



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2022 – 03:35 am GMT

PDB ID : 7QBF  
Title : TC:CD320 in complex with nanobody TC-Nb34  
Authors : Bloch, J.S.; Locher, K.P.  
Deposited on : 2021-11-19  
Resolution : 1.85 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

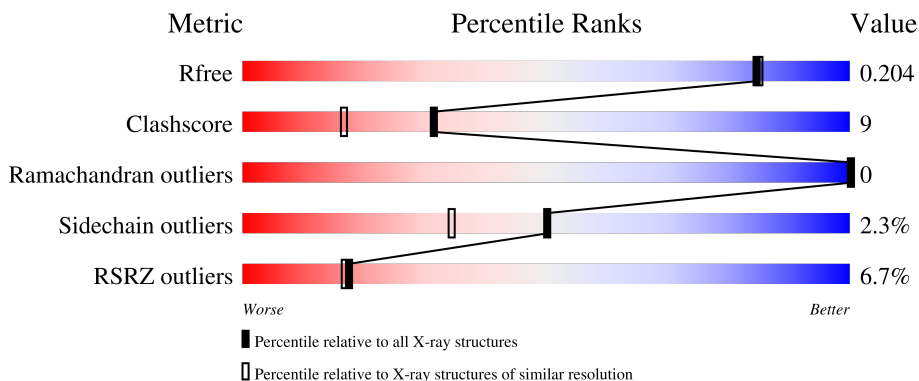
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	409	 5% 89% 10%
2	C	147	 6% 49% 47%
3	B	137	 9% 79% 10% 9%

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
5	EDO	A	517	-	-	X	-
5	EDO	A	520	-	-	X	-
5	EDO	A	529	-	-	X	-
6	CNC	A	536[A]	X	-	-	-
6	CNC	A	536[B]	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10278 atoms, of which 4733 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	409	6481	2079	3207	576	600	19	0	9	0

- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	C	78	1085	345	500	103	125	12	0	0	0

- Molecule 3 is a protein called Anti-transcobalamin-2 nanobody TC-Nb34.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	B	125	1831	599	864	170	192	6	0	3	0

- Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	12	Total	I	0	0
			12	12		
4	C	4	Total	I	0	0
			4	4		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



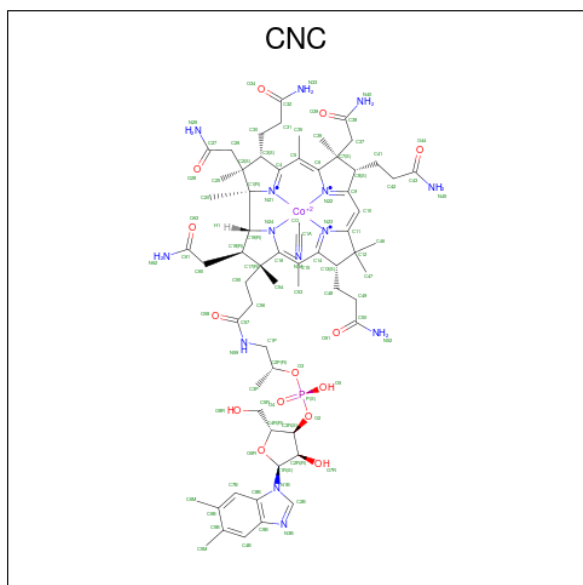
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		
5	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is CYANOCOBALAMIN (three-letter code: CNC) (formula: C<sub>63</sub>H<sub>89</sub>CoN<sub>14</sub>O<sub>14</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Co	N	O			P
6	A	1	186	126	2	28	28	2	0	1

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	C	2	2	2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	297	297	297	0	0
8	C	49	49	49	0	0
8	B	61	61	61	0	0





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.82Å 104.82Å 167.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.27 – 1.85 49.27 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.27-1.85) 99.7 (49.27-1.85)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 1.86Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.174 , 0.205 0.173 , 0.204	Depositor DCC
$R_{free}$ test set	3971 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CNC, CA, EDO, IOD

