



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:11 am BST

PDB ID : 2ZOF  
Title : Crystal structure of mouse carnosinase CN2 complexed with MN and bestatin  
Authors : Unno, H.; Yamashita, T.; Okumura, N.; Kusunoki, M.  
Deposited on : 2008-05-14  
Resolution : 2.30 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](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 : 1.8.5 (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

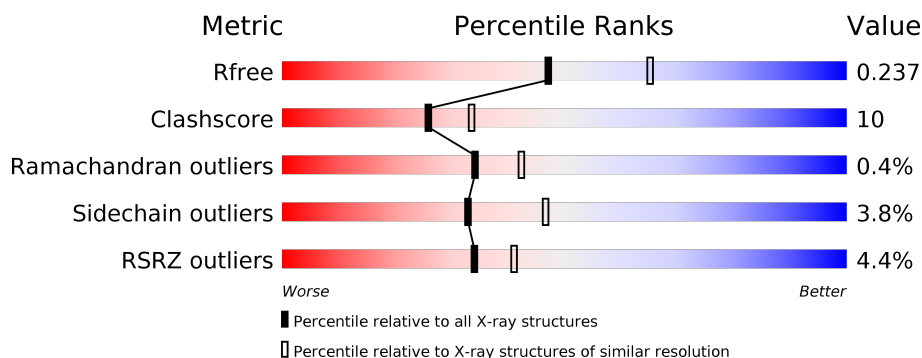
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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  $\geq 3$ , 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	479	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	479	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7978 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 Cytosolic non-specific dipeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	0	0	0
			3729	2373	626	709	21			
1	B	478	Total	C	N	O	S	0	0	0
			3729	2373	626	709	21			

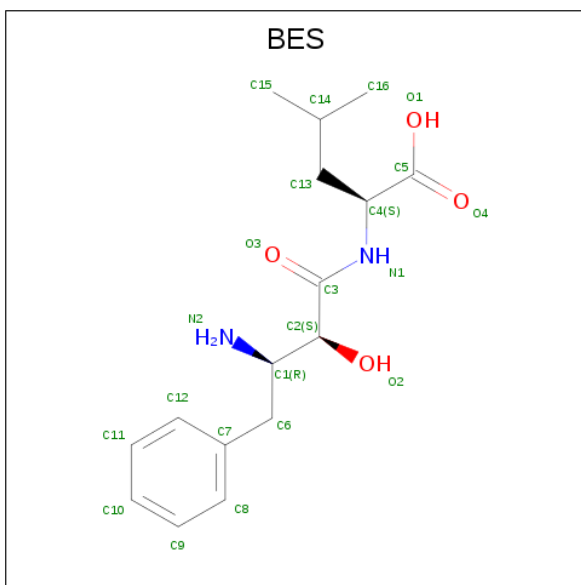
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	EXPRESSION TAG	UNP Q9D1A2
A	-2	PRO	-	EXPRESSION TAG	UNP Q9D1A2
A	-1	ASN	-	EXPRESSION TAG	UNP Q9D1A2
A	0	SER	-	EXPRESSION TAG	UNP Q9D1A2
B	-3	SER	-	EXPRESSION TAG	UNP Q9D1A2
B	-2	PRO	-	EXPRESSION TAG	UNP Q9D1A2
B	-1	ASN	-	EXPRESSION TAG	UNP Q9D1A2
B	0	SER	-	EXPRESSION TAG	UNP Q9D1A2

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: C<sub>16</sub>H<sub>24</sub>N<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	16	2	4		
3	B	1	Total	C	N	O	0	0
			22	16	2	4		

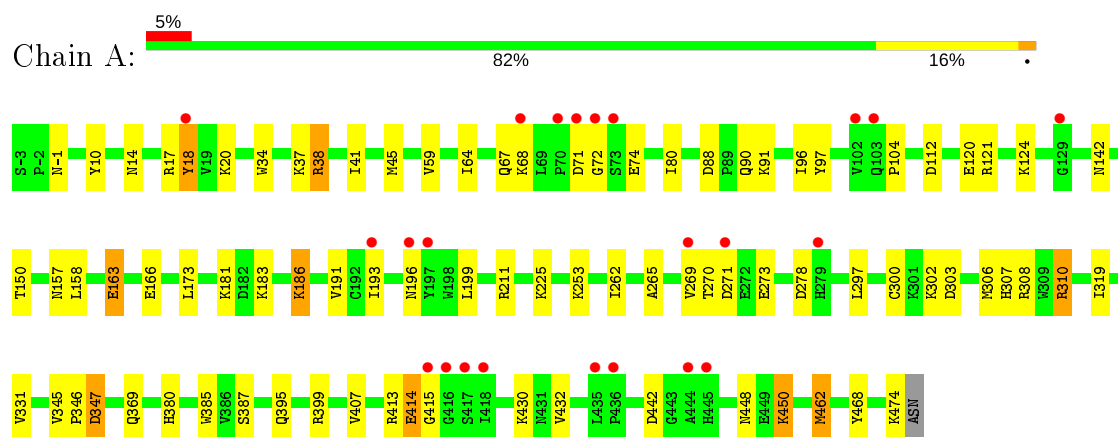
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	226	Total	O	0	0
			226	226		

