



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:00 PM UTC

PDB ID : 5V3O / pdb_00005v3o
Title : Cereblon in complex with DDB1 and CC-220
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Deposited on : 2017-03-07
Resolution : 3.20 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

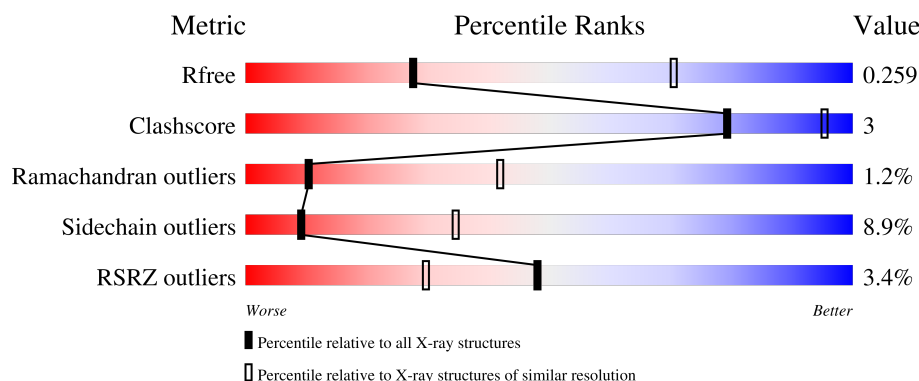
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	1140	3% 83% 11% • 5%
2	C	406	3% 75% 13% • 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ZN	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11175 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1087	Total	C	N	O	S	0	0	0
			8273	5266	1386	1575	46			

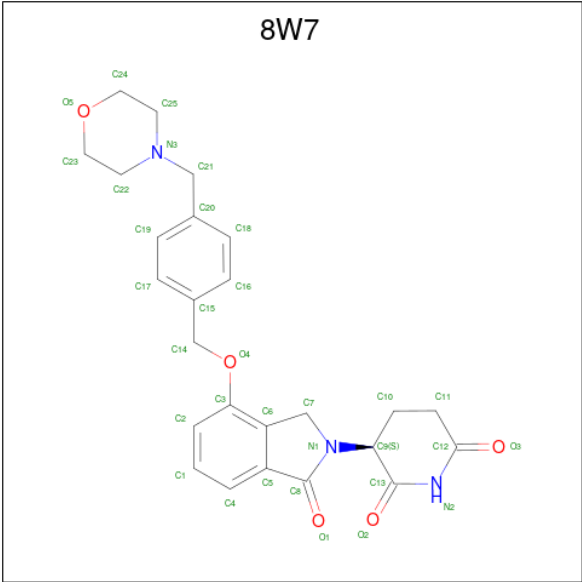
- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	363	Total	C	N	O	S	0	0	0
			2868	1839	487	519	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	GLY	-	expression tag	UNP Q96SW2
C	38	SER	-	expression tag	UNP Q96SW2
C	39	MET	-	expression tag	UNP Q96SW2

- Molecule 3 is (3S)-3-[4-({4-[(morpholin-4-yl)methyl]phenyl}methoxy)-1-oxo-1,3-dihydro-2H-isoindol-2-yl]piperidine-2,6-dione (CCD ID: 8W7) (formula: C₂₅H₂₇N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			33	25	3	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 1: DNA damage-binding protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.03Å 126.89Å 172.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.20 50.01 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.01-3.20) 99.9 (50.01-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.204 , 0.267 0.204 , 0.259	Depositor DCC
R_{free} test set	2023 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	79.3	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11175	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 8W7

