



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:42 PM UTC

PDB ID : 5HXB / pdb_00005hxb
Title : Cereblon in complex with DDB1, CC-885, and GSPT1
Authors : Chamberlain, P.P.; Matyskiela, M.; Pagarigan, B.
Deposited on : 2016-01-30
Resolution : 3.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

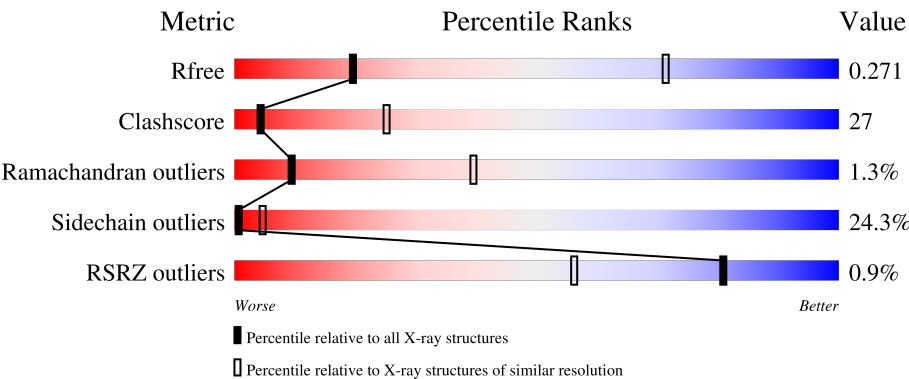
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	199	% 33%39%23%. .
1	X	199	% 28%41%21%9%. .
2	B	1140	% 49%36%9%. 6%
2	Y	1140	% 49%36%9%. 5%
3	C	406	% 47%35%9%. 9%

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Mol	Chain	Length	Quality of chain
3	Z	406	 % 46% 37% 9% • 6%

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	501	-	-	X	-
5	85C	Z	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25089 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 Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	195	Total	C	N	O	S	0	0	0
			1481	941	254	275	11			
1	A	196	Total	C	N	O	S	0	0	0
			1441	919	245	267	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	436	GLY	-	expression tag	UNP P15170
X	437	SER	-	expression tag	UNP P15170
A	436	GLY	-	expression tag	UNP P15170
A	437	SER	-	expression tag	UNP P15170

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	1080	Total	C	N	O	S	0	0	0
			8178	5215	1369	1550	44			
2	B	1075	Total	C	N	O	S	0	0	0
			8096	5164	1351	1536	45			

- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	380	Total	C	N	O	S	0	0	0
			2960	1891	502	544	23			
3	C	370	Total	C	N	O	S	0	0	0
			2869	1835	485	526	23			

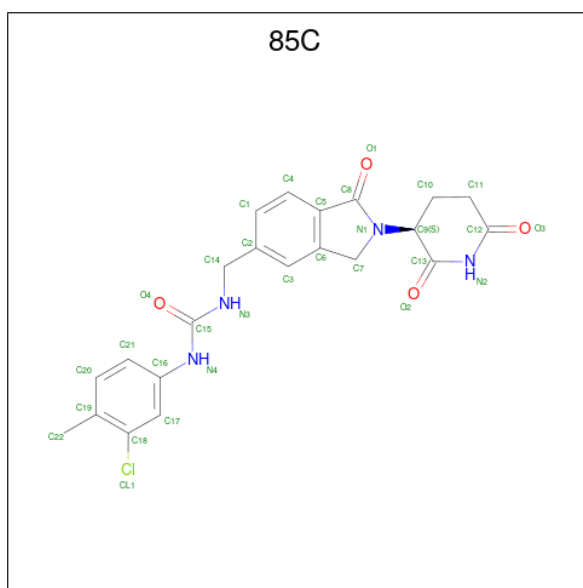
There are 6 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 5 is 1-(3-chloro-4-methylphenyl)-3-({2-[(3S)-2,6-dioxopiperidin-3-yl]-1-oxo-2,3-dihydro-1H-isindol-5-yl}methyl)urea (CCD ID: 85C) (formula: C₂₂H₂₁ClN₄O₄).

