



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2022 – 06:42 PM JST

PDB ID : 7EXH
Title : Crystal structure of D383A mutant from Arabidopsis thaliana complexed with Galactinol.
Authors : Chuankhayan, P.; Guan, H.H.; Lin, C.C.; Chen, N.C.; Huang, Y.C.; Yoshimura, M.; Nakagawa, A.; Lee, R.H.; Chen, C.J.
Deposited on : 2021-05-27
Resolution : 2.63 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
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)	:	2.31.3

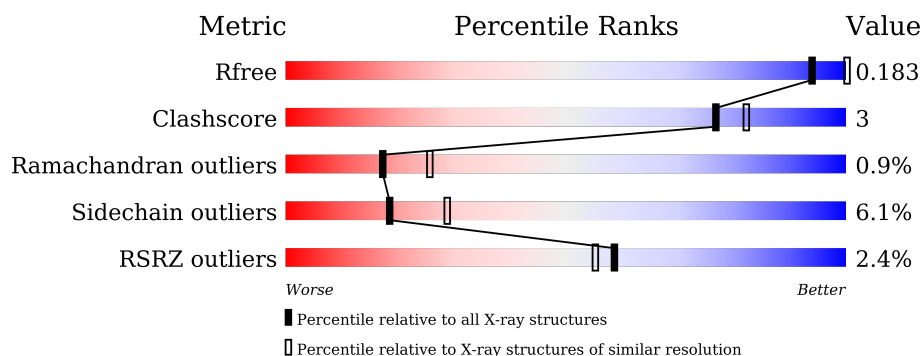
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 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	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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	749	<div> <div>4%</div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	B	749	<div> <div>%</div> <div>83%</div> <div>11%</div> <div>..</div> </div>

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
2	BQZ	A	801	X	-	-	-
2	BQZ	B	801	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11330 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.

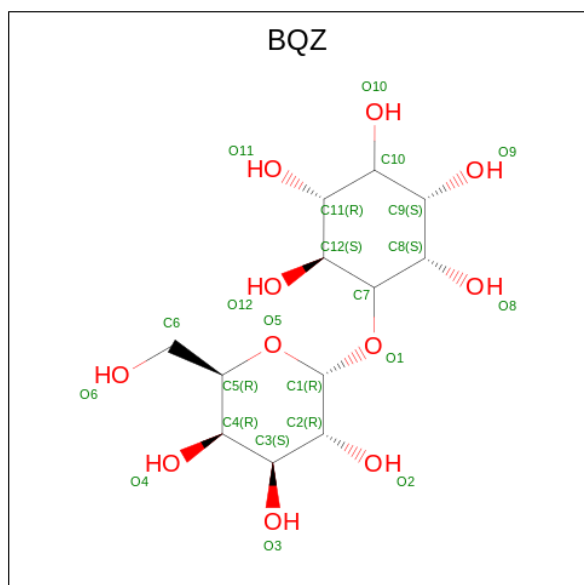
- Molecule 1 is a protein called Probable galactinol–sucrose galactosyltransferase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	717	Total	C	N	O	S	0	0	0
			5616	3570	968	1049	29			
1	A	717	Total	C	N	O	S	0	0	0
			5616	3570	968	1049	29			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	302	ARG	LYS	conflict	UNP Q8RX87
B	383	ALA	ASP	engineered mutation	UNP Q8RX87
A	302	ARG	LYS	conflict	UNP Q8RX87
A	383	ALA	ASP	engineered mutation	UNP Q8RX87

- Molecule 2 is galactinol (three-letter code: BQZ) (formula: $C_{12}H_{22}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			23	12	11		
2	A	1	Total	C	O	0	0
			23	12	11		

