Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:15 PM JST

PDB ID	:	7BVD
Title	:	Anthranilate synthase component I (TrpE)[Mycolicibacterium smegmatis]
Authors	:	Chen, Y.; Che, S.; Zhang, Q.; Bartlam, M.
Deposited on	:	2020-04-10
Resolution	:	1.70 Å(reported)

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

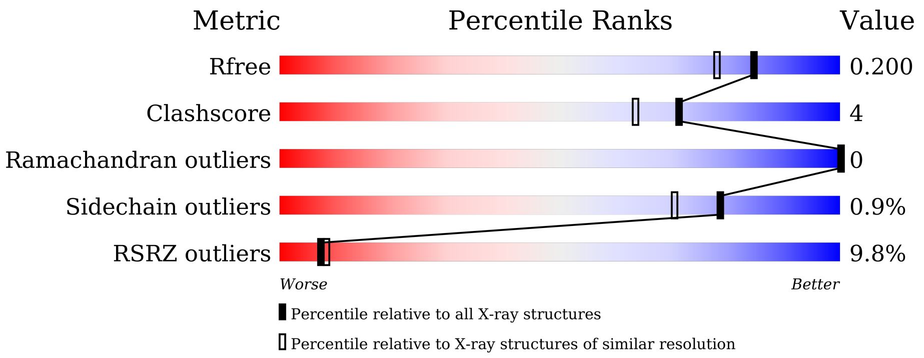
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

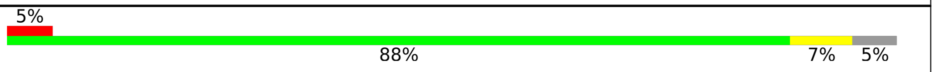
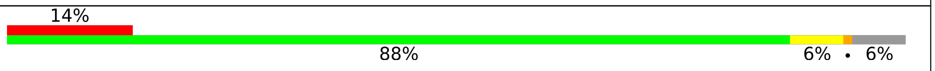
The reported resolution of this entry is 1.70 Å.

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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	524	
1	B	524	

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	PYR	A	604	-	X	-	-
5	GOL	B	603	-	-	-	X

2 Entry composition (i)

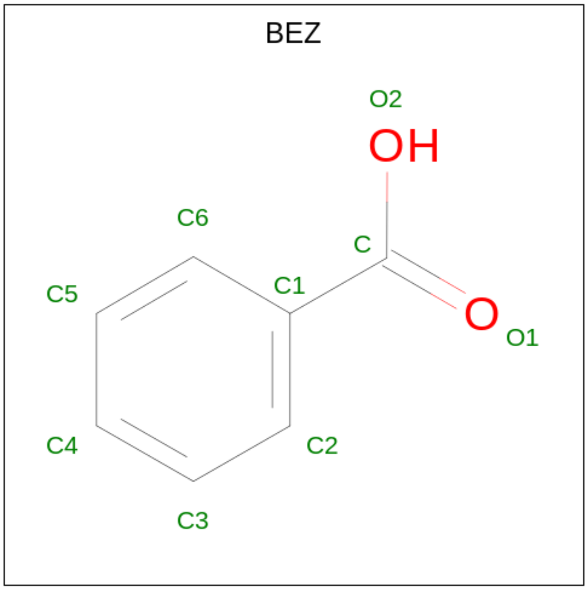
There are 6 unique types of molecules in this entry. The entry contains 15841 atoms, of which 7405 are hydrogens and 0 are deuteriums.

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 Anthranilate synthase component 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	499	Total 7473	C 2371	H 3688	N 662	O 739	S 13	0	0	0
1	B	495	Total 7414	C 2347	H 3672	N 654	O 728	S 13	0	0	0

- Molecule 2 is BENZOIC ACID (three-letter code: BEZ) (formula: $C_7H_6O_2$) (labeled as "Ligand of Interest" by depositor).

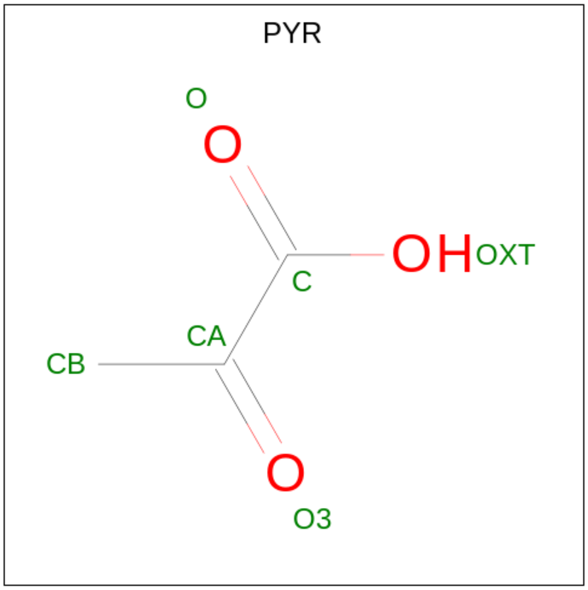


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 7	H 5	O 2	0	0
2	B	1	Total 14	C 7	H 5	O 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

