



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:46 PM UTC

PDB ID : 6H0G / pdb_00006h0g
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)

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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

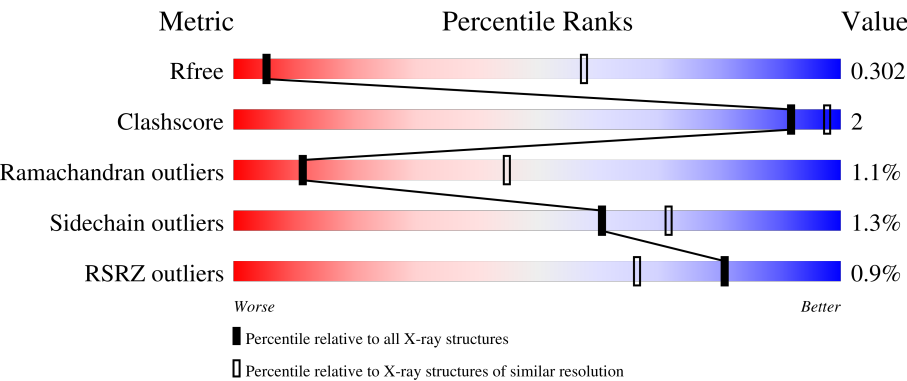
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

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 $\leq 5\%$. 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	% 92% • •
2	B	426	85% 8% • 6%
2	E	426	2% 85% 8% • 6%
3	C	31	81% 16% •

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Mol	Chain	Length	Quality of chain
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	C	H	N	O	S	6443	0	0
			12920	4100	6443	1092	1249	36			
1	D	825	Total	C	H	N	O	S	6443	0	0
			12920	4100	6443	1092	1249	36			

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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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	C	H	N	O	S	3225	0	0
			6457	2058	3225	551	598	25			
2	E	401	Total	C	H	N	O	S	3226	0	0
			6458	2058	3226	551	598	25			

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 441	C 140	H 208	N 48	O 42	S 3	208	0	0
3	F	30	Total 456	C 143	H 219	N 49	O 42	S 3	219	0	0

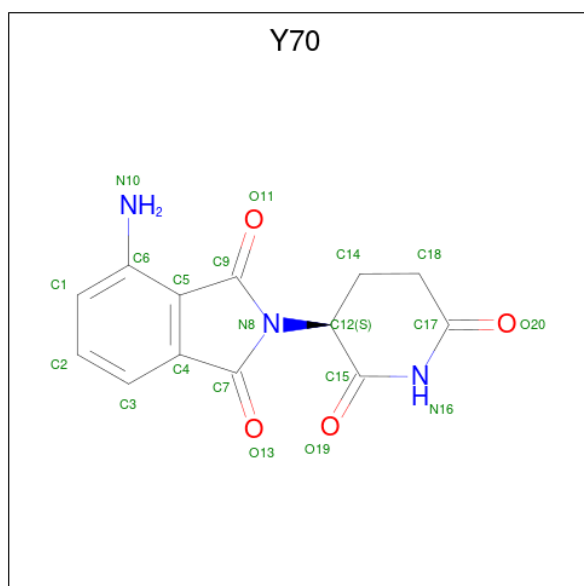
There are 6 discrepancies between the modelled and reference sequences:

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is S-Pomalidomide (CCD ID: Y70) (formula: C₁₃H₁₁N₃O₄).

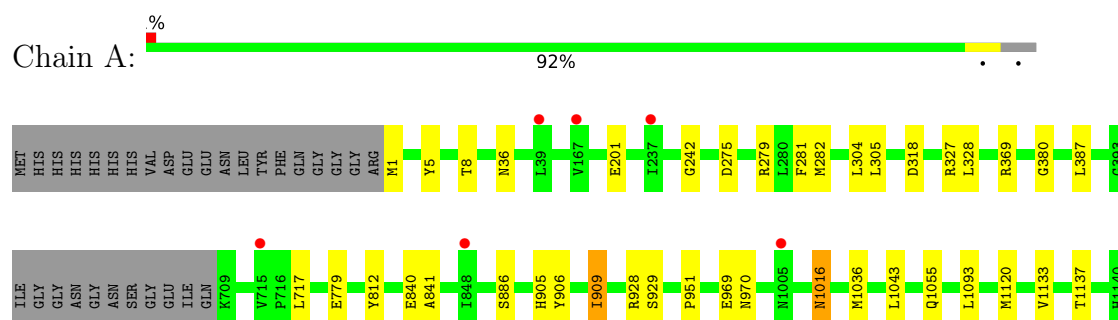


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 20 13 3 4	0	0
5	E	1	Total C N O 20 13 3 4	0	0

