



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:53 AM UTC

PDB ID : 8QN5 / pdb_00008qn5
Title : M. tuberculosis salicylate synthase MbtI in complex with methyl-AMT (new crystal form)
Authors : Mori, M.; Villa, S.; Meneghetti, M.; Bellinzoni, M.
Deposited on : 2023-09-25
Resolution : 1.54 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	:	4-5-2 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

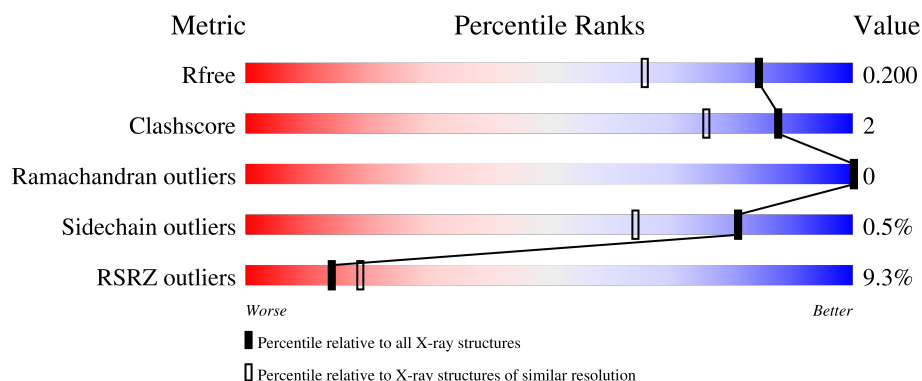
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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	1003 (1.54-1.54)
Clashscore	190562	1025 (1.54-1.54)
Ramachandran outliers	187476	1007 (1.54-1.54)
Sidechain outliers	187428	1007 (1.54-1.54)
RSRZ outliers	180081	1002 (1.54-1.54)

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	451	5% 88% 6% 7%
1	B	451	4% 93% . .
1	C	451	13% 88% 6% 6%
1	D	451	14% 90% . 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14520 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.

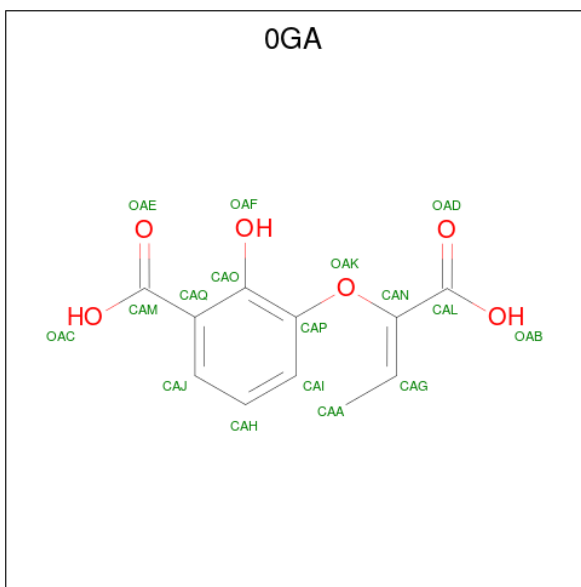
- Molecule 1 is a protein called Salicylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	8	0
			3234	2030	586	608	10			
1	B	436	Total	C	N	O	S	0	8	0
			3345	2096	605	634	10			
1	C	422	Total	C	N	O	S	0	4	0
			3187	2000	575	602	10			
1	D	424	Total	C	N	O	S	0	4	0
			3209	2016	574	609	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP P9WFX1
B	0	HIS	-	expression tag	UNP P9WFX1
C	0	HIS	-	expression tag	UNP P9WFX1
D	0	HIS	-	expression tag	UNP P9WFX1

- Molecule 2 is 3-{{(1Z)-1-carboxyprop-1-en-1-yl}oxy}-2-hydroxybenzoic acid (CCD ID: 0GA) (formula: C₁₁H₁₀O₆) (labeled as "Ligand of Interest" by depositor).



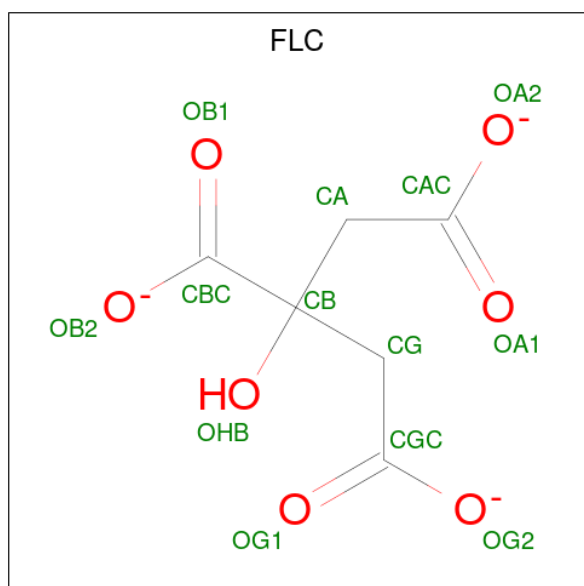
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			17	11	6		
2	B	1	Total	C	O	0	0
			17	11	6		
2	C	1	Total	C	O	0	0
			17	11	6		
2	D	1	Total	C	O	0	0
			17	11	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