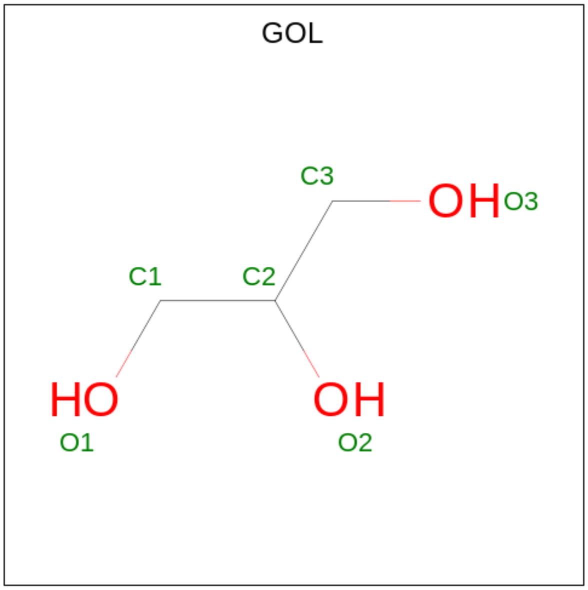
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	2	2	2	0	0
			Total	Mg		
3	B	1	1	1	0	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	9	3	3	3	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C H O 14 3 8 3	0	0
5	A	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0
5	B	1	Total C H O 14 3 8 3	0	0

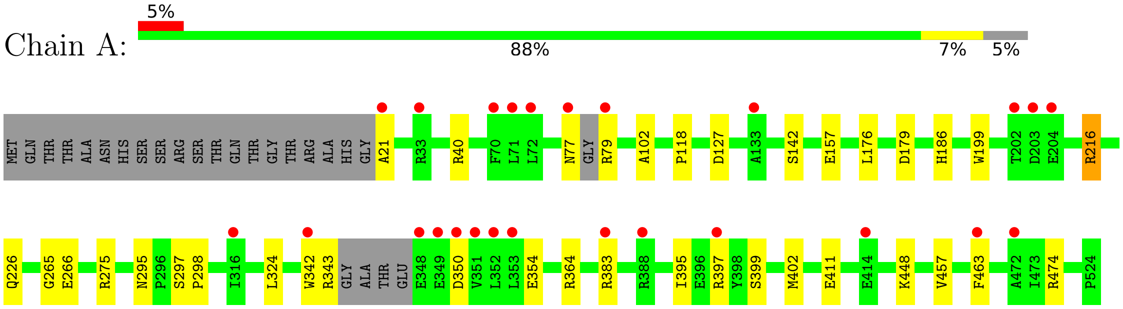
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	526	Total O 526 526	0	0
6	B	332	Total O 332 332	0	0

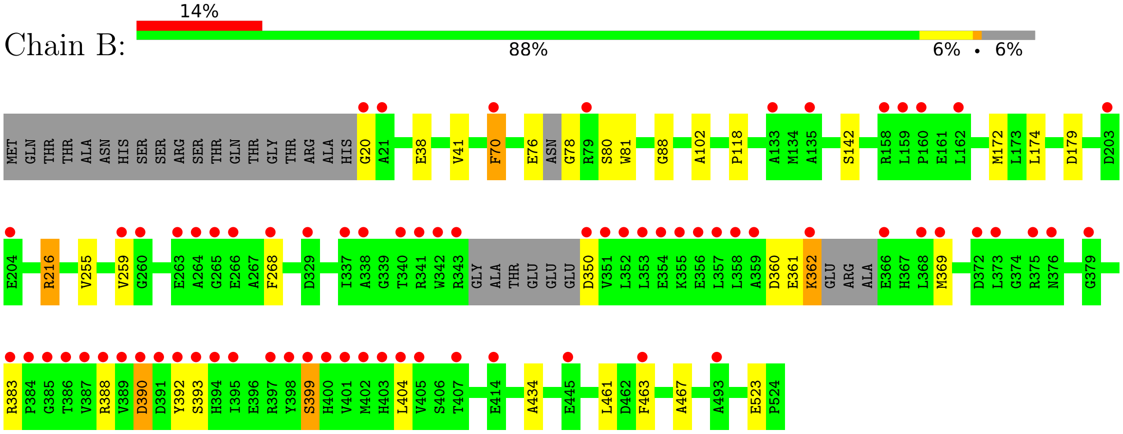
3 Residue-property plots

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: Anthranilate synthase component 1



