



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:25 pm BST

PDB ID : 4TZU
Title : Crystal Structure of Murine Cereblon in Complex with Pomalidomide
Authors : Chamberlain, P.P.; Pagarigan, B.; Delker, S.; Leon, B.
Deposited on : 2014-07-10
Resolution : 2.00 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

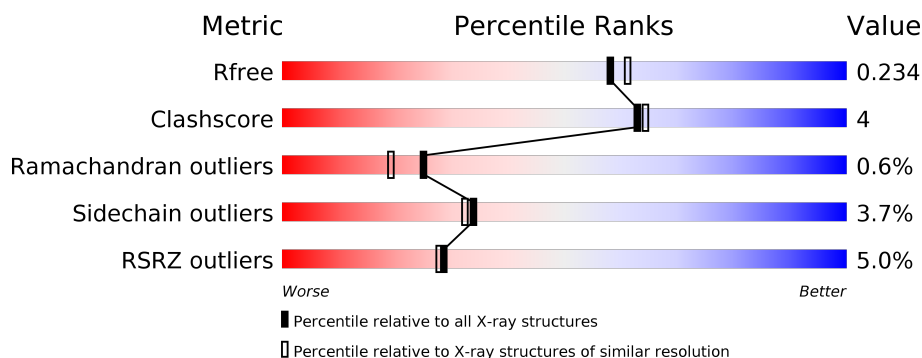
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	108	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>12%</div> <div>••</div> <div>17%</div> </div> </div>
1	B	108	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	108	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>12%</div> <div></div> <div>17%</div> </div> </div>
1	D	108	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>6%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3162 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	0	0	0
			711	457	119	129	6			
1	B	91	Total	C	N	O	S	0	0	0
			718	461	120	131	6			
1	C	90	Total	C	N	O	S	0	0	0
			711	457	119	129	6			
1	D	90	Total	C	N	O	S	0	1	0
			717	461	119	131	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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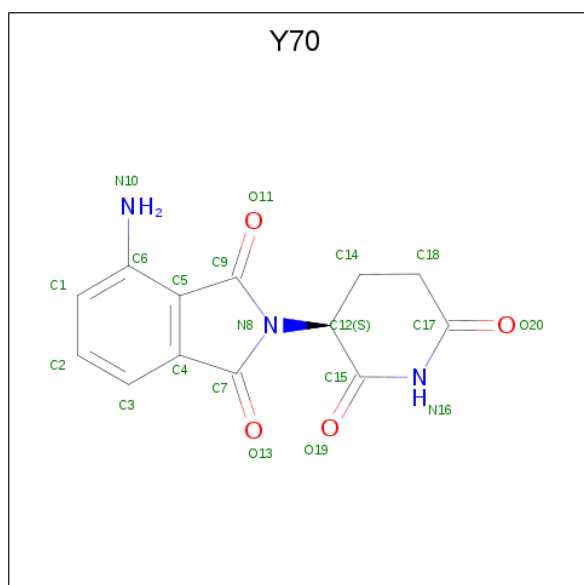
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is S-Pomalidomide (three-letter code: Y70) (formula: C₁₃H₁₁N₃O₄).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	53	Total	O	0	0
			53	53		
5	B	43	Total	O	0	0
			43	43		
5	C	29	Total	O	0	0
			29	29		
5	D	56	Total	O	0	0
			56	56		

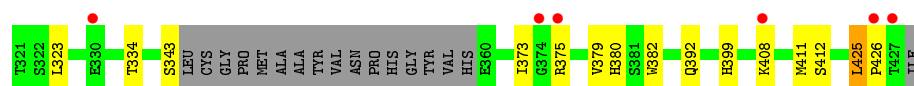
3 Residue-property plots [i](#)

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.

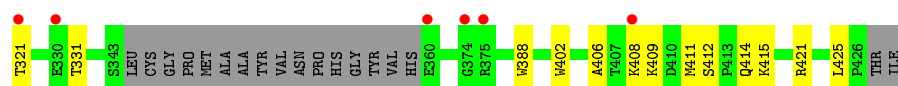
- Molecule 1: Protein cereblon



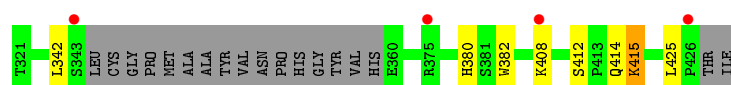
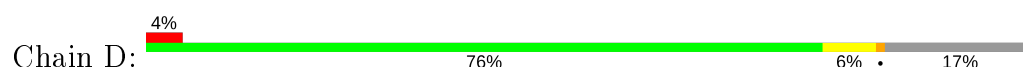
- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon