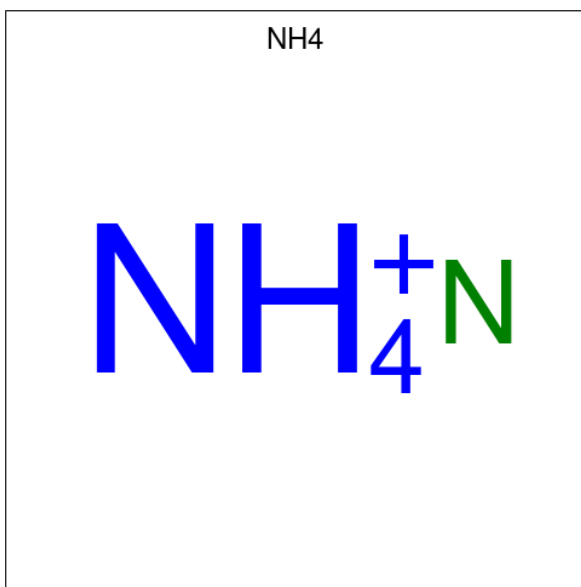
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is AMMONIUM ION (CCD ID: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0
5	C	1	Total N 1 1	0	0

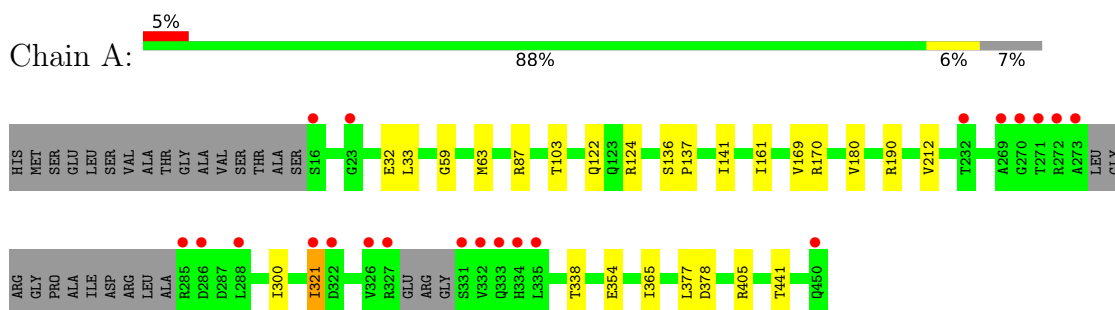
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	434	Total O 434 434	0	2
6	B	414	Total O 414 414	0	0
6	C	318	Total O 318 318	0	0
6	D	252	Total O 252 252	0	0

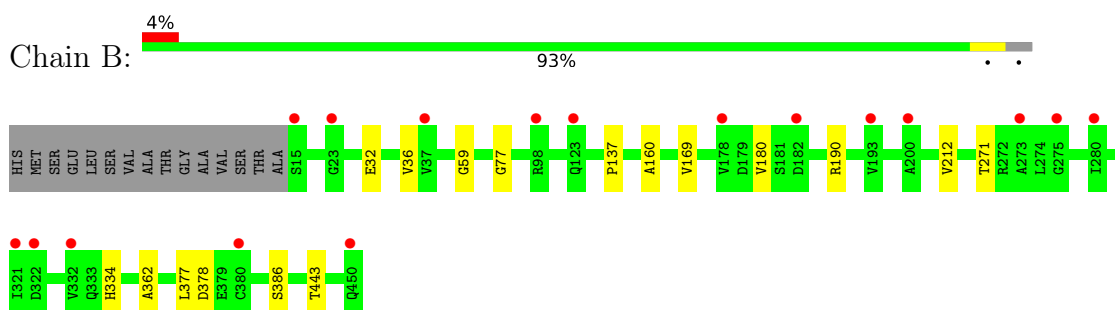
3 Residue-property plots [i](#)

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.