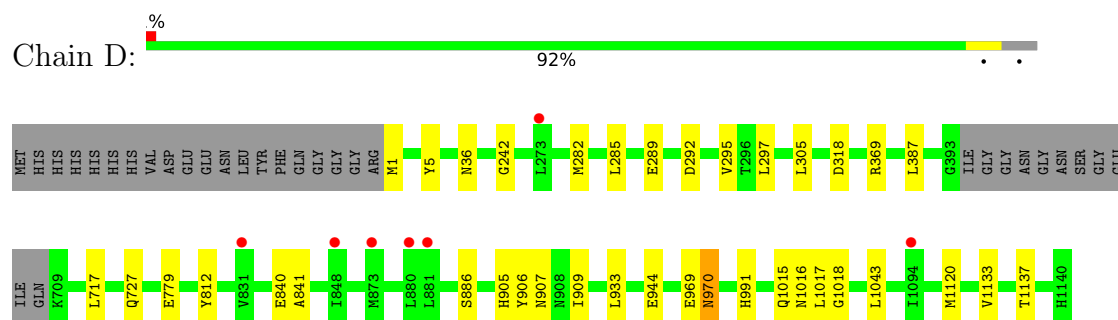
3 Residue-property plots [i](#)

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

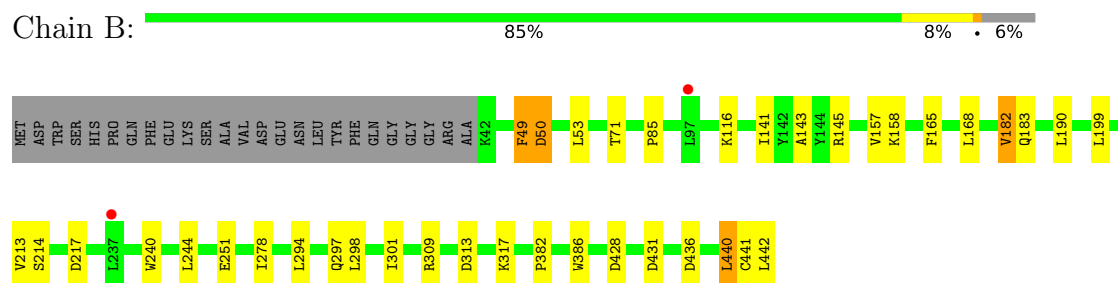
- Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DDB1 (DNA damage binding protein 1),DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1



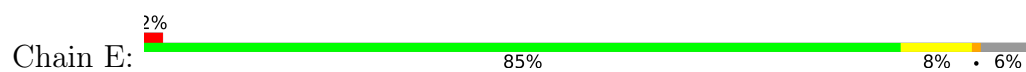
- Molecule 1: DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1,DDB1 (DNA damage binding protein 1),DNA damage-binding protein 1,DNA damage-binding protein 1,DNA damage-binding protein 1



