wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 03:03 PM EDT

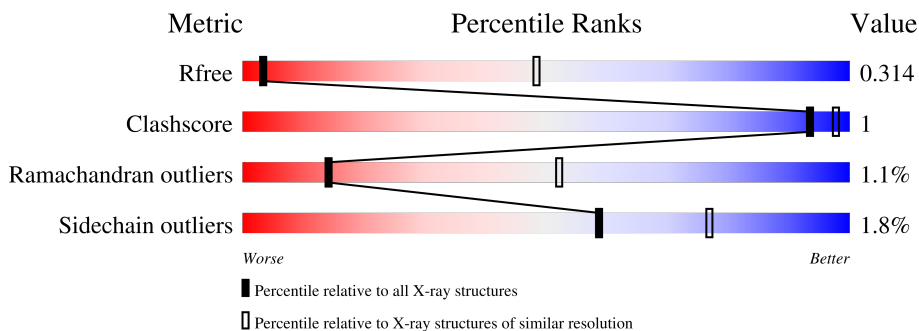|		
PDB ID	:	6H0G
Title	:	Structure of the DDB1-CRBN-pomalidomide complex bound to ZNF692(ZF4)
Authors	:	Bunker, R.D.; Petzold, G.; Thoma, N.H.
Deposited on	:	2018-07-09
Resolution	:	4.25 Å(reported)

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 4.25 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	Percentile Ranks	Value
Rfree		0.314
Clashscore		1
Ramachandran outliers		1.1%
Sidechain outliers		1.8%

Worse → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1017 (4.72-3.78)
Clashscore	141614	1059 (4.72-3.80)
Ramachandran outliers	138981	1014 (4.72-3.80)
Sidechain outliers	138945	1018 (4.72-3.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	856	92% · ·
1	D	856	92% · ·
2	B	426	85% 8% · 6%
2	E	426	86% 8% · 6%
3	C	31	81% 16% ·
3	F	31	90% 6% ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 39696 atoms, of which 19764 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,DDB1 (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	825	Total 12920	C 4100	H 6443	N 1092	O 1249	S 36	6443	0	0
1	D	825	Total 12920	C 4100	H 6443	N 1092	O 1249	S 36	6443	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q16531
A	-18	HIS	-	expression tag	UNP Q16531
A	-17	HIS	-	expression tag	UNP Q16531
A	-16	HIS	-	expression tag	UNP Q16531
A	-15	HIS	-	expression tag	UNP Q16531
A	-14	HIS	-	expression tag	UNP Q16531
A	-13	HIS	-	expression tag	UNP Q16531
A	-12	VAL	-	expression tag	UNP Q16531
A	-11	ASP	-	expression tag	UNP Q16531
A	-10	GLU	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	expression tag	UNP Q16531
A	-2	GLY	-	expression tag	UNP Q16531
A	-1	GLY	-	expression tag	UNP Q16531
A	0	ARG	-	expression tag	UNP Q16531
D	-19	MET	-	initiating methionine	UNP Q16531
D	-18	HIS	-	expression tag	UNP Q16531
D	-17	HIS	-	expression tag	UNP Q16531

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP Q16531
D	-15	HIS	-	expression tag	UNP Q16531
D	-14	HIS	-	expression tag	UNP Q16531
D	-13	HIS	-	expression tag	UNP Q16531
D	-12	VAL	-	expression tag	UNP Q16531
D	-11	ASP	-	expression tag	UNP Q16531
D	-10	GLU	-	expression tag	UNP Q16531
D	-9	GLU	-	expression tag	UNP Q16531
D	-8	ASN	-	expression tag	UNP Q16531
D	-7	LEU	-	expression tag	UNP Q16531
D	-6	TYR	-	expression tag	UNP Q16531
D	-5	PHE	-	expression tag	UNP Q16531
D	-4	GLN	-	expression tag	UNP Q16531
D	-3	GLY	-	expression tag	UNP Q16531
D	-2	GLY	-	expression tag	UNP Q16531
D	-1	GLY	-	expression tag	UNP Q16531
D	0	ARG	-	expression tag	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	401	Total 6457	C 2058	H 3225	N 551	O 598	S 25	3225	0	0
2	E	401	Total 6458	C 2058	H 3226	N 551	O 598	S 25	3226	0	0