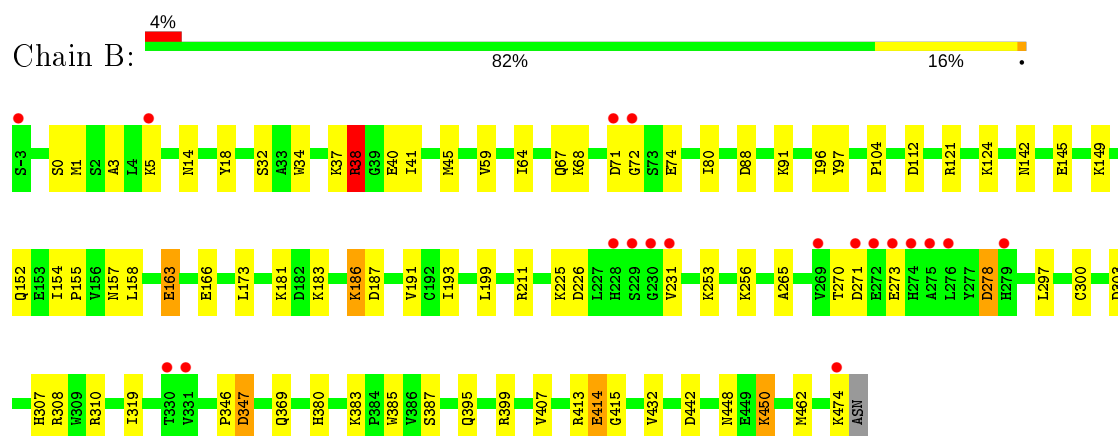
### 3 Residue-property plots [i](#)

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: Cytosolic non-specific dipeptidase



- Molecule 1: Cytosolic non-specific dipeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.50Å 199.18Å 55.22Å 90.00° 118.92° 90.00°	Depositor
Resolution (Å)	43.03 – 2.30 43.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	86.9 (43.03-2.30) 86.9 (43.02-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.96 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.192 , 0.239 0.191 , 0.237	Depositor DCC
$R_{free}$ test set	2016 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.026 for h,-k,-h-l 0.025 for -h-l,-k,l 0.028 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7978	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BES, MN

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	0.67	3/3813 (0.1%)	0.69	2/5153 (0.0%)
1	B	0.66	2/3813 (0.1%)	0.70	3/5153 (0.1%)
All	All	0.67	5/7626 (0.1%)	0.70	5/10306 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	GLU	CD-OE1	-6.22	1.18	1.25
1	B	163	GLU	CD-OE1	-5.81	1.19	1.25
1	A	18	TYR	CE2-CZ	-5.59	1.31	1.38
1	A	414	GLU	CG-CD	5.27	1.59	1.51
1	B	414	GLU	CG-CD	5.11	1.59	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	163	GLU	OE1-CD-OE2	-5.89	116.23	123.30
1	B	163	GLU	OE1-CD-OE2	-5.82	116.31	123.30
1	A	462	MET	CG-SD-CE	5.58	109.13	100.20
1	B	38	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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	3729	0	3692	85	0
1	B	3729	0	3692	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	22	0	22	3	0
3	B	22	0	22	1	0
4	A	246	0	0	25	0
4	B	226	0	0	15	0
All	All	7978	0	7428	156	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 10.