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	0.55	0/3363	0.74	4/4553 (0.1%)
2	C	0.50	0/595	0.71	0/807
3	B	0.51	1/995 (0.1%)	0.68	1/1347 (0.1%)
All	All	0.54	1/4953 (0.0%)	0.72	5/6707 (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
3	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	96	CYS	CB-SG	-7.20	1.70	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	MET	CG-SD-CE	-11.79	81.34	100.20
1	A	290	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	A	290	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	209	ARG	NE-CZ-NH2	-6.05	117.28	120.30
3	B	67	ARG	NE-CZ-NH2	-5.63	117.49	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	39[B]	GLN	Mainchain

## 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	3274	3207	3255	51	0
2	C	585	500	516	3	0
3	B	967	864	893	8	0
4	A	12	0	0	3	0
4	C	4	0	0	1	0
5	A	92	138	138	30	0
5	B	12	18	18	1	0
5	C	4	6	6	0	0
6	A	186	0	174	28	0
7	C	2	0	0	0	0
8	A	297	0	0	8	0
8	B	61	0	0	2	0
8	C	49	0	0	1	0
All	All	5545	4733	5000	92	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 9.

The worst 5 of 92 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:206:ARG:HD2	1:A:209:ARG:HH22	1.34	0.90
2:C:142:SER:OG	8:C:301:HOH:O	1.72	0.90
6:A:536[A]:CNC:C4	6:A:536[A]:CNC:H4B	2.18	0.74
5:A:525:EDO:O2	8:A:601:HOH:O	2.08	0.71
1:A:209:ARG:HH21	1:A:209:ARG:CB	2.04	0.71

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	416/409 (102%)	412 (99%)	4 (1%)	0	100	100
2	C	74/147 (50%)	72 (97%)	2 (3%)	0	100	100
3	B	124/137 (90%)	119 (96%)	5 (4%)	0	100	100
All	All	614/693 (89%)	603 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	357/348 (103%)	353 (99%)	4 (1%)	73	65
2	C	70/129 (54%)	69 (99%)	1 (1%)	67	55
3	B	101/108 (94%)	92 (91%)	9 (9%)	9	2
All	All	528/585 (90%)	514 (97%)	14 (3%)	50	29

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	B	39[A]	GLN
3	B	39[B]	GLN
3	B	131	HIS
3	B	109[B]	TRP
3	B	128	SER

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

Mol	Chain	Res	Type
1	A	138	GLN
3	B	13	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 47 ligands modelled in this entry, 18 are monoatomic - leaving 29 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	EDO	A	519	-	3,3,3	0.55	0	2,2,2	0.37	0
5	EDO	A	521	-	3,3,3	0.61	0	2,2,2	0.29	0
5	EDO	B	201	-	3,3,3	0.42	0	2,2,2	0.38	0
5	EDO	A	530	-	3,3,3	0.56	0	2,2,2	0.59	0
5	EDO	B	203	-	3,3,3	0.82	0	2,2,2	0.25	0
5	EDO	A	516	-	3,3,3	0.69	0	2,2,2	1.11	0
5	EDO	A	517	-	3,3,3	0.75	0	2,2,2	0.96	0
5	EDO	A	520	-	3,3,3	0.43	0	2,2,2	0.32	0
5	EDO	A	528	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	524	-	3,3,3	0.49	0	2,2,2	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	EDO	A	514	-	3,3,3	0.43	0	2,2,2	0.53	0
5	EDO	A	525	-	3,3,3	0.30	0	2,2,2	0.22	0
5	EDO	A	523	-	3,3,3	0.55	0	2,2,2	0.22	0
5	EDO	A	533	-	3,3,3	0.66	0	2,2,2	0.29	0
5	EDO	A	534	-	3,3,3	0.44	0	2,2,2	0.67	0
6	CNC	A	536[B]	-	90,103,103	3.26	36 (40%)	139,171,171	3.98	55 (39%)
5	EDO	A	515	-	3,3,3	0.57	0	2,2,2	0.71	0
5	EDO	A	513	-	3,3,3	0.42	0	2,2,2	0.36	0
5	EDO	A	529	-	3,3,3	0.57	0	2,2,2	0.94	0
6	CNC	A	536[A]	-	90,103,103	3.40	34 (37%)	139,171,171	4.21	51 (36%)
5	EDO	A	531	-	3,3,3	0.45	0	2,2,2	0.08	0
5	EDO	A	535	-	3,3,3	0.71	0	2,2,2	0.44	0
5	EDO	C	207	-	3,3,3	0.51	0	2,2,2	0.04	0
5	EDO	A	527	-	3,3,3	0.52	0	2,2,2	0.51	0
5	EDO	A	522	-	3,3,3	0.51	0	2,2,2	0.31	0
5	EDO	A	526	-	3,3,3	0.29	0	2,2,2	0.75	0
5	EDO	A	532	-	3,3,3	0.58	0	2,2,2	0.28	0
5	EDO	A	518	-	3,3,3	1.01	0	2,2,2	0.36	0
5	EDO	B	202	-	3,3,3	0.48	0	2,2,2	0.50	0