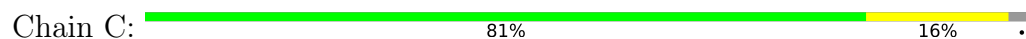
- Molecule 2: Protein cereblon



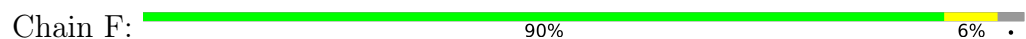
- Molecule 2: Protein cereblon



- Molecule 3: Zinc finger protein 692



- Molecule 3: Zinc finger protein 692



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 48.60 – 4.25	Depositor EDS
% Data completeness (in resolution range)	93.3 (48.60-4.25) 93.3 (48.60-4.25)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.16 (at 4.29Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.221 , 0.256 (Not available) , 0.302	Depositor DCC
R_{free} test set	1140 reflections (4.57%)	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)	0.26 , 168.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.68	0/6594	0.85	3/8919 (0.0%)
1	D	0.67	0/6594	0.85	5/8919 (0.1%)
2	B	0.73	0/3308	0.86	1/4487 (0.0%)
2	E	0.71	0/3308	0.84	0/4487
3	C	0.78	0/238	0.99	0/319
3	F	0.70	0/242	1.01	0/323
All	All	0.69	0/20284	0.86	9/27454 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	909	ILE	N-CA-C	-6.69	106.48	111.90
1	A	909	ILE	N-CA-C	-6.58	106.57	111.90
1	A	970	ASN	CA-CB-CG	5.70	118.30	112.60
1	D	970	ASN	CA-CB-CG	5.61	118.21	112.60
2	B	431	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	1016	ASN	CA-CB-CG	5.46	118.06	112.60
1	D	292	ASP	CA-CB-CG	5.38	117.98	112.60
1	D	1017	LEU	N-CA-C	-5.37	102.37	110.70
1	D	1015	GLN	N-CA-CB	5.21	117.51	110.38

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	6477	6443	6445	18	0
1	D	6477	6443	6445	12	0
2	B	3232	3225	3228	20	0
2	E	3232	3226	3230	18	0
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	65	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 2.

All (65) 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:440:LEU:C	2:E:440:LEU:HD23	2.32	0.55
2:E:298:LEU:HD12	2:E:301:ILE:HD12	1.88	0.55
2:E:313:ASP:HB2	2:E:442:LEU:HD12	1.88	0.55
1:A:886:SER:OG	2:B:442:LEU:HD21	2.06	0.55
2:B:313:ASP:HB2	2:B:442:LEU:HD12	1.89	0.54
2:B:386:TRP:CD1	5:B:502:Y70:H181	2.43	0.53
1:A:1055:GLN:HG3	1:A:1093:LEU:HD23	1.93	0.51
1:D:285:LEU:HB3	1:D:297:LEU:HD11	1.93	0.51
2:B:309:ARG:NH1	2:B:442:LEU:HD13	2.26	0.50
2:E:309:ARG:NH1	2:E:442:LEU:HD13	2.27	0.49
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.93	0.48
1:D:5:TYR:HB2	1:D:1043:LEU:HD11	1.94	0.48
1:D:282:MET:HB2	1:D:305:LEU:HD11	1.95	0.48
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.95	0.48
1:A:281:PHE:CE1	1:A:304:LEU:HD13	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.95	0.47
2:B:168:LEU:HD11	2:B:183:GLN:HB2	1.96	0.46
2:B:297:GLN:HB3	2:B:440:LEU:HD21	1.98	0.46
2:B:53:LEU:HD22	2:B:382:PRO:HG2	1.98	0.45
2:B:240:TRP:HB3	2:B:244:LEU:HD23	1.97	0.45
2:E:168:LEU:HD11	2:E:183:GLN:HB2	1.97	0.45
2:E:310:CYS:SG	2:E:440:LEU:HD21	2.55	0.45
2:E:53:LEU:HD22	2:E:382:PRO:HG2	1.98	0.45
1:D:282:MET:HE2	1:D:305:LEU:HD11	1.99	0.45
2:B:294:LEU:HD22	2:B:440:LEU:HB3	1.99	0.44
1:A:905:HIS:ND1	1:A:906:TYR:N	2.66	0.44
1:A:282:MET:HE2	1:A:305:LEU:HD11	1.99	0.44
1:A:327:ARG:HD3	2:B:199:LEU:HD22	2.00	0.44
3:C:415:ARG:HB2	3:C:416:PRO:HD2	2.00	0.44
2:E:165:PHE:HB2	2:E:182:VAL:HG13	2.01	0.43
1:A:886:SER:O	1:A:906:TYR:O	2.36	0.43
1:A:909:ILE:O	2:B:442:LEU:HD22	2.18	0.43
1:A:928:ARG:O	1:A:929:SER:C	2.61	0.43
2:B:278:ILE:N	2:B:278:ILE:HD12	2.33	0.43
2:E:141:ILE:HG23	2:E:157:VAL:HG13	2.00	0.43
1:A:275:ASP:OD1	1:A:279:ARG:N	2.49	0.43
2:B:49:PHE:O	2:B:50:ASP:CB	2.67	0.43
2:B:213:VAL:HG22	2:B:214:SER:N	2.34	0.43
1:D:886:SER:O	1:D:906:TYR:O	2.36	0.43
2:B:141:ILE:HG23	2:B:157:VAL:HG13	2.00	0.43
1:D:1133:VAL:O	1:D:1137:THR:HG23	2.18	0.43
1:D:387:LEU:HG	1:D:717:LEU:HD11	2.01	0.42
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.19	0.42
2:E:143:ALA:HB3	2:E:158:LYS:HB2	2.01	0.42
2:E:440:LEU:C	2:E:440:LEU:CD2	2.93	0.42
1:D:905:HIS:ND1	1:D:906:TYR:N	2.67	0.42
2:E:278:ILE:HD12	2:E:278:ILE:N	2.34	0.42
2:E:49:PHE:O	2:E:50:ASP:CB	2.68	0.42
2:E:250:ALA:HB3	2:E:251:GLU:OE2	2.20	0.42
1:A:387:LEU:HG	1:A:717:LEU:HD11	2.02	0.41
2:E:247:LEU:O	2:E:253:LEU:HD21	2.21	0.41
1:A:328:LEU:O	1:A:380:GLY:HA2	2.21	0.41
2:B:165:PHE:HB2	2:B:182:VAL:HG13	2.01	0.41
2:E:417:LEU:HB2	2:E:422:LEU:HD11	2.02	0.41
1:A:8:THR:HG23	1:A:1036:MET:HE2	2.03	0.41
1:A:909:ILE:HD12	1:A:928:ARG:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:933:LEU:HD23	1:D:944:GLU:HA	2.03	0.41
1:D:906:TYR:O	1:D:907:ASN:C	2.64	0.41
1:D:1016:ASN:C	1:D:1018:GLY:N	2.78	0.40
2:E:89:MET:HE1	2:E:91:LEU:HD13	2.02	0.40
2:E:209:PRO:O	2:E:210:SER:C	2.64	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	821/856 (96%)	753 (92%)	62 (8%)	6 (1%)	18	55
1	D	821/856 (96%)	751 (92%)	64 (8%)	6 (1%)	18	55
2	B	399/426 (94%)	372 (93%)	21 (5%)	6 (2%)	8	38
2	E	399/426 (94%)	375 (94%)	17 (4%)	7 (2%)	6	33
3	C	28/31 (90%)	20 (71%)	7 (25%)	1 (4%)	2	20
3	F	28/31 (90%)	23 (82%)	3 (11%)	2 (7%)	1	11
All	All	2496/2626 (95%)	2294 (92%)	174 (7%)	28 (1%)	11	45