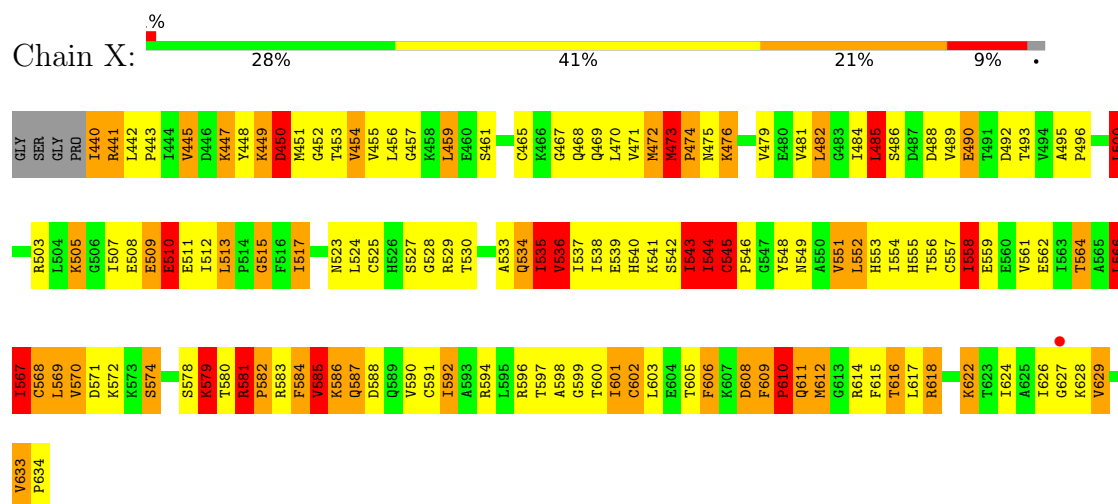


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Z	1	Total C Cl N O 31 22 1 4 4	0	0
5	C	1	Total C Cl N O 31 22 1 4 4	0	0

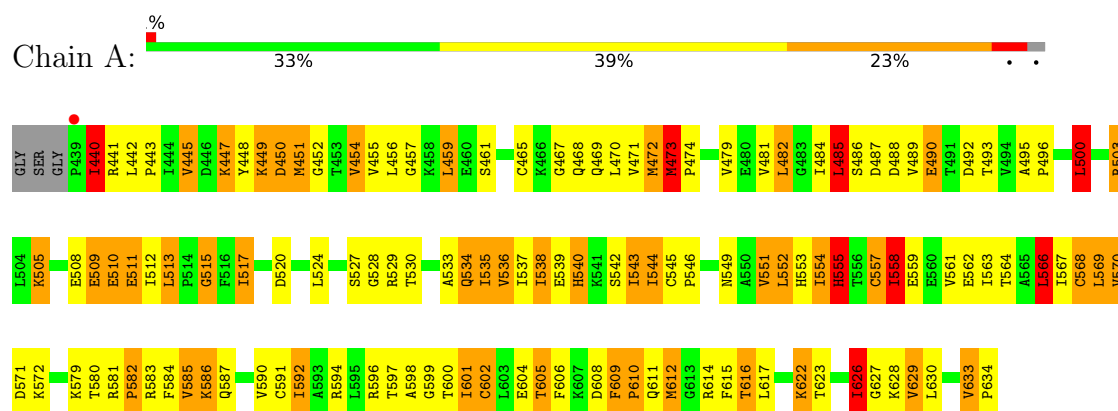
3 Residue-property plots

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 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.

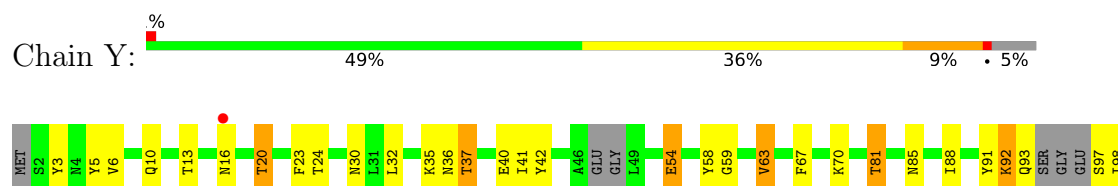
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