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	EDO	A	519	-	-	0/1/1/1	-
5	EDO	A	521	-	-	1/1/1/1	-
5	EDO	B	201	-	-	1/1/1/1	-
5	EDO	A	530	-	-	1/1/1/1	-
5	EDO	B	203	-	-	1/1/1/1	-
5	EDO	A	516	-	-	0/1/1/1	-
5	EDO	A	517	-	-	0/1/1/1	-
5	EDO	A	520	-	-	1/1/1/1	-
5	EDO	A	528	-	-	1/1/1/1	-
5	EDO	A	524	-	-	0/1/1/1	-
5	EDO	A	514	-	-	1/1/1/1	-
5	EDO	A	525	-	-	0/1/1/1	-
5	EDO	A	523	-	-	1/1/1/1	-
5	EDO	A	533	-	-	0/1/1/1	-
5	EDO	A	534	-	-	0/1/1/1	-
6	CNC	A	536[B]	-	1/1/36/38	1/52/235/235	0/3/11/11

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	515	-	-	0/1/1/1	-
5	EDO	A	513	-	-	1/1/1/1	-
5	EDO	A	529	-	-	0/1/1/1	-
6	CNC	A	536[A]	-	1/1/36/38	5/52/235/235	0/3/11/11
5	EDO	A	531	-	-	1/1/1/1	-
5	EDO	A	535	-	-	0/1/1/1	-
5	EDO	C	207	-	-	1/1/1/1	-
5	EDO	A	527	-	-	0/1/1/1	-
5	EDO	A	522	-	-	1/1/1/1	-
5	EDO	A	526	-	-	0/1/1/1	-
5	EDO	A	532	-	-	1/1/1/1	-
5	EDO	A	518	-	-	0/1/1/1	-
5	EDO	B	202	-	-	1/1/1/1	-

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	536[A]	CNC	C2R-C1R	-11.21	1.36	1.53
6	A	536[B]	CNC	C2R-C1R	-10.78	1.37	1.53
6	A	536[B]	CNC	C10-C11	9.26	1.64	1.37
6	A	536[A]	CNC	C10-C9	9.25	1.65	1.39
6	A	536[A]	CNC	C10-C11	9.01	1.63	1.37

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	536[A]	CNC	C3-C4-C5	-20.17	89.82	123.81
6	A	536[A]	CNC	C36-C7-C37	-15.26	85.65	110.80
6	A	536[B]	CNC	C9-C10-C11	-14.79	104.05	125.88
6	A	536[B]	CNC	C3-C4-C5	-14.10	100.06	123.81
6	A	536[B]	CNC	C36-C7-C37	-13.67	88.28	110.80

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	536[A]	CNC	N24
6	A	536[B]	CNC	N24

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	536[A]	CNC	C2R-C3R-O2-P

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Mol	Chain	Res	Type	Atoms
6	A	536[A]	CNC	C4R-C3R-O2-P
5	A	520	EDO	O1-C1-C2-O2
5	A	523	EDO	O1-C1-C2-O2
5	A	532	EDO	O1-C1-C2-O2