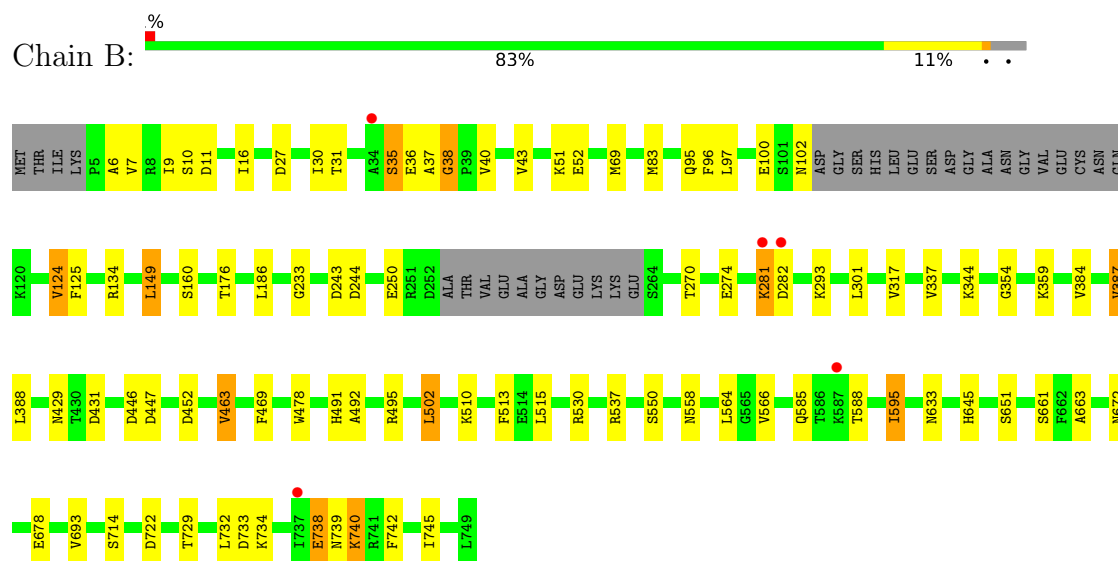
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	30	Total	O	0	0
			30	30		
3	A	22	Total	O	0	0
			22	22		

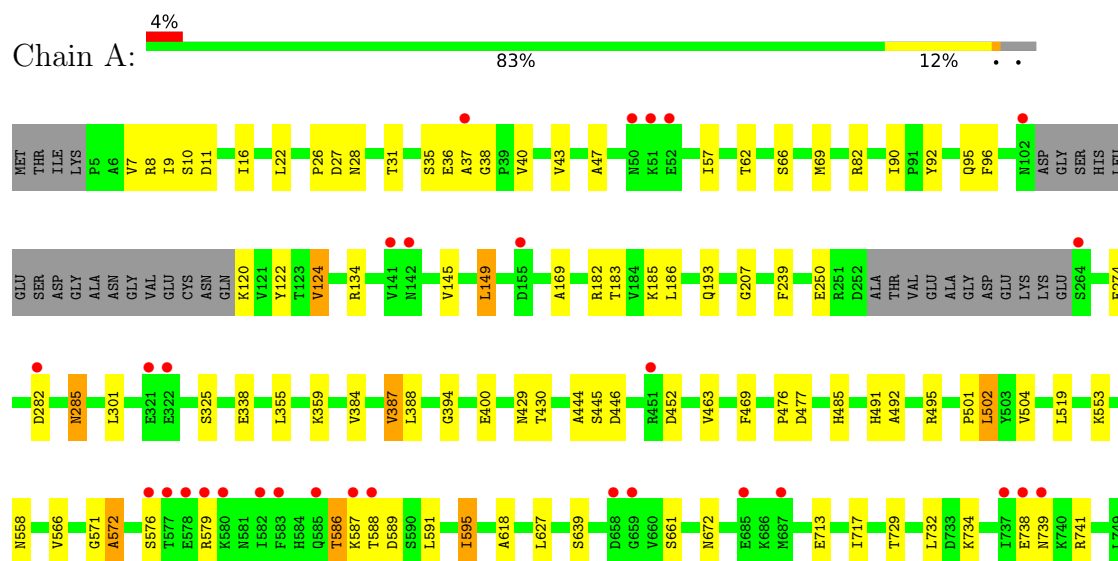
3 Residue-property plots

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: Probable galactinol–sucrose galactosyltransferase 6



- Molecule 1: Probable galactinol–sucrose galactosyltransferase 6



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.52Å 103.65Å 182.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.22 – 2.63 30.67 – 2.63	Depositor EDS
% Data completeness (in resolution range)	99.4 (91.22-2.63) 99.5 (30.67-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.183 , 0.246 0.186 , 0.183	Depositor DCC
R_{free} test set	2690 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 24.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11330	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: BQZ