All (156) 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:10:TYR:HB2	4:A:2235:HOH:O	1.58	1.04
1:A:308:ARG:HB3	4:A:2240:HOH:O	1.58	1.03
1:A:90:GLN:HG3	4:A:2227:HOH:O	1.57	1.01
1:B:199:LEU:CD1	1:B:308:ARG:HH12	1.73	1.01
1:B:18:TYR:CE1	1:B:142:ASN:HB3	1.95	1.01
1:A:199:LEU:CD1	1:A:308:ARG:HH12	1.73	1.00
1:A:18:TYR:CE1	1:A:142:ASN:HB3	1.97	0.99
1:A:18:TYR:HE1	1:A:142:ASN:HB3	1.31	0.95
1:A:20:LYS:HB3	4:A:2231:HOH:O	1.68	0.94
1:A:150:THR:CG2	4:A:2235:HOH:O	2.14	0.94
1:B:14:ASN:O	1:B:18:TYR:HD2	1.53	0.91
1:A:14:ASN:O	1:A:18:TYR:HD2	1.54	0.91
1:B:18:TYR:HE1	1:B:142:ASN:HB3	1.30	0.90
1:A:265:ALA:O	1:A:347:ASP:HB2	1.74	0.88
1:B:14:ASN:CB	1:B:18:TYR:HE2	1.88	0.87
1:B:265:ALA:O	1:B:347:ASP:HB2	1.76	0.85
1:A:14:ASN:CB	1:A:18:TYR:HE2	1.90	0.85
1:A:17:ARG:NH2	4:A:2238:HOH:O	1.90	0.85
1:B:383:LYS:HE2	4:B:3080:HOH:O	1.76	0.84
1:A:150:THR:HG21	4:A:2235:HOH:O	1.77	0.84
1:B:270:THR:CG2	1:B:273:GLU:HB2	2.10	0.82
1:A:270:THR:CG2	1:A:273:GLU:HB2	2.11	0.81
1:B:14:ASN:HB3	1:B:18:TYR:HE2	1.42	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASN:HB3	1:A:18:TYR:HE2	1.45	0.80
1:A:199:LEU:HD12	1:A:308:ARG:HH12	1.46	0.80
1:A:38:ARG:NH2	1:A:67:GLN:OE1	2.15	0.80
1:A:319:ILE:HD12	1:B:319:ILE:HD12	1.62	0.79
1:A:211:ARG:HD2	1:A:415:GLY:HA2	1.65	0.78
1:A:14:ASN:O	1:A:18:TYR:CD2	2.36	0.78
1:B:14:ASN:O	1:B:18:TYR:CD2	2.35	0.78
1:A:308:ARG:HG2	4:B:3100:HOH:O	1.83	0.78
1:B:38:ARG:NH2	1:B:67:GLN:OE1	2.14	0.77
1:A:121:ARG:HD3	4:A:2187:HOH:O	1.82	0.77
1:B:211:ARG:HD2	1:B:415:GLY:HA2	1.64	0.76
1:B:278:ASP:HB3	4:B:3047:HOH:O	1.85	0.76
1:A:150:THR:HG22	4:A:2235:HOH:O	1.76	0.76
1:B:199:LEU:HD12	1:B:308:ARG:HH12	1.50	0.76
1:B:270:THR:HG23	1:B:273:GLU:HB2	1.70	0.73
1:B:474:LYS:HG3	4:B:3062:HOH:O	1.87	0.73
4:A:2073:HOH:O	1:B:308:ARG:HG2	1.89	0.72
1:A:88:ASP:N	1:A:157:ASN:HD21	1.87	0.72
1:B:163:GLU:OE2	1:B:173:LEU:HD22	1.92	0.69
1:A:270:THR:HG23	1:A:273:GLU:HB2	1.72	0.69
1:B:88:ASP:N	1:B:157:ASN:HD21	1.91	0.68
1:A:17:ARG:NE	4:A:2238:HOH:O	2.13	0.68
1:B:14:ASN:HB3	1:B:18:TYR:CE2	2.29	0.68
1:B:199:LEU:CD1	1:B:308:ARG:NH1	2.55	0.67
1:B:5:LYS:HD2	4:B:3210:HOH:O	1.95	0.66
1:A:18:TYR:HD1	1:A:142:ASN:ND2	1.93	0.66
1:B:18:TYR:HD1	1:B:142:ASN:ND2	1.93	0.66
1:A:163:GLU:OE2	1:A:173:LEU:HD22	1.95	0.66
1:A:199:LEU:CD1	1:A:308:ARG:NH1	2.54	0.65
1:A:120:GLU:HB2	4:A:2172:HOH:O	1.96	0.64