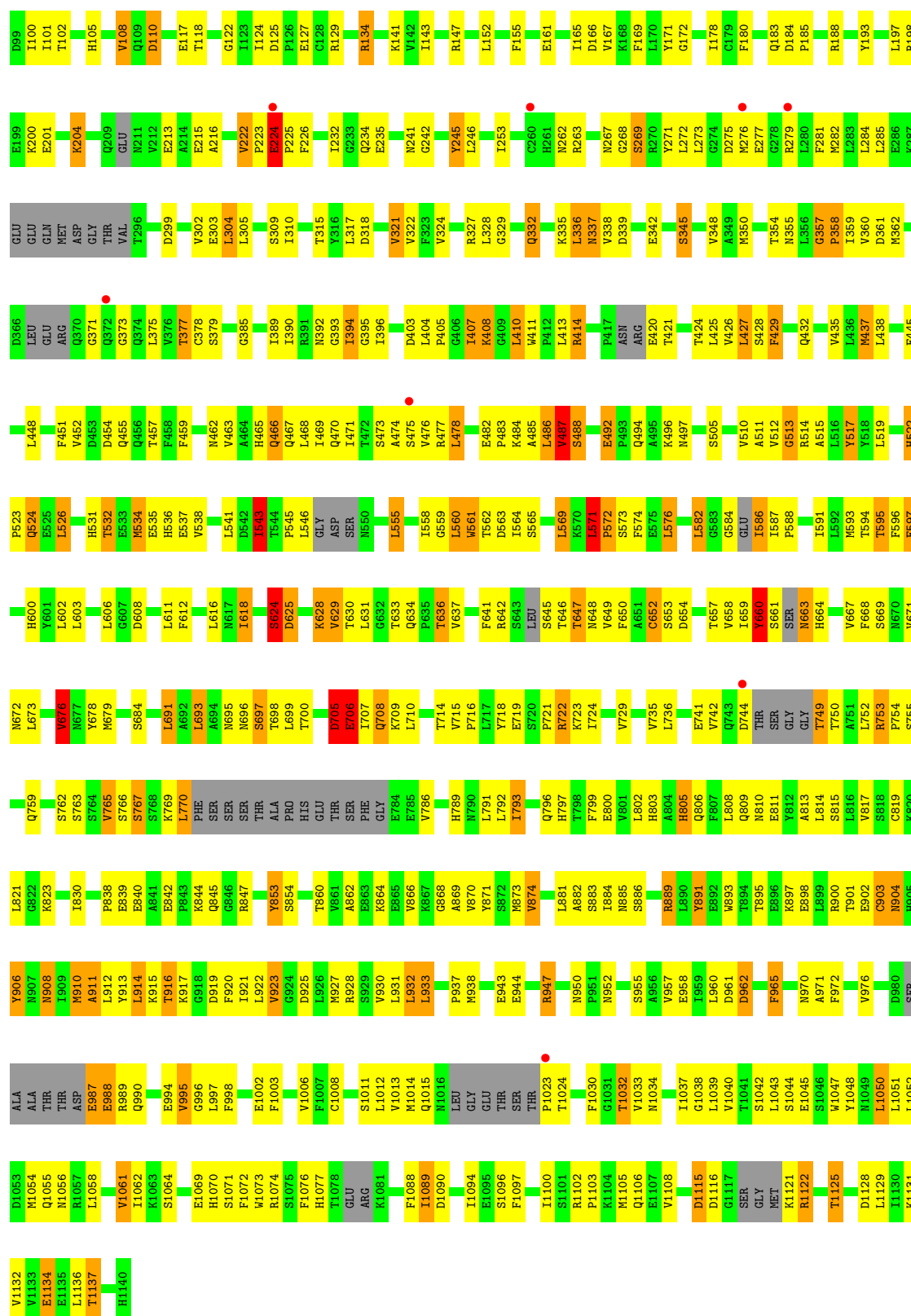


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



- Molecule 2: DNA damage-binding protein 1





• Molecule 2: DNA damage-binding protein 1



L1136	M1054	ALA	E840	S766	Y678	L611	H536	A464	L304	L101	MET
T1137	Q1055	THR	A441	S767	M679	F612	E537	H465	L305	T102	S2
H1140	L1058	ASP	E842	S768	S684		V538	Q466			Y3
		THR	P843	L770	L691	L616	L541	Q467	S309	V108	N4
	I1062	E987	K844	PHE	A692	N617	D542	L468	I310	D10	Y5
	K1083	E988	G846	SER	E693	E618	E543	L469	T315	E17	V6
	S1064	R889	R847	SER	L693	E619	E544	Q470	T316	T118	V7
		Q990	E848	SER	A694	T620	T544	L471	T317	G19	Q10
		H991	T648	THR	N695	T620	L546	L472	D318		T13
	E1069	L992	V849	ALA	N696	L623	A474	S473	L404		
	H1070	G924		PRO	S697	S624	A475	A474	V321	G122	N16
	S1071	Q993	H853	THR	R898	D625	V476	Q405	V322		T20
	F1072	E994	S854	HIS	T700	R626	R477	G406	V322	D125	
	W1073	G996	T860	GLU	L699	R627	L478	I407	F323	F126	
	R1074	L997		THR	T700	K628	V479	Q408	V324	E127	T24
	S1075	F998		SER		V629	G128	G409	R327	R129	
	H1076	V930	E863	PHE	Q708	T630	G129	L410	R328		N30
	F1077	L931	K864	GLY	K709	G559	Q481	G129	R328		L31
	T1078	L932	E865	E784	L631	L560	E482	G129	R328		L32
	GLU	L933	V866	E785	G632	W561	P483	G129	Q332	R134	N36
	ARG		R867		T633	T562	K484	G129	VAL		T37
	K1081		G868		P635	I564	L486	G129	ASP	L152	E40
			A869		T636		V487	G129	ASN	F155	I41
	F1088		H871		V637		S488	G129	ARG	Y42	Y42
	I1089		S872		R642		E492	G129	ASN		
	D1090		M873		S643		P493	G129	GLU	E161	A46
	L1093		E874		LEU		Q494	G129	Q343	I165	GLU
	I1094		N877		S645		K495	G129	R270	D166	GLY
	S1096		L881		T646		K496	G129	G344	L49	L49
	F1097		L802		T647			G129	S345	F169	E54
			L803		T648		A501	G129	V348	L170	Y58
	I1100		A882		T649		S502	G129	M350	G172	G59
	R1101		S883		F650		S505	G129	T354	I178	V63
	P1103		L884		R652		V510	G129	N355	F180	K70
	K1104		T885		A651		V512	G129	G357	Q183	T81