All (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
1	A	841	ALA
2	B	49	PHE

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Mol	Chain	Res	Type
2	B	428	ASP
1	D	369	ARG
1	D	841	ALA
2	E	49	PHE
2	E	213	VAL
2	E	215	ARG
2	B	317	LYS
1	D	840	GLU
1	A	36	ASN
1	A	242	GLY
1	D	36	ASN
1	D	242	GLY
2	B	116	LYS
1	D	970	ASN
2	E	116	LYS
3	F	428	GLN
3	C	414	GLY
2	B	85	PRO
2	E	85	PRO
3	F	414	GLY
2	E	427	PRO

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%)	713 (99%)	7 (1%)	68	75
1	D	720/744 (97%)	711 (99%)	9 (1%)	61	71
2	B	365/385 (95%)	357 (98%)	8 (2%)	45	64
2	E	365/385 (95%)	362 (99%)	3 (1%)	73	77
3	C	23/25 (92%)	21 (91%)	2 (9%)	9	30
3	F	24/25 (96%)	24 (100%)	0	100	100
All	All	2217/2308 (96%)	2188 (99%)	29 (1%)	61	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	201	GLU
1	A	318	ASP
1	A	779	GLU
1	A	812	TYR
1	A	969	GLU
1	A	1120	MET
2	B	71	THR
2	B	145	ARG
2	B	182	VAL
2	B	217	ASP
2	B	251	GLU
2	B	436	ASP
2	B	440	LEU
2	B	441	CYS
3	C	426	CYS
3	C	432	LEU
1	D	1	MET
1	D	289	GLU
1	D	318	ASP
1	D	727	GLN
1	D	779	GLU
1	D	812	TYR
1	D	969	GLU
1	D	991	HIS
1	D	1120	MET
2	E	71	THR
2	E	145	ARG
2	E	182	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	332	GLN
1	A	372	GLN
1	A	711	HIS
1	A	759	GLN
1	A	1009	HIS
2	B	179	GLN
2	B	233	HIS