- Molecule 1: Protein cereblon



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	143.34Å 143.34Å 143.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.4 (30.00-2.00) 91.4 (29.26-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.239 0.192 , 0.234	Depositor DCC
R_{free} test set	1536 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3162	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 63.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.2997e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, 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	0.97	2/729 (0.3%)	0.79	3/988 (0.3%)
1	B	0.93	1/736 (0.1%)	0.73	1/998 (0.1%)
1	C	0.82	2/729 (0.3%)	0.69	0/988
1	D	1.02	1/738 (0.1%)	0.74	0/1000
All	All	0.94	6/2932 (0.2%)	0.74	4/3974 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TRP	CD2-CE2	5.92	1.48	1.41
1	B	382	TRP	CD2-CE2	5.79	1.48	1.41
1	D	382	TRP	CD2-CE2	5.56	1.48	1.41
1	A	388	TRP	CD2-CE2	5.39	1.47	1.41
1	C	388	TRP	CD2-CE2	5.20	1.47	1.41
1	C	402	TRP	CD2-CE2	5.12	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	LEU	C-N-CD	-5.73	108.00	120.60
1	A	342	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	425	LEU	C-N-CD	-5.59	108.30	120.60
1	A	425	LEU	CA-CB-CG	5.29	127.47	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	412	SER	Mainchain,Peptide
1	A	425	LEU	Peptide
1	B	412	SER	Mainchain,Peptide
1	B	425	LEU	Peptide
1	C	412	SER	Mainchain,Peptide
1	C	425	LEU	Peptide
1	D	412	SER	Mainchain,Peptide
1	D	425	LEU	Peptide

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	711	0	708	8	0
1	B	718	0	715	6	0
1	C	711	0	708	7	0
1	D	717	0	714	3	0
2	A	10	0	0	2	0
2	B	15	0	0	1	0
2	C	10	0	0	1	0
2	D	5	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	20	0	11	0	0
4	B	20	0	11	0	0
4	C	20	0	11	0	0
4	D	20	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	53	0	0	4	0
5	B	43	0	0	0	0
5	C	29	0	0	2	0
5	D	56	0	0	0	0
All	All	3162	0	2889	25	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 4.

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:LYS:H	1:A:411:MET:CE	1.84	0.89
1:A:408:LYS:H	1:A:411:MET:HE3	1.40	0.85
1:C:408:LYS:H	1:C:411:MET:CE	2.04	0.70
1:A:321:THR:N	5:A:626:HOH:O	2.26	0.69
2:A:502:SO4:O3	5:A:624:HOH:O	2.14	0.66
1:B:373:ILE:HD11	1:B:392:GLN:NE2	2.14	0.62
1:A:408:LYS:N	1:A:411:MET:HE3	2.16	0.59
1:A:369:ASN:OD1	1:A:394:LYS:NZ	2.36	0.58
1:D:380:HIS:ND1	2:D:501:SO4:O3	2.25	0.56
1:A:408:LYS:N	1:A:411:MET:CE	2.65	0.55
1:C:421:ARG:NH1	5:C:628:HOH:O	2.39	0.54
1:B:408:LYS:H	1:B:411:MET:CE	2.21	0.54
1:C:406:ALA:HB1	1:C:411:MET:HE3	1.93	0.51
1:C:409:LYS:HD3	1:C:409:LYS:HA	1.62	0.48
1:B:323:LEU:HD12	1:B:334:THR:HG23	1.98	0.44
1:C:408:LYS:H	1:C:411:MET:HE1	1.80	0.44
1:B:379:VAL:HG12	1:B:380:HIS:CD2	2.54	0.43
1:A:366:LYS:HE2	2:B:502:SO4:O3	2.19	0.43
1:B:408:LYS:HB2	1:B:411:MET:CE	2.48	0.42
2:A:501:SO4:O4	1:D:414:GLN:HB2	2.19	0.42
1:A:343:SER:HA	5:A:622:HOH:O	2.19	0.42
1:C:414:GLN:HB2	2:C:501:SO4:O4	2.21	0.41
5:A:625:HOH:O	1:D:415:LYS:HD3	2.20	0.41
1:C:321:THR:N	5:C:627:HOH:O	2.53	0.41
1:B:408:LYS:HB2	1:B:411:MET:HE2	2.02	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	86/108 (80%)	84 (98%)	1 (1%)	1 (1%)	13	7
1	B	87/108 (81%)	84 (97%)	2 (2%)	1 (1%)	14	8
1	C	86/108 (80%)	83 (96%)	3 (4%)	0	100	100
1	D	87/108 (81%)	84 (97%)	3 (3%)	0	100	100
All	All	346/432 (80%)	335 (97%)	9 (3%)	2 (1%)	25	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	426	PRO
1	A	413	PRO