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	0.73	0/8421	0.93	13/11439 (0.1%)
2	C	0.71	0/2937	0.94	2/3992 (0.1%)
All	All	0.72	0/11358	0.94	15/15431 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	PRO	CA-N-CD	-8.56	100.02	112.00
1	A	357	GLY	C-N-CD	7.31	136.68	120.60
2	C	410	SER	C-N-CD	7.10	136.22	120.60
1	A	359	ILE	N-CA-C	-6.66	98.05	108.23
1	A	180	PHE	N-CA-C	6.01	118.29	108.55
1	A	205	GLY	CA-C-N	5.80	127.10	119.84
1	A	205	GLY	C-N-CA	5.80	127.10	119.84
1	A	207	TRP	N-CA-C	5.72	116.11	108.38
1	A	484	LYS	N-CA-C	5.58	118.44	110.24
1	A	382	PHE	CB-CA-C	-5.45	103.85	111.80
1	A	561	TRP	N-CA-C	5.27	119.43	112.89
1	A	393	GLY	N-CA-C	5.07	118.38	110.88
2	C	240	TRP	N-CA-C	5.06	116.44	108.55
1	A	356	LEU	N-CA-C	5.04	116.85	111.36
1	A	633	THR	N-CA-C	5.03	118.52	112.38

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	8273	0	8033	41	0
2	C	2868	0	2818	24	0
3	C	33	0	0	0	0
4	C	1	0	0	2	0
All	All	11175	0	10851	60	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 3.

All (60) 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:C:391:CYS:HG	4:C:502:ZN:ZN	0.64	0.96
2:C:326:CYS:SG	2:C:394:CYS:HB3	2.18	0.82
1:A:482:GLU:OE2	1:A:483:PRO:HD2	1.84	0.77
1:A:572:PRO:HD2	1:A:573:SER:H	1.54	0.70
1:A:572:PRO:CD	1:A:573:SER:H	2.05	0.70
1:A:482:GLU:HG3	1:A:483:PRO:HD2	1.82	0.61
1:A:927:MET:HE1	2:C:305:ILE:HB	1.82	0.61
2:C:391:CYS:SG	4:C:502:ZN:ZN	1.79	0.58
2:C:199:LEU:CD1	2:C:237:LEU:HD11	2.37	0.55
1:A:356:LEU:HD21	1:A:712:ILE:HD13	1.89	0.53
1:A:481:GLN:HA	1:A:481:GLN:OE1	2.07	0.53
1:A:382:PHE:O	1:A:383:LYS:CB	2.57	0.53
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.45	0.52
1:A:1032:THR:HG21	1:A:1036:MET:HB3	1.91	0.52
1:A:572:PRO:CD	1:A:573:SER:N	2.71	0.52
1:A:866:VAL:CG1	1:A:884:ILE:HG21	2.39	0.52
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.92	0.52
2:C:250:ALA:HB2	2:C:305:ILE:HD11	1.92	0.51
1:A:338:VAL:O	1:A:340:SER:N	2.43	0.51
1:A:328:LEU:HD21	2:C:237:LEU:HD21	1.92	0.51
1:A:482:GLU:CG	1:A:483:PRO:HD2	2.41	0.50
2:C:383:GLY:HA3	2:C:409:MET:HE1	1.93	0.50
1:A:102:THR:OG1	1:A:1065:VAL:O	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:CYS:SG	2:C:394:CYS:CB	2.92	0.49
2:C:383:GLY:CA	2:C:409:MET:HE1	2.42	0.49
1:A:382:PHE:O	1:A:383:LYS:HB3	2.13	0.48
1:A:134:ARG:HD2	1:A:134:ARG:C	2.38	0.48
1:A:356:LEU:O	1:A:379:SER:HB3	2.14	0.47
2:C:165:PHE:HB2	2:C:182:VAL:HG13	1.95	0.47
2:C:81:ILE:HG22	2:C:120:PHE:HA	1.96	0.47
1:A:20:THR:HG23	1:A:315:THR:HG21	1.96	0.47
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.96	0.47
1:A:374:GLN:NE2	1:A:391:ARG:CB	2.77	0.47
1:A:509:VAL:HG21	1:A:543:ILE:HD13	1.96	0.47
1:A:913:TYR:CE1	2:C:240:TRP:CH2	3.03	0.47
2:C:394:CYS:O	2:C:395:ALA:HB3	2.15	0.46
2:C:199:LEU:HD13	2:C:237:LEU:HD11	1.97	0.46
2:C:290:ILE:O	2:C:419:ARG:NH2	2.46	0.46
2:C:172:THR:HA	2:C:178:GLN:HA	1.99	0.45
2:C:67:PHE:CZ	2:C:114:ILE:HG23	2.52	0.44
1:A:722:ARG:NH1	2:C:238:THR:O	2.50	0.44
1:A:532:THR:OG1	1:A:533:GLU:N	2.51	0.43
1:A:482:GLU:CD	1:A:483:PRO:HD2	2.44	0.43
1:A:257:THR:HB	1:A:276:MET:CE	2.49	0.43
1:A:10:GLN:HB3	1:A:1037:ILE:HB	1.99	0.43
1:A:695:ASN:OD1	1:A:695:ASN:C	2.62	0.42
2:C:359:THR:HG21	2:C:380:TRP:CZ3	2.54	0.42
1:A:374:GLN:HE21	1:A:391:ARG:CB	2.32	0.42
1:A:710:LEU:HD23	1:A:710:LEU:HA	1.87	0.42
1:A:913:TYR:CE1	2:C:240:TRP:HH2	2.37	0.42
1:A:317:LEU:O	1:A:318:ASP:HB2	2.20	0.41
2:C:406:LYS:HE3	2:C:409:MET:HE3	2.02	0.41
2:C:367:ASN:HA	2:C:392:LYS:HE3	2.02	0.41
1:A:64:MET:HG3	1:A:77:LEU:HD11	2.02	0.41
1:A:118:THR:HB	1:A:134:ARG:HH22	1.85	0.41
1:A:480:SER:OG	1:A:484:LYS:HA	2.20	0.41
1:A:572:PRO:CG	1:A:573:SER:N	2.83	0.40
1:A:670:ASN:HB3	1:A:1014:MET:HE2	2.03	0.40
1:A:43:VAL:HG23	1:A:52:VAL:HG21	2.02	0.40
2:C:398:ILE:O	2:C:418:THR:HG22	2.22	0.40

