEU:HD22	1:J:280:LEU:HD11	1.78	0.64
1:A:1056:ASN:ND2	2:E:410:SER:HB3	2.18	0.57
1:G:912:LEU:HD21	2:H:244:LEU:HD11	1.87	0.57
1:A:912:LEU:HD21	2:B:244:LEU:HD11	1.85	0.57
1:D:912:LEU:HD21	2:E:244:LEU:HD11	1.93	0.51
1:J:118:THR:CG2	2:K:204:LYS:HA	2.40	0.51
2:H:118:ARG:CG	2:H:118:ARG:HH11	2.28	0.47
1:J:912:LEU:HD21	2:K:244:LEU:HD11	1.95	0.47
1:A:1086:THR:HG22	2:E:408:ASP:OD2	2.15	0.47
1:J:118:THR:HG23	2:K:207:ILE:CD1	2.47	0.45
2:B:207:ILE:C	2:B:208:PHE:CA	2.85	0.45
2:B:81:ILE:HD11	2:B:138:THR:HG22	1.98	0.44
1:D:1109:VAL:HG12	1:D:1129:LEU:HD22	1.99	0.44
1:G:59:GLY:HA2	1:G:1073:TRP:CZ3	2.53	0.44
1:A:1056:ASN:HD21	2:E:410:SER:HB3	1.83	0.43
1:D:118:THR:HG23	2:E:207:ILE:CD1	2.48	0.43
1:G:239:TYR:CD2	1:G:297:LEU:HD23	2.54	0.43
2:K:141:ILE:HG23	2:K:157:VAL:HG13	2.00	0.42
2:B:331:ILE:HD12	2:B:368:LEU:HD21	2.02	0.41
1:A:912:LEU:HD21	2:B:244:LEU:CD1	2.49	0.41
2:B:320:SER:OG	2:B:333:THR:HG22	2.21	0.41
1:G:181:VAL:HG23	1:G:219:VAL:CG2	2.51	0.41
2:B:81:ILE:CD1	2:B:138:THR:HG22	2.51	0.41
2:B:141:ILE:HG23	2:B:157:VAL:HG13	2.03	0.41
2:K:110:VAL:HG11	2:K:157:VAL:HG21	2.02	0.40
1:J:1030:PHE:CZ	1:J:1038:GLY:HA3	2.56	0.40
1:G:1109:VAL:HG12	1:G:1129:LEU:HD22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	209	GLN
2	E	71	THR
2	H	116	LYS
1	J	291	MET
1	A	291	MET
1	A	1021	SER
1	D	291	MET
1	G	291	MET
1	G	295	VAL
1	G	1021	SER
1	J	112	ILE
1	J	209	GLN
1	J	295	VAL
1	J	371	GLY
1	J	1021	SER
1	A	112	ILE
1	A	208	LYS
1	A	295	VAL

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Mol	Chain	Res	Type
1	A	371	GLY
1	D	112	ILE
1	D	295	VAL
1	G	112	ILE
1	G	371	GLY
1	J	-9	GLU
1	A	36	ASN
1	A	367	LEU
1	D	36	ASN
1	D	371	GLY
1	G	36	ASN
1	J	36	ASN
1	J	1118	SER
1	J	1120	MET
2	B	116	LYS
2	B	410	SER
2	E	410	SER
2	H	410	SER
1	J	367	LEU
2	K	410	SER
2	K	175	ASP
1	J	242	GLY
1	D	242	GLY
2	B	213	VAL
2	E	213	VAL
2	H	213	VAL
2	K	213	VAL

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

All (233) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	70	LYS
1	A	74	LYS
1	A	112	ILE
1	A	118	THR
1	A	208	LYS
1	A	224	GLU
1	A	234	GLN
1	A	287	LYS
1	A	288	GLU
1	A	294	THR
1	A	295	VAL
1	A	318	ASP
1	A	345	SER
1	A	368	GLU
1	A	372	GLN
1	A	728	GLU
1	A	745	THR
1	A	786	VAL
1	A	902	GLU
1	A	914	LEU
1	A	928	ARG
1	A	938	MET
1	A	957	VAL
1	A	977	CYS