1:A:88:ASP:H	1:A:157:ASN:HD21	1.44	0.64
1:A:199:LEU:HD11	1:A:308:ARG:HH12	1.63	0.64
1:A:163:GLU:OE1	1:A:166:GLU:N	2.32	0.63
1:A:18:TYR:CD1	1:A:142:ASN:ND2	2.67	0.62
1:A:262:ILE:O	4:A:2236:HOH:O	2.16	0.62
4:A:2073:HOH:O	1:B:308:ARG:CG	2.46	0.62
1:B:380:HIS:HD2	4:B:3198:HOH:O	1.83	0.62
1:B:199:LEU:HD11	1:B:308:ARG:HH12	1.63	0.62
1:B:270:THR:HG22	1:B:273:GLU:HB2	1.80	0.62
1:A:308:ARG:CG	4:B:3100:HOH:O	2.45	0.61
1:A:124:LYS:HD3	4:A:2234:HOH:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:TYR:CD1	1:B:142:ASN:ND2	2.69	0.61
1:A:91:LYS:HB2	1:A:157:ASN:OD1	2.01	0.61
1:A:270:THR:HG22	1:A:273:GLU:HB2	1.80	0.61
1:A:414:GLU:HG2	4:A:2107:HOH:O	2.02	0.60
1:A:14:ASN:HB3	1:A:18:TYR:CE2	2.32	0.58
1:B:163:GLU:OE1	1:B:166:GLU:N	2.36	0.58
1:B:88:ASP:H	1:B:157:ASN:HD21	1.49	0.58
1:B:187:ASP:OD1	4:B:3084:HOH:O	2.18	0.56
1:A:166:GLU:O	3:A:1080:BES:H152	2.06	0.56
1:A:331:VAL:HG11	4:A:2134:HOH:O	2.05	0.56
1:B:152:GLN:NE2	4:B:3164:HOH:O	2.38	0.56
1:A:14:ASN:HB2	1:A:18:TYR:HE2	1.70	0.55
1:B:3:ALA:O	4:B:3042:HOH:O	2.19	0.54
1:B:91:LYS:HB2	1:B:157:ASN:OD1	2.07	0.53
1:B:14:ASN:HB2	1:B:18:TYR:HE2	1.70	0.52
1:A:199:LEU:HD11	1:A:308:ARG:NH1	2.24	0.52
1:A:88:ASP:H	1:A:157:ASN:ND2	2.06	0.52
1:B:395:GLN:O	1:B:399:ARG:HG3	2.10	0.51
1:B:414:GLU:OE1	3:B:1081:BES:H10	2.11	0.51
1:B:64:ILE:HG21	1:B:80:ILE:HD12	1.93	0.50
1:B:14:ASN:CB	1:B:18:TYR:CE2	2.81	0.50
1:B:96:ILE:HD11	1:B:158:LEU:HD22	1.93	0.50
1:B:88:ASP:H	1:B:157:ASN:ND2	2.10	0.50
1:B:199:LEU:HD11	1:B:308:ARG:NH1	2.25	0.50
1:A:64:ILE:HG21	1:A:80:ILE:HD12	1.94	0.49
1:B:145:GLU:OE1	4:B:3213:HOH:O	2.20	0.49
1:A:97:TYR:HB3	1:A:193:ILE:HG12	1.93	0.49
1:B:346:PRO:HG2	1:B:413:ARG:NH2	2.27	0.49
1:A:121:ARG:O	1:A:124:LYS:HB2	2.14	0.48
1:B:121:ARG:O	1:B:124:LYS:HB2	2.14	0.47
1:A:-1:ASN:HB3	1:A:468:TYR:OH	2.15	0.46
1:A:395:GLN:O	1:A:399:ARG:HG3	2.15	0.46
1:B:18:TYR:CD1	1:B:142:ASN:CG	2.90	0.45
1:A:253:LYS:HE3	1:B:369:GLN:NE2	2.30	0.45
1:A:18:TYR:CD1	1:A:142:ASN:CG	2.89	0.45
1:A:96:ILE:HD11	1:A:158:LEU:HD22	1.98	0.45
1:B:34:TRP:HE3	1:B:37:LYS:HG3	1.81	0.45
1:A:38:ARG:HD3	4:A:2022:HOH:O	2.17	0.45
1:B:442:ASP:HA	1:B:450:LYS:HD2	1.98	0.45
1:A:14:ASN:CB	1:A:18:TYR:CE2	2.82	0.45
1:A:269:VAL:HG23	4:A:2201:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LYS:O	1:A:186:LYS:HG2	2.17	0.45
1:B:380:HIS:HE1	4:B:3184:HOH:O	1.98	0.45
