



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:03 PM UTC

PDB ID : 8RW3 / pdb_00008rw3
Title : Crystal Structure of Agd31B, alpha-transglucosylase, complexed with a non-covalent 1,2- Cyclophellitol aziridine
Authors : Moran, E.; Davies, G.; Ofamn, T.; Heming, J.; Nin-Hill, A.; Kullmer, F.; Steneker, R.; Klein, A.; Bennett, M.; Ruijgrok, G.; Kok, K.; Aerts, J.; Van der Marel, G.; Rovira, C.; Artola, M.; Codee, J.; Overkleeft, H.
Deposited on : 2024-02-02
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

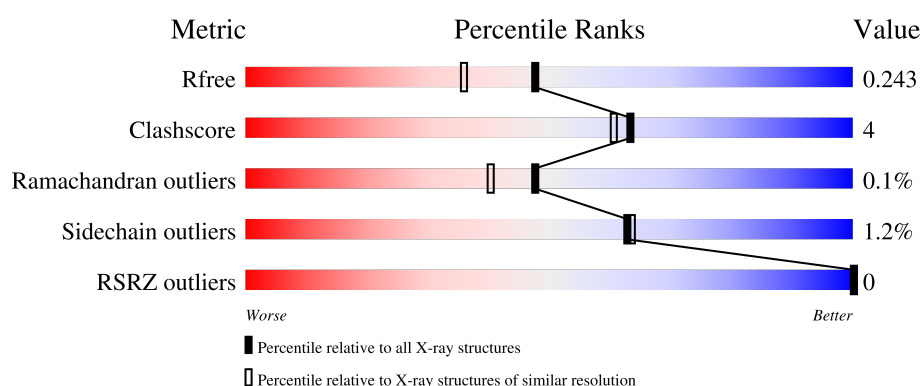
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	817	
1	B	817	
1	C	817	

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
3	OXL	A	907	-	X	-	-
3	OXL	B	903	-	X	-	-
3	OXL	C	902	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 19733 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.

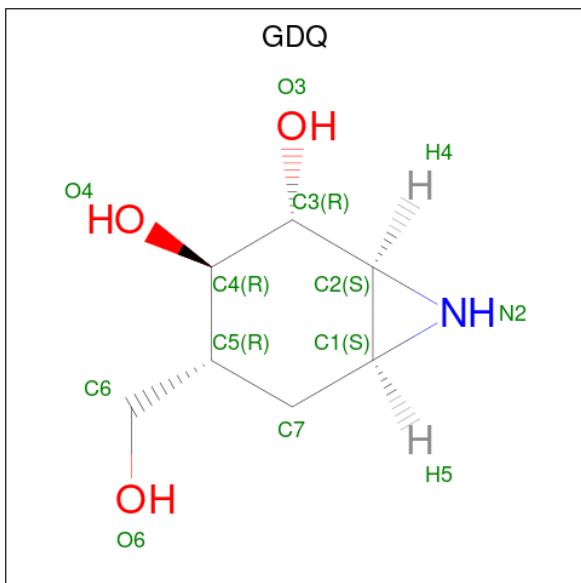
- Molecule 1 is a protein called Oligosaccharide 4-alpha-D-glucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	781	Total	C	N	O	S	0	0	0
			6172	3953	1045	1153	21			
1	A	781	Total	C	N	O	S	0	2	0
			6198	3969	1054	1154	21			
1	B	781	Total	C	N	O	S	0	1	0
			6207	3973	1053	1160	21			

There are 3 discrepancies between the modelled and reference sequences:

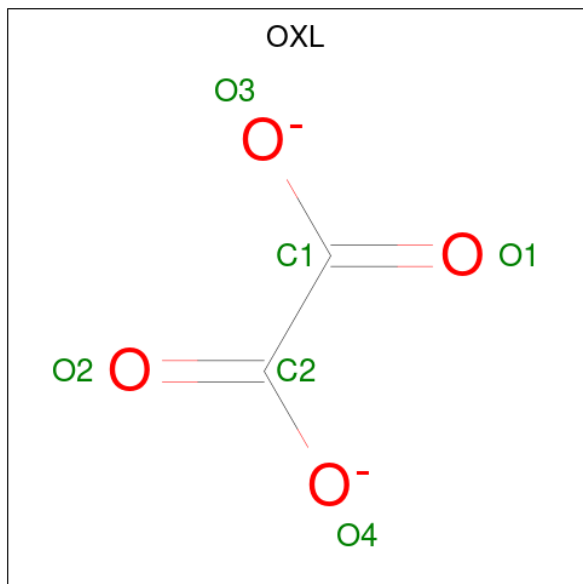
Chain	Residue	Modelled	Actual	Comment	Reference
C	817	LYS	-	expression tag	UNP B3PEE6
A	817	LYS	-	expression tag	UNP B3PEE6
B	817	LYS	-	expression tag	UNP B3PEE6

- Molecule 2 is (1 {S},2 {R},3 {R},4 {R},6 {S})-4-(hydroxymethyl)-7-azabicyclo[4.1.0]heptane-2,3-diol (CCD ID: GDQ) (formula: C₇H₁₃NO₃) (labeled as "Ligand of Interest" by depositor).