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Mol	Chain	Res	Type
1	A	985	THR
1	A	1016	ASN
1	A	1078	THR
1	A	1106	GLN
1	A	1120	MET
2	B	71	THR
2	B	72	LEU
2	B	78	CYS
2	B	95	GLN
2	B	145	ARG
2	B	149	ASP
2	B	154	ILE
2	B	171	ARG
2	B	175	ASP
2	B	182	VAL
2	B	199	LEU
2	B	211	LYS
2	B	213	VAL
2	B	225	GLN
2	B	239	SER
2	B	251	GLU
2	B	269	LYS
2	B	283	ARG
2	B	298	LEU
2	B	329	THR
2	B	334	LYS
2	B	339	SER
2	B	342	LEU
2	B	358	GLU
2	B	409	MET
2	B	410	SER
2	B	413	LYS
3	C	155	THR
1	D	54	GLU
1	D	70	LYS
1	D	74	LYS
1	D	112	ILE
1	D	118	THR
1	D	234	GLN
1	D	288	GLU
1	D	294	THR
1	D	295	VAL

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Mol	Chain	Res	Type
1	D	318	ASP
1	D	345	SER
1	D	368	GLU
1	D	372	GLN
1	D	728	GLU
1	D	745	THR
1	D	786	VAL
1	D	902	GLU
1	D	914	LEU
1	D	928	ARG
1	D	938	MET
1	D	957	VAL
1	D	977	CYS
1	D	985	THR
1	D	1079	GLU
1	D	1080	ARG
1	D	1121	LYS
2	E	78	CYS
2	E	81	ILE
2	E	95	GLN
2	E	118	ARG
2	E	145	ARG
2	E	149	ASP
2	E	154	ILE
2	E	175	ASP
2	E	177	ILE
2	E	182	VAL
2	E	211	LYS
2	E	213	VAL
2	E	225	GLN
2	E	239	SER
2	E	251	GLU
2	E	269	LYS
2	E	283	ARG
2	E	298	LEU
2	E	339	SER
2	E	340	LEU
2	E	342	LEU
2	E	358	GLU
2	E	387	THR
2	E	409	MET
2	E	410	SER

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Mol	Chain	Res	Type
2	E	413	LYS
1	G	1	MET
1	G	54	GLU
1	G	70	LYS
1	G	74	LYS
1	G	112	ILE
1	G	118	THR
1	G	207	TRP
1	G	210	GLU
1	G	224	GLU
1	G	234	GLN
1	G	288	GLU
1	G	291	MET
1	G	292	ASP
1	G	318	ASP
1	G	341	ASN
1	G	345	SER
1	G	372	GLN
1	G	728	GLU
1	G	745	THR
1	G	769	LYS
1	G	786	VAL
1	G	902	GLU
1	G	914	LEU
1	G	928	ARG
1	G	938	MET
1	G	957	VAL
1	G	977	CYS
1	G	985	THR
1	G	1015	GLN
2	H	71	THR
2	H	72	LEU
2	H	78	CYS
2	H	81	ILE
2	H	95	GLN
2	H	114	ILE
2	H	118	ARG
2	H	145	ARG
2	H	149	ASP
2	H	154	ILE
2	H	171	ARG
2	H	182	VAL

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Mol	Chain	Res	Type
2	H	204	LYS
2	H	211	LYS
2	H	213	VAL
2	H	225	GLN
2	H	239	SER
2	H	269	LYS
2	H	283	ARG
2	H	298	LEU
2	H	334	LYS
2	H	339	SER
2	H	342	LEU
2	H	358	GLU
2	H	387	THR
2	H	409	MET
2	H	410	SER
2	H	413	LYS
2	H	419	ARG
2	H	442	LEU
1	J	54	GLU
1	J	74	LYS
1	J	112	ILE
1	J	118	THR
1	J	129	ARG
1	J	148	ASP
1	J	224	GLU
1	J	234	GLN
1	J	287	LYS
1	J	294	THR
1	J	318	ASP
1	J	345	SER
1	J	368	GLU
1	J	372	GLN
1	J	707	ILE
1	J	728	GLU
1	J	745	THR
1	J	766	SER
1	J	769	LYS
1	J	786	VAL
1	J	790	ASN
1	J	867	LYS
1	J	902	GLU
1	J	914	LEU

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Mol	Chain	Res	Type
1	J	928	ARG
1	J	938	MET
1	J	957	VAL
1	J	977	CYS
1	J	980	ASP
1	J	981	SER
1	J	985	THR
1	J	994	GLU
1	J	1054	MET
1	J	1079	GLU
1	J	1120	MET
2	K	72	LEU
2	K	78	CYS
2	K	81	ILE
2	K	95	GLN
2	K	145	ARG
2	K	149	ASP
2	K	154	ILE
2	K	172	THR
2	K	177	ILE
2	K	182	VAL
2	K	211	LYS
2	K	213	VAL
2	K	225	GLN
2	K	239	SER
2	K	251	GLU
2	K	269	LYS
2	K	283	ARG
2	K	298	LEU
2	K	320	SER
2	K	334	LYS
2	K	339	SER
2	K	342	LEU
2	K	358	GLU
2	K	409	MET
2	K	410	SER
2	K	413	LYS
2	K	442	LEU
3	L	140	ARG
3	L	164	ILE

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 (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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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.