			S886		G652		G513	G129	P358	D184	N85
	M1105		L889		S653		R514	G129	I359	P185	L88
	Q1106		E890		D654		P588	G129	V360	Y193	Y91
			R889		T657		L591	G129	D361	L197	Q93
	D1115		T893		V658		L519	G129	M362	E201	SER
	D1116		T894		N663		T594	G129	LEU	Q209	GLY
	G1117		T895		H664		F596	G129	GLN	E210	S97
	SER		E896		L666		E597	G129	MET	A216	D99
	GLY		K897		V667		S598	G129	ASP	S217	I100
	GLY		E898		P668			G129	GLY		
	GLY		L899		P669			G129	THR		
	GLY		R900		N670			G129	VAL		
	GLY		T901		V671			G129	T296		
	GLY		E902		L602			G129	D299		
	GLY		C903		L603			G129	V302		
	GLY		N904					G129	C378		
	GLY		N907					G129	S379		
	GLY		N908					G129			
	GLY		N909					G129			
	GLY		N910					G129			
	GLY		N911					G129			
	GLY		N912					G129			
	GLY		N913					G129			
	GLY		N914					G129			
	GLY		N915					G129			
	GLY		N916					G129			
	GLY		N917					G129			
	GLY		N918					G129			
	GLY		N919					G129			
	GLY		N920					G129			
	GLY		N921					G129			
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	GLY		N927					G129			
	GLY		N928					G129			
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	GLY		N930					G129			
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	GLY		N1001					G129			
	GLY		N1002					G129			
	GLY		N1003					G129			
	GLY		N1004					G129			
	GLY		N1005					G129			
	GLY		N1006					G129			
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	GLY		N1009					G129			
	GLY		N1010					G129			
	GLY		N1011					G129			
	GLY		N1012					G129			
	GLY		N1013					G129			
	GLY		N1014					G129			
	GLY		N1015					G129			
	GLY		N1016					G129			
	GLY		N1017					G129			
	GLY		N1018					G129			
	GLY		N1019					G129			
	GLY		N1020					G129			
	GLY		N1021					G129			
	GLY		N1022					G129			
	GLY		N1023					G129			
	GLY		N1024					G129			
	GLY		N1025					G129			
	GLY		N1026					G129			
	GLY		N1027					G129			
	GLY		N1028					G129			
	GLY		N1029					G129			