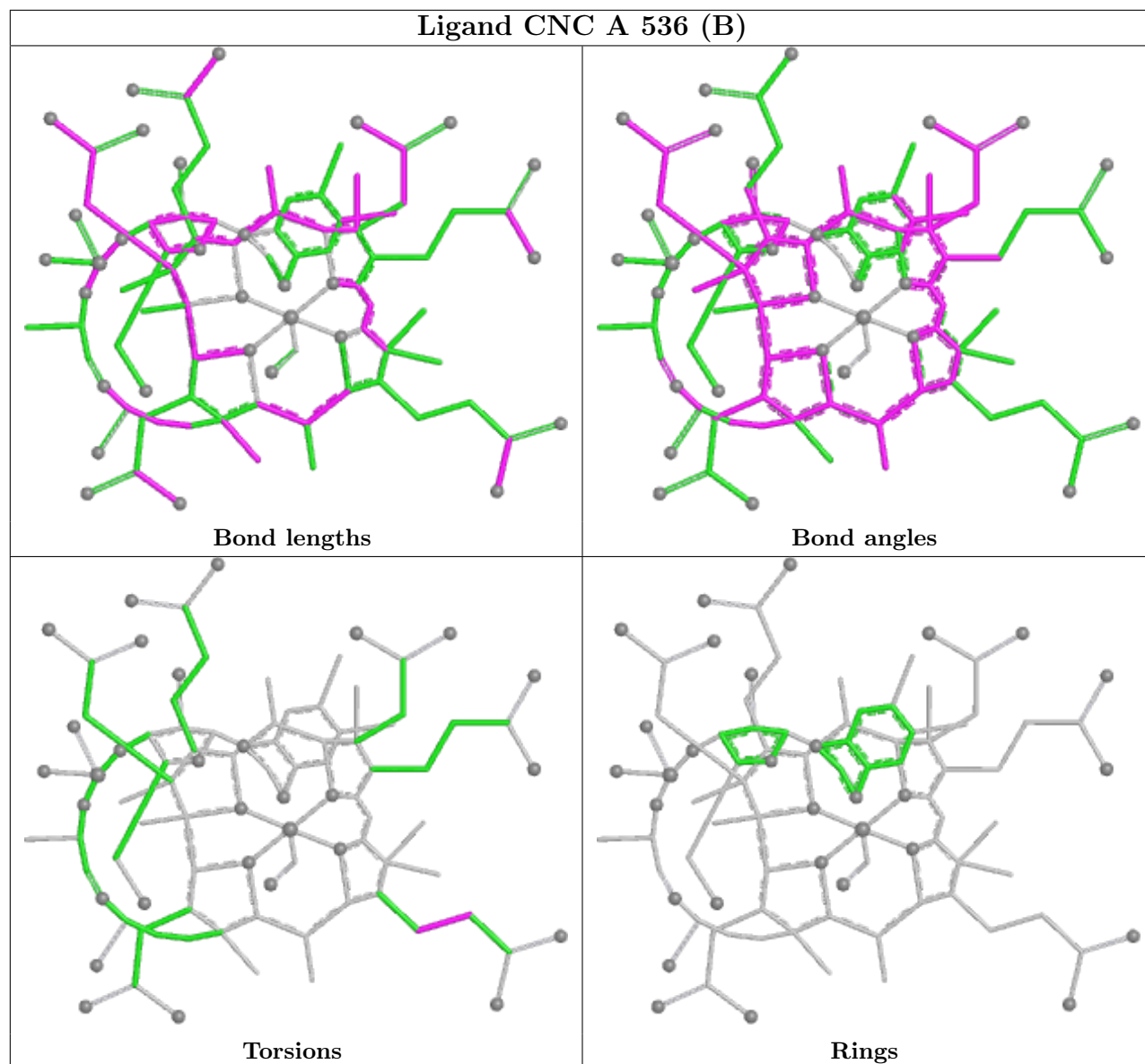
There are no ring outliers.