- Molecule 1: Anthranilate synthase component 1



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.82Å 66.08Å 80.72Å 81.88° 72.73° 70.88°	Depositor
Resolution (Å)	38.49 – 1.70 38.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (38.49-1.70) 96.9 (38.49-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.91 (at 1.70Å)	Xtriage
Refinement program	PHENIX version 1.17.1-3660	Depositor
R, R_{free}	0.164 , 0.200 0.165 , 0.200	Depositor DCC
R_{free} test set	1998 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å^2)	21.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15841	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, PYR, BEZ, MG

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	0.51	0/3855	0.70	4/5250 (0.1%)
1	B	0.44	1/3811 (0.0%)	0.64	2/5189 (0.0%)
All	All	0.48	1/7666 (0.0%)	0.67	6/10439 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	PHE	CE2-CZ	6.02	1.48	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	A	216	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	275	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	216	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	216	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	275	ARG	NE-CZ-NH1	5.87	123.23	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	3785	3688	3733	28	0
1	B	3742	3672	3696	27	0
2	A	9	5	5	0	0
2	B	9	5	5	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	6	3	0	0	0
5	A	12	16	16	1	0
5	B	12	16	16	0	0
6	A	526	0	0	10	0
6	B	332	0	0	5	0
All	All	8436	7405	7471	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (53) 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:B:523:GLU:OE1	6:B:701:HOH:O	1.81	0.96
1:A:295:ASN:O	6:A:701:HOH:O	1.93	0.87
1:B:350:ASP:N	6:B:702:HOH:O	2.12	0.83
1:B:383:ARG:NH2	6:B:703:HOH:O	2.14	0.80
1:A:157:GLU:OE1	6:A:702:HOH:O	2.05	0.75
1:A:21:ALA:N	6:A:706:HOH:O	2.24	0.70
1:A:266:GLU:OE1	6:A:703:HOH:O	2.14	0.65
1:B:76:GLU:O	1:B:78:GLY:HA2	1.99	0.61
1:A:350:ASP:OD2	1:A:397:ARG:NH2	2.37	0.57
1:B:70:PHE:CE2	1:B:88:GLY:HA3	2.40	0.56
1:B:20:GLY:HA2	6:B:724:HOH:O	2.04	0.56
1:B:390:ASP:HB3	1:B:393:SER:HB3	1.88	0.56
1:A:448:LYS:NZ	6:A:716:HOH:O	2.39	0.55
1:A:383:ARG:NH1	6:A:712:HOH:O	2.33	0.55
1:A:226:GLN:NE2	6:A:707:HOH:O	2.25	0.53
1:B:360:ASP:OD1	1:B:362:LYS:HB2	2.08	0.53
1:A:186:HIS:CE1	1:B:399:SER:HB2	2.44	0.52
1:A:383:ARG:NH2	1:A:411:GLU:OE1	2.38	0.50
1:A:77:ASN:O	1:A:79:ARG:N	2.45	0.49
1:A:354:GLU:OE1	1:A:397:ARG:NH1	2.46	0.48
1:B:41:VAL:HG11	1:B:463:PHE:HD2	1.78	0.48
1:A:176:LEU:CD1	1:A:463:PHE:HZ	2.25	0.48
1:A:186:HIS:CD2	1:B:80:SER:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASP:OD1	1:A:216:ARG:HD2	2.14	0.47
1:A:324:LEU:HD22	1:A:457:VAL:HG11	1.97	0.47
1:B:102:ALA:HB2	1:B:118:PRO:HA	1.98	0.46
1:B:179:ASP:OD1	1:B:216:ARG:HD2	2.15	0.46
1:B:268:PHE:HB2	1:B:369:MET:SD	2.56	0.46
1:A:176:LEU:HD11	1:A:463:PHE:HZ	1.82	0.45
1:A:265:GLY:O	5:A:605:GOL:H2	2.17	0.45
1:A:127:ASP:OD1	6:A:704:HOH:O	2.21	0.45
1:B:172:MET:CE	1:B:174:LEU:HD12	2.47	0.45
1:A:342:TRP:O	1:A:343:ARG:HB2	2.17	0.45
1:B:142:SER:HB2	1:B:463:PHE:CE2	2.52	0.44
1:B:76:GLU:C	1:B:78:GLY:HA2	2.38	0.44
1:A:364:ARG:HD3	6:A:714:HOH:O	2.18	0.44
1:B:255:VAL:O	1:B:259:VAL:HG23	2.17	0.43
1:B:172:MET:HE3	1:B:174:LEU:CD1	2.48	0.43
1:B:461:LEU:HD23	1:B:467:ALA:HB2	2.00	0.43
1:B:80:SER:OG	1:B:81:TRP:N	2.50	0.43
1:B:392:TYR:HD2	1:B:404:LEU:HD21	1.84	0.42
1:B:369:MET:SD	1:B:434:ALA:HB3	2.59	0.42
1:A:395:ILE:HG21	1:A:402:MET:HE2	2.01	0.42
1:A:142:SER:HB2	1:A:463:PHE:CD2	2.54	0.42
1:B:392:TYR:CD1	1:B:392:TYR:N	2.88	0.42
1:A:297:SER:HB2	1:A:298:PRO:HD2	2.01	0.42
1:A:40:ARG:NH2	1:A:199:TRP:O	2.53	0.41
1:A:102:ALA:HB2	1:A:118:PRO:HA	2.02	0.41
1:B:369:MET:HB2	1:B:369:MET:HE3	1.91	0.41
1:A:474:ARG:HA	6:A:879:HOH:O	2.20	0.41
1:B:20:GLY:CA	6:B:724:HOH:O	2.66	0.41
1:A:142:SER:OG	1:A:463:PHE:HD2	2.04	0.40
1:B:172:MET:HE3	1:B:174:LEU:HD12	2.02	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	493/524 (94%)	485 (98%)	8 (2%)	0	100	100
1	B	487/524 (93%)	473 (97%)	14 (3%)	0	100	100
All	All	980/1048 (94%)	958 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	390/408 (96%)	389 (100%)	1 (0%)	92	89
1	B	385/408 (94%)	379 (98%)	6 (2%)	62	48
All	All	775/816 (95%)	768 (99%)	7 (1%)	78	70