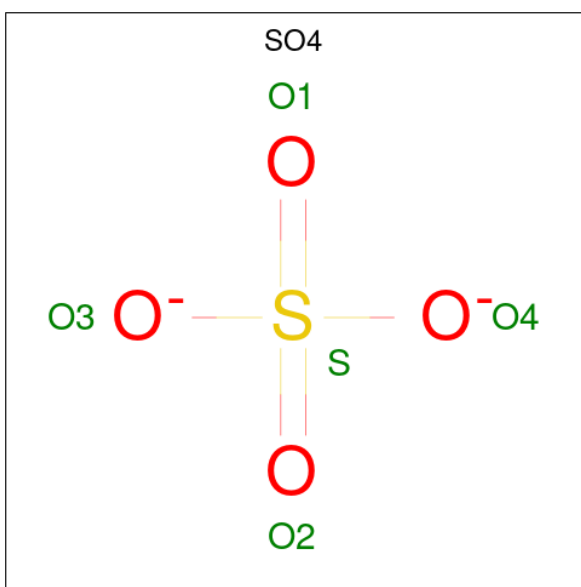
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			11	7	1	3		
2	A	1	Total	C	N	O	0	0
			11	7	1	3		
2	B	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 3 is OXALATE ION (CCD ID: OXL) (formula: C_2O_4).



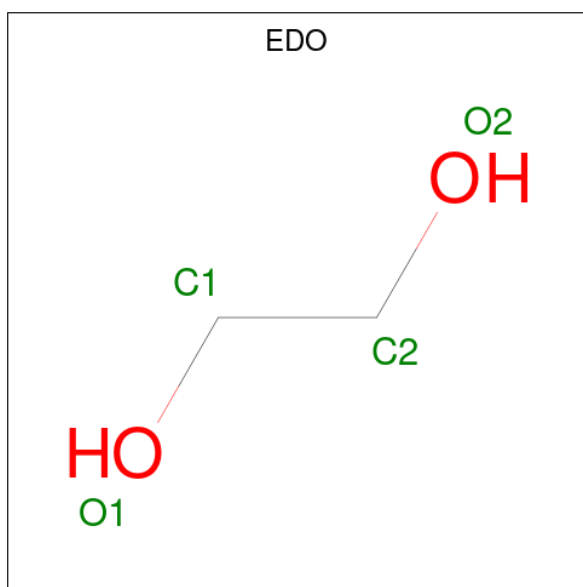
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	2	4		
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



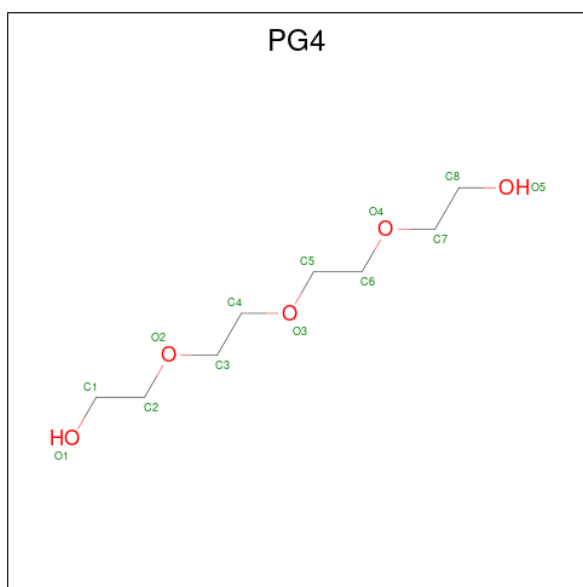
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		

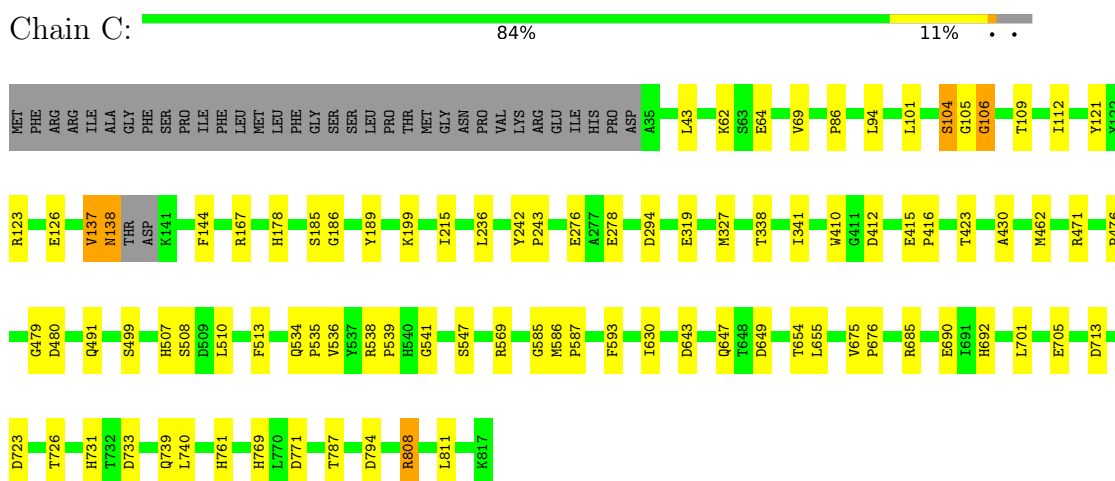
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	332	Total	O	0	0
			332	332		
7	A	338	Total	O	0	0
			338	338		
7	B	324	Total	O	0	0
			324	324		