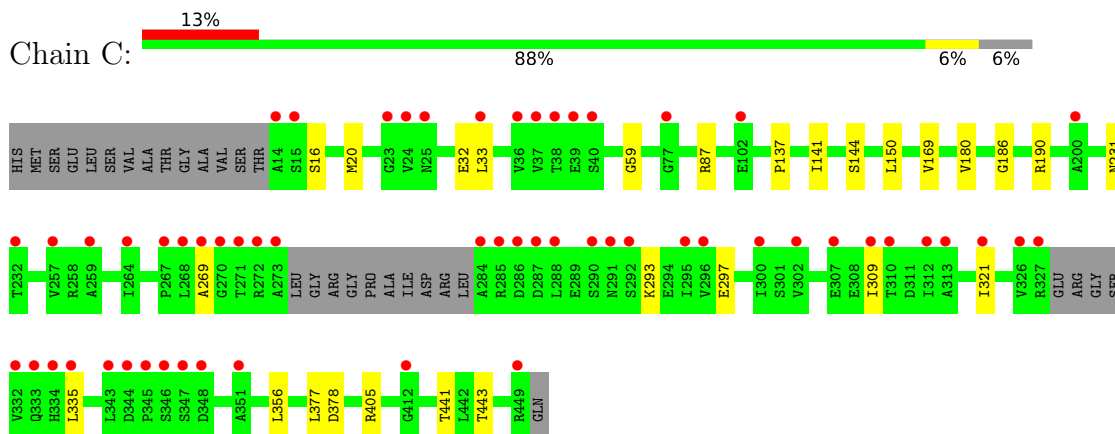
- Molecule 1: Salicylate synthase



- Molecule 1: Salicylate synthase



- Molecule 1: Salicylate synthase



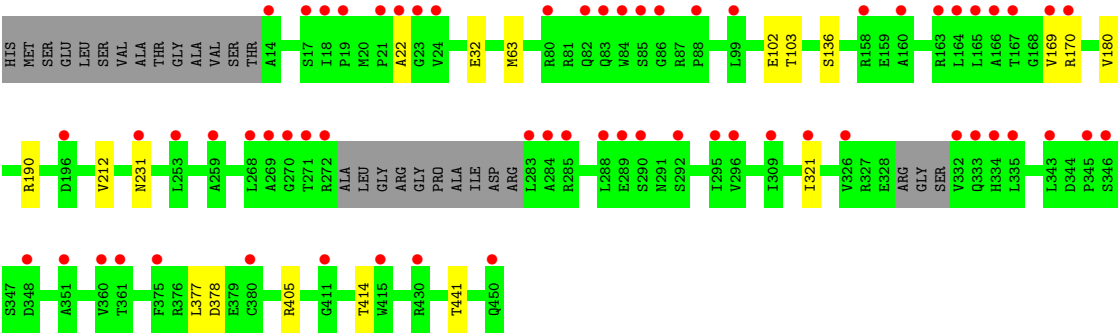
- Molecule 1: Salicylate synthase

Chain D:

14%

90%

6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.64Å 83.06Å 126.26Å 90.00° 111.66° 90.00°	Depositor
Resolution (Å)	117.34 – 1.54 117.34 – 1.54	Depositor EDS
% Data completeness (in resolution range)	78.6 (117.34-1.54) 78.6 (117.34-1.54)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 1.55Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.183 , 0.208 0.178 , 0.200	Depositor DCC
R_{free} test set	10546 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14520	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.99% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, OGA, NH4, GOL

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	0.86	2/3314 (0.1%)	0.93	1/4502 (0.0%)
1	B	0.81	0/3425	0.93	0/4657
1	C	0.78	0/3251	0.92	0/4421
1	D	0.74	1/3275 (0.0%)	0.92	1/4454 (0.0%)
All	All	0.80	3/13265 (0.0%)	0.92	2/18034 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	MET	SD-CE	-6.52	1.63	1.79
1	D	63	MET	SD-CE	-5.36	1.66	1.79
1	A	321	ILE	CA-C	5.19	1.58	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ARG	CA-CB-CG	-5.34	103.41	114.10
1	D	22	ALA	N-CA-C	5.21	117.38	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3234	0	3229	19	0
1	B	3345	0	3346	10	0
1	C	3187	0	3149	14	1
1	D	3209	0	3180	12	1
2	A	17	0	7	0	0
2	B	17	0	7	0	0
2	C	17	0	7	0	0
2	D	17	0	7	0	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	3	0
4	A	13	0	5	0	0
4	D	13	0	5	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
6	A	434	0	0	0	0
6	B	414	0	0	0	0
6	C	318	0	0	0	0
6	D	252	0	0	0	0
All	All	14520	0	12982	53	1

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 2.