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	399	SER
1	B	38	GLU
1	B	361	GLU
1	B	362	LYS
1	B	388	ARG
1	B	390	ASP
1	B	399	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	GOL	A	605	-	5,5,5	0.56	0	5,5,5	0.68	0
5	GOL	A	606	-	5,5,5	0.40	0	5,5,5	0.65	0
2	BEZ	B	601	-	9,9,9	0.88	1 (11%)	11,11,11	0.97	1 (9%)
2	BEZ	A	601	-	9,9,9	0.72	0	11,11,11	1.01	1 (9%)
5	GOL	B	604	-	5,5,5	0.30	0	5,5,5	0.22	0
5	GOL	B	603	-	5,5,5	0.29	0	5,5,5	0.39	0
4	PYR	A	604	-	5,5,5	3.26	3 (60%)	3,6,6	0.80	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	GOL	A	605	-	-	3/4/4/4	-
5	GOL	A	606	-	-	0/4/4/4	-

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Mol	**Type**	**Chain**	**Res**	**Link**	**Chirals**	**Torsions**	**Rings**
2	BEZ	B	601	-	-	0/4/4/4	0/1/1/1
2	BEZ	A	601	-	-	0/4/4/4	0/1/1/1
5	GOL	B	604	-	-	4/4/4/4	-
5	GOL	B	603	-	-	2/4/4/4	-
4	PYR	A	604	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(Å)**	**Ideal(Å)**
4	A	604	PYR	O-C	4.46	1.34	1.22
4	A	604	PYR	CA-C	-4.21	1.39	1.54
4	A	604	PYR	O3-CA	3.95	1.32	1.23
2	B	601	BEZ	O2-C	-2.13	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**	**Z**	**Observed(^{o})**	**Ideal(^{o})**
2	B	601	BEZ	O2-C-O1	-2.14	118.59	123.35
2	A	601	BEZ	O2-C-C1	2.09	120.27	114.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	**Chain**	**Res**	**Type**	**Atoms**
4	A	604	PYR	O-C-CA-CB
4	A	604	PYR	OXT-C-CA-CB
5	A	605	GOL	O1-C1-C2-C3
5	B	603	GOL	C1-C2-C3-O3
5	B	604	GOL	O1-C1-C2-C3
5	B	604	GOL	C1-C2-C3-O3
5	B	603	GOL	O2-C2-C3-O3
5	B	604	GOL	O1-C1-C2-O2
5	B	604	GOL	O2-C2-C3-O3
5	A	605	GOL	O1-C1-C2-O2
4	A	604	PYR	OXT-C-CA-O3
5	A	605	GOL	C1-C2-C3-O3