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	80/94 (85%)	76 (95%)	4 (5%)	24	20
1	B	81/94 (86%)	78 (96%)	3 (4%)	34	32
1	C	80/94 (85%)	78 (98%)	2 (2%)	47	49
1	D	81/94 (86%)	78 (96%)	3 (4%)	34	32
All	All	322/376 (86%)	310 (96%)	12 (4%)	34	32

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	342	LEU
1	A	362	LEU
1	A	415	LYS
1	A	425	LEU
1	B	343	SER
1	B	375	ARG
1	B	399	HIS
1	C	331	THR
1	C	415	LYS
1	D	342	LEU
1	D	408	LYS
1	D	415	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	HIS
1	B	369	ASN
1	B	371	ASN
1	B	392	GLN
1	C	371	ASN
1	C	399	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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$
2	SO4	B	501	-	4,4,4	0.44	0	6,6,6	1.58	1 (16%)
2	SO4	A	501	-	4,4,4	0.60	0	6,6,6	1.07	0
2	SO4	D	501	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	C	502	-	4,4,4	0.15	0	6,6,6	0.48	0
2	SO4	A	502	-	4,4,4	0.40	0	6,6,6	0.55	0
2	SO4	C	501	-	4,4,4	0.30	0	6,6,6	1.05	0
4	Y70	B	505	-	22,22,22	2.14	5 (22%)	31,33,33	1.80	11 (35%)
2	SO4	B	503	-	4,4,4	0.29	0	6,6,6	0.34	0
4	Y70	D	503	-	22,22,22	2.07	4 (18%)	31,33,33	1.74	10 (32%)
2	SO4	B	502	-	4,4,4	0.20	0	6,6,6	0.20	0
4	Y70	C	504	-	22,22,22	2.16	4 (18%)	31,33,33	1.72	9 (29%)
4	Y70	A	504	-	22,22,22	2.13	4 (18%)	31,33,33	1.76	9 (29%)

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
4	Y70	C	504	-	-	0/4/33/33	0/3/3/3
4	Y70	A	504	-	-	0/4/33/33	0/3/3/3
4	Y70	B	505	-	-	0/4/33/33	0/3/3/3
4	Y70	D	503	-	-	0/4/33/33	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	Y70	C4-C7	-5.78	1.39	1.48
4	D	503	Y70	C4-C7	-5.61	1.39	1.48
4	B	505	Y70	C4-C7	-5.56	1.39	1.48
4	B	505	Y70	C5-C9	-5.41	1.39	1.49
4	C	504	Y70	C5-C9	-5.33	1.40	1.49
4	A	504	Y70	C5-C9	-5.25	1.40	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	Y70	C4-C7	-5.23	1.40	1.48
4	D	503	Y70	C5-C9	-5.13	1.40	1.49
4	A	504	Y70	C9-N8	-3.90	1.32	1.40
4	C	504	Y70	C7-N8	-3.64	1.33	1.40
4	D	503	Y70	C7-N8	-3.54	1.33	1.40
4	C	504	Y70	C9-N8	-3.49	1.33	1.40
4	A	504	Y70	C7-N8	-3.41	1.33	1.40
4	D	503	Y70	C9-N8	-3.41	1.33	1.40
4	B	505	Y70	C9-N8	-3.36	1.33	1.40
4	B	505	Y70	C7-N8	-3.29	1.33	1.40
4	B	505	Y70	C18-C17	2.32	1.55	1.50