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:A:405:ARG:HH11	1:A:441:THR:HG21	1.24	0.99
1:A:405:ARG:HH11	1:A:441:THR:CG2	1.86	0.88
1:A:405:ARG:NH1	1:A:441:THR:HG21	1.91	0.86
1:A:405:ARG:NH1	1:A:441:THR:CG2	2.45	0.78
1:B:271:THR:HG22	1:B:334:HIS:ND1	2.03	0.73
1:C:33:LEU:HD21	1:C:141:ILE:HD13	1.76	0.66
1:A:103:THR:HG21	1:A:136:SER:HB2	1.78	0.64
1:C:231:ASN:OD1	1:C:441:THR:HG23	2.00	0.62
1:D:231:ASN:OD1	1:D:441:THR:HG23	2.04	0.58
1:A:103:THR:HG21	1:A:136:SER:CB	2.36	0.56
1:A:405:ARG:HD3	1:A:441:THR:HG21	1.88	0.55
1:A:405:ARG:NH1	1:A:441:THR:HG23	2.23	0.54
1:D:103:THR:HG21	1:D:136:SER:HB2	1.88	0.54
1:C:32:GLU:HG3	1:C:169:VAL:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:405:ARG:HB3	1:D:441:THR:HG21	1.92	0.52
1:C:16:SER:HB2	1:C:150:LEU:HD13	1.92	0.51
1:C:20:MET:HG3	1:C:144:SER:O	2.11	0.51
1:D:103:THR:HG21	1:D:136:SER:CB	2.41	0.51
1:C:405:ARG:NH1	1:C:441:THR:OG1	2.43	0.50
1:A:33:LEU:HD21	1:A:141:ILE:HD13	1.94	0.50
1:A:122[A]:GLN:HE21	1:C:186:GLY:HA3	1.77	0.49
1:D:32:GLU:HG3	1:D:169:VAL:HB	1.96	0.47
1:A:321:ILE:HG13	1:A:338:THR:HB	1.96	0.46
1:B:180:VAL:HG12	1:B:212:VAL:HG11	1.97	0.46
1:C:405:ARG:HB3	1:C:441:THR:HG21	1.98	0.46
1:A:180:VAL:HG12	1:A:212:VAL:HG11	1.98	0.46
1:C:190:ARG:HD2	1:C:377:LEU:O	2.16	0.46
1:A:32:GLU:HG3	1:A:169:VAL:HB	1.97	0.46
1:B:32:GLU:HG3	1:B:169:VAL:HB	1.98	0.46
1:C:293:LYS:O	1:C:297:GLU:HG2	2.15	0.46
1:B:180:VAL:HG11	1:B:443:THR:HG21	1.98	0.45
1:D:414:THR:HB	3:D:802:GOL:H12	1.99	0.45
1:D:414:THR:CB	3:D:802:GOL:H12	2.47	0.45
1:A:300:ILE:HG21	1:A:365:ILE:HG21	1.99	0.45
1:D:180:VAL:HG12	1:D:212:VAL:HG11	1.98	0.45
1:D:32:GLU:OE1	1:D:170:ARG:HG2	2.17	0.44
1:C:309:ILE:HG12	1:C:356:LEU:HD21	2.00	0.44
1:A:141:ILE:HD13	1:A:161:ILE:HD11	2.00	0.43
1:D:405:ARG:NH1	1:D:441:THR:OG1	2.50	0.43
1:B:190:ARG:HD2	1:B:377:LEU:O	2.19	0.42
1:A:170:ARG:HD3	1:B:77:GLY:HA3	2.00	0.42
1:A:190:ARG:HD2	1:A:377:LEU:O	2.20	0.42
1:D:190:ARG:HD2	1:D:377:LEU:O	2.20	0.42
1:A:59:GLY:O	1:A:137:PRO:HA	2.20	0.41
1:B:59:GLY:O	1:B:137:PRO:HA	2.20	0.41
1:B:36:VAL:HG12	1:B:160:ALA:HB1	2.02	0.41
1:D:414:THR:OG1	3:D:802:GOL:H12	2.20	0.41
1:C:59:GLY:O	1:C:137:PRO:HA	2.20	0.41
1:C:180:VAL:HG11	1:C:443:THR:HG21	2.02	0.41
1:A:87:ARG:NH1	1:A:354:GLU:OE1	2.53	0.41
1:C:269:ALA:O	1:C:335:LEU:HB2	2.20	0.41
1:B:362:ALA:HB1	1:B:386:SER:HB2	2.02	0.41
1:B:362:ALA:CB	1:B:386:SER:HB2	2.51	0.40

All (1) 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)
1:C:87:ARG:NH2	1:D:102:GLU:OE1[2_454]	2.19	0.01