Chain Z:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 111.52Å 175.06Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-3.60) 94.4 (50.00-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.271	Depositor DCC
R_{free} test set	3289 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25089	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% 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: 85C, ZN

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	1.28	6/1463 (0.4%)	1.24	16/1987 (0.8%)
1	X	1.35	7/1502 (0.5%)	1.37	19/2032 (0.9%)
2	B	1.14	21/8235 (0.3%)	1.13	28/11187 (0.3%)
2	Y	1.15	17/8319 (0.2%)	1.14	29/11295 (0.3%)
3	C	1.08	5/2937 (0.2%)	1.16	15/4003 (0.4%)
3	Z	1.12	6/3030 (0.2%)	1.20	15/4125 (0.4%)
All	All	1.16	62/25486 (0.2%)	1.17	122/34629 (0.4%)

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	13
1	X	0	16
2	B	0	17
2	Y	0	19
3	C	0	5
3	Z	0	5
All	All	0	75

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	676	VAL	C-O	-8.93	1.14	1.24
2	Y	624	SER	C-O	8.64	1.30	1.24
2	B	676	VAL	C-O	-8.11	1.15	1.24
2	Y	769	LYS	CA-C	7.75	1.62	1.53
2	B	669	SER	CA-C	-7.55	1.44	1.52

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	606	PHE	N-CA-C	-12.43	95.12	110.41
1	X	510	GLU	N-CA-C	-11.94	92.26	108.74
2	Y	576	LEU	N-CA-C	10.62	122.44	111.07
2	Y	767	SER	N-CA-C	9.79	123.95	109.07
1	A	555	HIS	CB-CA-C	-9.67	103.12	115.89

There are no chirality outliers.

5 of 75 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	472	MET	Peptide
1	X	473	MET	Peptide
1	X	500	LEU	Peptide
1	X	509	GLU	Peptide
1	X	515	GLY	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	1441	0	1439	160	2
1	X	1481	0	1519	216	0
2	B	8096	0	7807	358	0
2	Y	8178	0	7930	358	0
3	C	2869	0	2758	131	0
3	Z	2960	0	2851	151	2
4	C	1	0	0	2	0
4	Z	1	0	0	0	0
5	C	31	0	0	4	0
5	Z	31	0	0	10	0
All	All	25089	0	24304	1326	2

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 27.

The worst 5 of 1326 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:X:606:PHE:CD2	1:X:628:LYS:HG2	1.44	1.49
1:A:606:PHE:CE2	1:A:628:LYS:HG2	1.50	1.47
1:A:606:PHE:CD2	1:A:628:LYS:HG2	1.48	1.45
1:X:606:PHE:CE2	1:X:628:LYS:HG2	1.64	1.30
3:Z:352:PRO:HG3	3:Z:378:HIS:ND1	1.44	1.29

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:103:HIS:CD2	1:A:542:SER:OG[2_546]	2.05	0.15
3:Z:116:LYS:CB	1:A:448:TYR:CB[1_544]	2.18	0.02

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	194/199 (98%)	155 (80%)	30 (16%)	9 (5%)	2	17
1	X	193/199 (97%)	152 (79%)	33 (17%)	8 (4%)	2	19
2	B	1039/1140 (91%)	955 (92%)	76 (7%)	8 (1%)	16	49
2	Y	1046/1140 (92%)	959 (92%)	78 (8%)	9 (1%)	14	46
3	C	360/406 (89%)	322 (89%)	32 (9%)	6 (2%)	7	35
3	Z	372/406 (92%)	332 (89%)	37 (10%)	3 (1%)	16	49
All	All	3204/3490 (92%)	2875 (90%)	286 (9%)	43 (1%)	9	39