There are 48 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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	36	GLN	-	expression tag	UNP Q96SW2
B	37	GLY	-	expression tag	UNP Q96SW2
B	38	GLY	-	expression tag	UNP Q96SW2
B	39	GLY	-	expression tag	UNP Q96SW2
B	40	ARG	-	expression tag	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	36	GLN	-	expression tag	UNP Q96SW2
E	37	GLY	-	expression tag	UNP Q96SW2
E	38	GLY	-	expression tag	UNP Q96SW2
E	39	GLY	-	expression tag	UNP Q96SW2
E	40	ARG	-	expression tag	UNP Q96SW2

- Molecule 3 is a protein called Zinc finger protein 692.

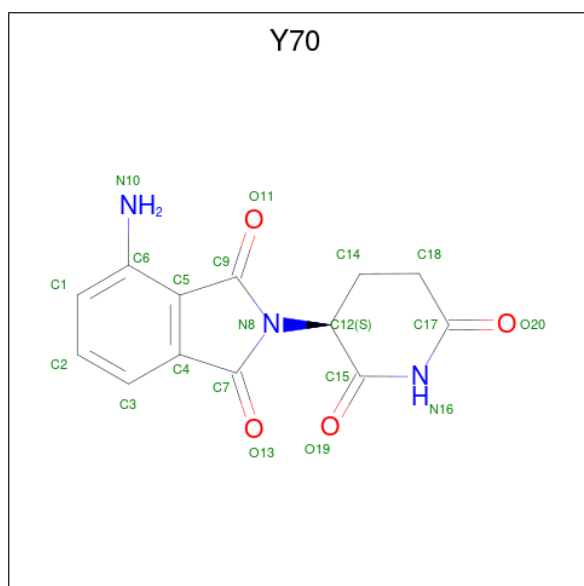| Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	30	Total	C	H	N	O	S	208	0	0
			441	140	208	48	42	3			
3	F	30	Total	C	H	N	O	S	219	0	0
			456	143	219	49	42	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	GLY	-	expression tag	UNP Q9BU19
C	414	GLY	GLU	conflict	UNP Q9BU19
C	415	ARG	LYS	conflict	UNP Q9BU19
F	412	GLY	-	expression tag	UNP Q9BU19
F	414	GLY	GLU	conflict	UNP Q9BU19
F	415	ARG	LYS	conflict	UNP Q9BU19