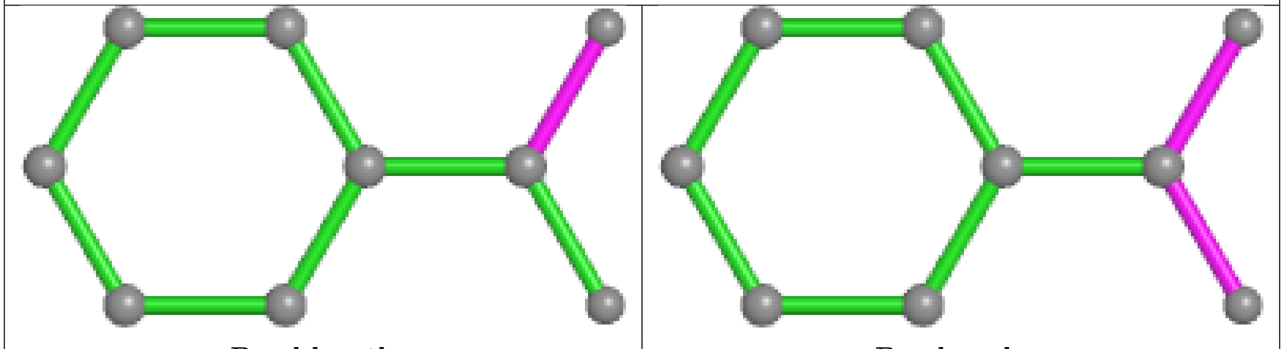
There are no ring outliers.

1 monomer is involved in 1 short contact:

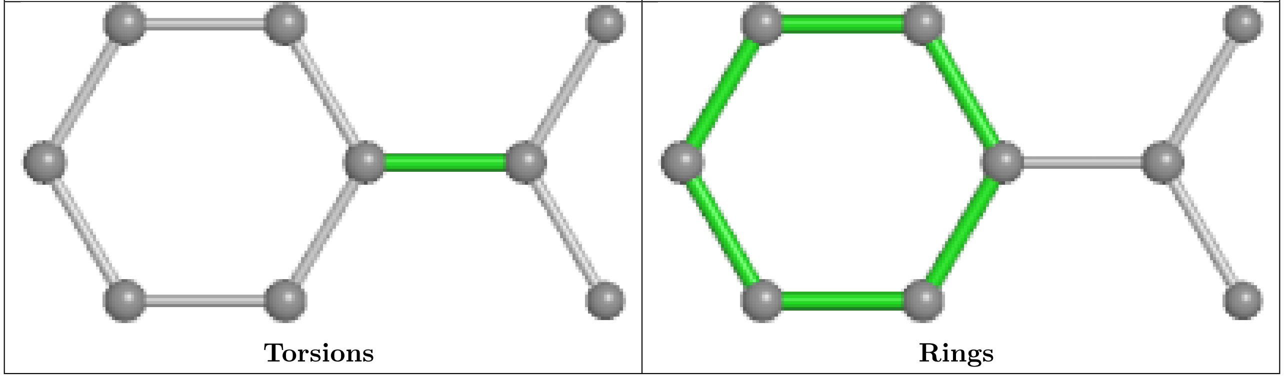
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	605	GOL	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand BEZ B 601