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	474	PRO
1	X	610	PRO
2	Y	224	GLU

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Mol	Chain	Res	Type
2	Y	358	PRO
2	Y	483	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	153/175 (87%)	110 (72%)	43 (28%)	0	3
1	X	165/175 (94%)	111 (67%)	54 (33%)	0	2
2	B	855/999 (86%)	670 (78%)	185 (22%)	1	7
2	Y	868/999 (87%)	674 (78%)	194 (22%)	1	6
3	C	306/368 (83%)	220 (72%)	86 (28%)	0	3
3	Z	316/368 (86%)	232 (73%)	84 (27%)	0	3
All	All	2663/3084 (86%)	2017 (76%)	646 (24%)	1	5

5 of 646 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	854	SER
3	C	301	ILE
2	B	904	ASN
2	B	845	GLN
3	C	64	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	803	HIS
3	C	95	GLN
2	B	852	GLN
2	B	1055	GLN
3	C	206	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	85C	Z	502	-	34,34,34	1.51	3 (8%)	49,49,49	2.34	11 (22%)
5	85C	C	502	-	34,34,34	1.54	3 (8%)	49,49,49	2.32	12 (24%)

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	85C	Z	502	-	-	2/13/38/38	0/4/4/4
5	85C	C	502	-	-	1/13/38/38	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	85C	C5-C8	-5.86	1.39	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Z	502	85C	C5-C8	-5.42	1.40	1.48
5	Z	502	85C	C16-N4	-4.24	1.33	1.41
5	C	502	85C	C16-N4	-3.95	1.33	1.41
5	C	502	85C	C8-N1	-3.37	1.32	1.36

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	502	85C	C5-C8-N1	8.19	111.63	106.42
5	C	502	85C	C7-N1-C8	-8.05	109.76	113.15
5	Z	502	85C	C7-N1-C8	-7.25	110.09	113.15
5	C	502	85C	C5-C8-N1	7.09	110.93	106.42
5	C	502	85C	C10-C9-N1	-4.53	109.07	114.03

There are no chirality outliers.

All (3) torsion outliers are listed below:

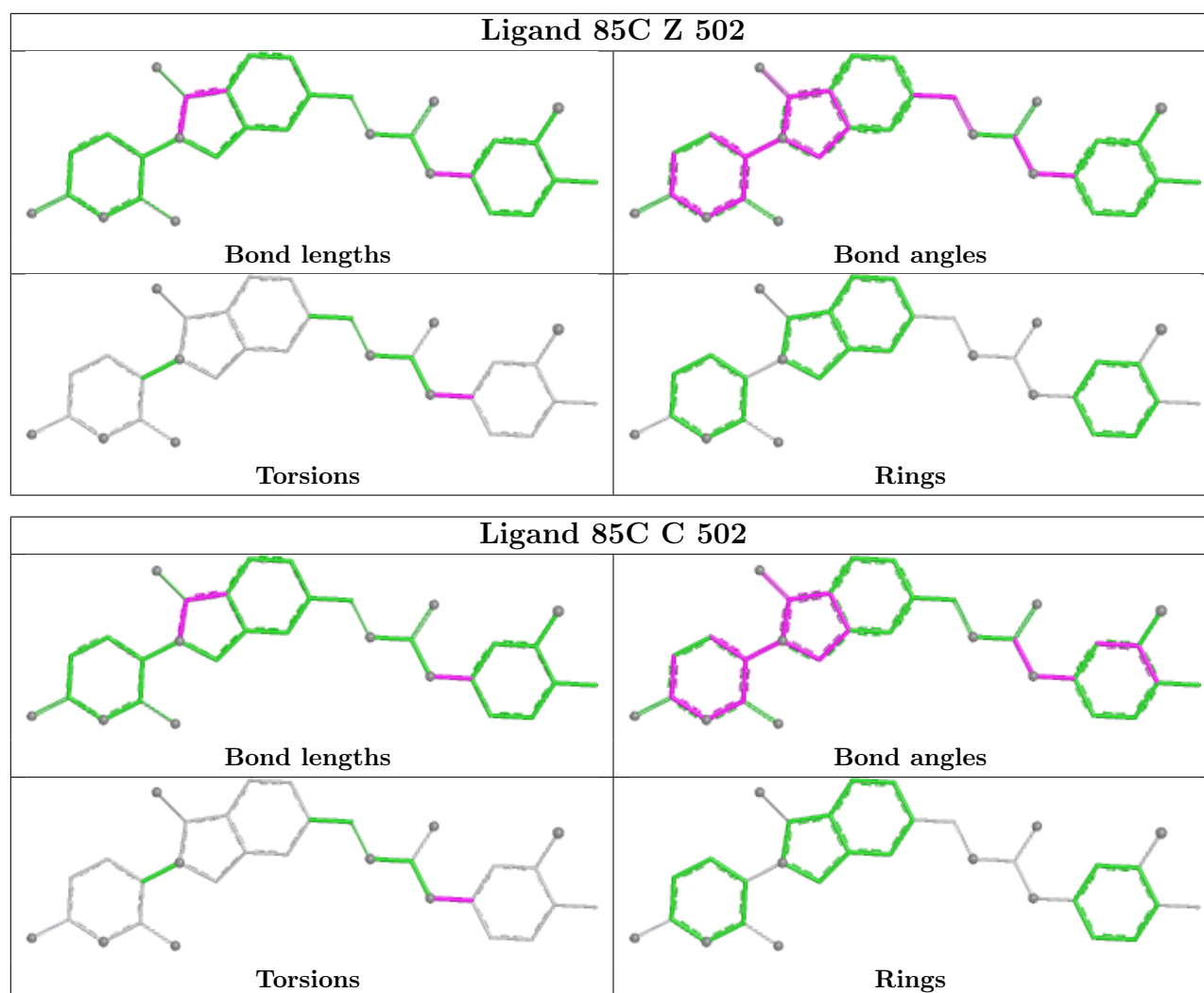
Mol	Chain	Res	Type	Atoms
5	Z	502	85C	C17-C16-N4-C15
5	Z	502	85C	C21-C16-N4-C15
5	C	502	85C	C21-C16-N4-C15