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

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

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

Y70

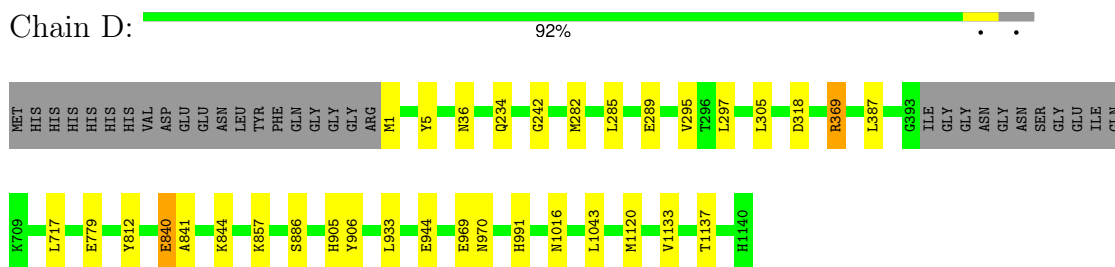| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 20	C 13	N 3	O 4	0	0
5	E	1	Total 20	C 13	N 3	O 4	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.
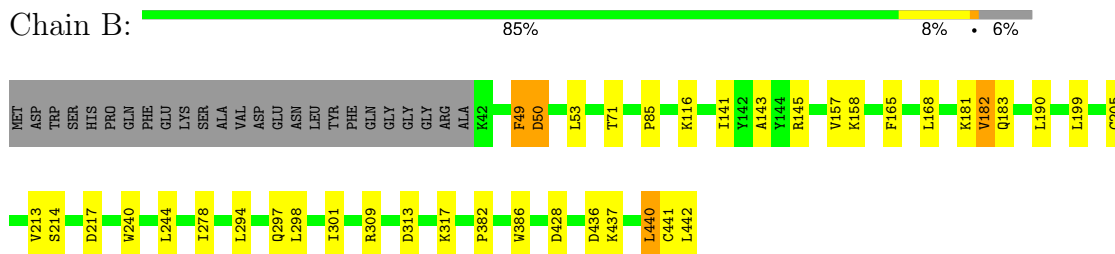
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DDB1 (DNA damage binding protein 1),DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1
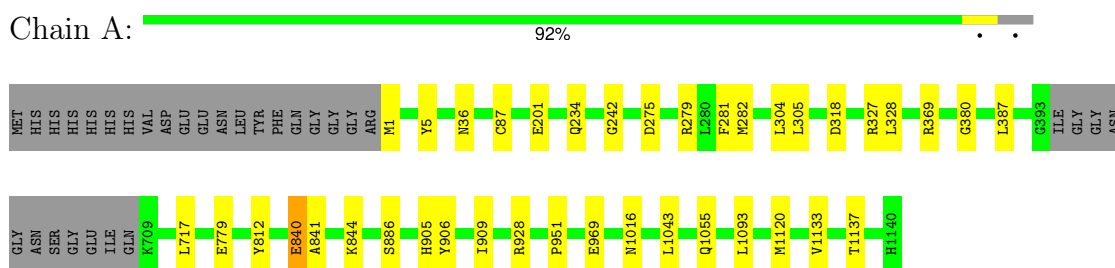
• Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DDB1 (DNA damage binding protein 1),DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1
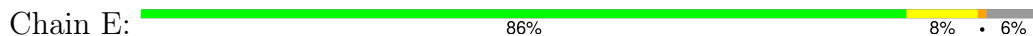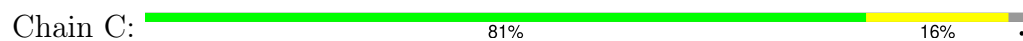

• Molecule 2: Protein cereblon

• Molecule 2: Protein cereblon

MET ASP TRP SER HIS PRO GLN PHE GLU LYS SER ALA VAL ASP GLU ASN LEU TYR PHE GLN GLY GLY ARG ALA K42 F49 D50 L53 T71 P85 K116 I141 Y142 A143 Y144 R145 V157 K158 F165 L168 K181 V182 Q183 V213 S214 R215 E216 D217

L247 A250 E251 T252 L253 I278 L298 I301 R309 C310 D313 P382 L417 L422 P427 L440 C441 L442

- Molecule 3: Zinc finger protein 692

Chain C:

81%   16%

GLY G413 G414 R415 P416 C426 L432 T442

- Molecule 3: Zinc finger protein 692

Chain F:

90%   6%

GLY G413 G414 Q428 T442
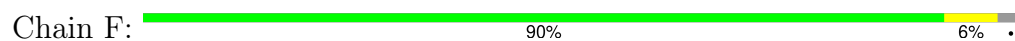
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.51Å 99.53Å 166.94Å 90.00° 108.49° 90.00°	Depositor
Resolution (Å)	48.60 – 4.25 48.97 – 4.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (48.60-4.25) 93.3 (48.97-4.25)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 4.29Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.221 , 0.256 0.278 , 0.314	Depositor DCC
R_{free} test set	1140 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	169.8	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 90.5	EDS
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.084 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	39696	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	0.44	0/6594	0.53	0/8919
1	D	0.43	0/6594	0.54	1/8919 (0.0%)
2	B	0.47	0/3308	0.51	0/4487
2	E	0.46	0/3308	0.50	0/4487
3	C	0.52	0/238	0.59	0/319
3	F	0.43	0/242	0.60	0/323
All	All	0.44	0/20284	0.53	1/27454 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1016	ASN	N-CA-CB	5.07	119.73	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6477	6443	6445	15	0
1	D	6477	6443	6445	9	0
2	B	3232	3225	3228	20	0
2	E	3232	3226	3230	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	233	208	208	1	0
3	F	237	219	219	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
5	B	20	0	11	1	0
5	E	20	0	11	0	0
All	All	19932	19764	19797	56	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 1.