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	505	Y70	C17-N16-C15	-4.04	120.98	126.61
4	C	504	Y70	C17-N16-C15	-4.02	121.01	126.61
4	A	504	Y70	C17-N16-C15	-3.79	121.33	126.61
4	D	503	Y70	C17-N16-C15	-3.62	121.57	126.61
4	B	505	Y70	C18-C17-N16	3.53	120.62	116.65
4	A	504	Y70	C18-C17-N16	3.50	120.58	116.65
4	D	503	Y70	C4-C7-N8	3.40	109.66	105.96
4	A	504	Y70	C5-C9-N8	3.32	109.79	105.82
4	C	504	Y70	C4-C7-N8	3.30	109.56	105.96
4	D	503	Y70	C18-C17-N16	3.28	120.33	116.65
4	C	504	Y70	C18-C17-N16	3.26	120.31	116.65
4	B	505	Y70	C4-C7-N8	3.13	109.37	105.96
4	B	505	Y70	C12-C15-N16	3.11	120.43	116.25
4	A	504	Y70	C4-C7-N8	3.10	109.34	105.96
4	B	505	Y70	C5-C9-N8	3.06	109.48	105.82
4	C	504	Y70	C12-C15-N16	3.03	120.32	116.25
4	D	503	Y70	C5-C9-N8	3.02	109.43	105.82
4	D	503	Y70	C12-C15-N16	2.99	120.27	116.25
4	A	504	Y70	C12-C15-N16	2.75	119.95	116.25
2	B	501	SO4	O4-S-O1	-2.61	95.68	109.31
4	C	504	Y70	C5-C9-N8	2.60	108.93	105.82
4	A	504	Y70	C3-C4-C7	2.58	133.84	129.63
4	B	505	Y70	O11-C9-C5	-2.54	125.47	129.09
4	D	503	Y70	C14-C18-C17	-2.52	109.66	114.12
4	C	504	Y70	C5-C4-C7	-2.42	105.87	108.32
4	B	505	Y70	C9-N8-C7	-2.33	108.85	111.53
4	C	504	Y70	O11-C9-C5	-2.32	125.79	129.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	Y70	C5-C4-C7	-2.32	105.98	108.32
4	D	503	Y70	C9-N8-C7	-2.31	108.87	111.53
4	C	504	Y70	C3-C4-C7	2.31	133.40	129.63
4	B	505	Y70	C3-C4-C7	2.30	133.38	129.63
4	A	504	Y70	C9-N8-C7	-2.21	109.00	111.53
4	D	503	Y70	C3-C4-C7	2.15	133.14	129.63
4	D	503	Y70	C5-C4-C7	-2.15	106.15	108.32
4	D	503	Y70	C4-C5-C9	-2.10	105.89	108.15
4	C	504	Y70	C14-C18-C17	-2.10	110.41	114.12
4	A	504	Y70	C4-C5-C9	-2.09	105.90	108.15
4	B	505	Y70	C5-C4-C7	-2.08	106.22	108.32
4	B	505	Y70	C14-C18-C17	-2.06	110.47	114.12
4	B	505	Y70	O13-C7-C4	-2.02	124.76	128.68

There are no chirality outliers.

There are no torsion outliers.

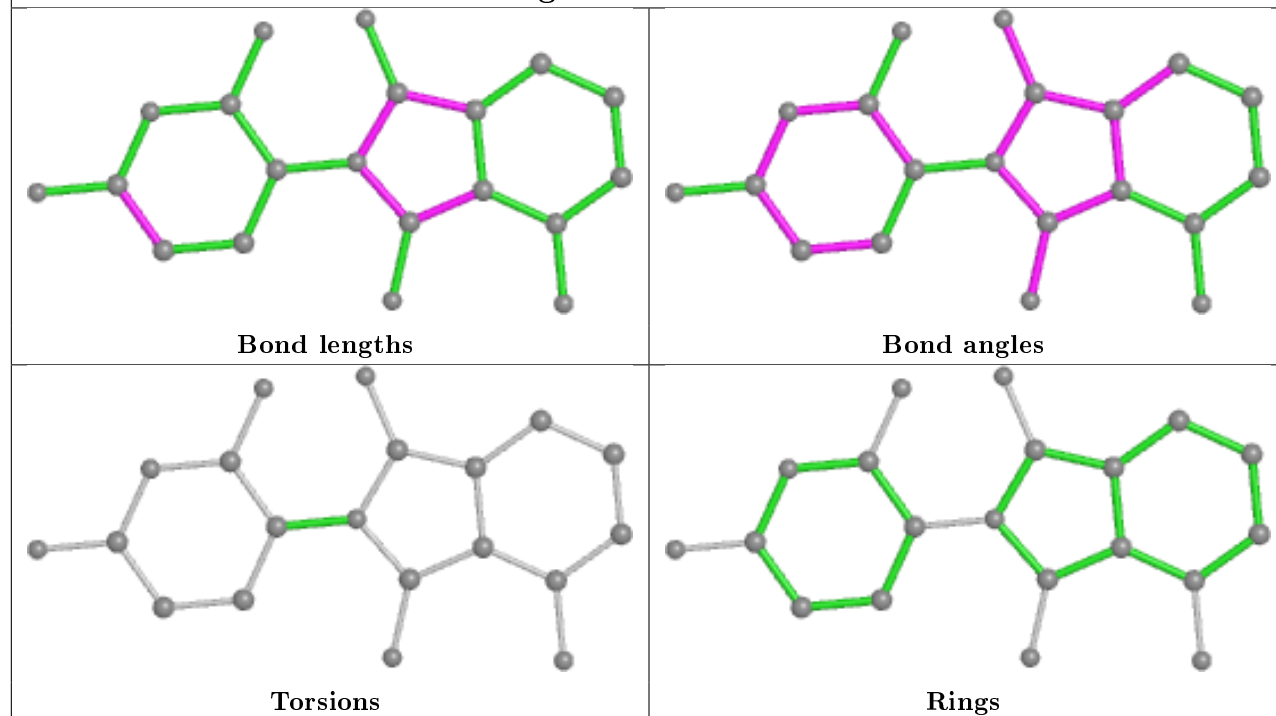
There are no ring outliers.