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Mol	Chain	Res	Type
2	B	267	ASN
2	B	325	GLN
2	B	335	ASN
1	D	203	ASN
1	D	262	ASN
1	D	332	GLN
1	D	711	HIS
1	D	759	GLN
1	D	789	HIS
1	D	796	GLN
1	D	797	HIS
1	D	952	ASN
1	D	1009	HIS
1	D	1059	ASN
2	E	105	GLN
2	E	179	GLN
2	E	233	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

All (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
5	E	502	Y70	C5-C9	3.64	1.56	1.49
5	E	502	Y70	C9-N8	3.55	1.47	1.40
5	B	502	Y70	C7-N8	3.44	1.47	1.40
5	E	502	Y70	C7-N8	3.32	1.46	1.40
5	B	502	Y70	C4-C7	3.11	1.53	1.48
5	B	502	Y70	C5-C9	2.89	1.54	1.49
5	B	502	Y70	C9-N8	2.56	1.45	1.40
5	B	502	Y70	C6-N10	2.35	1.45	1.38
5	E	502	Y70	C6-N10	2.28	1.45	1.38
5	E	502	Y70	C18-C17	2.27	1.54	1.50
5	B	502	Y70	O19-C15	-2.27	1.19	1.23
5	B	502	Y70	O20-C17	-2.24	1.18	1.23
5	E	502	Y70	O19-C15	-2.22	1.19	1.23
5	B	502	Y70	C12-C15	2.15	1.56	1.51

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	502	Y70	C5-C6-N10	5.23	129.91	121.99
5	B	502	Y70	C14-C12-C15	4.24	118.80	111.56
5	B	502	Y70	C9-N8-C7	-3.17	107.94	111.55
5	B	502	Y70	O13-C7-C4	-3.04	122.76	128.66
5	E	502	Y70	C14-C12-N8	-3.01	106.89	113.60
5	B	502	Y70	C18-C14-C12	3.01	115.20	109.77
5	B	502	Y70	C17-N16-C15	-2.86	122.92	126.69
5	E	502	Y70	C12-C15-N16	-2.75	112.22	116.24
5	B	502	Y70	C14-C12-N8	-2.70	107.58	113.60
5	B	502	Y70	O13-C7-N8	2.55	128.58	124.99
5	B	502	Y70	C4-C7-N8	2.40	108.61	105.96
5	E	502	Y70	C9-N8-C7	-2.38	108.85	111.55
5	E	502	Y70	O11-C9-C5	-2.21	125.79	129.15
5	E	502	Y70	C18-C17-N16	-2.09	114.47	116.69
5	E	502	Y70	O19-C15-C12	2.06	124.96	120.69

There are no chirality outliers.