The worst 5 of 56 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:440:LEU:O	2:B:440:LEU:HD13	1.99	0.63
1:D:295:VAL:HG23	1:D:295:VAL:O	2.04	0.57
2:B:298:LEU:HD12	2:B:301:ILE:HD12	1.88	0.56
1:A:951:PRO:O	2:B:190:LEU:HD21	2.06	0.56
2:E:298:LEU:HD12	2:E:301:ILE:HD12	1.88	0.55

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	821/856 (96%)	753 (92%)	62 (8%)	6 (1%)	22	62
1	D	821/856 (96%)	751 (92%)	64 (8%)	6 (1%)	22	62
2	B	399/426 (94%)	372 (93%)	21 (5%)	6 (2%)	10	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	399/426 (94%)	375 (94%)	17 (4%)	7 (2%)	8	42
3	C	28/31 (90%)	20 (71%)	7 (25%)	1 (4%)	3	28
3	F	28/31 (90%)	23 (82%)	3 (11%)	2 (7%)	1	16
All	All	2496/2626 (95%)	2294 (92%)	174 (7%)	28 (1%)	14	52

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	ARG
1	A	1016	ASN
2	B	50	ASP
2	E	50	ASP
1	A	840	GLU

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	720/744 (97%)	709 (98%)	11 (2%)	65	80
1	D	720/744 (97%)	707 (98%)	13 (2%)	59	77
2	B	365/385 (95%)	355 (97%)	10 (3%)	44	66
2	E	365/385 (95%)	360 (99%)	5 (1%)	67	80
3	C	23/25 (92%)	21 (91%)	2 (9%)	10	34
3	F	24/25 (96%)	24 (100%)	0	100	100
All	All	2217/2308 (96%)	2176 (98%)	41 (2%)	59	77

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	779	GLU
1	D	1120	MET
1	D	812	TYR
1	D	857	LYS

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Mol	Chain	Res	Type
2	E	145	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1059	ASN
2	E	57	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	E	502	-	22,22,22	2.86	9 (40%)	31,33,33	1.96	8 (25%)
5	Y70	B	502	-	22,22,22	2.73	10 (45%)	31,33,33	2.50	11 (35%)

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

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	502	Y70	C17-N16	7.34	1.49	1.37
5	B	502	Y70	C17-N16	6.78	1.48	1.37
5	B	502	Y70	C15-N16	6.60	1.49	1.37
5	E	502	Y70	C15-N16	6.42	1.48	1.37
5	E	502	Y70	C4-C7	4.32	1.55	1.48

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	Y70	C5-C6-N10	6.14	131.29	121.99
5	B	502	Y70	C1-C6-N10	-5.46	109.42	120.11
5	B	502	Y70	C18-C17-N16	-5.32	111.03	116.69
5	E	502	Y70	C1-C6-N10	-5.27	109.80	120.11
5	E	502	Y70	C5-C6-N10	5.23	129.91	121.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	Y70	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand Y70 E 502