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	423/451 (94%)	421 (100%)	2 (0%)	0	100	100
1	B	442/451 (98%)	436 (99%)	6 (1%)	0	100	100
1	C	420/451 (93%)	418 (100%)	2 (0%)	0	100	100
1	D	422/451 (94%)	418 (99%)	4 (1%)	0	100	100
All	All	1707/1804 (95%)	1693 (99%)	14 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	336/359 (94%)	335 (100%)	1 (0%)	86	74
1	B	349/359 (97%)	348 (100%)	1 (0%)	86	74
1	C	324/359 (90%)	322 (99%)	2 (1%)	78	59
1	D	329/359 (92%)	327 (99%)	2 (1%)	78	59
All	All	1338/1436 (93%)	1332 (100%)	6 (0%)	81	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ASP
1	B	378	ASP
1	C	321	ILE
1	C	378	ASP
1	D	321	ILE
1	D	378	ASP

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

Mol	Chain	Res	Type
1	A	333	GLN
1	B	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are modelled with single atom - leaving 11 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	$\# Z > 2$
4	FLC	A	803	-	12,12,12	0.99	0	17,17,17	1.02	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	0GA	A	801	-	17,17,17	0.76	0	21,23,23	1.11	3 (14%)
2	0GA	D	801	-	17,17,17	0.73	0	21,23,23	1.10	1 (4%)
3	GOL	A	802	-	5,5,5	0.22	0	5,5,5	0.17	0
3	GOL	C	802	-	5,5,5	0.10	0	5,5,5	0.13	0
3	GOL	D	802	-	5,5,5	0.15	0	5,5,5	0.37	0
3	GOL	B	802	-	5,5,5	0.16	0	5,5,5	0.17	0
2	0GA	B	801	-	17,17,17	0.90	0	21,23,23	0.88	1 (4%)
3	GOL	A	804	-	5,5,5	0.15	0	5,5,5	0.48	0
4	FLC	D	803	-	12,12,12	0.97	0	17,17,17	1.01	0
2	0GA	C	801	-	17,17,17	0.80	0	21,23,23	0.90	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
4	FLC	A	803	-	-	0/16/16/16	-
2	0GA	A	801	-	-	2/14/14/14	0/1/1/1
2	0GA	D	801	-	-	2/14/14/14	0/1/1/1
3	GOL	A	802	-	-	0/4/4/4	-
3	GOL	C	802	-	-	0/4/4/4	-
3	GOL	D	802	-	-	0/4/4/4	-
3	GOL	B	802	-	-	0/4/4/4	-
2	0GA	B	801	-	-	2/14/14/14	0/1/1/1
3	GOL	A	804	-	-	2/4/4/4	-
4	FLC	D	803	-	-	2/16/16/16	-
2	0GA	C	801	-	-	2/14/14/14	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	0GA	OAK-CAN-CAL	-3.12	106.03	114.54
2	B	801	0GA	OAK-CAN-CAL	-2.64	107.35	114.54
2	C	801	0GA	OAK-CAN-CAL	-2.54	107.60	114.54
2	A	801	0GA	OAD-CAL-CAN	-2.40	114.69	120.57
4	A	803	FLC	OB1-CBC-CB	-2.30	117.64	122.09
2	A	801	0GA	OAB-CAL-CAN	2.29	119.25	114.06
2	A	801	0GA	OAK-CAN-CAL	-2.18	108.59	114.54

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	0GA	CAA-CAG-CAN-OAK
2	A	801	0GA	CAG-CAN-OAK-CAP
2	B	801	0GA	CAA-CAG-CAN-OAK
2	B	801	0GA	CAG-CAN-OAK-CAP
2	C	801	0GA	CAA-CAG-CAN-OAK
2	C	801	0GA	CAG-CAN-OAK-CAP
2	D	801	0GA	CAA-CAG-CAN-OAK
2	D	801	0GA	CAG-CAN-OAK-CAP
3	A	804	GOL	C1-C2-C3-O3
3	A	804	GOL	O2-C2-C3-O3
4	D	803	FLC	CB-CG-CGC-OG1
4	D	803	FLC	CB-CG-CGC-OG2