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	0/5750	0.85	4/7787 (0.1%)
1	B	0.74	0/5750	0.90	9/7787 (0.1%)
All	All	0.70	0/11500	0.88	13/15574 (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
1	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	B	530	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	149	LEU	CA-CB-CG	6.90	131.17	115.30
1	B	387	VAL	CB-CA-C	-6.34	99.36	111.40
1	B	244	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	37	ALA	N-CA-C	6.00	127.21	111.00
1	A	149	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	738	GLU	C-N-CA	5.77	136.12	121.70
1	B	722	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	82	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	37	ALA	CA-C-N	5.37	126.94	116.20
1	B	738	GLU	CA-C-N	5.05	128.31	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	VAL	CB-CA-C	-5.05	101.81	111.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	SER	Peptide
1	A	394	GLY	Peptide
1	A	445	SER	Peptide
1	A	586	THR	Peptide
1	B	281	LYS	Peptide
1	B	35	SER	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	5616	0	5537	36	0
1	B	5616	0	5537	32	0
2	A	23	0	0	0	0
2	B	23	0	0	2	0
3	A	22	0	0	1	0
3	B	30	0	0	0	0
All	All	11330	0	11074	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (68) 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:558:ASN:HD21	1:B:672:ASN:HD21	1.41	0.66
1:B:738:GLU:HB3	1:B:739:ASN:HB2	1.77	0.65
1:A:558:ASN:HD21	1:A:672:ASN:HD21	1.45	0.62
1:B:693:VAL:HG21	1:B:745:ILE:HD12	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ALA:HB1	1:A:627:LEU:HD11	1.85	0.59
1:B:95:GLN:HE22	1:B:429:ASN:HA	1.67	0.58
1:B:693:VAL:CG2	1:B:745:ILE:HD12	2.32	0.58
1:A:90:ILE:HD12	1:A:145:VAL:HG22	1.87	0.55
1:A:495:ARG:HB3	1:A:502:LEU:HD22	1.88	0.54
1:A:40:VAL:HG21	1:A:183:THR:HG23	1.91	0.52
1:A:95:GLN:HE21	1:A:134:ARG:HH21	1.57	0.52
1:B:463:VAL:HG13	1:B:478:TRP:CE2	2.45	0.51
1:A:444:ALA:HB2	1:A:476:PRO:HB3	1.94	0.50
1:B:566:VAL:O	1:B:645:HIS:HA	2.11	0.50
1:B:96:PHE:HB3	1:B:469:PHE:CE2	2.47	0.50
1:A:95:GLN:NE2	1:A:430:THR:HG23	2.27	0.49
1:B:95:GLN:HE21	1:B:134:ARG:HH21	1.59	0.49
1:B:35:SER:O	1:B:38:GLY:HA2	2.13	0.49
1:B:651:SER:HB3	1:B:663:ALA:HB1	1.94	0.48
1:A:9:ILE:HD12	1:A:31:THR:HG21	1.94	0.48
1:A:576:SER:O	1:A:579:ARG:NH1	2.47	0.48
1:B:97:LEU:HB3	1:B:125:PHE:HB2	1.95	0.48
1:B:738:GLU:HB3	1:B:739:ASN:CB	2.42	0.48
1:A:738:GLU:HB3	1:A:739:ASN:HB3	1.96	0.47
1:A:553:LYS:HD3	1:A:595:ILE:HD12	1.96	0.47
1:B:738:GLU:HB2	1:B:740:LYS:HB2	1.96	0.47
1:A:96:PHE:HB3	1:A:469:PHE:CE2	2.50	0.47
1:A:477:ASP:HA	1:A:501:PRO:HD2	1.97	0.47
1:A:338:GLU:O	1:A:579:ARG:NE	2.48	0.46
1:A:285:ASN:N	1:A:285:ASN:OD1	2.48	0.46
1:B:492:ALA:CB	1:B:515:LEU:HD21	2.46	0.46
1:A:588:THR:HG22	1:A:589:ASP:H	1.80	0.46
1:B:95:GLN:NE2	1:B:134:ARG:HH21	2.13	0.45
1:A:7:VAL:HG13	1:A:16:ILE:CD1	2.47	0.45
1:B:678:GLU:HG3	1:B:742:PHE:CE1	2.52	0.45
1:A:207:GLY:HA3	1:A:239:PHE:CZ	2.53	0.44
1:B:495:ARG:HB3	1:B:502:LEU:HD22	1.99	0.44
1:B:7:VAL:HG13	1:B:16:ILE:CD1	2.48	0.43
1:A:22:LEU:HA	1:A:62:THR:O	2.19	0.43
1:A:90:ILE:CD1	1:A:145:VAL:HG22	2.46	0.43
1:B:250:GLU:HB2	1:B:270:THR:HG21	1.99	0.43
1:B:9:ILE:HD12	1:B:31:THR:CG2	2.48	0.43
1:A:558:ASN:ND2	1:A:672:ASN:HD21	2.15	0.43
1:B:124:VAL:HG23	1:B:176:THR:HG22	2.00	0.43
1:B:463:VAL:HG22	1:B:478:TRP:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:HIS:O	1:A:495:ARG:HG2	2.18	0.42
1:A:384:VAL:O	1:A:387:VAL:HG22	2.19	0.42
1:A:571:GLY:O	1:A:572:ALA:HB2	2.19	0.42
1:B:233:GLY:HA3	1:B:513:PHE:CE1	2.55	0.42
1:A:325:SER:HA	1:A:355:LEU:O	2.19	0.42
1:A:492:ALA:HB1	1:A:519:LEU:HD11	2.01	0.42
1:A:28:ASN:O	1:A:47:ALA:HA	2.20	0.41
1:A:95:GLN:HE22	1:A:429:ASN:HA	1.85	0.41
1:A:122:TYR:O	1:A:169:ALA:HA	2.19	0.41
1:B:491:HIS:HD1	1:B:495:ARG:HH12	1.68	0.41
1:B:515:LEU:HD23	1:B:515:LEU:O	2.19	0.41
1:A:250:GLU:CB	3:A:905:HOH:O	2.68	0.41
1:A:185:LYS:NZ	1:A:193:GLN:HE21	2.19	0.41
1:B:243:ASP:OD2	2:B:801:BQZ:O4	2.38	0.41
1:B:337:VAL:HG13	1:B:344:LYS:HE3	2.01	0.41
1:A:92:TYR:CE1	1:A:338:GLU:HG2	2.55	0.41
1:A:384:VAL:O	1:A:384:VAL:HG12	2.21	0.41
1:B:447:ASP:OD1	2:B:801:BQZ:O2	2.40	0.40
1:A:37:ALA:N	1:A:38:GLY:HA2	2.37	0.40
1:B:124:VAL:CG2	1:B:176:THR:HG22	2.51	0.40
1:B:317:VAL:O	1:B:354:GLY:HA3	2.22	0.40
1:A:566:VAL:HG22	1:A:595:ILE:HD11	2.03	0.40
1:B:564:LEU:HD21	1:B:595:ILE:HG13	2.04	0.40