All (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
5	H	502	Y70	C15-C12-N8	2.25	111.13	109.08
5	B	502	Y70	C15-C12-N8	2.24	111.12	109.08
5	E	502	Y70	C15-C12-N8	2.02	110.92	109.08

There are no chirality outliers.

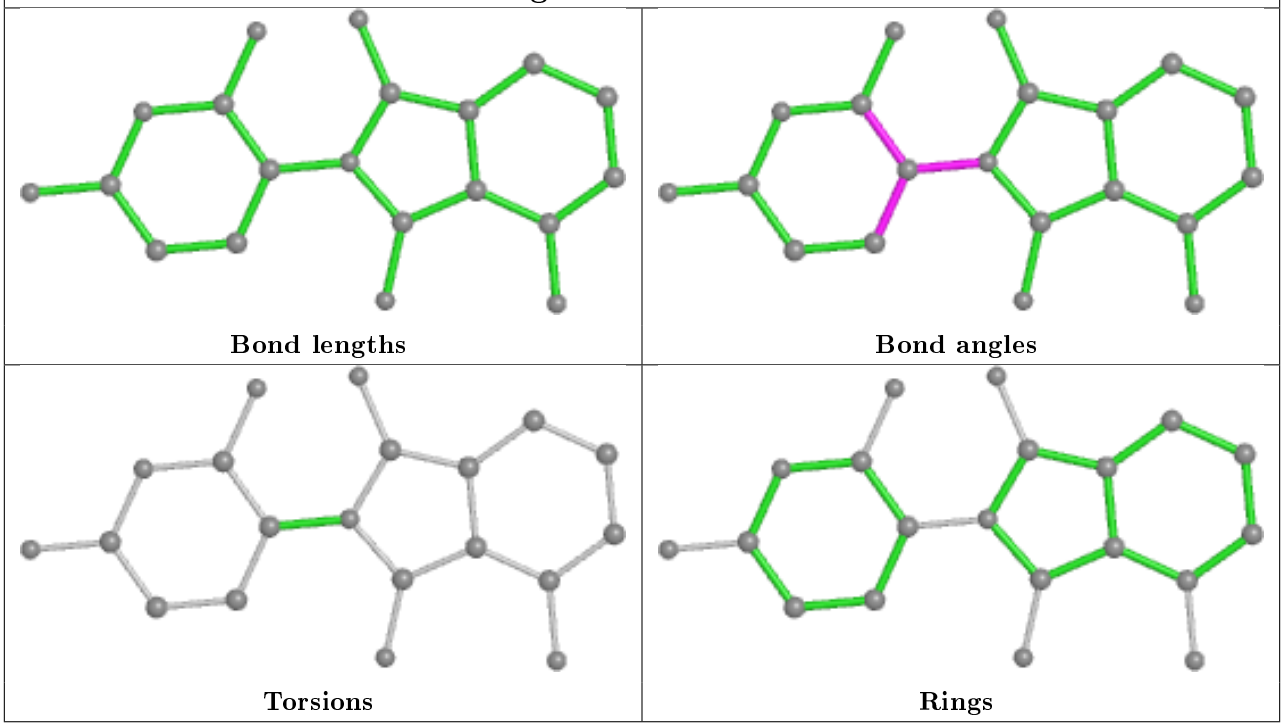
There are no torsion outliers.

There are no ring outliers.