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	1067/1140 (94%)	992 (93%)	60 (6%)	15 (1%)	9	39
2	C	355/406 (87%)	330 (93%)	23 (6%)	2 (1%)	21	56
All	All	1422/1546 (92%)	1322 (93%)	83 (6%)	17 (1%)	10	42

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	PRO
1	A	572	PRO
1	A	255	GLN
1	A	339	ASP
1	A	383	LYS
1	A	1090	ASP
1	A	761	LEU
2	C	68	HIS
2	C	392	LYS
1	A	36	ASN
1	A	297	LEU
1	A	524	GLN
1	A	632	GLY
1	A	768	SER
1	A	951	PRO
1	A	242	GLY
1	A	1065	VAL

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	883/999 (88%)	809 (92%)	74 (8%)	10	38
2	C	312/368 (85%)	280 (90%)	32 (10%)	7	28
All	All	1195/1367 (87%)	1089 (91%)	106 (9%)	9	34

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	19	VAL
1	A	118	THR
1	A	120	ILE
1	A	125	ASP
1	A	129	ARG
1	A	134	ARG
1	A	147	ARG
1	A	189	HIS
1	A	190	VAL
1	A	197	LEU
1	A	198	ARG
1	A	212	VAL
1	A	213	GLU
1	A	238	THR
1	A	255	GLN
1	A	257	THR
1	A	318	ASP
1	A	351	GLU
1	A	360	VAL
1	A	410	LEU
1	A	452	VAL
1	A	483	PRO
1	A	496	LYS
1	A	519	LEU
1	A	525	GLU
1	A	526	LEU
1	A	531	HIS
1	A	532	THR
1	A	534	MET
1	A	538	VAL
1	A	555	LEU
1	A	558	ILE
1	A	564	ILE