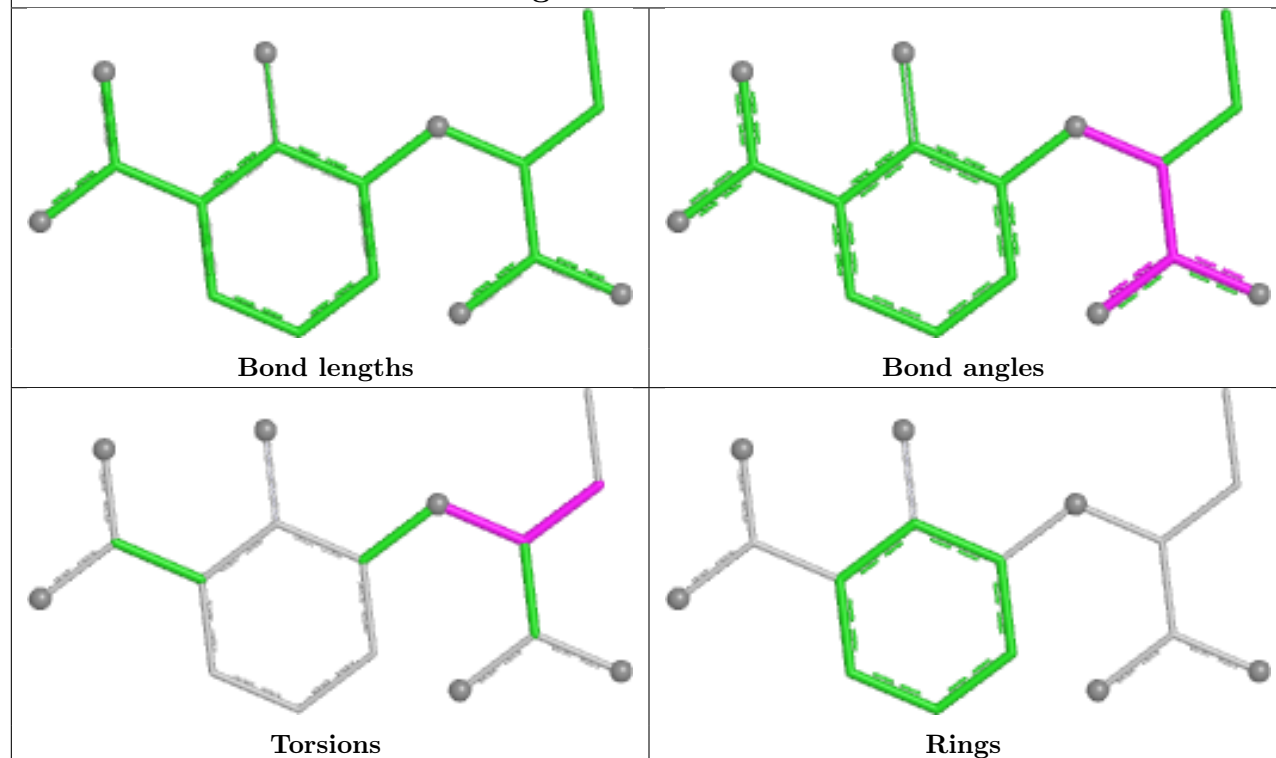
There are no ring outliers.

1 monomer is involved in 3 short contacts:

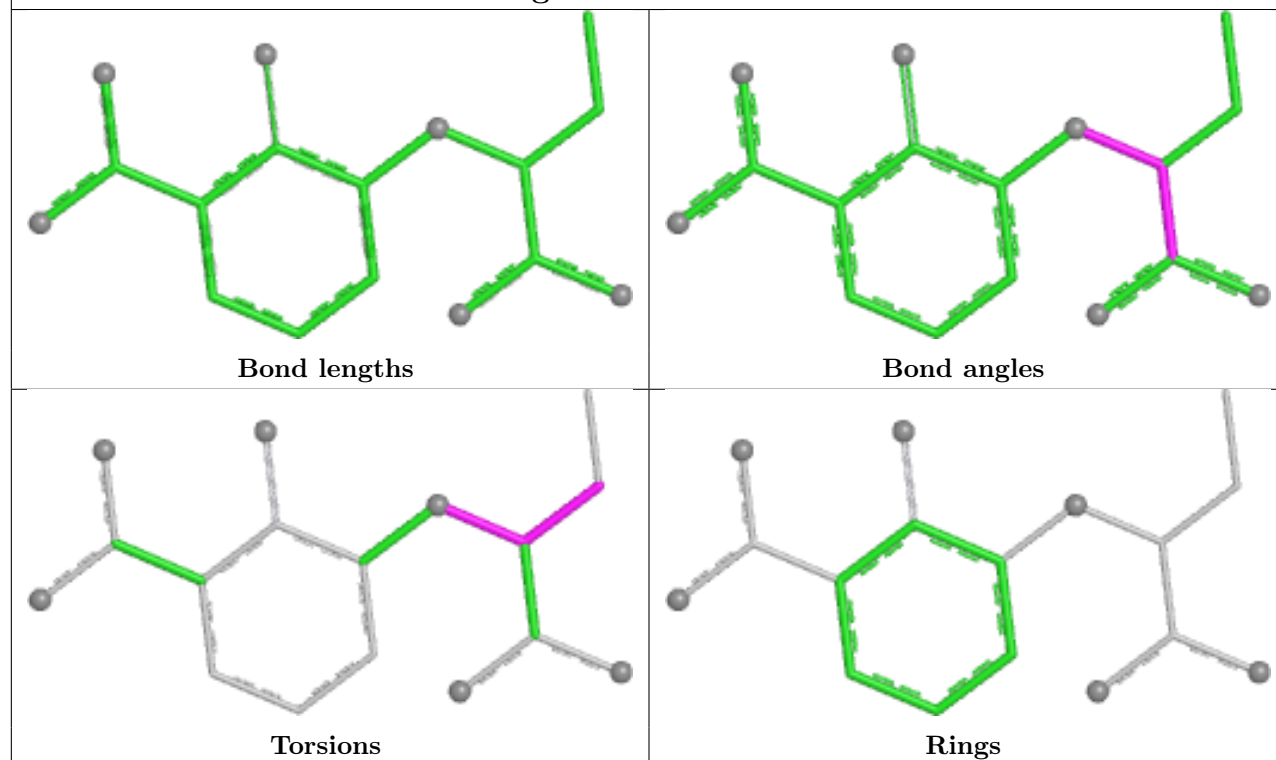
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	802	GOL	3	0