Bond lengths

Bond angles

Torsions

Rings

Ligand Y70 B 502

Bond lengths

Bond angles

Torsions

Rings
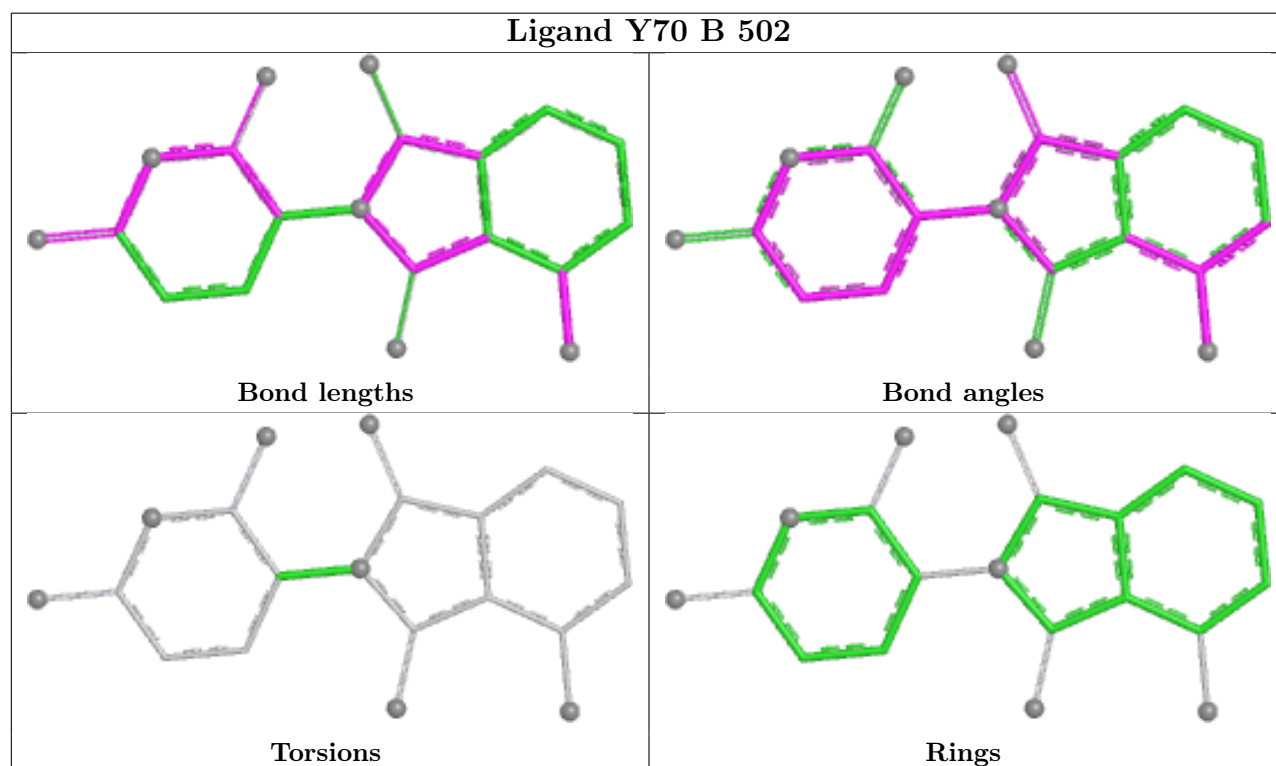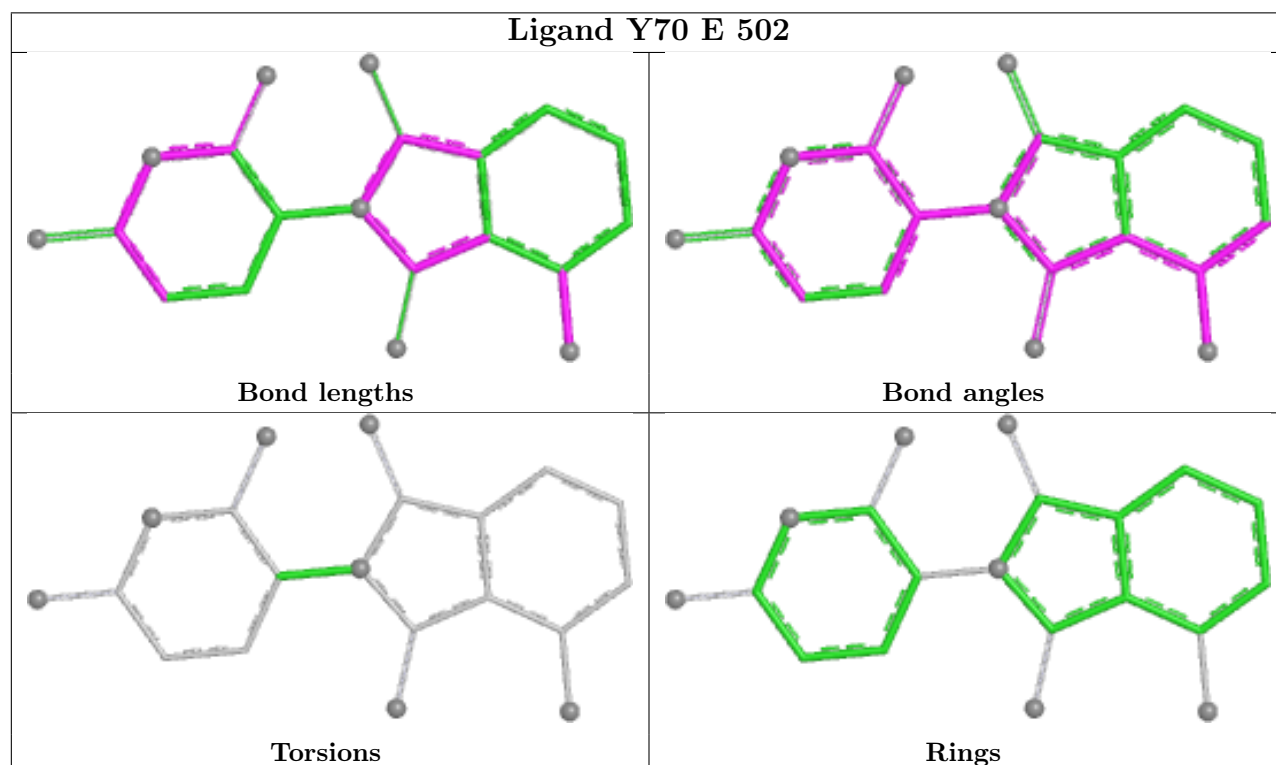
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