5 monomers are involved in 5 short contacts:

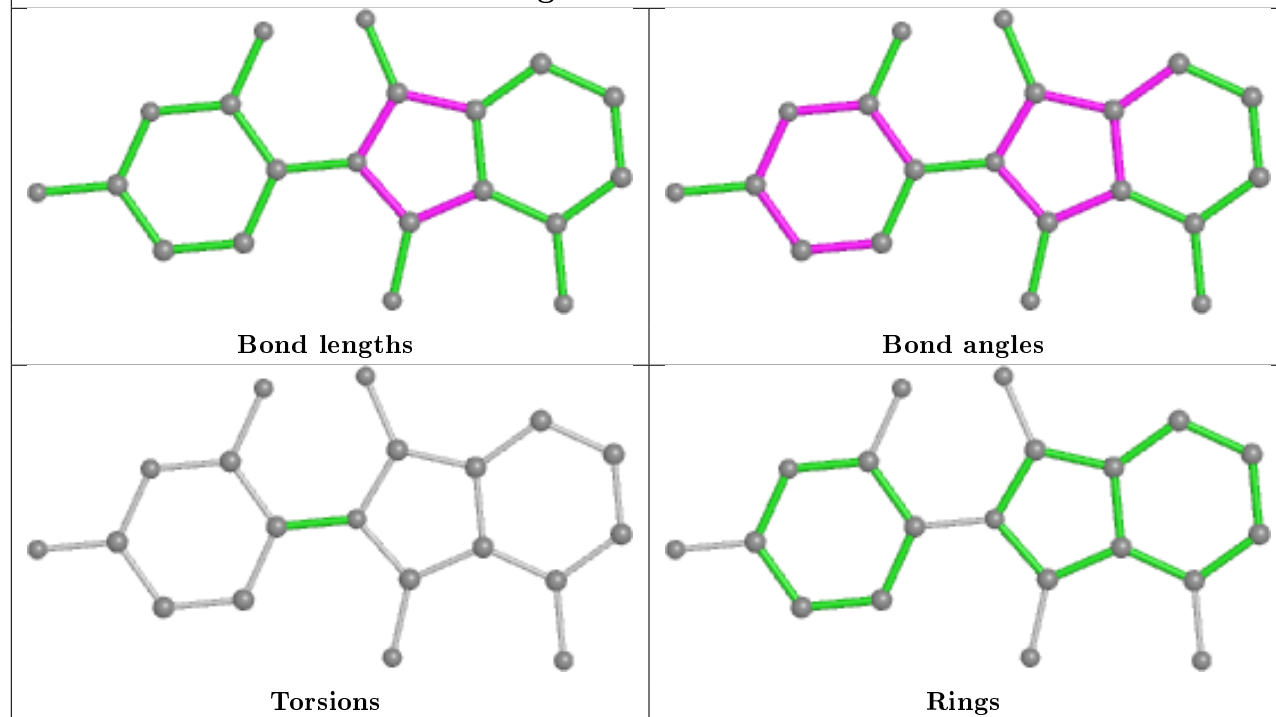
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	D	501	SO4	1	0
2	A	502	SO4	1	0
2	C	501	SO4	1	0
2	B	502	SO4	1	0