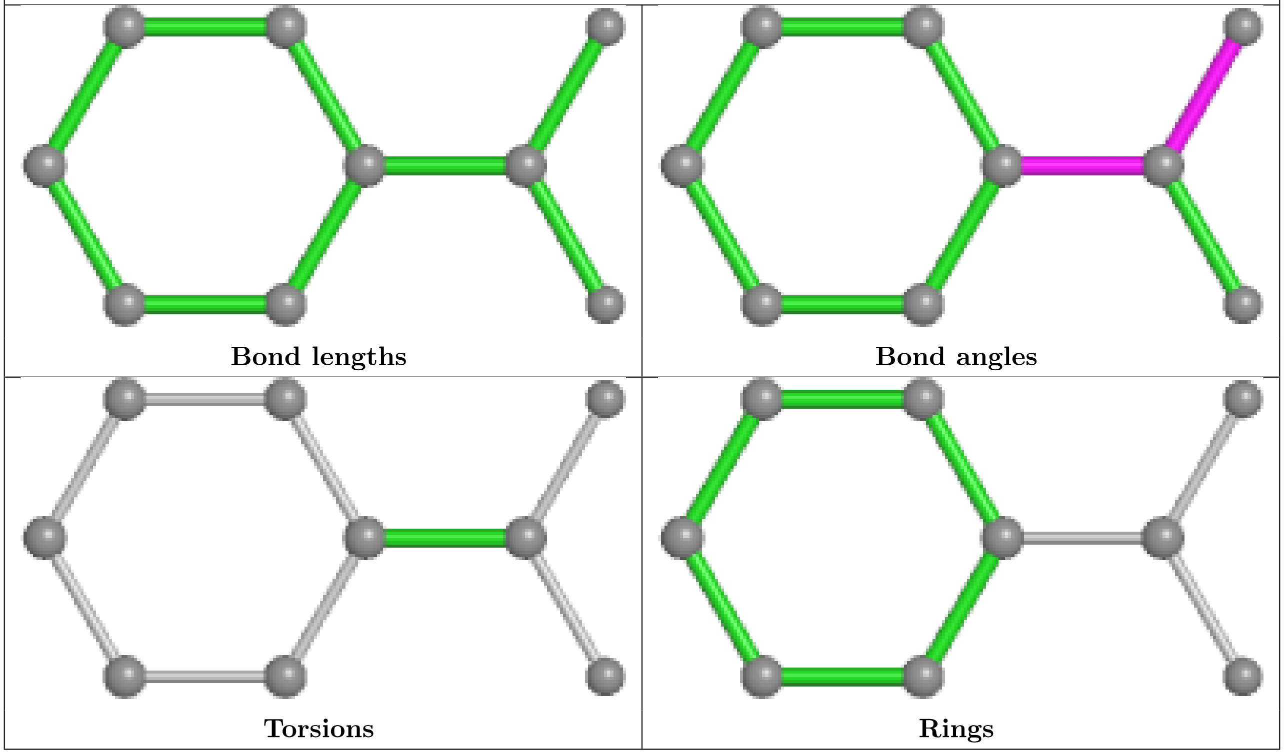


Bond lengths **Bond angles**



Torsions **Rings**

Ligand BEZ A 601



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	499/524 (95%)	0.11	25 (5%)	28	32	16, 25, 53, 76	0
1	B	495/524 (94%)	0.70	72 (14%)	2	2	16, 32, 81, 125	0
All	All	994/1048 (94%)	0.40	97 (9%)	7	8	16, 28, 71, 125	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	LEU	11.1
1	B	392	TYR	10.6
1	B	353	LEU	10.5
1	B	358	LEU	9.3
1	B	351	VAL	8.8
1	B	368	LEU	8.3
1	B	395	ILE	7.6
1	B	357	LEU	7.2
1	B	391	ASP	7.1
1	B	342	TRP	6.8
1	B	397	ARG	6.3
1	A	352	LEU	6.3
1	A	353	LEU	6.2
1	A	79	ARG	6.0
1	B	350	ASP	5.9
1	B	390	ASP	5.9
1	B	354	GLU	5.6
1	B	268	PHE	5.5
1	B	393	SER	5.5
1	B	400	HIS	5.3
1	A	351	VAL	5.1
1	B	388	ARG	5.1
1	B	355	LYS	5.0
1	B	265	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	79	ARG	4.9
1	B	20	GLY	4.9
1	B	158	ARG	4.7
1	B	463	PHE	4.4
1	B	405	VAL	4.4
1	B	394	HIS	4.3
1	B	386	THR	4.3
1	A	348	GLU	4.3
1	A	77	ASN	4.2
1	B	402	MET	4.2
1	B	362	LYS	4.2
1	B	383	ARG	4.1
1	B	389	VAL	4.1
1	B	407	THR	4.1
1	B	70	PHE	4.0
1	B	162	LEU	3.9
1	B	375	ARG	3.8
1	A	70	PHE	3.8
1	A	463	PHE	3.8
1	B	369	MET	3.7
1	A	21	ALA	3.7
1	B	398	TYR	3.7
1	A	342	TRP	3.7
1	A	133	ALA	3.6
1	B	343	ARG	3.6
1	A	350	ASP	3.6
1	B	338	ALA	3.5
1	B	404	LEU	3.5
1	B	160	PRO	3.5
1	A	349	GLU	3.4
1	B	399	SER	3.4
1	A	203	ASP	3.4
1	B	341	ARG	3.3
1	B	356	GLU	3.3
1	B	376	ASN	3.3
1	B	385	GLY	3.3
1	B	379	GLY	3.2
1	B	21	ALA	3.1
1	B	337	ILE	3.0
1	B	387	VAL	3.0
1	B	403	HIS	2.9
1	B	359	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	372	ASP	2.8
1	B	264	ALA	2.8
1	A	202	THR	2.8
1	B	260	GLY	2.8
1	B	159	LEU	2.7
1	A	204	GLU	2.7
1	B	414	GLU	2.7
1	A	388	ARG	2.6
1	B	329	ASP	2.6
1	B	384	PRO	2.6
1	A	397	ARG	2.5
1	B	133	ALA	2.5
1	A	71	LEU	2.3
1	A	72	LEU	2.3
1	B	259	VAL	2.3
1	B	340	THR	2.3
1	A	414	GLU	2.3
1	B	263	GLU	2.3
1	B	373	LEU	2.3
1	A	33	ARG	2.2
1	A	316	ILE	2.2
1	B	366	GLU	2.2
1	A	472	ALA	2.2
1	B	493	ALA	2.2
1	B	204	GLU	2.2
1	B	135	ALA	2.1
1	B	401	VAL	2.1
1	B	266	GLU	2.0
1	B	445	GLU	2.0
1	B	203	ASP	2.0
1	A	383	ARG	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)