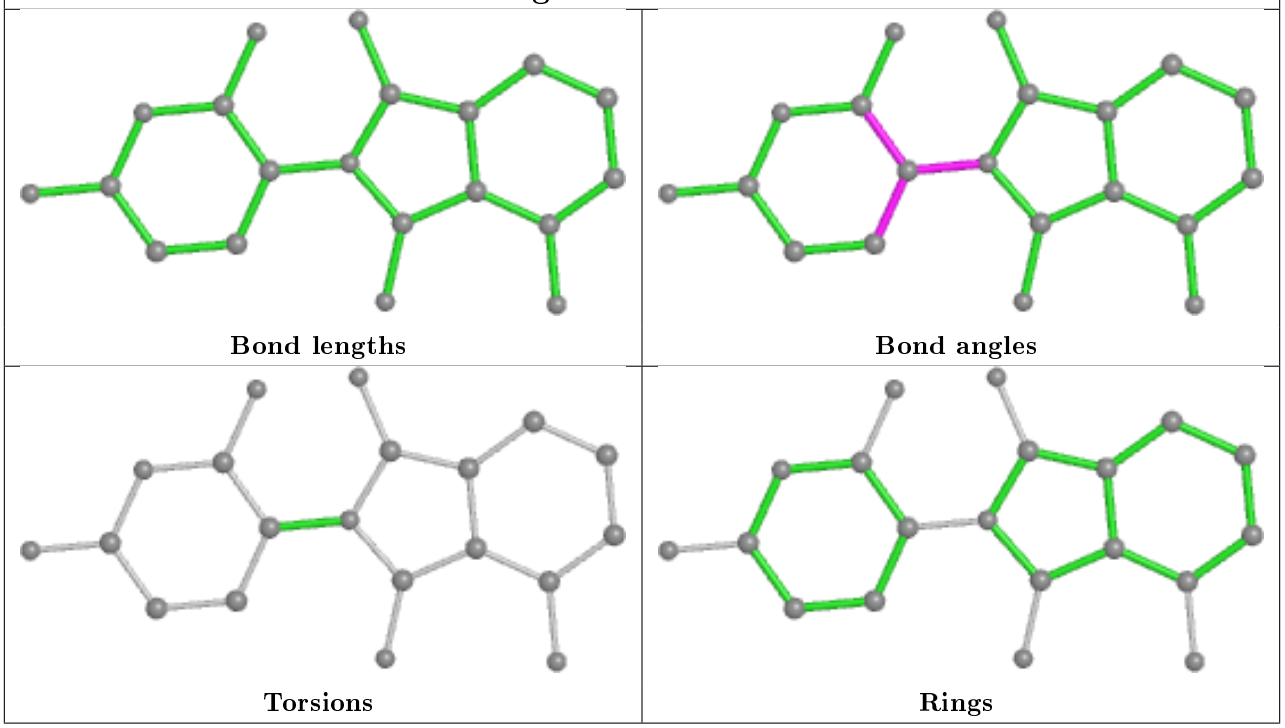
No monomer is involved in short contacts.

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.