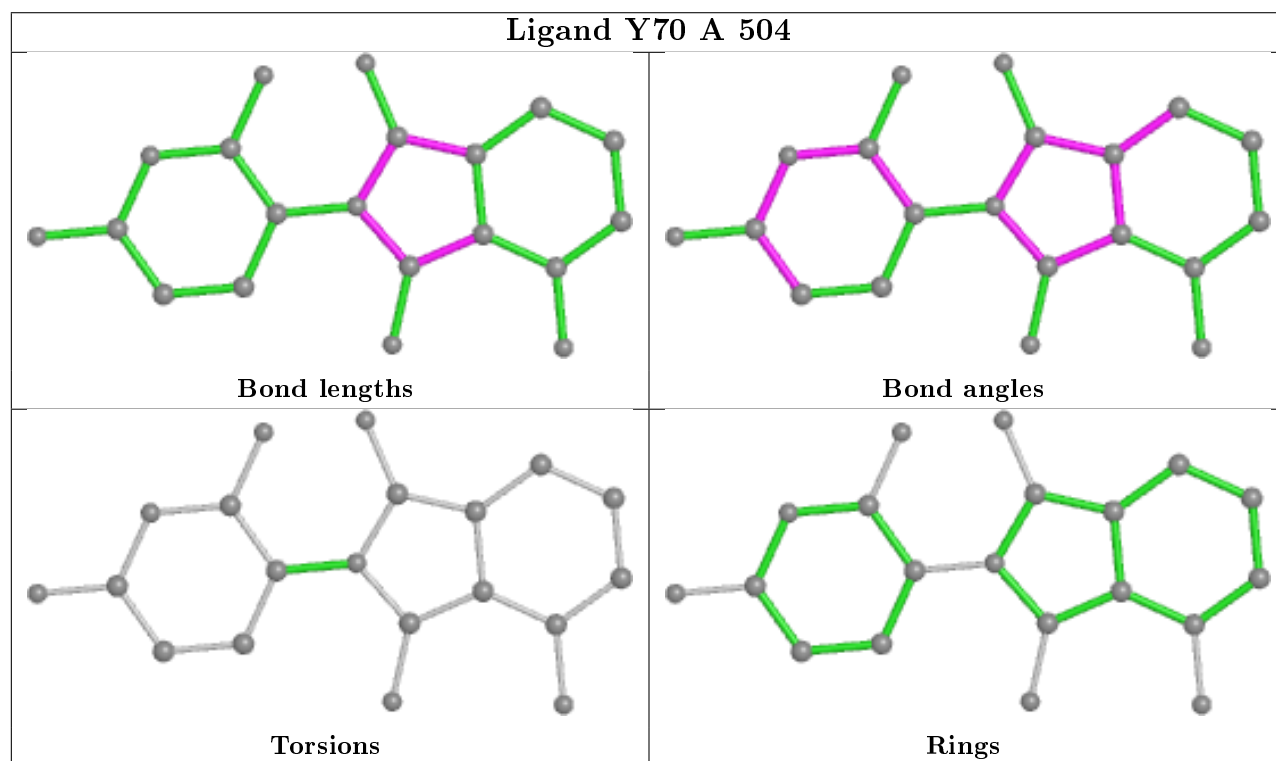
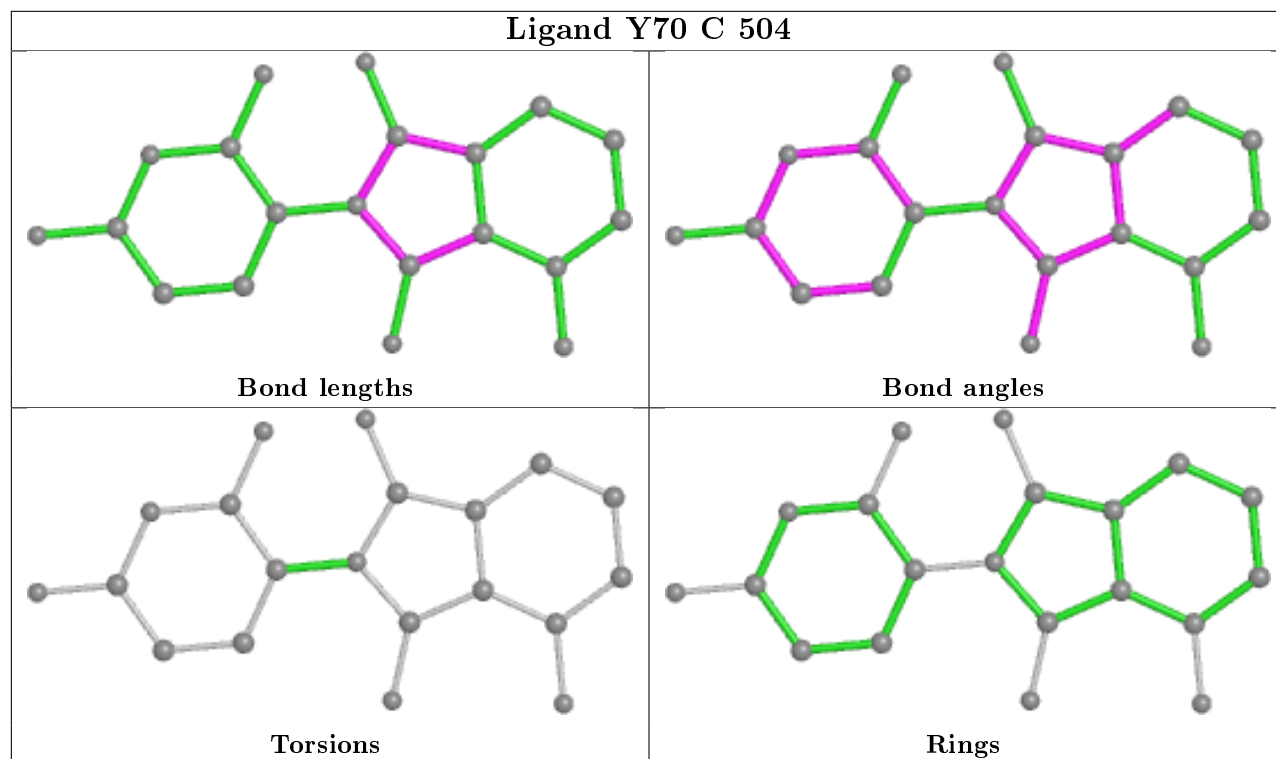
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand Y70 B 505