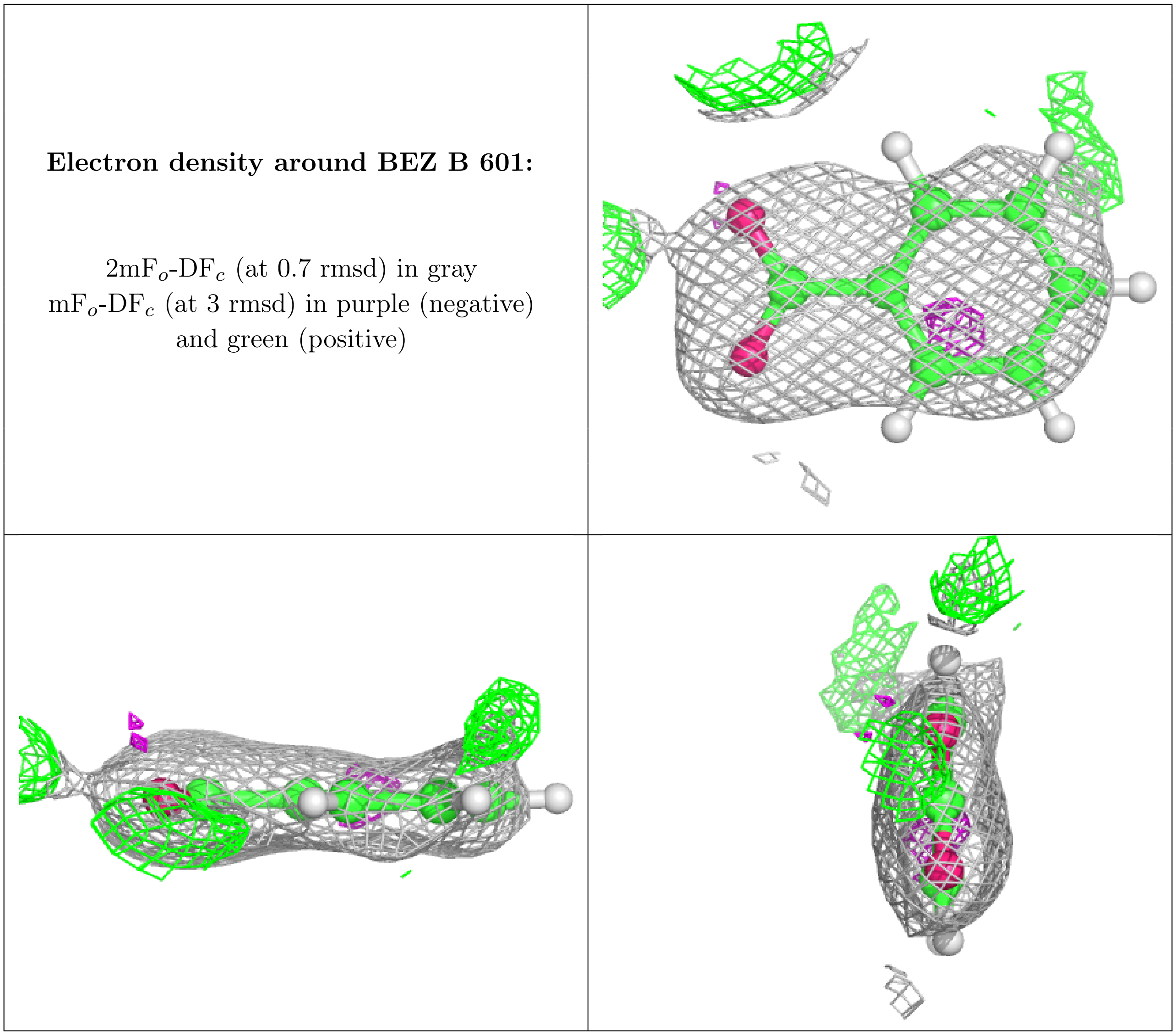
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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^{th} 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	GOL	B	603	6/6	0.71	0.42	52,63,67,68	0
3	MG	B	602	1/1	0.81	0.17	57,57,57,57	0
5	GOL	B	604	6/6	0.84	0.16	32,45,55,55	0
4	PYR	A	604	6/6	0.88	0.10	36,39,47,47	0
5	GOL	A	605	6/6	0.88	0.10	32,38,46,50	0
2	BEZ	B	601	9/9	0.92	0.12	32,49,59,62	0
3	MG	A	603	1/1	0.94	0.20	41,41,41,41	0
2	BEZ	A	601	9/9	0.98	0.10	21,30,39,41	0
5	GOL	A	606	6/6	0.98	0.07	22,29,37,37	0
3	MG	A	602	1/1	0.99	0.04	28,28,28,28	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.