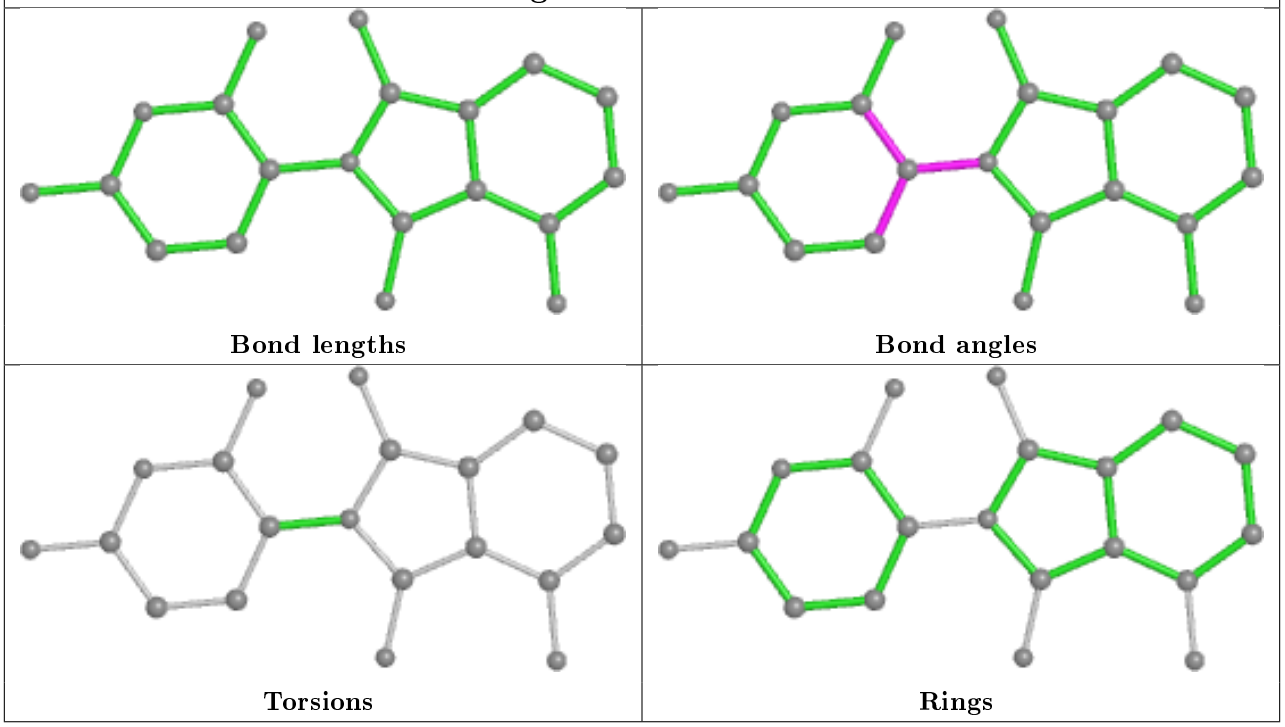
Ligand Y70 H 502



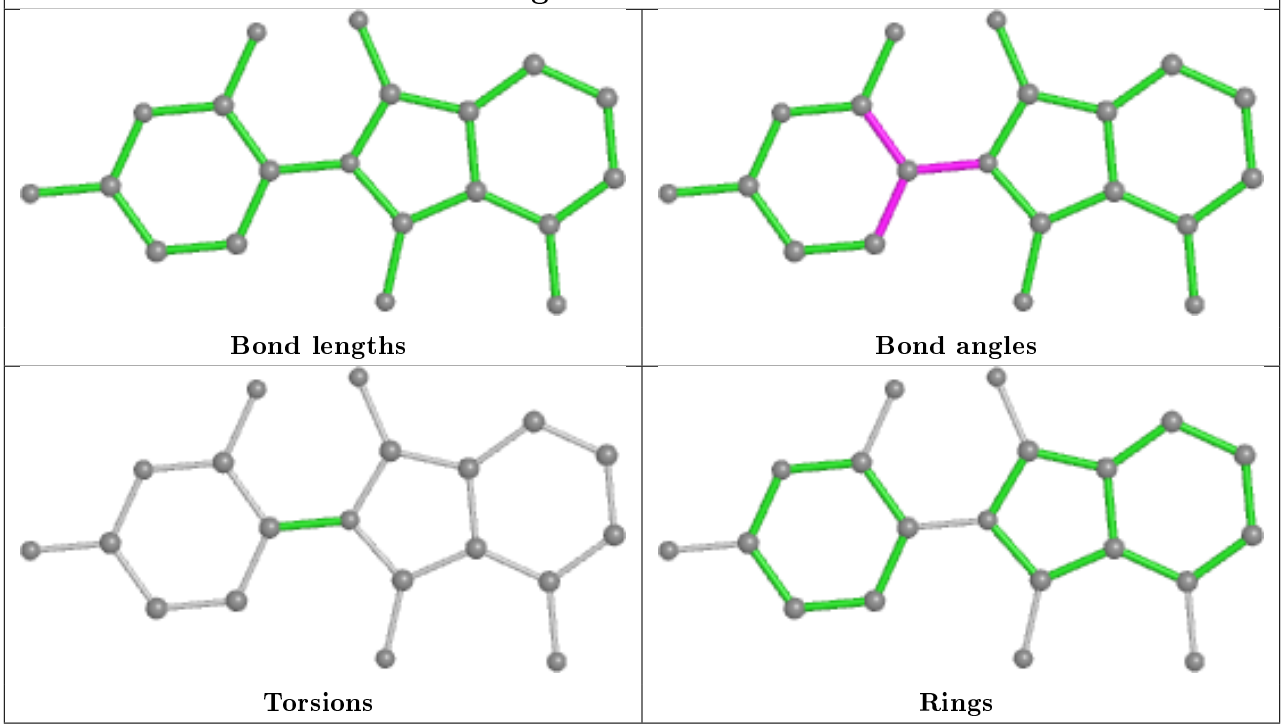
Ligand Y70 E 502



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

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

All (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
2	E	219	CYS	5.8
1	J	1120	MET	5.4
1	D	1118	SER	5.3
1	J	1019	GLU	5.2
1	D	1123	GLU	4.9
3	F	138	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	773	SER	4.8
2	K	219	CYS	4.8
1	D	774	SER	4.7
1	D	775	THR	4.7
1	J	1022	THR	4.5
1	J	1114	TYR	4.4
2	B	219	CYS	4.4
1	J	1018	GLY	4.4
1	G	777	PRO	4.2
1	J	777	PRO	4.1
1	J	705	GLY	3.9
2	B	70	ARG	3.9
2	K	69	GLY	3.9
2	E	69	GLY	3.9
2	E	220	SER	3.9
1	A	1111	ASN	3.8
2	H	434	SER	3.8
2	K	71	THR	3.8
2	E	433	ILE	3.8
2	B	433	ILE	3.8
1	G	1115	ASP	3.7
2	H	219	CYS	3.7
1	G	1119	GLY	3.7
2	B	216	GLU	3.7
1	J	776	ALA	3.7
1	A	1020	THR	3.6
1	G	1	MET	3.6
2	H	216	GLU	3.6
1	G	776	ALA	3.6
2	H	433	ILE	3.6
1	J	1119	GLY	3.5
1	J	745	THR	3.5
1	D	1024	THR	3.4
1	D	1122	ARG	3.4
2	B	213	VAL	3.4
1	G	1020	THR	3.4
2	E	239	SER	3.4
2	B	220	SER	3.4
2	H	213	VAL	3.4
1	J	209	GLN	3.3
1	D	821	LEU	3.3
1	J	746	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	778	HIS	3.3
1	G	982	ALA	3.3
1	D	1126	ALA	3.2
1	J	775	THR	3.1
1	J	1021	SER	3.0
2	K	432	GLU	3.0
1	D	209	GLN	3.0
2	E	270	ASP	3.0
1	D	1114	TYR	3.0
1	D	771	PHE	3.0
1	G	775	THR	3.0
1	D	1108	VAL	3.0
2	E	271	ASP	3.0
1	G	1018	GLY	3.0
2	E	218	GLN	3.0
1	D	862	ALA	3.0
1	G	1130	ILE	2.9
1	D	776	ALA	2.9
1	J	1121	LYS	2.9
1	J	1129	LEU	2.9
1	G	778	HIS	2.9
1	D	1097	PHE	2.9
2	B	215	ARG	2.9
1	A	1019	GLU	2.8
1	D	897	LYS	2.8
1	J	1017	LEU	2.8
1	D	981	SER	2.8
2	B	434	SER	2.8
1	A	1016	ASN	2.7