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	711/749 (95%)	672 (94%)	32 (4%)	7 (1%)	15 22
1	B	711/749 (95%)	675 (95%)	30 (4%)	6 (1%)	19 28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1422/1498 (95%)	1347 (95%)	62 (4%)	13 (1%)	17	26

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	GLU
1	A	282	ASP
1	A	446	ASP
1	A	572	ALA
1	A	741	ARG
1	B	6	ALA
1	B	282	ASP
1	A	11	ASP
1	A	36	GLU
1	B	446	ASP
1	B	38	GLY
1	B	281	LYS
1	A	26	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	615/640 (96%)	581 (94%)	34 (6%)	21	33
1	B	615/640 (96%)	574 (93%)	41 (7%)	16	24
All	All	1230/1280 (96%)	1155 (94%)	75 (6%)	18	29

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	SER
1	B	11	ASP
1	B	27	ASP
1	B	30	ILE
1	B	40	VAL

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Mol	Chain	Res	Type
1	B	43	VAL
1	B	51	LYS
1	B	52	GLU
1	B	69	MET
1	B	83	MET
1	B	100	GLU
1	B	102	ASN
1	B	124	VAL
1	B	149	LEU
1	B	160	SER
1	B	186	LEU
1	B	274	GLU
1	B	293	LYS
1	B	301	LEU
1	B	359	LYS
1	B	384	VAL
1	B	387	VAL
1	B	388	LEU
1	B	431	ASP
1	B	452	ASP
1	B	463	VAL
1	B	502	LEU
1	B	510	LYS
1	B	537	ARG
1	B	550	SER
1	B	585	GLN
1	B	588	THR
1	B	595	ILE
1	B	633	ASN
1	B	661	SER
1	B	714	SER
1	B	729	THR
1	B	732	LEU
1	B	733	ASP
1	B	734	LYS
1	B	740	LYS
1	A	8	ARG
1	A	10	SER
1	A	27	ASP
1	A	43	VAL
1	A	57	ILE
1	A	66	SER

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Mol	Chain	Res	Type
1	A	69	MET
1	A	120	LYS
1	A	124	VAL
1	A	149	LEU
1	A	186	LEU
1	A	274	GLU
1	A	285	ASN
1	A	301	LEU
1	A	359	LYS
1	A	387	VAL
1	A	388	LEU
1	A	400	GLU
1	A	452	ASP
1	A	463	VAL
1	A	485	HIS
1	A	502	LEU
1	A	504	VAL
1	A	586	THR
1	A	587	LYS
1	A	591	LEU
1	A	595	ILE
1	A	639	SER
1	A	661	SER
1	A	713	GLU
1	A	717	ILE
1	A	729	THR
1	A	732	LEU
1	A	734	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	56	HIS
1	B	95	GLN
1	B	138	GLN
1	B	175	GLN
1	B	193	GLN
1	B	385	GLN
1	B	406	HIS
1	B	456	HIS
1	B	482	HIS
1	B	558	ASN