1:B:191:VAL:HB	1:B:432:VAL:HG22	1.99	0.45
1:A:191:VAL:HB	1:A:432:VAL:HG22	1.99	0.44
1:B:34:TRP:CZ2	1:B:104:PRO:HB3	2.52	0.44
1:A:346:PRO:HG2	1:A:413:ARG:NH2	2.32	0.44
1:A:414:GLU:OE1	3:A:1080:BES:H10	2.17	0.44
1:B:385:TRP:CZ2	1:B:387:SER:HB2	2.53	0.44
1:A:17:ARG:CZ	4:A:2238:HOH:O	2.32	0.44
1:A:41:ILE:O	1:A:45:MET:HG2	2.17	0.44
1:B:183:LYS:O	1:B:186:LYS:HG2	2.17	0.44
1:B:112:ASP:CG	1:B:448:ASN:HD21	2.20	0.44
1:A:303:ASP:O	1:A:307:HIS:HD2	2.00	0.44
1:A:18:TYR:HD1	1:A:142:ASN:HD22	1.66	0.44
1:B:303:ASP:O	1:B:307:HIS:HD2	2.00	0.44
1:A:163:GLU:OE1	1:A:166:GLU:CA	2.66	0.43
1:B:41:ILE:O	1:B:45:MET:HG2	2.18	0.43
1:B:256:LYS:HB3	4:B:3050:HOH:O	2.18	0.43
1:A:18:TYR:CD1	1:A:142:ASN:HB3	2.48	0.43
1:A:380:HIS:HD2	4:A:2054:HOH:O	2.01	0.43
1:A:442:ASP:HA	1:A:450:LYS:HD2	2.00	0.43
1:B:97:TYR:HB3	1:B:193:ILE:HG12	1.99	0.43
1:B:18:TYR:CD1	1:B:142:ASN:HB3	2.48	0.43
1:A:14:ASN:C	1:A:18:TYR:CD2	2.92	0.43
1:A:310:ARG:O	1:A:345:VAL:HG21	2.19	0.43
1:A:34:TRP:HE3	1:A:37:LYS:HG3	1.83	0.43
1:B:18:TYR:CE1	1:B:142:ASN:CB	2.85	0.43
1:A:369:GLN:NE2	1:B:253:LYS:HE3	2.33	0.42
1:A:196:ASN:HB2	4:A:2076:HOH:O	2.18	0.42
1:B:14:ASN:C	1:B:18:TYR:CD2	2.92	0.42
1:A:34:TRP:CZ2	1:A:104:PRO:HB3	2.53	0.42
1:B:14:ASN:HB2	1:B:18:TYR:CE2	2.53	0.42
1:A:120:GLU:CB	4:A:2172:HOH:O	2.60	0.42
1:A:302:LYS:O	1:A:306:MET:HG3	2.20	0.42
1:A:88:ASP:N	1:A:157:ASN:ND2	2.62	0.42
1:B:154:ILE:HA	1:B:155:PRO:HD3	1.91	0.42
3:A:1080:BES:H11	1:B:231:VAL:CG2	2.49	0.42
1:A:385:TRP:CZ2	1:A:387:SER:HB2	2.54	0.42
1:A:90:GLN:NE2	4:A:2227:HOH:O	2.26	0.42
1:B:67:GLN:O	1:B:74:GLU:HA	2.20	0.41
1:B:32:SER:HA	1:B:41:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:GLU:OE1	1:B:166:GLU:CA	2.68	0.41
1:B:40:GLU:HG2	4:B:3199:HOH:O	2.21	0.41
1:A:270:THR:HG23	1:A:273:GLU:H	1.85	0.41
1:A:67:GLN:O	1:A:74:GLU:HA	2.20	0.41
1:B:270:THR:HG23	1:B:273:GLU:H	1.85	0.41
1:A:112:ASP:CG	1:A:448:ASN:HD21	2.24	0.41
1:A:474:LYS:C	4:A:2218:HOH:O	2.59	0.40
1:B:149:LYS:HD3	1:B:149:LYS:HA	1.74	0.40
1:B:1:MET:HB3	4:B:3214:HOH:O	2.21	0.40
1:A:430:LYS:HD3	1:A:430:LYS:HA	1.88	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	476/479 (99%)	463 (97%)	11 (2%)	2 (0%)	34	42
1	B	476/479 (99%)	463 (97%)	11 (2%)	2 (0%)	34	42
All	All	952/958 (99%)	926 (97%)	22 (2%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	ASP
1	B	347	ASP
1	A	72	GLY
1	B	72	GLY