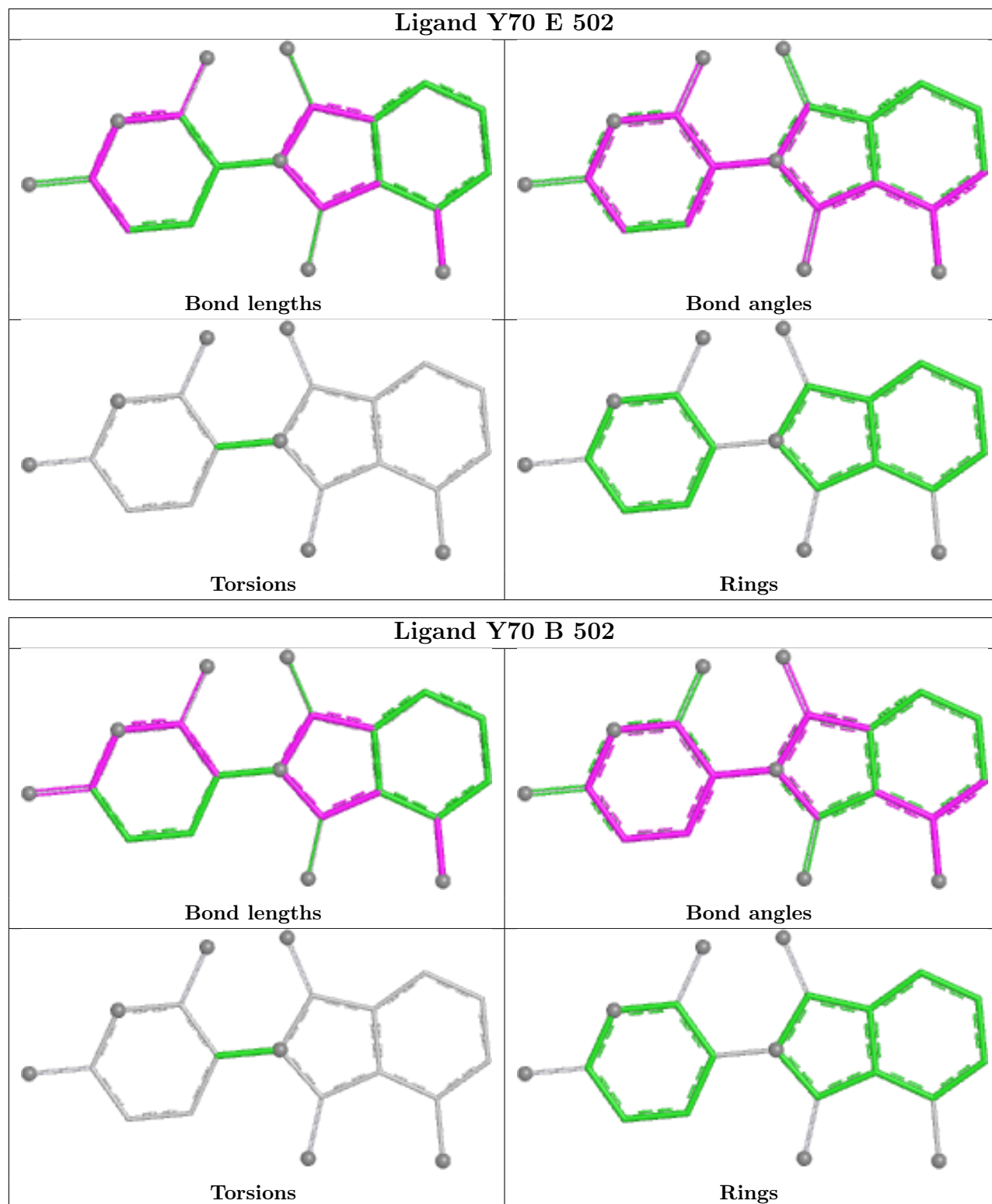
There are no torsion outliers.

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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	825/856 (96%)	-0.39	6 (0%) 84 70	44, 79, 122, 176	0
1	D	825/856 (96%)	-0.43	7 (0%) 82 68	25, 74, 121, 172	0
2	B	401/426 (94%)	-0.47	2 (0%) 87 75	40, 69, 114, 179	0
2	E	401/426 (94%)	-0.36	7 (1%) 69 54	35, 69, 120, 165	0
3	C	30/31 (96%)	-0.42	0 100 100	37, 53, 101, 120	0
3	F	30/31 (96%)	-0.67	0 100 100	59, 83, 121, 125	0
All	All	2512/2626 (95%)	-0.41	22 (0%) 81 66	25, 74, 121, 179	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ILE	4.2
1	D	848	ILE	4.0
2	E	415	TRP	3.6
1	D	1094	ILE	3.3
1	D	880	LEU	3.3
2	E	417	LEU	3.2
1	A	167	VAL	2.8
2	E	416	GLY	2.7
1	D	881	LEU	2.6
1	A	39	LEU	2.4
1	D	273	LEU	2.3
2	B	237	LEU	2.2
2	E	360	LEU	2.2
1	A	715	VAL	2.2
1	D	873	MET	2.2
2	B	97	LEU	2.2
1	A	848	ILE	2.1
2	E	120	PHE	2.1
1	D	831	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	83	VAL	2.0
2	E	359	THR	2.0
1	A	1005	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