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Mol	Chain	Res	Type
1	A	18	ASN
1	A	95	GLN
1	A	175	GLN
1	A	193	GLN
1	A	385	GLN
1	A	406	HIS
1	A	456	HIS
1	A	482	HIS
1	A	558	ASN
1	A	633	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	BQZ	A	801	-	24,24,24	1.04	2 (8%)	36,36,36	1.80	11 (30%)
2	BQZ	B	801	-	24,24,24	1.19	2 (8%)	36,36,36	2.26	14 (38%)

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
2	BQZ	A	801	-	7/7/11/11	0/6/50/50	0/2/2/2
2	BQZ	B	801	-	7/7/11/11	1/6/50/50	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BQZ	O3-C3	2.54	1.48	1.43
2	A	801	BQZ	O3-C3	2.11	1.48	1.43
2	A	801	BQZ	C2-C3	-2.04	1.47	1.52
2	B	801	BQZ	C6-C5	-2.00	1.45	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BQZ	C3-C4-C5	5.37	119.82	110.24
2	B	801	BQZ	C9-C8-C7	4.32	119.55	109.68
2	B	801	BQZ	C9-C10-C11	-4.05	103.75	110.82
2	A	801	BQZ	C3-C4-C5	3.97	117.33	110.24
2	B	801	BQZ	C11-C12-C7	-3.97	100.61	109.68
2	A	801	BQZ	O5-C1-C2	-3.94	102.01	110.35
2	B	801	BQZ	O1-C7-C12	3.85	117.53	107.28
2	A	801	BQZ	O5-C5-C4	3.72	116.45	109.69
2	B	801	BQZ	O11-C11-C10	3.55	118.56	110.35
2	A	801	BQZ	O1-C1-O5	-3.27	101.53	110.67
2	B	801	BQZ	O5-C5-C4	3.25	115.59	109.69
2	B	801	BQZ	O1-C7-C8	3.22	115.86	107.28
2	A	801	BQZ	O2-C2-C1	3.10	117.57	110.05
2	A	801	BQZ	O1-C7-C12	2.83	114.80	107.28
2	B	801	BQZ	O1-C1-O5	-2.59	103.43	110.67
2	B	801	BQZ	O11-C11-C12	2.54	116.23	110.35
2	A	801	BQZ	O1-C1-C2	2.46	114.48	108.10
2	A	801	BQZ	C2-C3-C4	2.40	115.01	110.82
2	B	801	BQZ	O3-C3-C2	2.26	115.57	110.35
2	B	801	BQZ	O1-C1-C2	2.16	113.71	108.10
2	A	801	BQZ	C9-C8-C7	2.13	114.54	109.68
2	B	801	BQZ	O10-C10-C11	2.12	115.24	110.35
2	A	801	BQZ	O5-C5-C6	2.11	111.68	106.44
2	A	801	BQZ	C1-O5-C5	2.05	117.71	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BQZ	O8-C8-C9	2.03	115.04	110.35

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	801	BQZ	C5
2	B	801	BQZ	C11
2	B	801	BQZ	C4
2	B	801	BQZ	C8
2	B	801	BQZ	C12
2	B	801	BQZ	C1
2	B	801	BQZ	C3
2	A	801	BQZ	C5
2	A	801	BQZ	C11
2	A	801	BQZ	C4
2	A	801	BQZ	C8
2	A	801	BQZ	C12
2	A	801	BQZ	C1
2	A	801	BQZ	C3