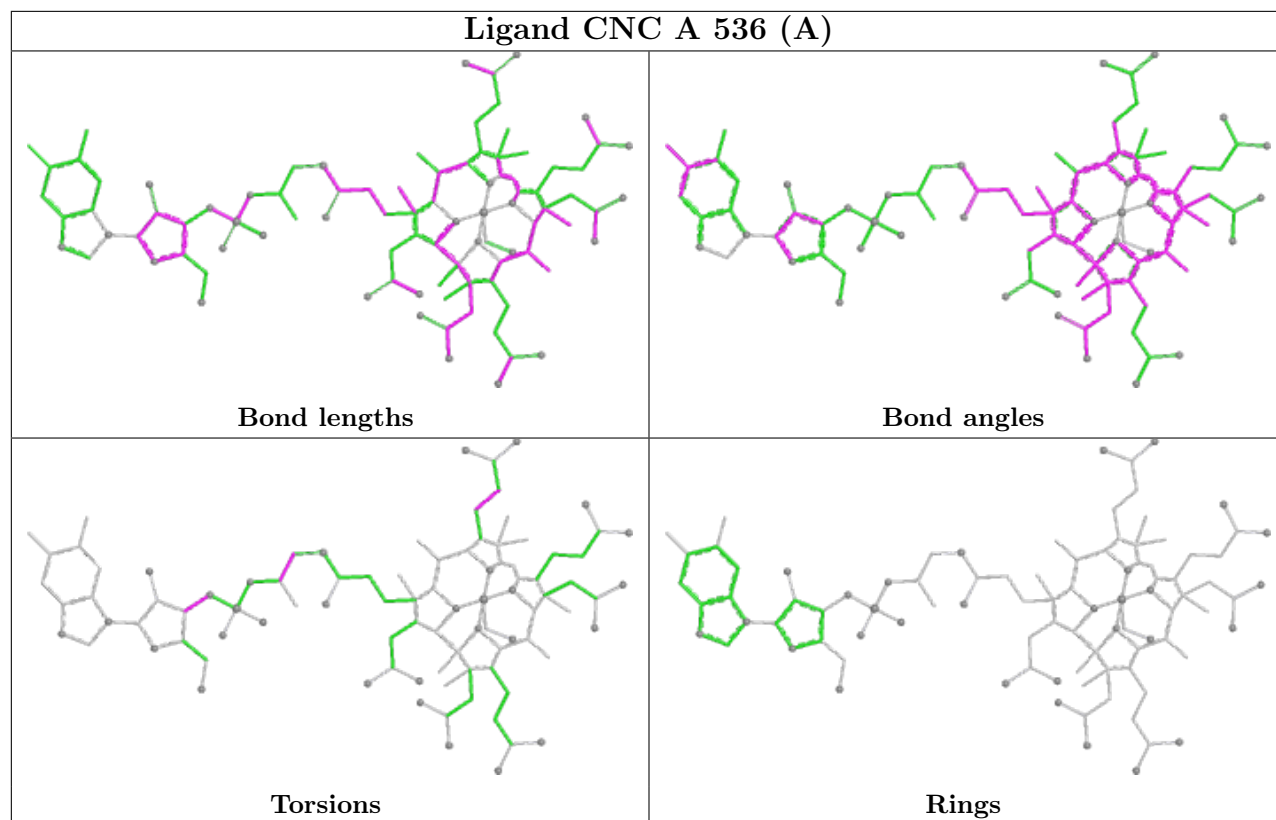
15 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	203	EDO	1	0
5	A	516	EDO	3	0
5	A	517	EDO	4	0
5	A	520	EDO	5	0
5	A	524	EDO	1	0
5	A	514	EDO	2	0
5	A	525	EDO	1	0
5	A	533	EDO	1	0
5	A	534	EDO	2	0
6	A	536[B]	CNC	13	0
5	A	513	EDO	3	0
5	A	529	EDO	4	0
6	A	536[A]	CNC	15	0
5	A	535	EDO	2	0
5	A	526	EDO	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	409/409 (100%)	0.38	19 (4%) 32 31	22, 32, 59, 134	0
2	C	78/147 (53%)	0.47	9 (11%) 4 4	25, 38, 67, 100	0
3	B	125/137 (91%)	0.75	13 (10%) 6 6	32, 45, 73, 102	0
All	All	612/693 (88%)	0.47	41 (6%) 17 17	22, 36, 65, 134	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	THR	7.9
1	A	305	ILE	7.5
1	A	306	PRO	7.2
3	B	131	HIS	6.2
1	A	303	GLU	6.0

### 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 monosaccharides 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, 95<sup>th</sup> 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.