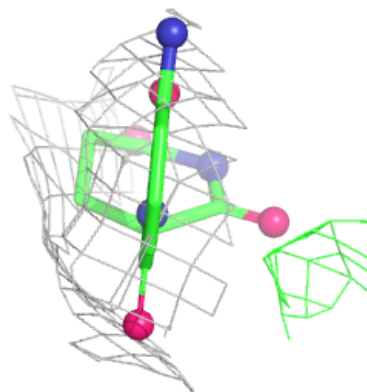
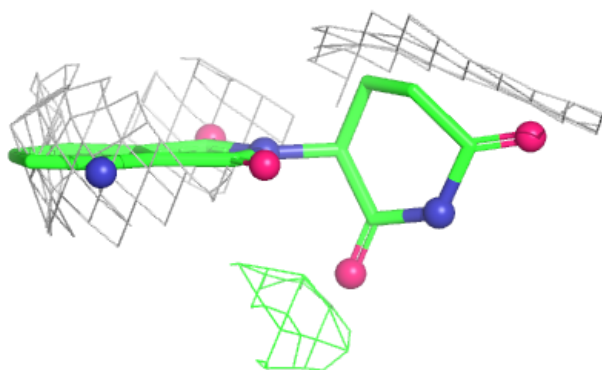
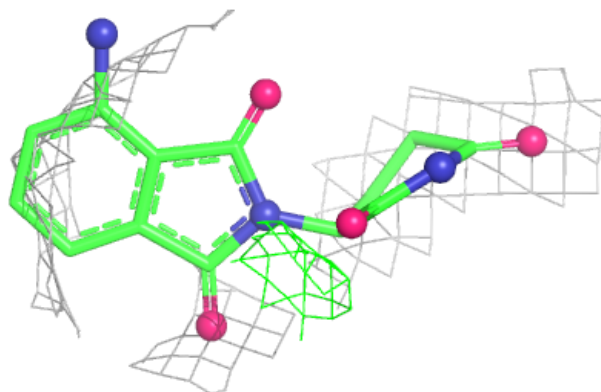
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.94	0.07	75,75,75,75	0
5	Y70	E	502	20/20	0.94	0.05	75,75,75,75	0
4	ZN	B	501	1/1	0.99	0.04	75,75,75,75	0
4	ZN	E	501	1/1	0.99	0.02	75,75,75,75	0
4	ZN	C	501	1/1	1.00	0.09	75,75,75,75	0
4	ZN	F	501	1/1	1.00	0.08	75,75,75,75	0

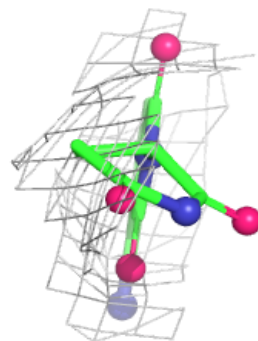
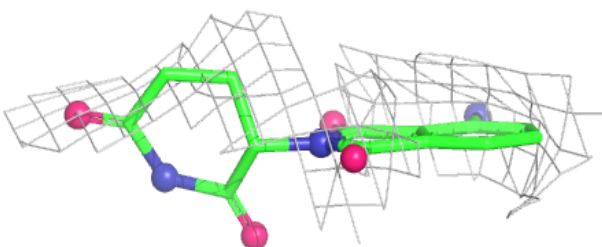
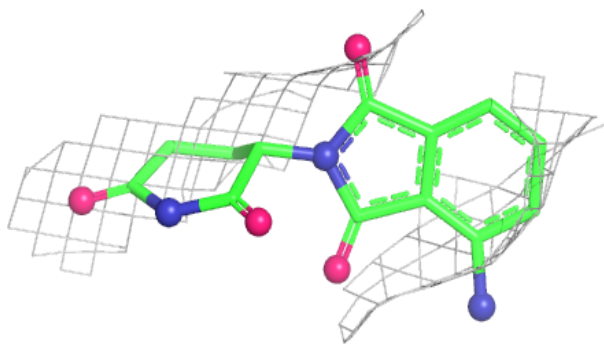
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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