Ligand Y70 D 503





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

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	90/108 (83%)	0.30	2 (2%) 62 60	17, 26, 50, 65	0
1	B	91/108 (84%)	0.46	6 (6%) 18 17	16, 30, 50, 91	0
1	C	90/108 (83%)	0.48	6 (6%) 17 17	22, 35, 54, 78	0
1	D	90/108 (83%)	0.17	4 (4%) 34 33	14, 23, 50, 69	0
All	All	361/432 (83%)	0.35	18 (4%) 28 28	14, 29, 53, 91	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	THR	9.0
1	A	343	SER	8.7
1	D	343	SER	5.3
1	C	408	LYS	3.2
1	C	321	THR	3.2
1	B	330	GLU	3.1
1	C	375	ARG	3.1
1	B	426	PRO	2.6
1	C	360	GLU	2.5
1	B	375	ARG	2.4
1	B	408	LYS	2.4
1	C	374	GLY	2.4
1	D	426	PRO	2.3
1	B	374	GLY	2.2
1	D	408	LYS	2.1
1	A	374	GLY	2.1
1	D	375	ARG	2.1
1	C	330	GLU	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](#)

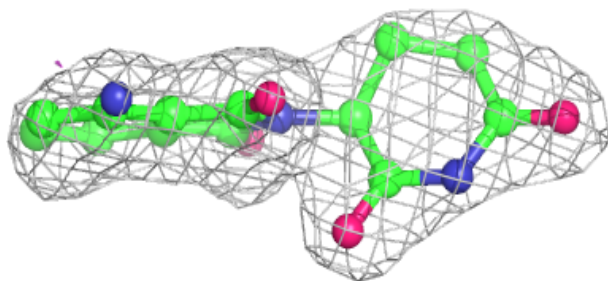
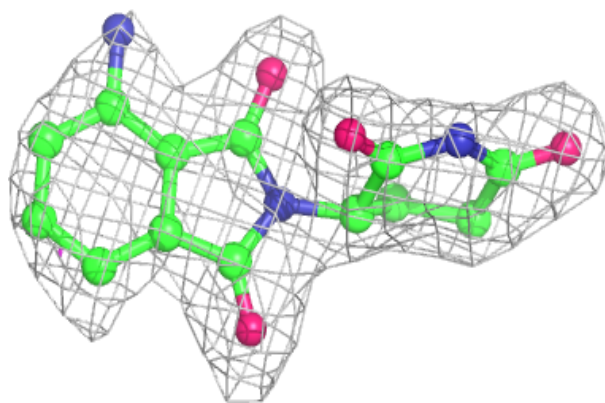
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	Y70	C	504	20/20	0.92	0.18	25,36,50,51	0
4	Y70	B	505	20/20	0.93	0.15	24,35,47,49	0
2	SO4	B	503	5/5	0.94	0.12	57,59,71,71	0
4	Y70	D	503	20/20	0.94	0.12	24,33,46,48	0
3	ZN	C	503	1/1	0.94	0.07	39,39,39,39	0
4	Y70	A	504	20/20	0.94	0.12	24,34,40,44	0
2	SO4	A	501	5/5	0.95	0.14	33,36,37,38	0
2	SO4	D	501	5/5	0.95	0.10	53,55,65,70	0
2	SO4	C	501	5/5	0.97	0.15	28,32,37,49	0
3	ZN	B	504	1/1	0.97	0.08	34,34,34,34	0
2	SO4	B	501	5/5	0.97	0.16	27,30,37,39	0
2	SO4	C	502	5/5	0.99	0.11	19,21,22,32	5
3	ZN	D	502	1/1	0.99	0.06	18,18,18,18	0
2	SO4	B	502	5/5	0.99	0.14	26,28,30,36	0
2	SO4	A	502	5/5	0.99	0.11	25,29,31,35	0
3	ZN	A	503	1/1	0.99	0.07	21,21,21,21	0