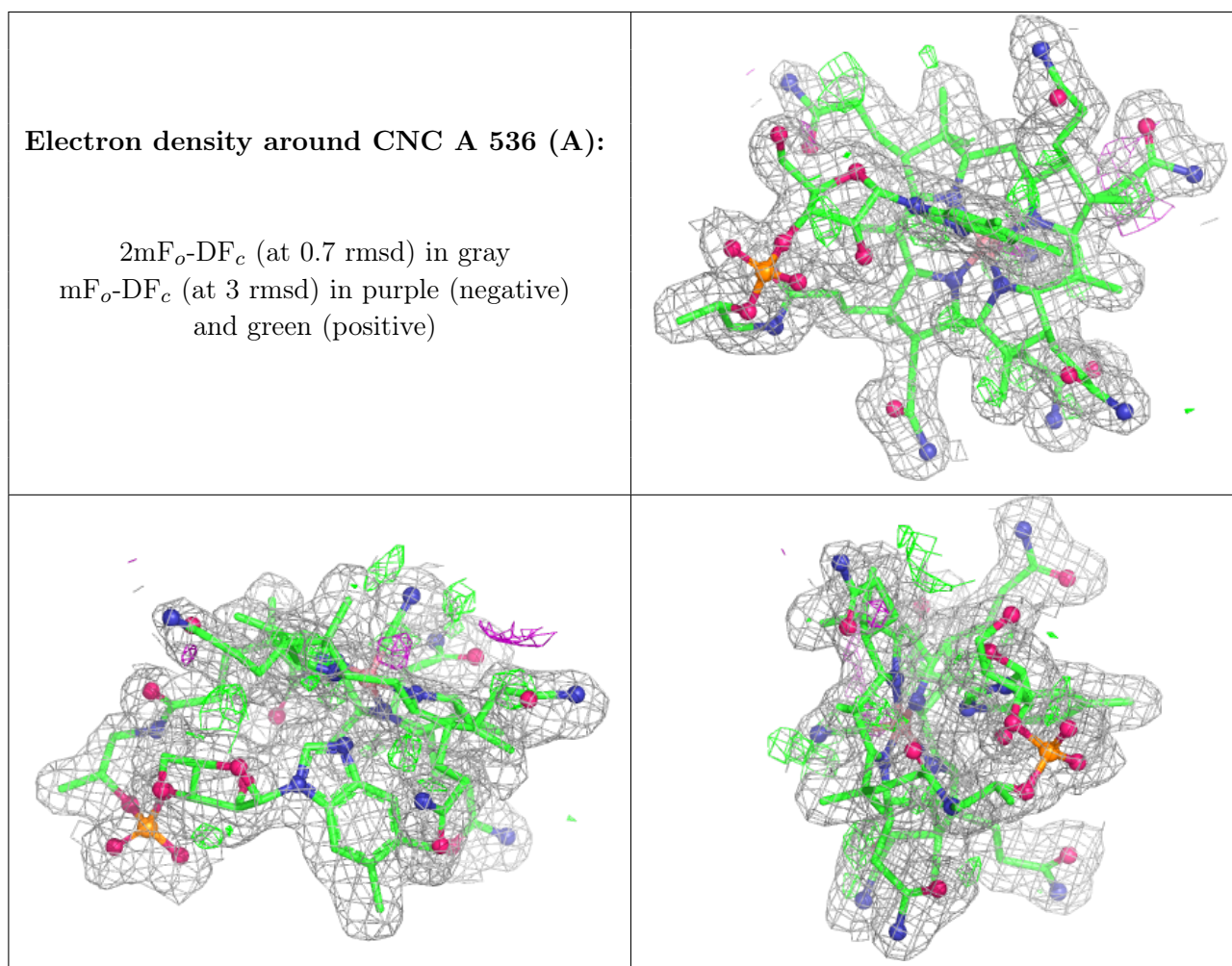
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	IOD	A	507	1/1	0.36	0.14	208,208,208,208	0
5	EDO	A	517	4/4	0.61	0.36	32,51,61,63	0
5	EDO	A	535	4/4	0.64	0.38	44,55,57,66	0
5	EDO	B	203	4/4	0.65	0.30	51,61,69,69	0
4	IOD	A	509	1/1	0.76	0.22	153,153,153,153	0
5	EDO	A	522	4/4	0.77	0.28	60,72,82,82	0
5	EDO	A	518	4/4	0.79	0.25	30,46,55,55	0
5	EDO	A	523	4/4	0.80	0.27	46,66,84,88	0
5	EDO	A	520	4/4	0.81	0.50	42,51,62,62	0
5	EDO	A	529	4/4	0.83	0.24	43,52,67,67	0
4	IOD	A	511	1/1	0.83	0.17	122,122,122,122	0
5	EDO	A	524	4/4	0.83	0.23	43,57,68,69	0
5	EDO	A	521	4/4	0.84	0.26	41,50,72,86	0
5	EDO	A	532	4/4	0.84	0.20	45,54,60,72	0
5	EDO	A	516	4/4	0.88	0.31	31,42,57,57	0
4	IOD	A	510	1/1	0.88	0.09	118,118,118,118	0
5	EDO	A	534	4/4	0.89	0.20	29,45,66,66	0
5	EDO	A	528	4/4	0.90	0.14	43,52,60,68	0
4	IOD	A	502	1/1	0.90	0.18	126,126,126,126	0
5	EDO	A	513	4/4	0.90	0.18	29,38,65,78	0