### 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	404/405 (100%)	389 (96%)	15 (4%)	34	48
1	B	404/405 (100%)	388 (96%)	16 (4%)	31	44
All	All	808/810 (100%)	777 (96%)	31 (4%)	33	47

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	59	VAL
1	A	68	LYS
1	A	71	ASP
1	A	181	LYS
1	A	186	LYS
1	A	225	LYS
1	A	271	ASP
1	A	278	ASP
1	A	297	LEU
1	A	300	CYS
1	A	310	ARG
1	A	407	VAL
1	A	450	LYS
1	A	462	MET
1	B	0	SER
1	B	38	ARG
1	B	59	VAL
1	B	68	LYS
1	B	71	ASP
1	B	181	LYS
1	B	186	LYS
1	B	225	LYS
1	B	271	ASP
1	B	278	ASP
1	B	297	LEU
1	B	300	CYS

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Mol	Chain	Res	Type
1	B	310	ARG
1	B	407	VAL
1	B	450	LYS
1	B	462	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	307	HIS
1	A	369	GLN
1	A	380	HIS
1	A	455	ASN
1	B	157	ASN
1	B	307	HIS
1	B	369	GLN
1	B	380	HIS
1	B	431	ASN
1	B	455	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 carbohydrates in this entry.

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

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BES	A	1080	2	19,22,22	1.29	3 (15%)	23,29,29	1.39	3 (13%)
3	BES	B	1081	2	19,22,22	0.88	0	23,29,29	1.32	1 (4%)

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	BES	A	1080	2	-	4/20/24/24	0/1/1/1
3	BES	B	1081	2	-	5/20/24/24	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1080	BES	C13-C4	-3.27	1.50	1.53
3	A	1080	BES	C2-C3	-2.67	1.47	1.52
3	A	1080	BES	C2-C1	-2.07	1.51	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1081	BES	C13-C4-N1	-5.07	100.76	109.80
3	A	1080	BES	C13-C4-N1	-4.20	102.32	109.80
3	A	1080	BES	O2-C2-C3	-2.49	105.27	110.63
3	A	1080	BES	C12-C7-C8	2.08	121.44	118.17

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1081	BES	O2-C2-C3-N1
3	A	1080	BES	C14-C13-C4-C5
3	A	1080	BES	C14-C13-C4-N1
3	B	1081	BES	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1081	BES	C14-C13-C4-N1
3	B	1081	BES	C13-C4-N1-C3
3	A	1080	BES	O2-C2-C3-N1
3	A	1080	BES	O2-C2-C3-O3
3	B	1081	BES	C14-C13-C4-C5

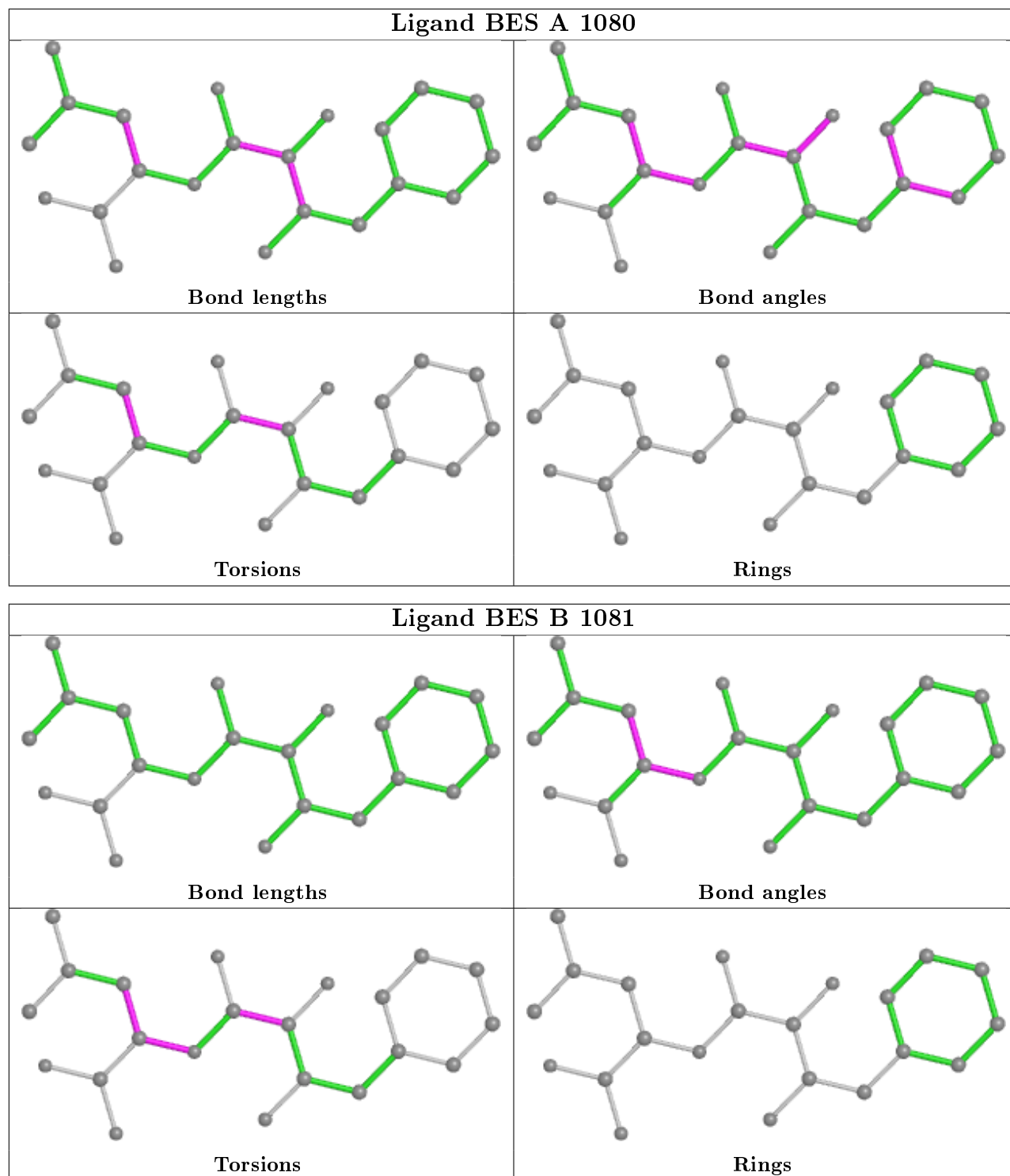
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1080	BES	3	0
3	B	1081	BES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	478/479 (99%)	0.22	23 (4%) 30 37	27, 45, 63, 90	0
1	B	478/479 (99%)	0.05	19 (3%) 38 45	27, 45, 64, 83	0
All	All	956/958 (99%)	0.14	42 (4%) 34 41	27, 45, 64, 90	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	GLU	4.1
1	A	71	ASP	4.0
1	A	197	TYR	3.6
1	B	231	VAL	3.6
1	A	418	ILE	3.4
1	B	272	GLU	3.4
1	A	70	PRO	3.4
1	B	275	ALA	3.4
1	B	71	ASP	3.3
1	A	279	HIS	3.2
1	A	271	ASP	2.9
1	A	416	GLY	2.9
1	B	474	LYS	2.9
1	B	228	HIS	2.9
1	A	415	GLY	2.8
1	B	72	GLY	2.8
1	A	68	LYS	2.8
1	B	-3	SER	2.8
1	B	269	VAL	2.7
1	B	331	VAL	2.7
1	B	330	THR	2.7
1	B	274	HIS	2.7
1	A	196	ASN	2.7
1	A	73	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	445	HIS	2.6
1	B	279	HIS	2.5
1	B	276	LEU	2.5
1	A	103	GLN	2.4
1	A	102	VAL	2.4
1	A	417	SER	2.4
1	B	230	GLY	2.4
1	A	444	ALA	2.4
1	A	436	PRO	2.4
1	A	129	GLY	2.3
1	A	269	VAL	2.3
1	A	18	TYR	2.3
1	A	435	LEU	2.2
1	B	5	LYS	2.1
1	A	193	ILE	2.1
1	B	229	SER	2.1
1	B	271	ASP	2.0
1	A	72	GLY	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, 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.