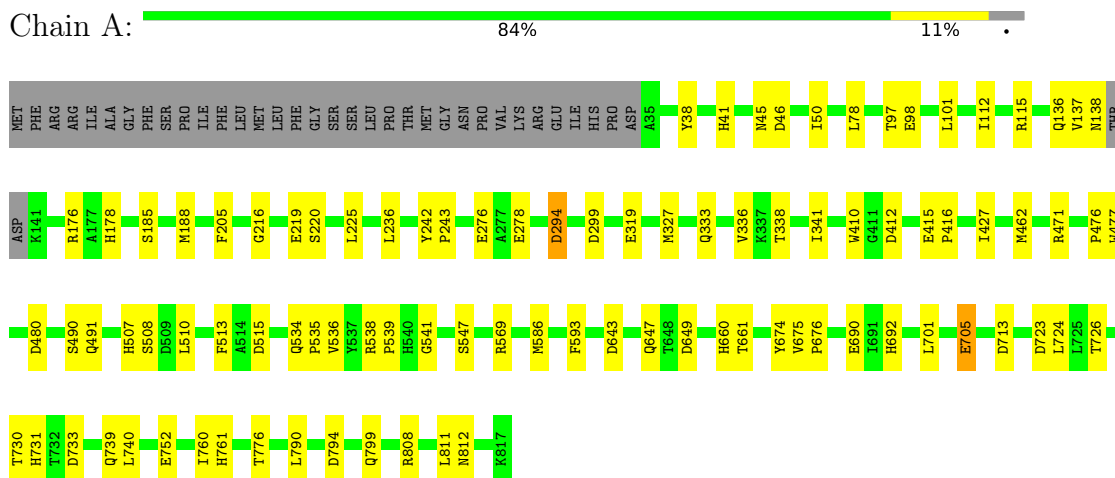
3 Residue-property plots

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.

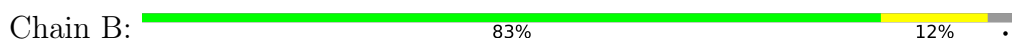
- Molecule 1: Oligosaccharide 4-alpha-D-glucosyltransferase



- Molecule 1: Oligosaccharide 4-alpha-D-glucosyltransferase



- Molecule 1: Oligosaccharide 4-alpha-D-glucosyltransferase



1691	T423	I112	ME1
H692	A430	Y121	ARG
L701	M462	R123	ILE
E705	P476	V137	ALA
D723	N477	M138	GLY
T726	D480	THR	PRO
H731	Q491	ASP	SER
T732	Y505	K141	ILE
D733	I506	M164	PHE
H737	R507	R176	LEU
F738	S508	A177	MET
Q739	S509	H178	GLY
E752	L510	S185	PHE
I760	G511	M188	SER
H761	F513	K199	LEU
H769	R526	P205	PRO
L770	S527	L225	THR
D771	Q529	L236	MET
D794	Q534	Y242	GLY
Q799	V535	P243	ASN
R808	Y537	E276	PRO
L811	P539	D294	VAL
N812	S540	D299	LVS
L813	G541	E319	ARG
R814	S547	M327	GLU
K817	R569	Q333	ILE
	T584	I341	HIS
	G585	D365	ASP
	M586	P366	PHE
	I630	Q369	ARG
	D643	P370	
	T654	W410	V69
	L655	G411	P86
	K667	D412	A89
	Y674	E415	Q93
	V675	D416	L94
	P676		L101
	S690		S104

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	197.02Å 341.25Å 102.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.82 – 1.90 49.82 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.82-1.90) 100.0 (49.82-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.217 , 0.261 (Not available) , 0.243	Depositor DCC
R_{free} test set	13898 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.477 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.470 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19733	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: GDQ, EDO, OXL, SO4, PG4

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	0.61	0/6365	1.07	18/8638 (0.2%)
1	B	0.61	0/6373	1.08	15/8647 (0.2%)
1	C	0.61	0/6338	1.08	18/8605 (0.2%)
All	All	0.61	0/19076	1.08	51/25890 (0.2%)

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	3
1	B	0	3
1	C	0	4
All	All	0	10

There are no bond length outliers.

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	726	THR	CA-CB-OG1	-8.05	97.52	109.60
1	A	726	THR	CA-CB-OG1	-7.59	98.21	109.60
1	B	723	ASP	CA-CB-CG	6.99	119.58	112.60
1	C	726	THR	CA-CB-OG1	-6.63	99.66	109.60
1	C	278	GLU	CB-CA-C	6.21	121.41	110.85

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	471	ARG	Sidechain
1	C	471	ARG	Sidechain
1	C	538	ARG	Sidechain
1	C	569	ARG	Sidechain
1	C	685	ARG	Sidechain

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	6198	0	5967	46	1
1	B	6207	0	5984	56	1
1	C	6172	0	5929	43	0
2	A	11	0	0	2	0
2	B	11	0	0	3	0
2	C	11	0	0	3	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
5	C	4	0	6	2	0
6	A	13	0	18	1	0
6	B	13	0	18	1	0
6	C	13	0	18	1	0
7	A	338	0	0	3	0
7	B	324	0	0	2	0
7	C	332	0	0	1	1
All	All	19733	0	17952	146	2

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

The worst 5 of 146 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:692:HIS:HD2	1:A:761:HIS:HE1	1.19	0.88
1:C:692:HIS:CD2	1:C:761:HIS:HE1	1.92	0.87
1:A:692:HIS:CD2	1:A:761:HIS:HE1	1.94	0.86
1:C:692:HIS:HD2	1:C:761:HIS:HE1	1.26	0.82
1:B:692:HIS:CD2	1:B:761:HIS:HE1	1.99	0.81

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:1332:HOH:O	7:C:1332:HOH:O[4_546]	1.95	0.25
1:A:812:ASN:ND2	1:B:369:GLN:OE1[8_545]	2.15	0.05

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	779/817 (95%)	747 (96%)	32 (4%)	0	100	100
1	B	778/817 (95%)	746 (96%)	32 (4%)	0	100	100
1	C	777/817 (95%)	746 (96%)	29 (4%)	2 (0%)	36	29
All	All	2334/2451 (95%)	2239 (96%)	93 (4%)	2 (0%)	48	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	106	GLY
1	C	137	VAL

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	642/690 (93%)	635 (99%)	7 (1%)	65	67
1	B	645/690 (94%)	636 (99%)	9 (1%)	59	59
1	C	637/690 (92%)	628 (99%)	9 (1%)	59	59
All	All	1924/2070 (93%)	1899 (99%)	25 (1%)	63	61