4	IOD	A	512	1/1	0.91	0.15	130,130,130,130	0
5	EDO	A	530	4/4	0.91	0.10	36,43,50,57	0
5	EDO	C	207	4/4	0.92	0.18	31,50,77,77	0
5	EDO	A	525	4/4	0.92	0.13	32,46,60,63	0
5	EDO	A	527	4/4	0.93	0.14	39,47,52,62	0
5	EDO	A	533	4/4	0.93	0.18	35,51,66,75	0
5	EDO	A	514	4/4	0.94	0.12	37,46,61,61	0
5	EDO	A	526	4/4	0.94	0.35	36,44,58,70	0
5	EDO	B	201	4/4	0.94	0.22	54,65,74,89	0
5	EDO	B	202	4/4	0.94	0.22	30,39,41,47	0
5	EDO	A	531	4/4	0.94	0.16	46,55,58,60	0
5	EDO	A	515	4/4	0.95	0.10	34,44,53,53	0
4	IOD	A	501	1/1	0.96	0.17	37,37,37,37	1
6	CNC	A	536[A]	93/93	0.96	0.16	20,23,27,34	93
6	CNC	A	536[B]	93/93	0.96	0.16	19,23,29,38	93
4	IOD	A	504	1/1	0.97	0.07	74,74,74,74	1
4	IOD	C	204	1/1	0.97	0.10	48,48,48,48	1
4	IOD	C	206	1/1	0.98	0.15	45,45,45,45	1
5	EDO	A	519	4/4	0.98	0.10	28,39,46,46	0
4	IOD	C	203	1/1	0.98	0.11	53,53,53,53	1
4	IOD	A	508	1/1	0.98	0.09	52,52,52,52	1
4	IOD	A	505	1/1	0.99	0.12	45,45,45,45	1
4	IOD	A	506	1/1	0.99	0.13	43,43,43,43	1