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	BQZ	C4-C5-C6-O6

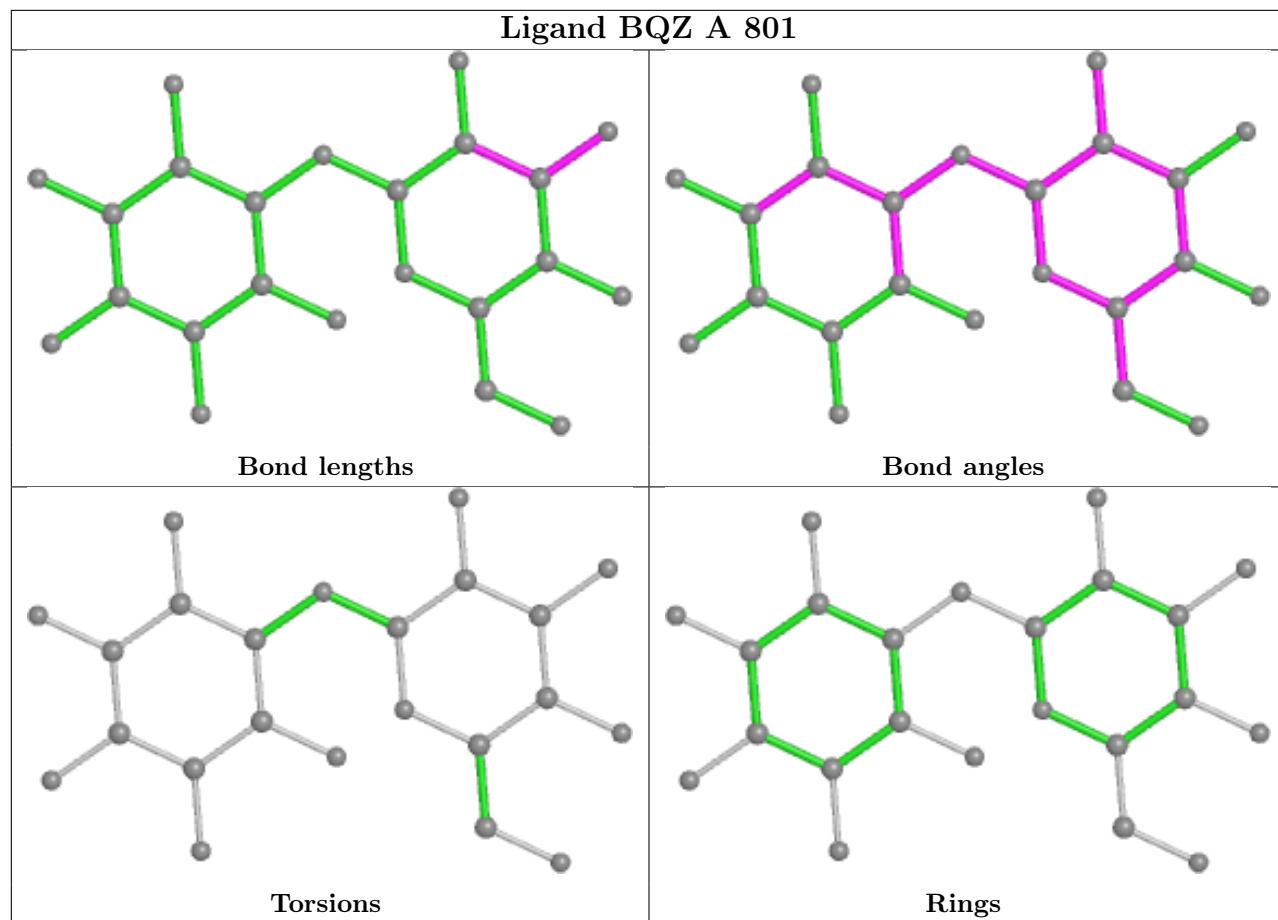
There are no ring outliers.

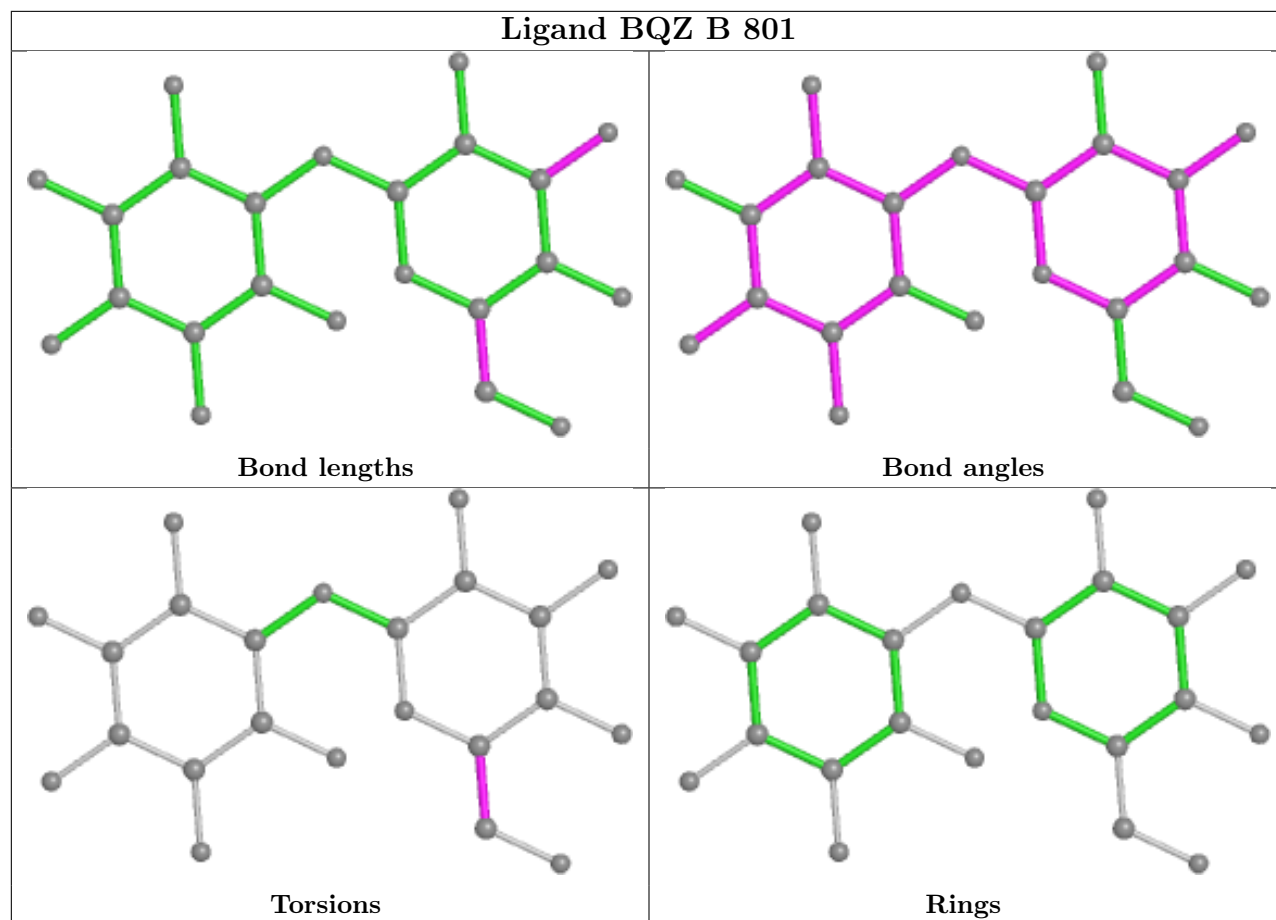
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	BQZ	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