3	F	139	GLY	2.7
1	D	893	TRP	2.7
2	H	212	PRO	2.7
1	A	1018	GLY	2.7
2	E	213	VAL	2.7
1	J	369	ARG	2.7
1	D	1127	ASP	2.7
1	D	979	LYS	2.7
2	K	342	LEU	2.7
1	D	978	GLN	2.7
1	J	743	GLN	2.6
1	G	1121	LYS	2.6
2	H	71	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	774	SER	2.6
2	K	176	GLY	2.5
1	J	1122	ARG	2.5
1	G	991	HIS	2.5
1	J	1020	THR	2.5
2	E	267	ASN	2.5
2	B	436	ASP	2.5
2	H	270	ASP	2.4
1	G	773	SER	2.4
1	D	768	SER	2.4
2	B	221	TYR	2.4
2	E	215	ARG	2.4
2	B	209	PRO	2.4
1	D	361	ASP	2.4
2	E	272	SER	2.4
1	D	27	GLU	2.4
2	H	70	ARG	2.4
1	J	1015	GLN	2.4
1	D	2	SER	2.4
2	E	71	THR	2.4
1	D	1115	ASP	2.3
1	D	828	TYR	2.3
1	A	1123	GLU	2.3
1	A	1017	LEU	2.3
1	D	992	LEU	2.3
2	K	215	ARG	2.3
1	J	1108	VAL	2.3
2	E	268	LEU	2.3
1	G	195	VAL	2.3
1	G	1021	SER	2.3
1	J	1097	PHE	2.3
2	K	213	VAL	2.3
1	G	1097	PHE	2.3
1	J	748	GLY	2.3
1	D	778	HIS	2.3
1	D	872	SER	2.3
1	G	782	PHE	2.3
1	D	991	HIS	2.3
1	G	1116	ASP	2.3
1	D	822	GLY	2.2
2	K	216	GLU	2.2
1	A	776	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	1117	GLY	2.2
1	A	1021	SER	2.2
1	D	370	GLN	2.2
1	D	982	ALA	2.2
2	B	212	PRO	2.2
1	G	1117	GLY	2.2
1	G	743	GLN	2.2
1	J	772	SER	2.2
1	D	980	ASP	2.2
2	E	216	GLU	2.2
1	G	149	ASN	2.2
1	G	1118	SER	2.1
1	D	1120	MET	2.1
1	G	1105	MET	2.1
2	B	214	SER	2.1
2	B	217	ASP	2.1
1	D	752	LEU	2.1
1	A	1126	ALA	2.1
1	G	783	GLY	2.1
1	D	345	SER	2.1
2	E	434	SER	2.1
1	D	208	LYS	2.1
1	J	111	ARG	2.1
1	D	861	VAL	2.1
2	B	410	SER	2.1
2	H	220	SER	2.1
1	D	98	ILE	2.1
2	K	271	ASP	2.1
1	G	1134	GLU	2.0
1	D	1013	VAL	2.0
2	K	268	LEU	2.0
1	G	148	ASP	2.0
1	D	726	TYR	2.0
1	D	1011	SER	2.0
1	G	987	GLU	2.0
2	K	210	SER	2.0
1	D	777	PRO	2.0
2	H	272	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