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	502	85C	10	0
5	C	502	85C	4	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	196/199 (98%)	-0.31	1 (0%) 87 66	56, 112, 160, 183	0
1	X	195/199 (97%)	-0.26	1 (0%) 87 66	66, 109, 160, 185	0
2	B	1075/1140 (94%)	-0.17	10 (0%) 81 56	39, 114, 185, 240	5 (0%)
2	Y	1080/1140 (94%)	-0.21	9 (0%) 82 58	38, 113, 174, 221	5 (0%)
3	C	370/406 (91%)	-0.10	5 (1%) 73 46	62, 111, 165, 225	0
3	Z	380/406 (93%)	-0.10	3 (0%) 82 58	64, 109, 169, 213	0
All	All	3296/3490 (94%)	-0.18	29 (0%) 81 56	38, 112, 174, 240	10 (0%)

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	475	SER	5.0
2	B	16	ASN	4.8
2	B	276	MET	4.3
2	B	260	CYS	4.2
3	C	318	CYS	4.2

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](#)

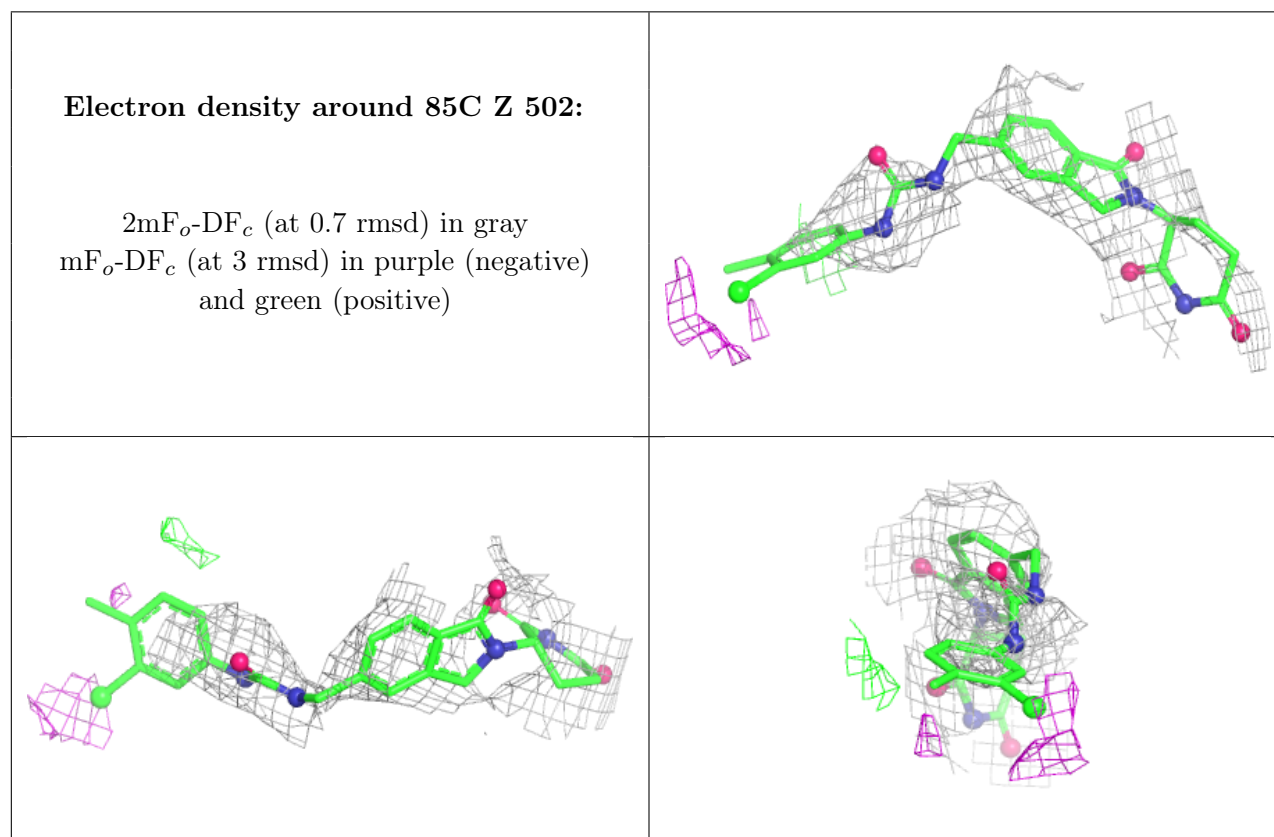
There are no oligosaccharides in this entry.

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.

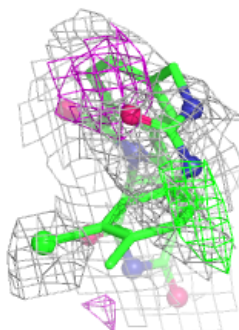
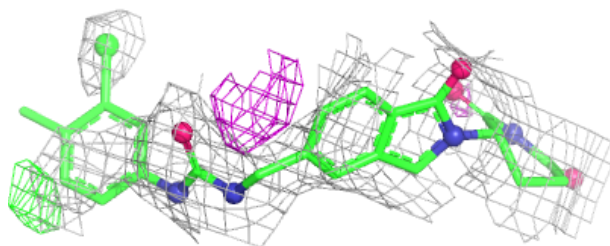
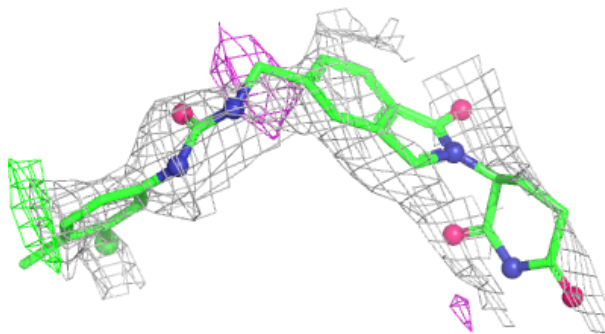
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	85C	Z	502	31/31	0.95	0.12	70,95,210,235	0
5	85C	C	502	31/31	0.96	0.10	61,90,177,227	0
4	ZN	C	501	1/1	0.97	0.07	187,187,187,187	0
4	ZN	Z	501	1/1	0.98	0.07	191,191,191,191	0

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 85C C 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.