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	701	LEU
1	B	93	GLN
1	B	705	GLU
1	B	40	GLU
1	B	123[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	452	GLN
1	B	761	HIS
1	B	529	GLN
1	B	692	HIS
1	B	769	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 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	GDQ	B	901	-	12,12,12	0.74	0	13,18,18	2.78	7 (53%)
4	SO4	C	903	-	4,4,4	0.32	0	6,6,6	0.12	0
5	EDO	A	902	-	3,3,3	0.49	0	2,2,2	0.67	0
4	SO4	B	908	-	4,4,4	0.28	0	6,6,6	0.11	0
6	PG4	C	907	-	12,12,12	0.40	0	11,11,11	0.32	0
4	SO4	B	905	-	4,4,4	0.34	0	6,6,6	0.14	0
4	SO4	A	904	-	4,4,4	0.35	0	6,6,6	0.16	0
4	SO4	C	905	-	4,4,4	0.36	0	6,6,6	0.12	0
4	SO4	B	906	-	4,4,4	0.28	0	6,6,6	0.14	0
6	PG4	B	904	-	12,12,12	0.31	0	11,11,11	0.22	0
2	GDQ	C	901	-	12,12,12	0.69	0	13,18,18	2.46	6 (46%)
3	OXL	A	907	-	5,5,5	1.90	2 (40%)	6,6,6	1.75	2 (33%)
3	OXL	C	902	-	5,5,5	2.19	2 (40%)	6,6,6	1.36	1 (16%)
3	OXL	B	903	-	5,5,5	2.67	2 (40%)	6,6,6	1.01	1 (16%)
4	SO4	B	902	-	4,4,4	0.35	0	6,6,6	0.14	0
5	EDO	B	907	-	3,3,3	0.42	0	2,2,2	0.15	0
4	SO4	A	908	-	4,4,4	0.29	0	6,6,6	0.09	0
5	EDO	C	906	-	3,3,3	0.34	0	2,2,2	0.59	0
4	SO4	A	906	-	4,4,4	0.35	0	6,6,6	0.12	0
4	SO4	C	904	-	4,4,4	0.34	0	6,6,6	0.10	0
4	SO4	C	908	-	4,4,4	0.31	0	6,6,6	0.14	0
4	SO4	A	903	-	4,4,4	0.36	0	6,6,6	0.15	0
6	PG4	A	905	-	12,12,12	0.33	0	11,11,11	0.23	0
2	GDQ	A	901	-	12,12,12	0.84	0	13,18,18	2.38	4 (30%)

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	GDQ	B	901	-	-	2/2/23/23	0/2/2/2
6	PG4	B	904	-	-	6/10/10/10	-
5	EDO	C	906	-	-	1/1/1/1	-
2	GDQ	C	901	-	-	2/2/23/23	0/2/2/2
5	EDO	A	902	-	-	0/1/1/1	-
3	OXL	A	907	-	-	4/4/4/4	-
3	OXL	C	902	-	-	4/4/4/4	-
3	OXL	B	903	-	-	4/4/4/4	-
6	PG4	C	907	-	-	7/10/10/10	-
5	EDO	B	907	-	-	1/1/1/1	-
6	PG4	A	905	-	-	8/10/10/10	-
2	GDQ	A	901	-	-	2/2/23/23	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	903	OXL	O3-C1	-4.62	1.18	1.30
3	C	902	OXL	O4-C2	-3.57	1.20	1.30
3	A	907	OXL	O4-C2	-3.27	1.21	1.30
3	C	902	OXL	O3-C1	-3.05	1.22	1.30
3	B	903	OXL	O4-C2	-3.04	1.22	1.30

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	GDQ	C5-C7-C1	6.19	116.52	108.53
2	C	901	GDQ	C5-C7-C1	6.18	116.52	108.53
2	A	901	GDQ	C5-C7-C1	5.96	116.22	108.53
2	A	901	GDQ	O4-C4-C3	-4.67	99.37	110.38
2	C	901	GDQ	O4-C4-C3	-3.89	101.21	110.38

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	GDQ	C4-C5-C6-O6
2	A	901	GDQ	C4-C5-C6-O6