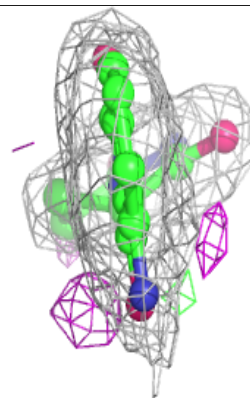
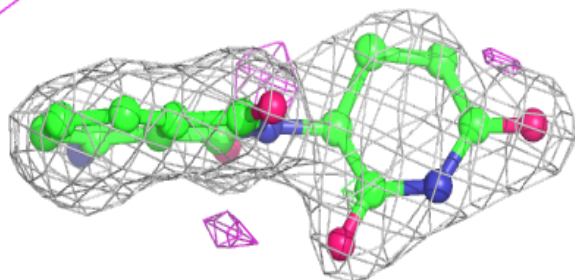
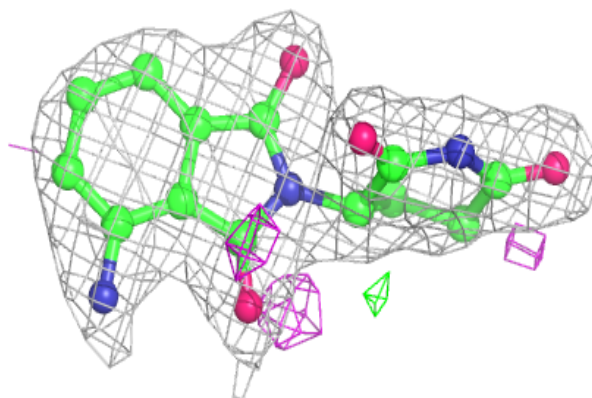
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Y70 C 504:

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

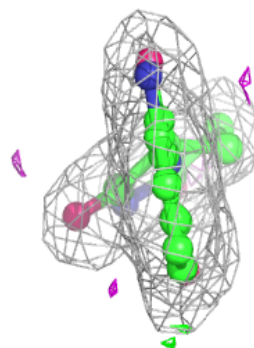
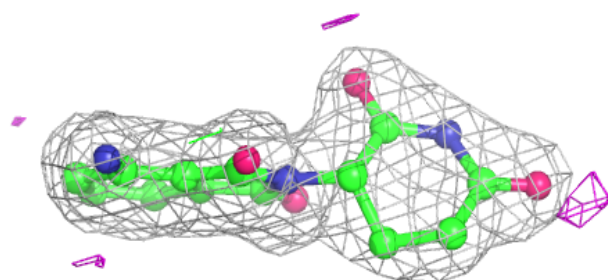
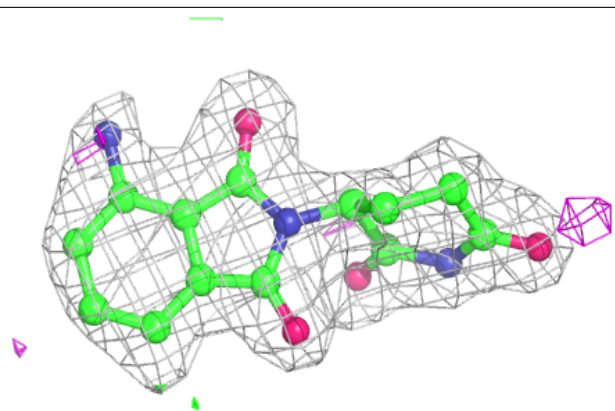
**Electron density around Y70 B 505:**

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

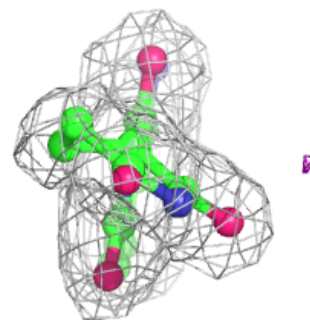
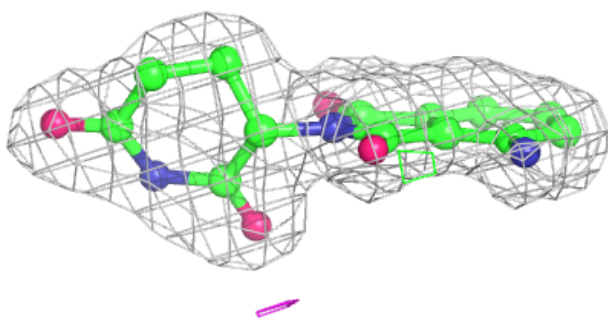
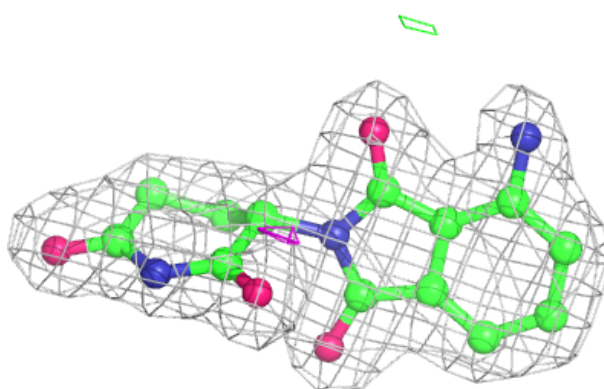


Electron density around Y70 D 503:

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

**Electron density around Y70 A 504:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.