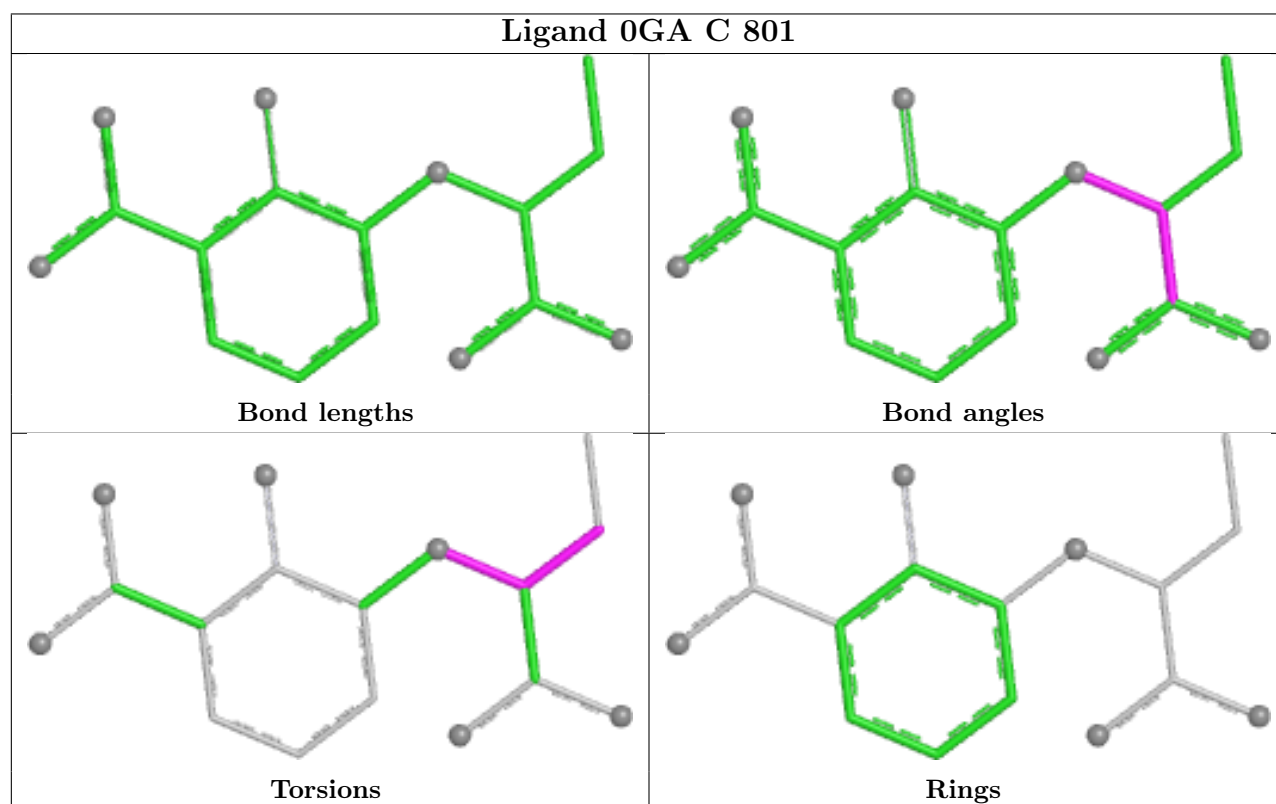
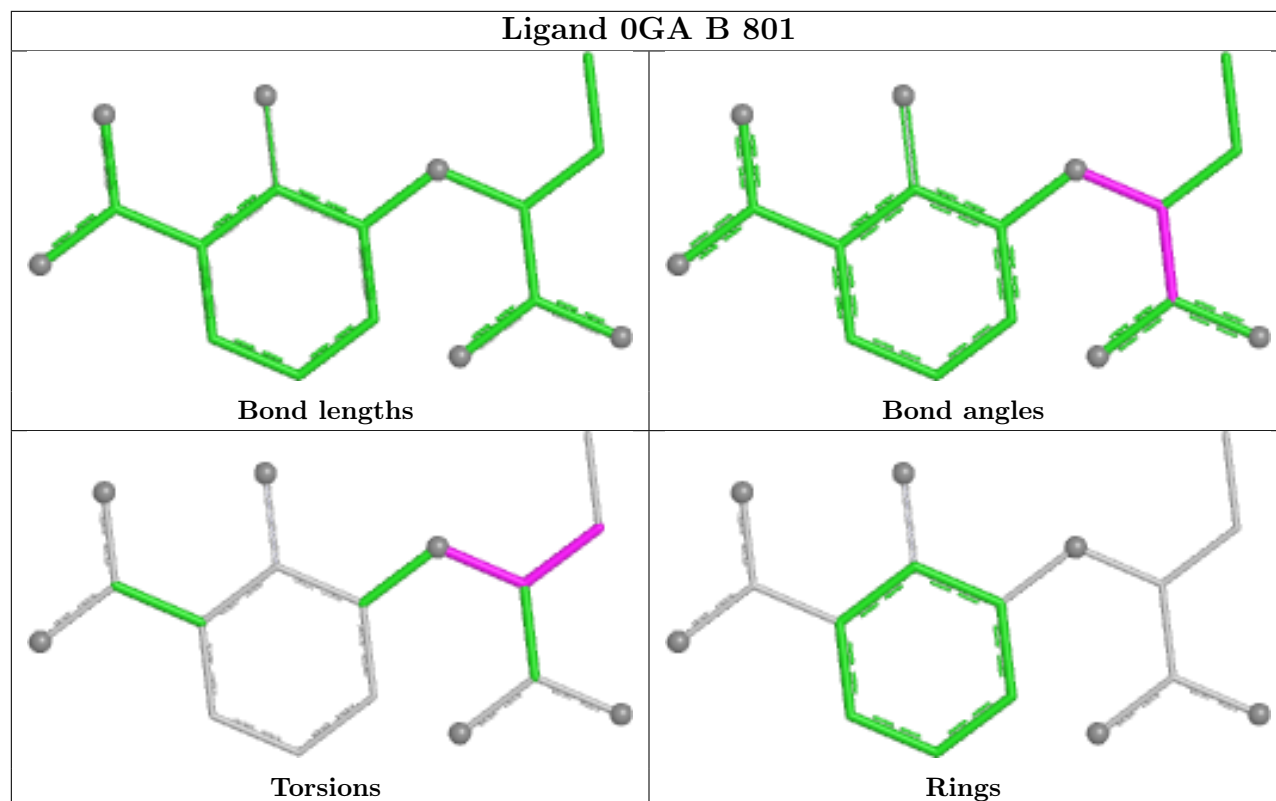
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 0GA A 801