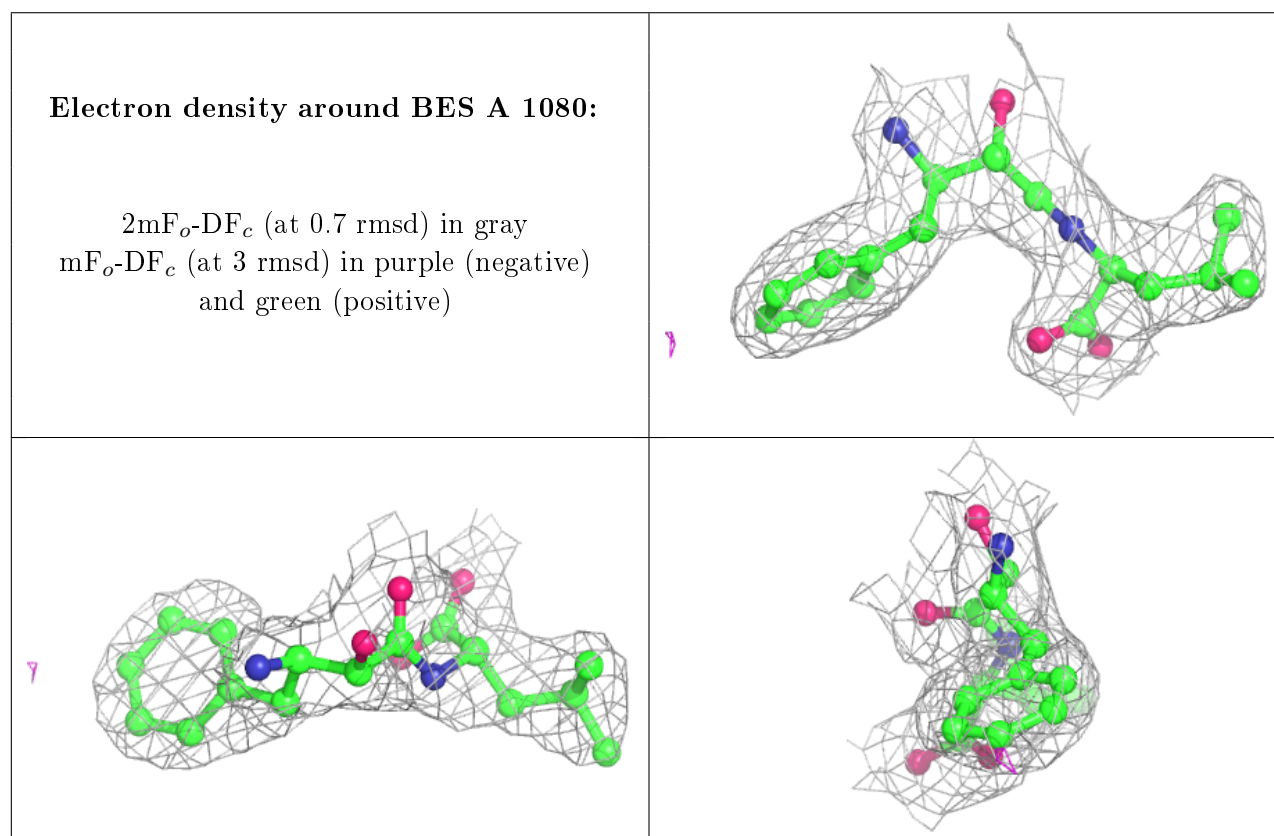
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BES	A	1080	22/22	0.97	0.32	26,30,37,38	0
3	BES	B	1081	22/22	0.98	0.16	24,34,39,39	0
2	MN	B	3002	1/1	0.99	0.14	32,32,32,32	0
2	MN	A	2002	1/1	1.00	0.18	33,33,33,33	0
2	MN	A	2001	1/1	1.00	0.15	30,30,30,30	0