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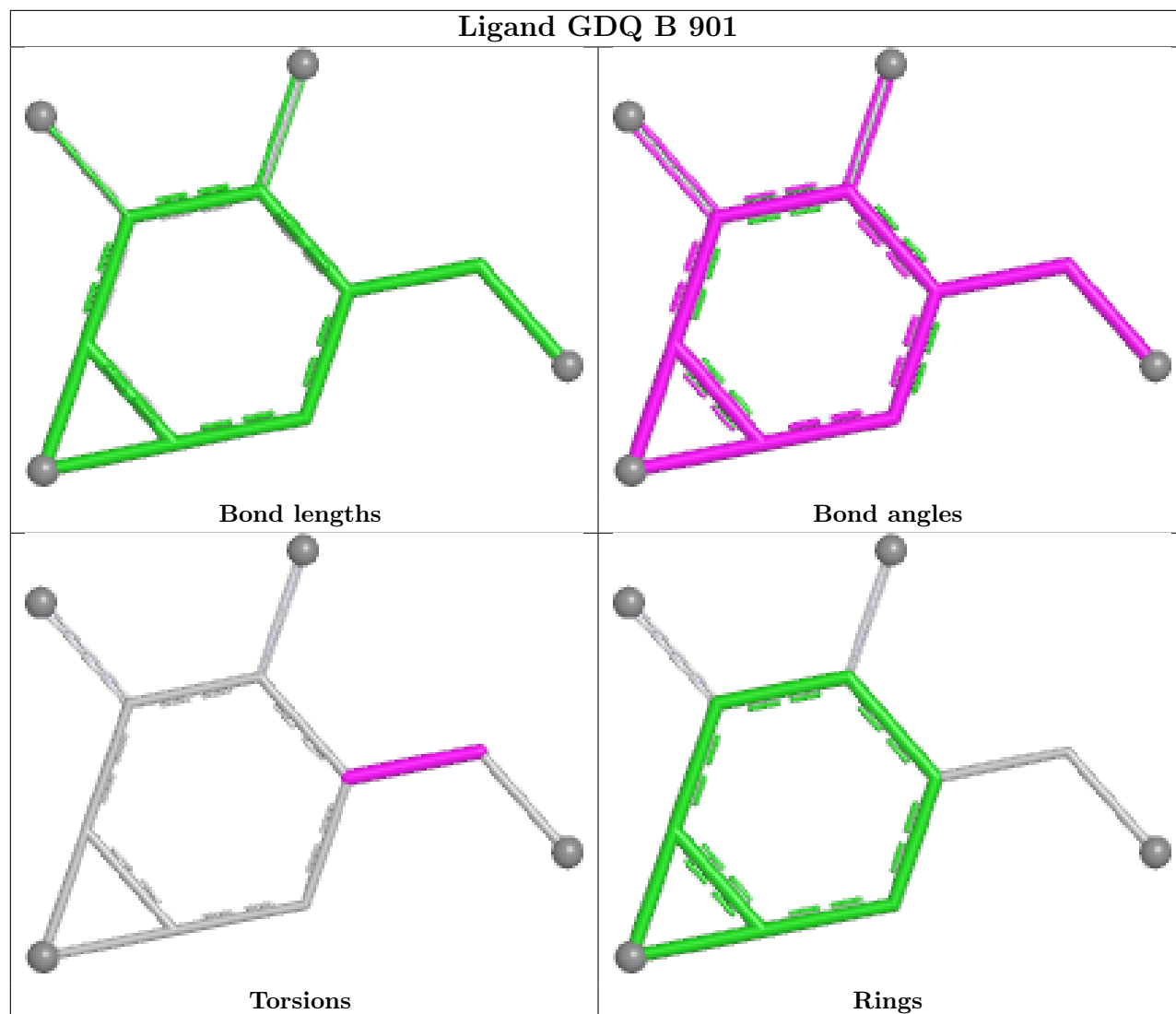
Mol	Chain	Res	Type	Atoms
3	A	907	OXL	O1-C1-C2-O2
3	A	907	OXL	O1-C1-C2-O4
3	A	907	OXL	O3-C1-C2-O2

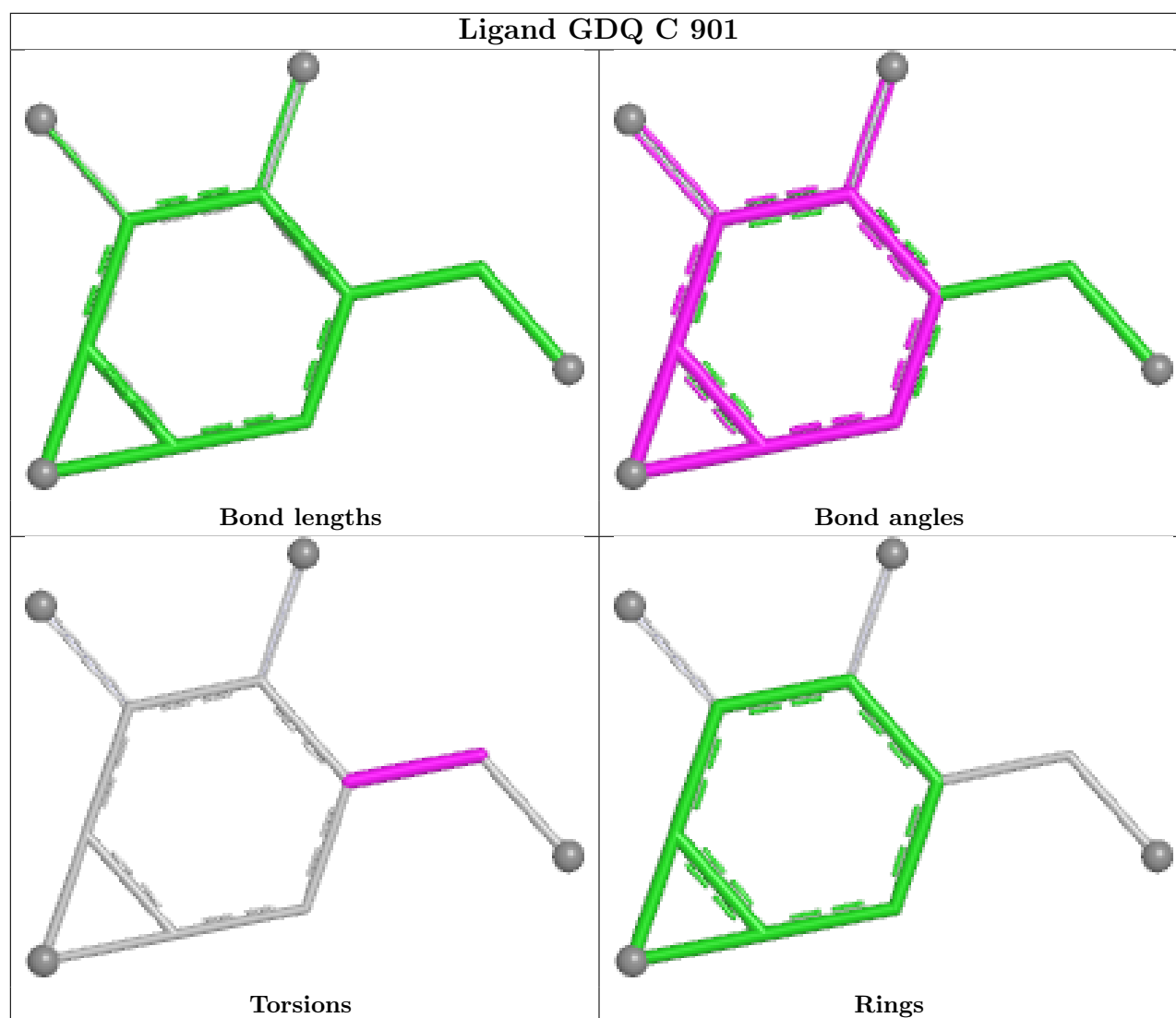
There are no ring outliers.