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Mol	Chain	Res	Type
1	A	565	SER
1	A	572	PRO
1	A	582	LEU
1	A	587	ILE
1	A	594	THR
1	A	598	SER
1	A	611	LEU
1	A	626	ARG
1	A	631	LEU
1	A	639	ARG
1	A	693	LEU
1	A	698	THR
1	A	728	GLU
1	A	738	SER
1	A	766	SER
1	A	800	GLU
1	A	815	SER
1	A	820	LYS
1	A	839	GLU
1	A	864	LYS
1	A	874	VAL
1	A	895	THR
1	A	927	MET
1	A	929	SER
1	A	930	VAL
1	A	947	ARG
1	A	957	VAL
1	A	988	GLU
1	A	991	HIS
1	A	993	GLN
1	A	1008	CYS
1	A	1032	THR
1	A	1052	LEU
1	A	1061	VAL
1	A	1064	SER
1	A	1086	THR
1	A	1100	ILE
1	A	1112	LEU
1	A	1122	ARG
1	A	1131	LYS
2	C	48	ASN
2	C	80	VAL

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Mol	Chain	Res	Type
2	C	81	ILE
2	C	91	LEU
2	C	96	THR
2	C	105	GLN
2	C	113	LEU
2	C	145	ARG
2	C	148	GLN
2	C	154	ILE
2	C	169	GLU
2	C	172	THR
2	C	182	VAL
2	C	183	GLN
2	C	189	VAL
2	C	221	TYR
2	C	246	SER
2	C	260	GLN
2	C	275	SER
2	C	283	ARG
2	C	284	VAL
2	C	293	VAL
2	C	295	ARG
2	C	299	LEU
2	C	303	SER
2	C	342	LEU
2	C	350	VAL
2	C	359	THR
2	C	364	LYS
2	C	371	ILE
2	C	373	ARG
2	C	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	397	HIS
1	A	520	GLN
1	A	600	HIS
1	A	907	ASN
1	A	1056	ASN
1	A	1059	ASN
1	A	1111	ASN

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Mol	Chain	Res	Type
2	C	73	HIS
2	C	115	GLN
2	C	228	GLN
2	C	233	HIS
2	C	236	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
3	8W7	C	501	-	37,37,37	1.44	3 (8%)	50,52,52	2.14	11 (22%)

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
3	8W7	C	501	-	-	3/13/46/46	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	8W7	C5-C8	-5.47	1.40	1.48
3	C	501	8W7	C14-C15	-4.63	1.39	1.50
3	C	501	8W7	C8-N1	-2.38	1.33	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	8W7	C5-C8-N1	8.18	111.62	106.42
3	C	501	8W7	C7-N1-C8	-5.94	110.64	113.15
3	C	501	8W7	C12-N2-C13	-4.18	121.18	126.69
3	C	501	8W7	O4-C14-C15	4.07	121.11	109.16
3	C	501	8W7	C10-C9-N1	-3.82	109.85	114.03
3	C	501	8W7	C11-C12-N2	3.52	120.44	116.69
3	C	501	8W7	C9-C13-N2	3.26	120.99	116.24
3	C	501	8W7	C9-N1-C8	2.39	125.50	121.86
3	C	501	8W7	O1-C8-C5	-2.34	124.14	128.66
3	C	501	8W7	O4-C3-C6	2.27	118.91	115.75
3	C	501	8W7	C4-C5-C8	2.14	133.17	129.59

There are no chirality outliers.

All (3) torsion outliers are listed below:

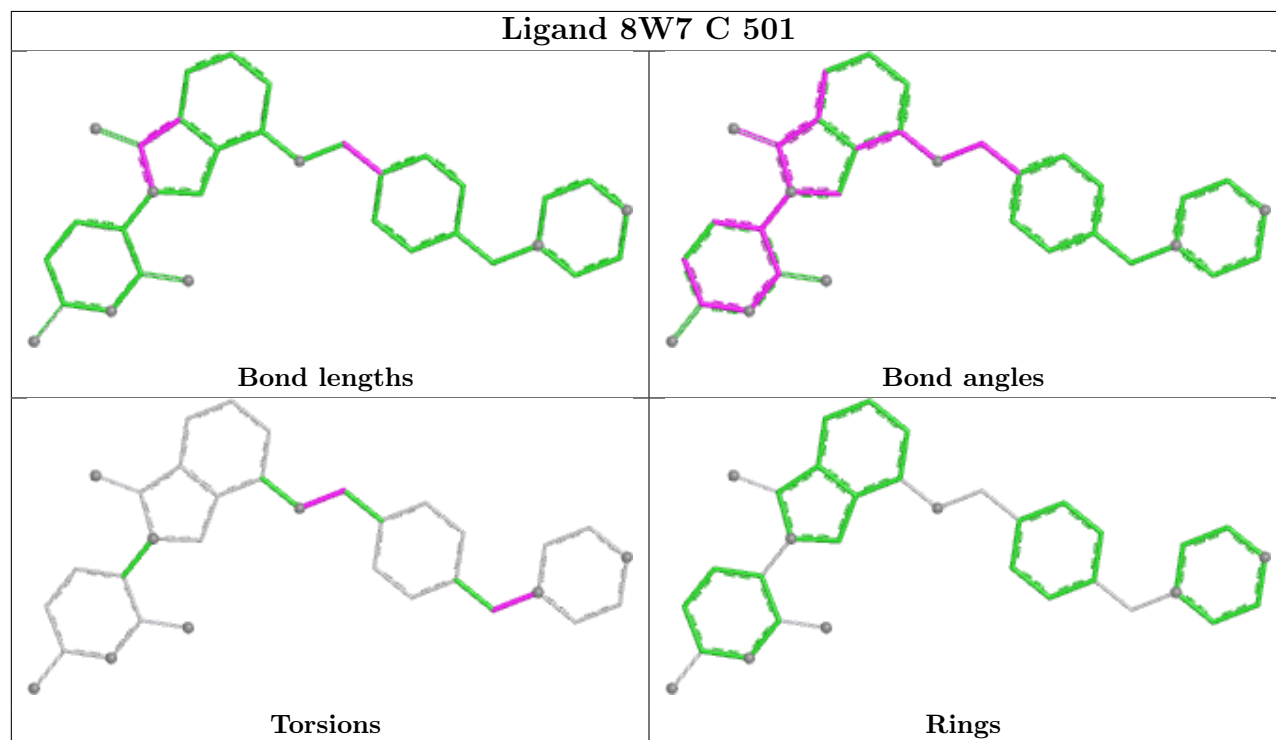
Mol	Chain	Res	Type	Atoms
3	C	501	8W7	C20-C21-N3-C25
3	C	501	8W7	C15-C14-O4-C3
3	C	501	8W7	C20-C21-N3-C22

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 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 [i](#)

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	1087/1140 (95%)	0.08	39 (3%)	46 28	32, 95, 147, 172	2 (0%)
2	C	363/406 (89%)	0.06	11 (3%)	52 33	64, 92, 147, 196	0
All	All	1450/1546 (93%)	0.07	50 (3%)	48 30	32, 94, 147, 196	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	270	ASP	5.3
1	A	475	SER	5.2
2	C	126	SER	5.1
1	A	279	ARG	4.9
1	A	744	ASP	4.6
1	A	535	GLU	4.3
1	A	341	ASN	4.1
1	A	340	SER	3.8
1	A	578	HIS	3.7
1	A	551	GLY	3.5
2	C	271	ASP	3.4
1	A	539	ALA	3.3
1	A	769	LYS	3.3
1	A	338	VAL	3.2
1	A	339	ASP	3.2
2	C	204	LYS	3.1
1	A	296	THR	3.1
1	A	618	ILE	3.1
1	A	572	PRO	2.9
1	A	855	ASP	2.9
1	A	563	ASP	2.8
1	A	211	ASN	2.8
1	A	784	GLU	2.7
2	C	318	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	574	PHE	2.6
1	A	576	LEU	2.6
1	A	536	HIS	2.6
1	A	620	THR	2.5
2	C	150	PHE	2.5
1	A	1014	MET	2.5
1	A	573	SER	2.4
1	A	1113	GLN	2.4
1	A	706	GLU	2.4
1	A	252	ILE	2.3
1	A	856	GLY	2.3
2	C	210	SER	2.3
1	A	575	GLU	2.2
1	A	251	PRO	2.2
1	A	403	ASP	2.2
2	C	68	HIS	2.1
1	A	634	GLN	2.1
2	C	152	ILE	2.1
1	A	1081	LYS	2.1
2	C	175	ASP	2.1
1	A	529	ILE	2.1
1	A	1063	LYS	2.0
1	A	486	LEU	2.0
1	A	896	GLU	2.0
1	A	1123	GLU	2.0
2	C	47	ILE	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](#)