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	717/749 (95%)	-0.22	30 (4%) 36 33	32, 55, 99, 134	0
1	B	717/749 (95%)	-0.39	5 (0%) 87 86	26, 42, 73, 118	0
All	All	1434/1498 (95%)	-0.31	35 (2%) 59 55	26, 49, 89, 134	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	658	ASP	5.1
1	A	587	LYS	4.4
1	A	578	GLU	4.1
1	A	577	THR	4.0
1	A	102	ASN	3.9
1	A	583	PHE	3.8
1	A	687	MET	3.8
1	A	659	GLY	3.6
1	A	685	GLU	3.5
1	A	585	GLN	3.4
1	A	737	ILE	3.3
1	A	264	SER	3.0
1	B	281	LYS	3.0
1	A	576	SER	3.0
1	A	37	ALA	2.9
1	A	739	ASN	2.8
1	B	587	LYS	2.7
1	A	451	ARG	2.5
1	A	579	ARG	2.5
1	A	588	THR	2.5
1	A	51	LYS	2.5
1	A	321	GLU	2.4
1	A	282	ASP	2.4
1	A	738	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	582	ILE	2.4
1	B	34	ALA	2.3
1	A	52	GLU	2.2
1	A	141	VAL	2.2
1	B	282	ASP	2.2
1	A	50	ASN	2.1
1	A	155	ASP	2.1
1	B	737	ILE	2.1
1	A	142	ASN	2.1
1	A	322	GLU	2.1
1	A	580	LYS	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 [i](#)

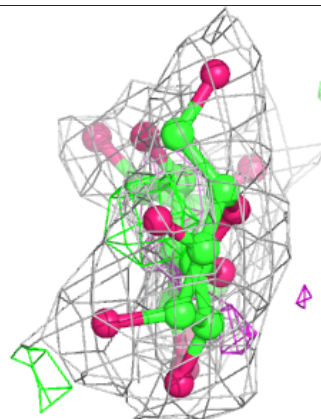
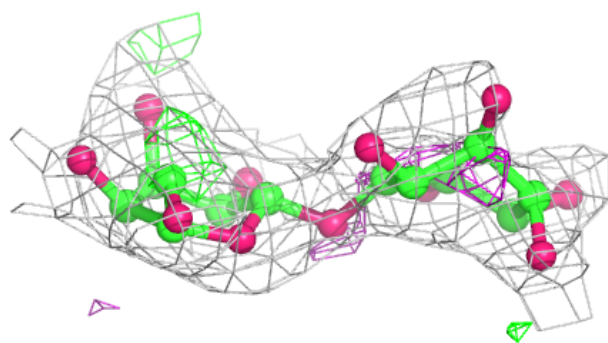
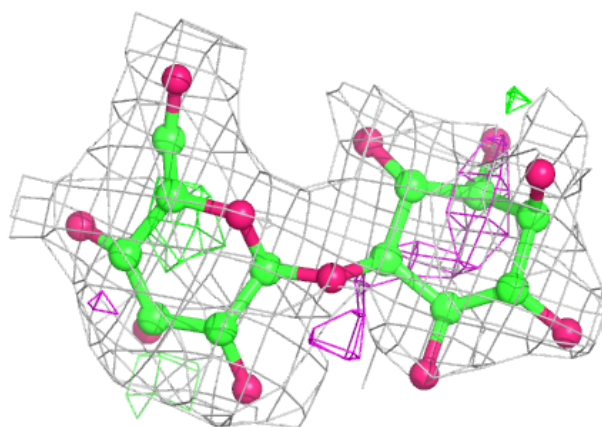
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