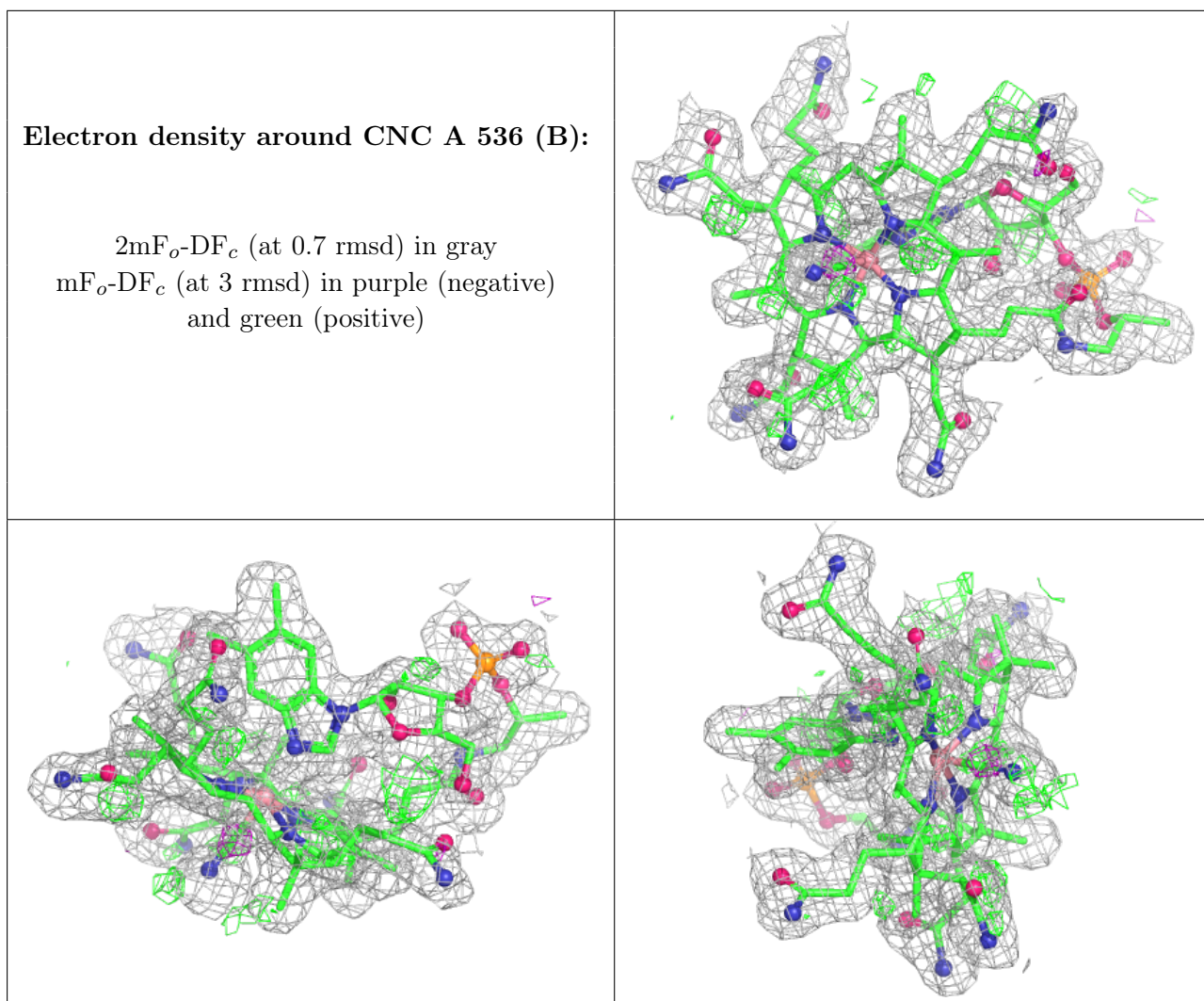
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	IOD	C	205	1/1	0.99	0.18	35,35,35,35	1
7	CA	C	202	1/1	0.99	0.13	30,30,30,30	0
7	CA	C	201	1/1	1.00	0.12	25,25,25,25	0
4	IOD	A	503	1/1	1.00	0.16	37,37,37,37	1

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 [\(i\)](#)

There are no such residues in this entry.