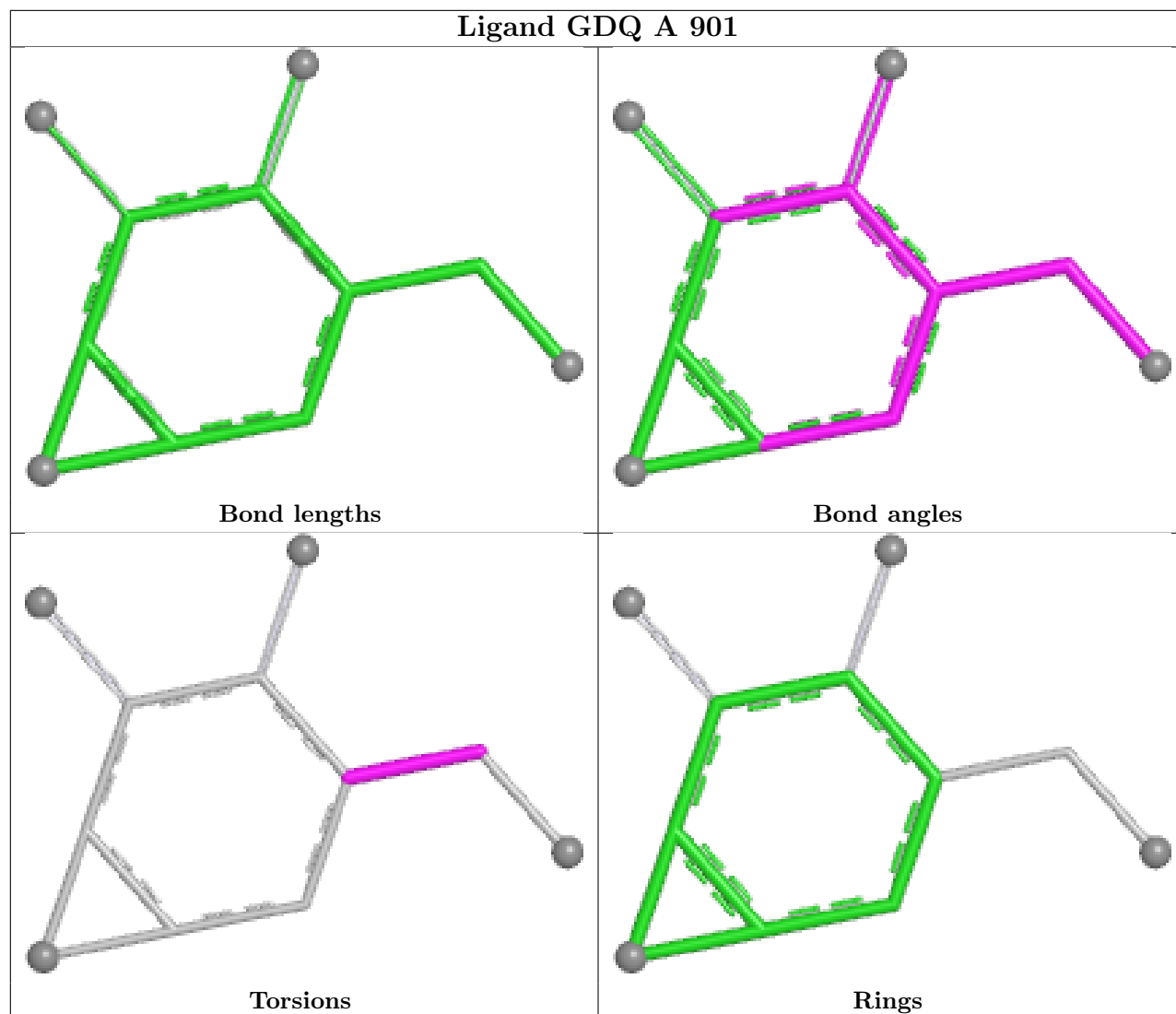
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	GDQ	3	0
6	C	907	PG4	1	0
6	B	904	PG4	1	0
2	C	901	GDQ	3	0
5	C	906	EDO	2	0
6	A	905	PG4	1	0
2	A	901	GDQ	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, 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	781/817 (95%)	-0.96	0 100 100	17, 33, 55, 79	10 (1%)
1	B	781/817 (95%)	-0.98	0 100 100	21, 33, 54, 87	19 (2%)
1	C	781/817 (95%)	-0.99	0 100 100	22, 33, 53, 72	17 (2%)
All	All	2343/2451 (95%)	-0.98	0 100 100	17, 33, 54, 87	46 (1%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDQ	A	901	11/11	0.97	0.08	27,29,31,32	11
2	GDQ	B	901	11/11	0.97	0.08	40,48,55,63	0
4	SO4	A	908	5/5	0.97	0.06	62,65,82,82	0
5	EDO	C	906	4/4	0.97	0.07	41,44,48,53	0
3	OXL	B	903	6/6	0.98	0.05	33,41,52,59	0