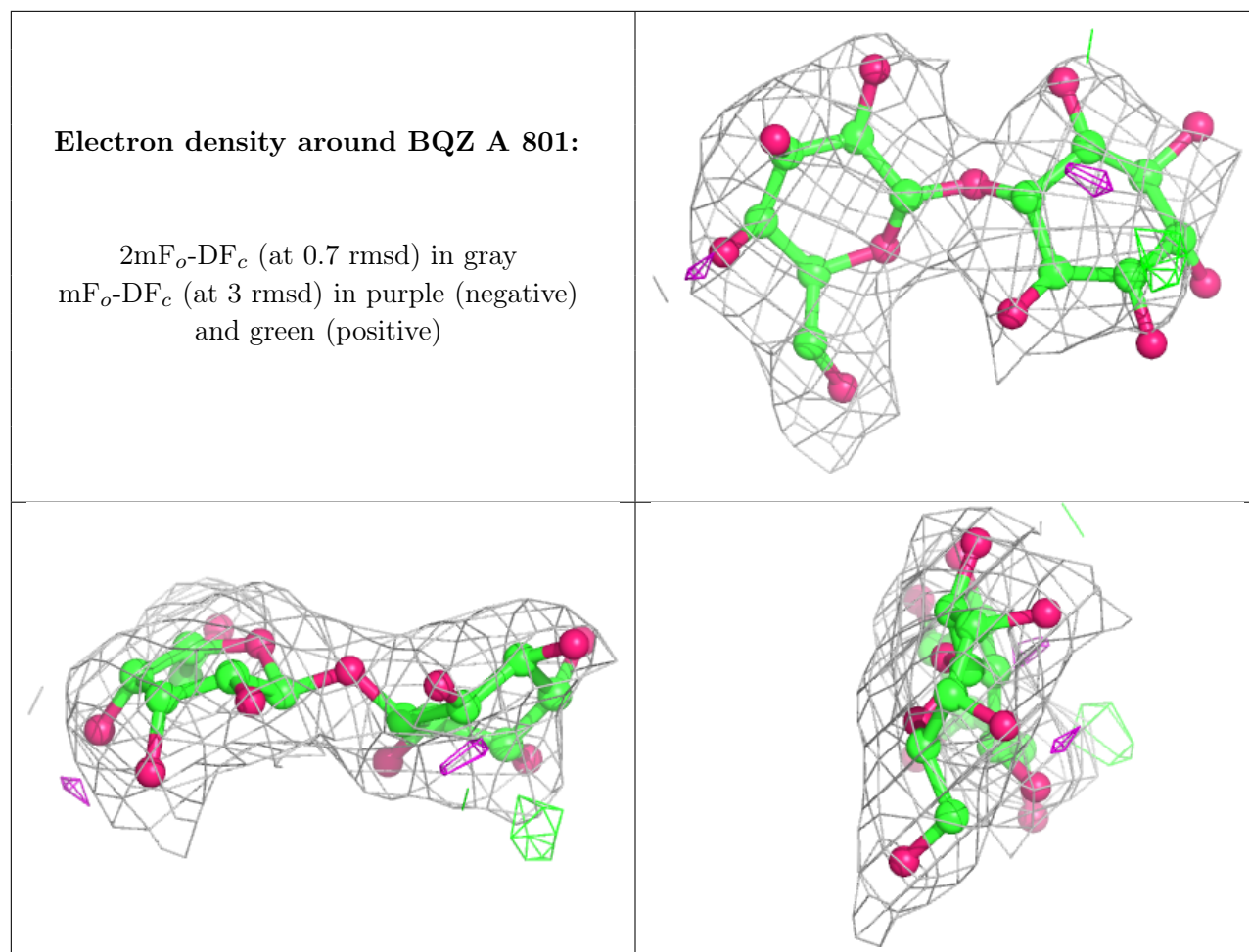
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BQZ	B	801	23/23	0.89	0.22	32,47,75,76	0
2	BQZ	A	801	23/23	0.91	0.21	41,60,84,93	0

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 BQZ B 801:

$2mF_o-DF_c$ (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.