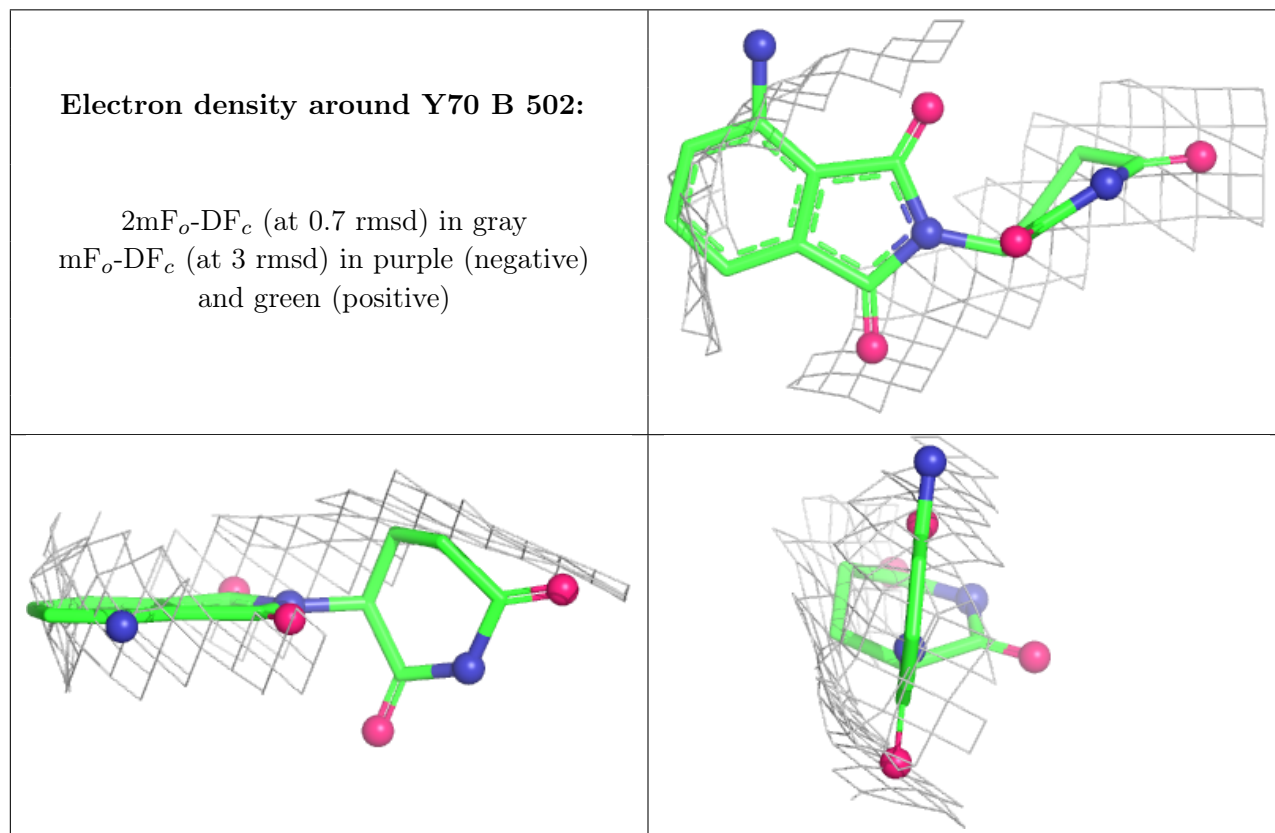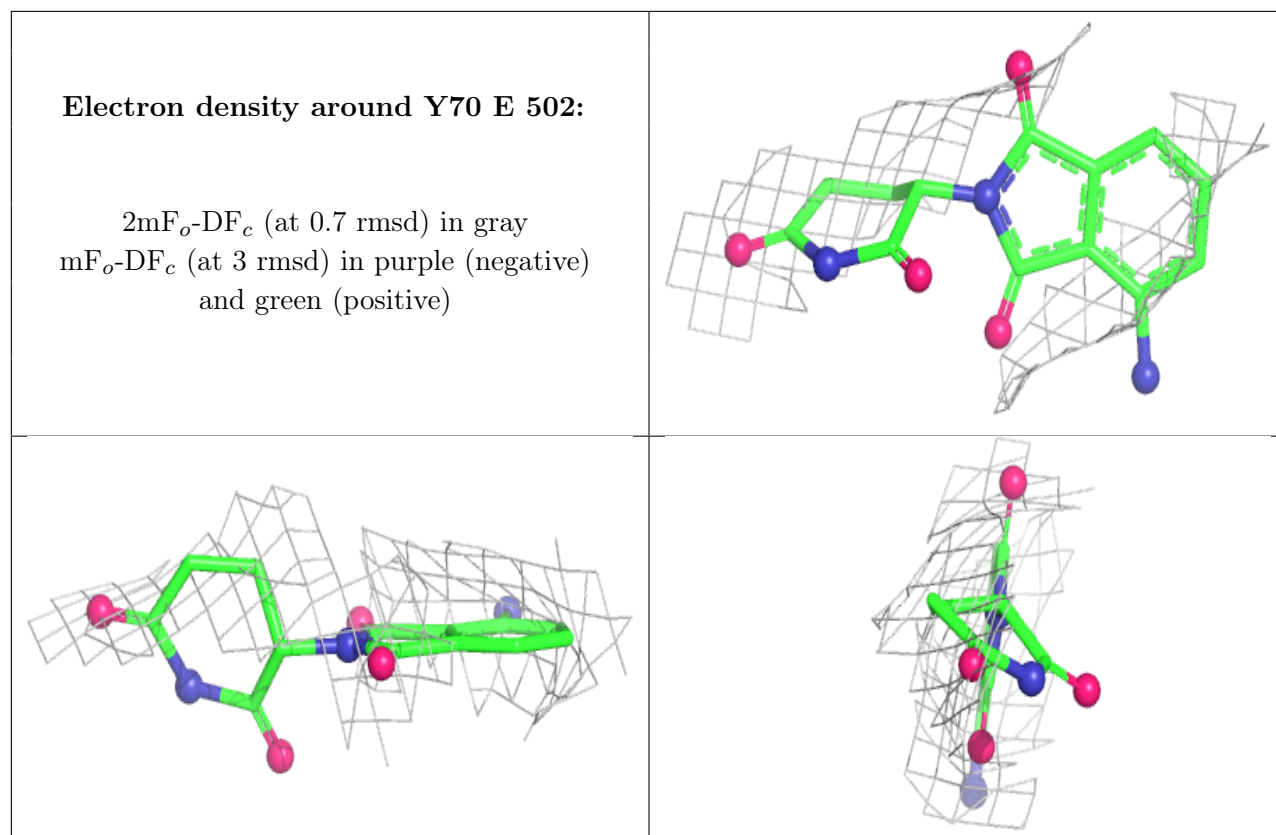Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.