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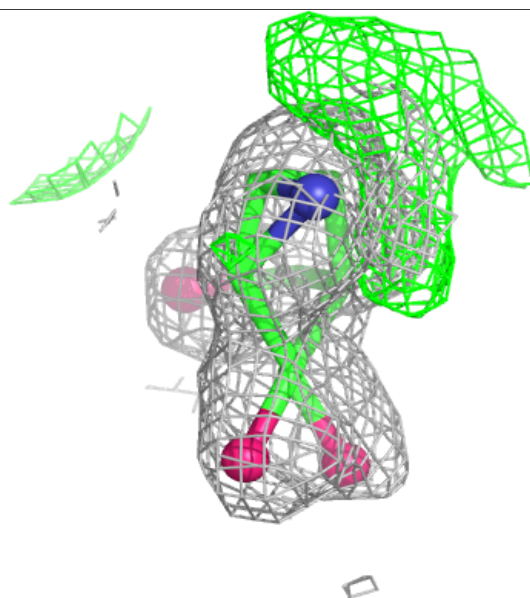
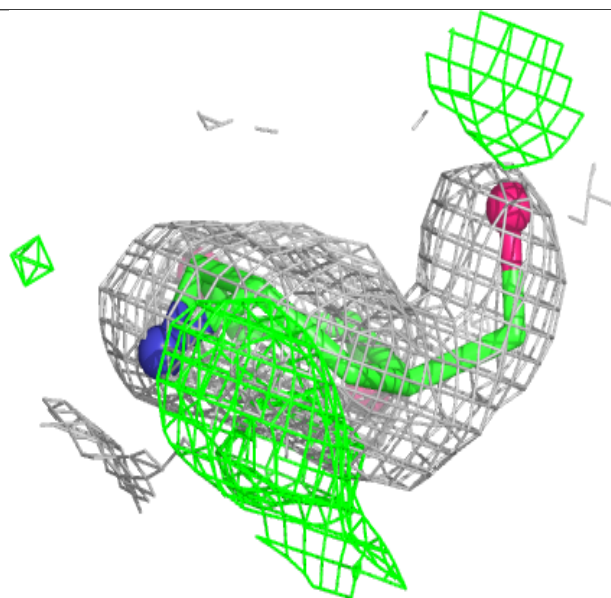
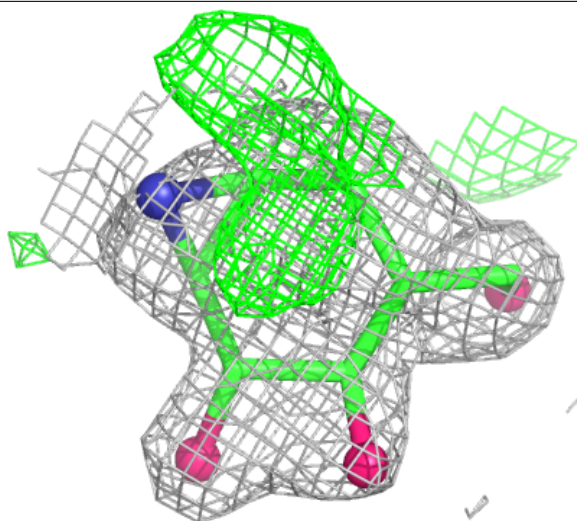
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	908	5/5	0.98	0.06	62,65,78,79	0
2	GDQ	C	901	11/11	0.98	0.07	41,49,55,57	0
4	SO4	B	908	5/5	0.98	0.06	63,67,84,86	0
3	OXL	C	902	6/6	0.98	0.07	39,49,63,63	0
5	EDO	A	902	4/4	0.98	0.05	41,43,45,46	0
5	EDO	B	907	4/4	0.98	0.06	42,46,54,60	0
6	PG4	C	907	13/13	0.98	0.06	41,47,62,64	0
6	PG4	B	904	13/13	0.98	0.06	41,49,61,62	0
4	SO4	C	903	5/5	0.99	0.05	40,42,45,45	0
4	SO4	B	902	5/5	0.99	0.06	38,41,44,47	0
4	SO4	B	905	5/5	0.99	0.04	66,67,72,73	0
4	SO4	B	906	5/5	0.99	0.04	50,53,57,64	0
4	SO4	C	904	5/5	0.99	0.03	65,66,71,73	0
4	SO4	C	905	5/5	0.99	0.03	52,52,58,66	0
3	OXL	A	907	6/6	0.99	0.06	40,48,57,64	0
4	SO4	A	903	5/5	0.99	0.04	66,66,70,71	0
4	SO4	A	904	5/5	0.99	0.03	49,53,57,64	0
6	PG4	A	905	13/13	0.99	0.06	42,53,63,66	0
4	SO4	A	906	5/5	0.99	0.06	38,41,42,47	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.