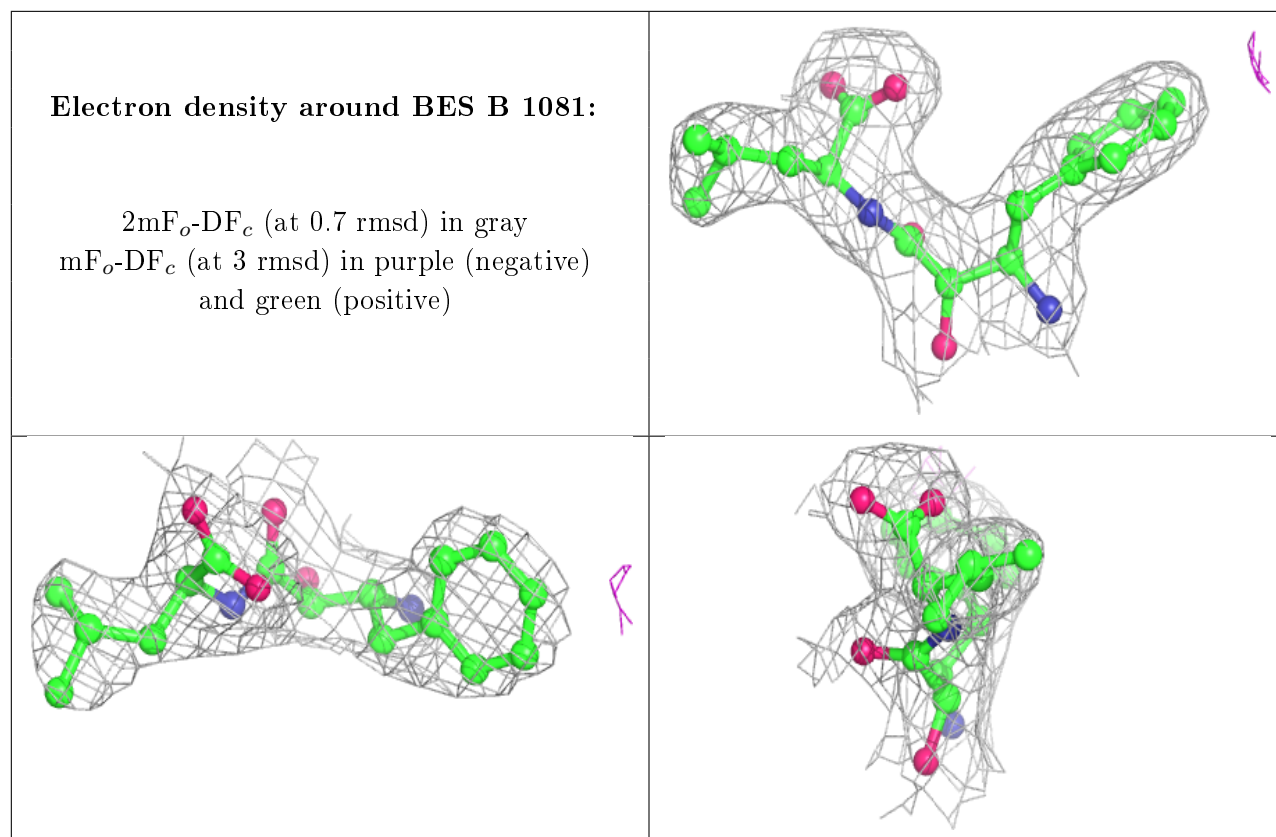
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MN	B	3001	1/1	1.00	0.16	31,31,31,31	0

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 [i](#)

There are no such residues in this entry.