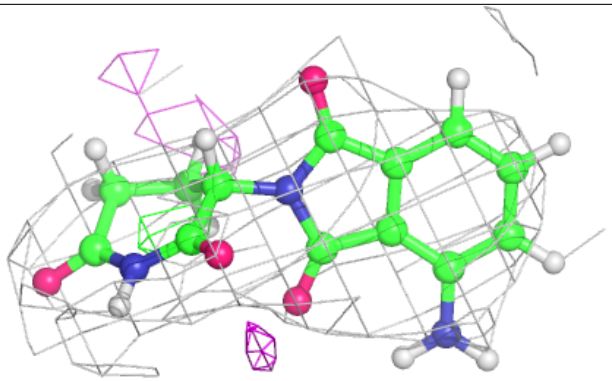
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

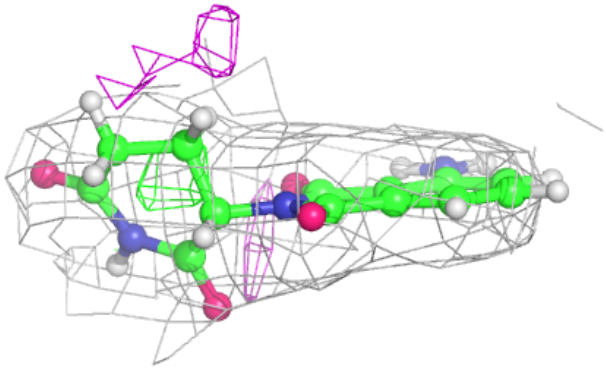
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	Y70	B	502	20/20	0.96	0.24	47,58,72,73	11
5	Y70	H	502	20/20	0.97	0.23	41,48,57,58	11
5	Y70	K	502	20/20	0.97	0.27	60,69,84,86	11
5	Y70	E	502	20/20	0.98	0.33	44,51,55,58	11
4	ZN	I	201	1/1	0.99	0.10	43,43,43,43	0
4	ZN	C	201	1/1	0.99	0.10	49,49,49,49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

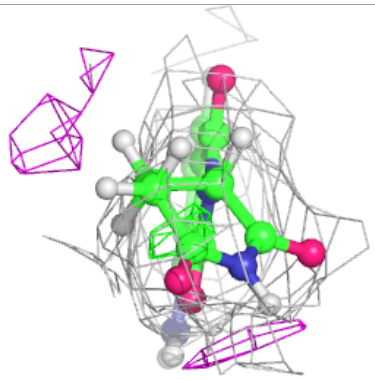
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

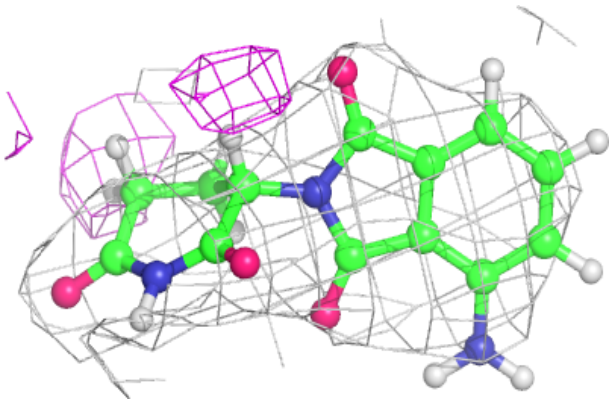


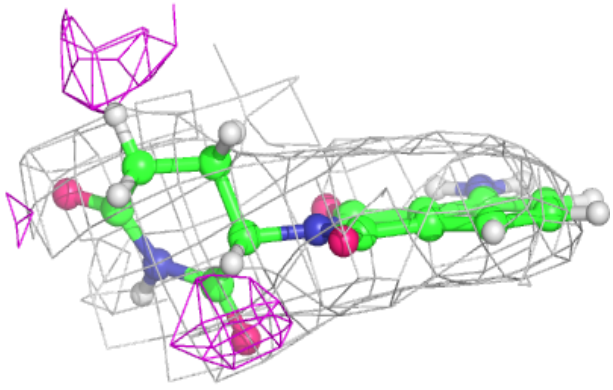


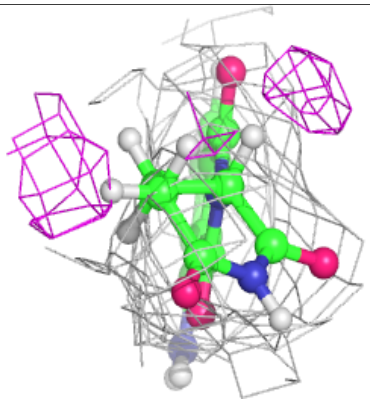


Electron density around Y70 H 502:

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

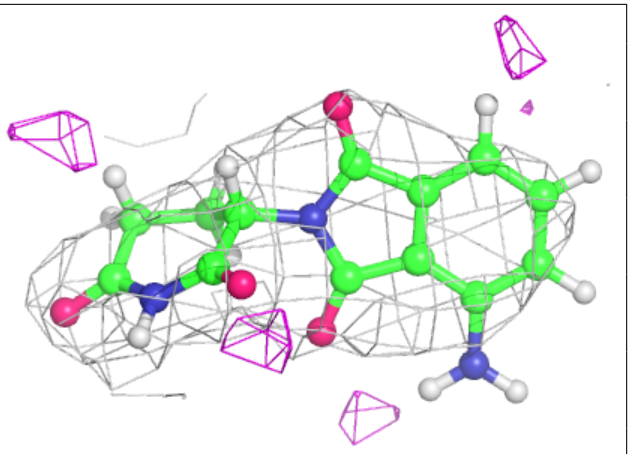


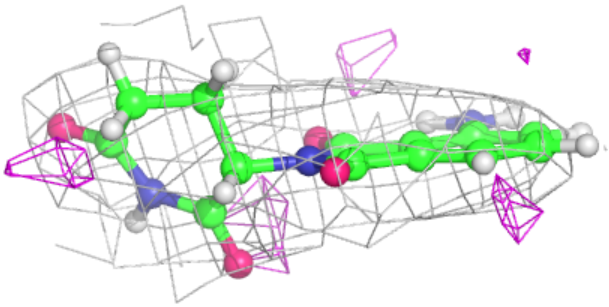


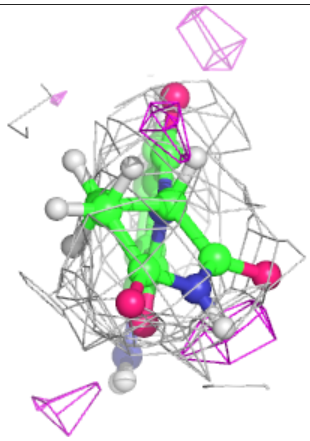


Electron density around Y70 K 502:

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

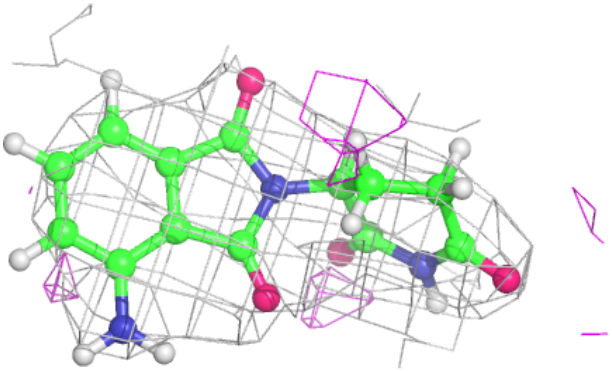


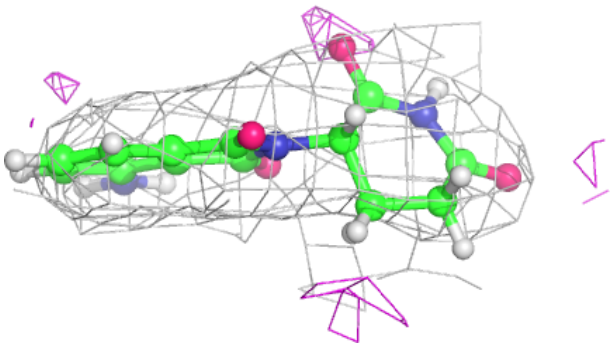


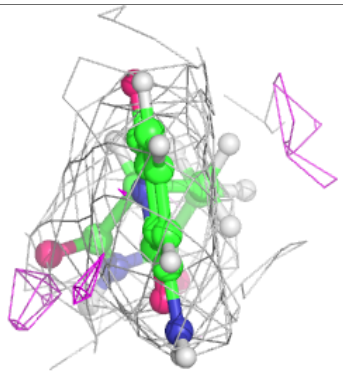


Electron density around Y70 E 502:

$2mF_o$-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.