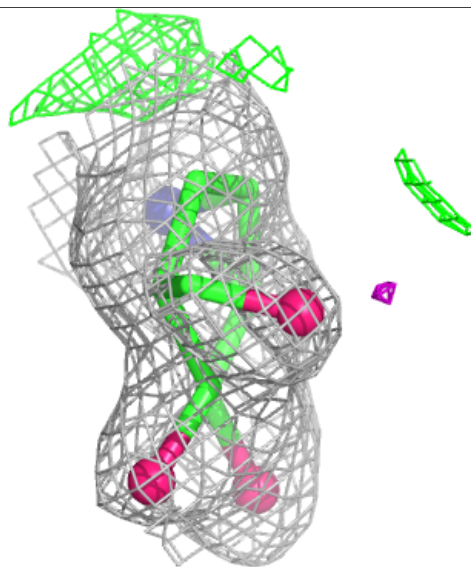
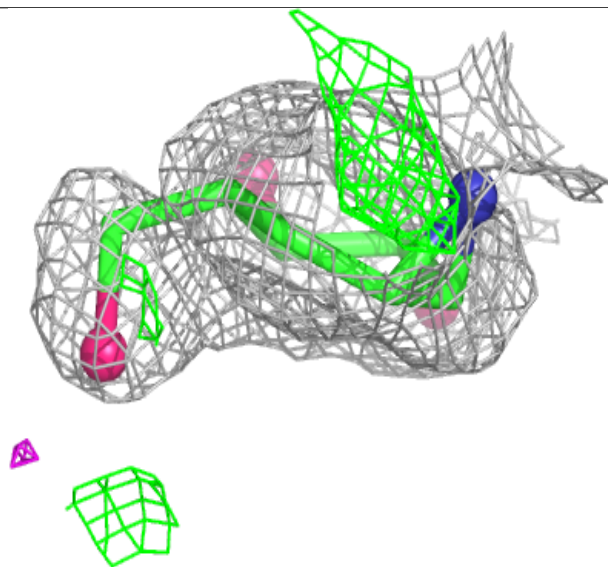
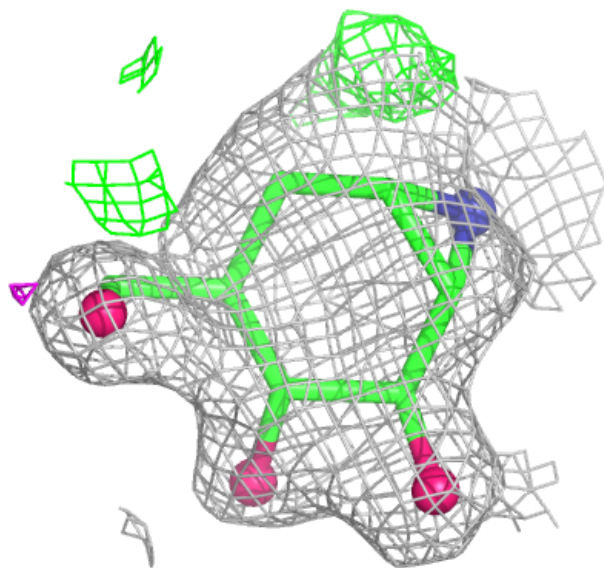
Electron density around GDQ A 901:

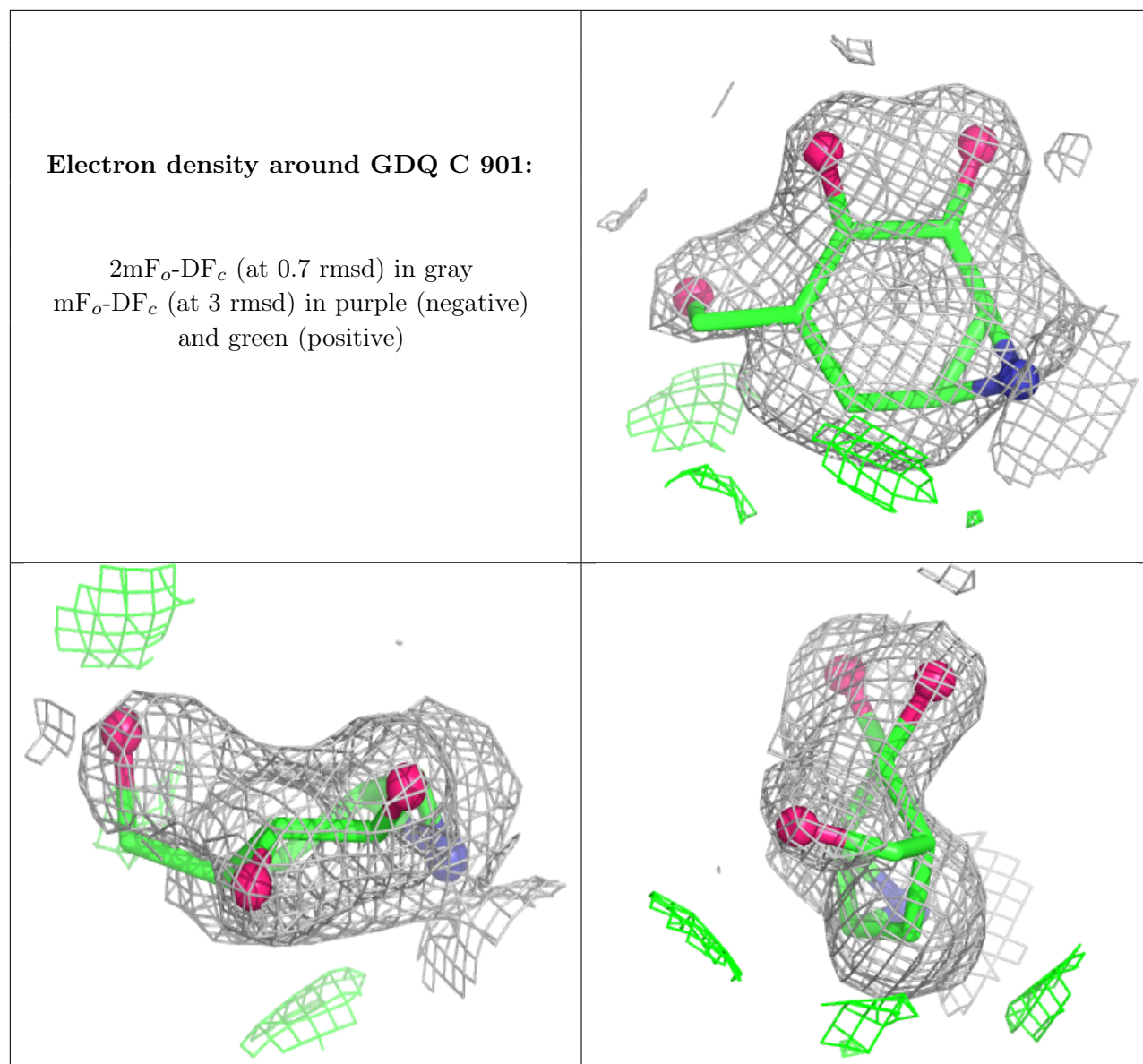
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GDQ B 901:

$2mF_o-DF_c$ (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.