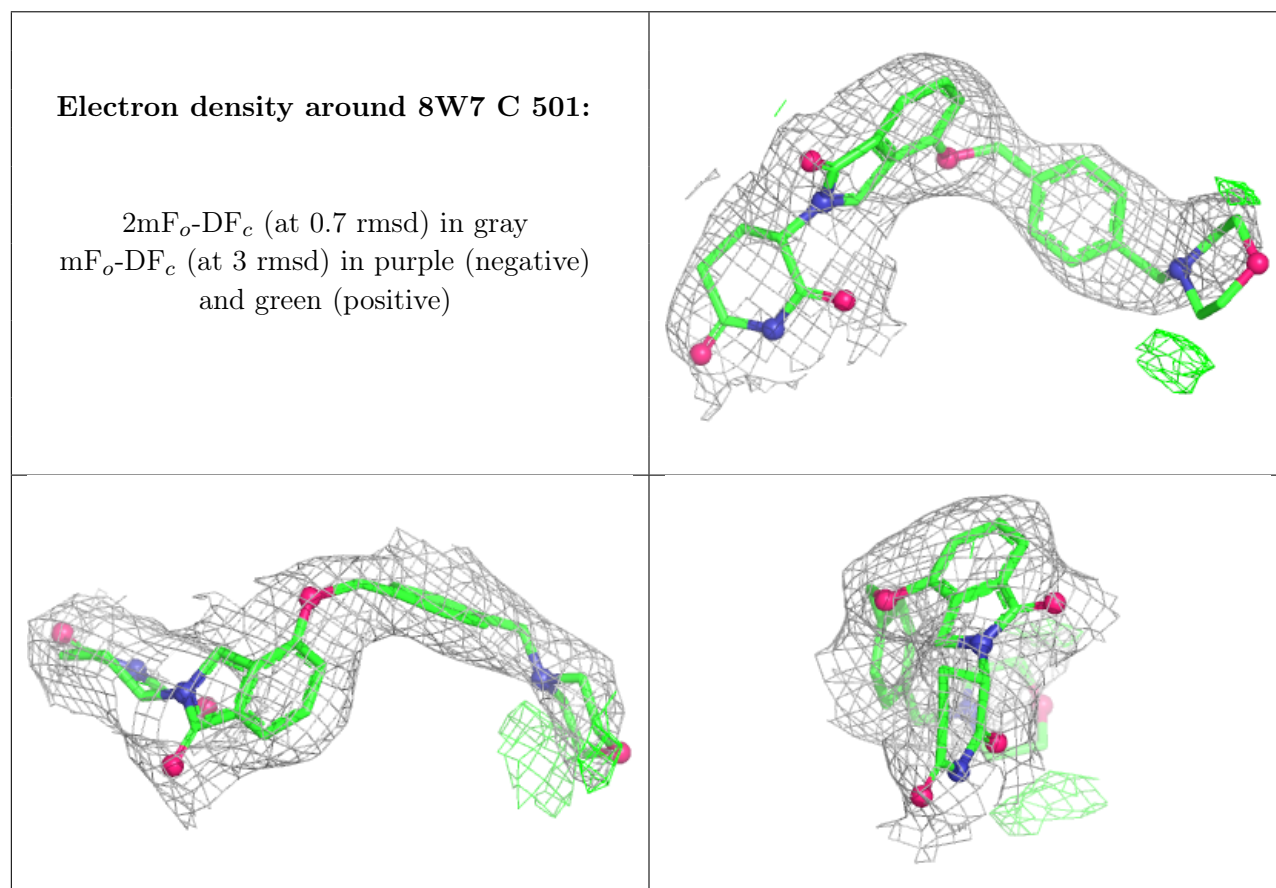
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	8W7	C	501	33/33	0.91	0.15	75,89,162,167	0
4	ZN	C	502	1/1	0.98	0.04	104,104,104,104	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.