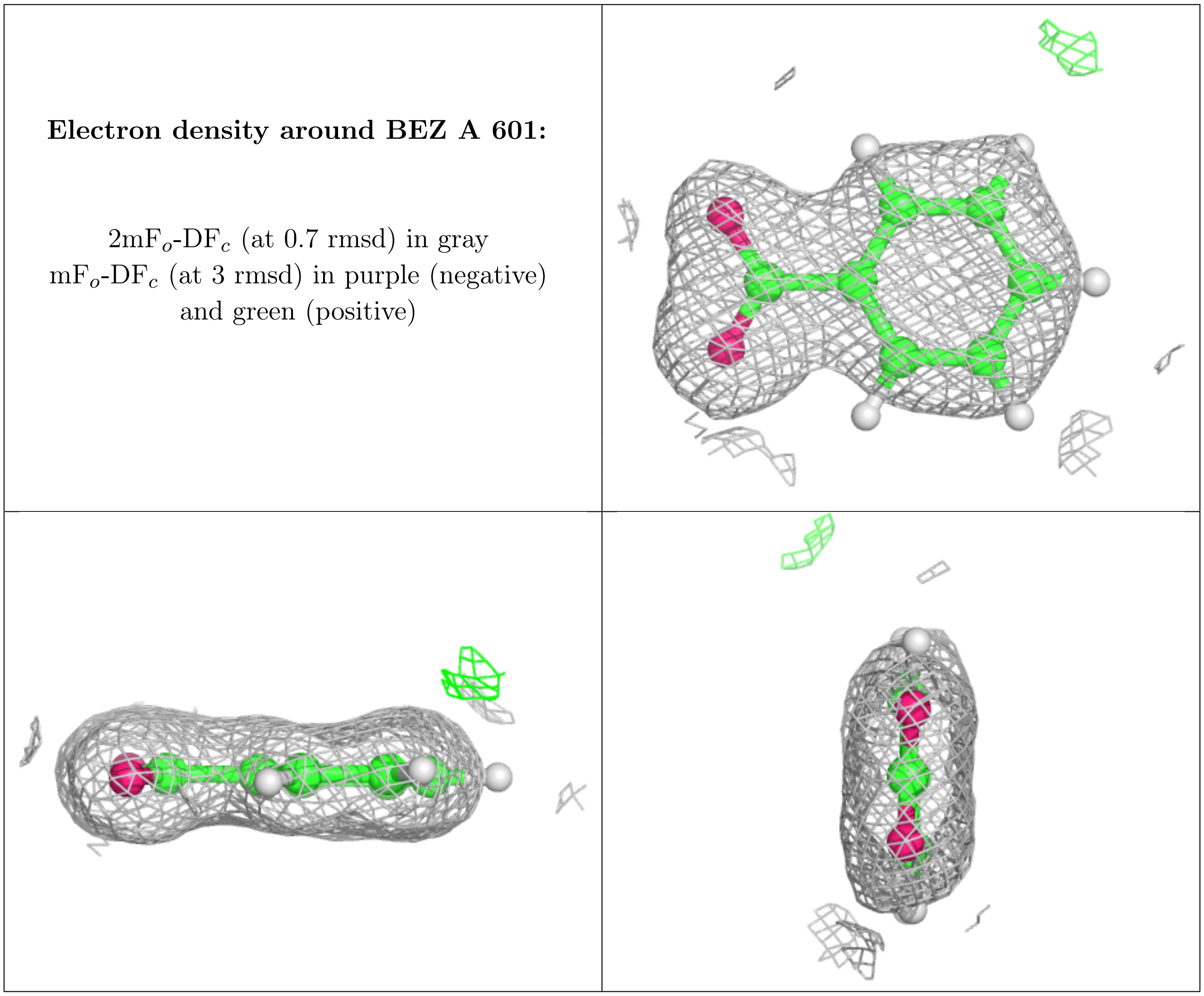


Electron density around BEZ B 601:

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

Electron density around BEZ A 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.