Ligand 0GA D 801





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, 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	421/451 (93%)	0.24	21 (4%) 34 42	11, 25, 46, 109	8 (1%)
1	B	436/451 (96%)	0.20	17 (3%) 43 52	8, 26, 52, 73	8 (1%)
1	C	422/451 (93%)	0.70	58 (13%) 6 8	10, 32, 79, 123	4 (0%)
1	D	424/451 (94%)	0.88	63 (14%) 5 7	17, 36, 67, 118	4 (0%)
All	All	1703/1804 (94%)	0.50	159 (9%) 14 19	8, 30, 61, 123	24 (1%)

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	ALA	8.7
1	A	273	ALA	8.2
1	D	283	LEU	7.5
1	C	332	VAL	7.0
1	C	271	THR	6.1
1	A	271	THR	6.1
1	D	332	VAL	6.0
1	C	269	ALA	5.9
1	C	334	HIS	5.7
1	A	332	VAL	5.5
1	C	335	LEU	5.2
1	C	343	LEU	5.1
1	C	273	ALA	5.1
1	C	284	ALA	5.0
1	D	22	ALA	4.9
1	D	271	THR	4.9
1	D	268	LEU	4.7
1	C	326	VAL	4.4
1	D	272	ARG	4.4
1	A	269	ALA	4.4
1	C	333	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	268	LEU	4.3
1	C	327	ARG	4.2
1	A	270	GLY	4.1
1	D	253	LEU	4.1
1	C	14	ALA	4.1
1	D	14	ALA	4.0
1	D	24	VAL	4.0
1	C	345	PRO	4.0
1	D	23	GLY	3.9
1	D	166	ALA	3.9
1	C	351	ALA	3.8
1	A	321	ILE	3.8
1	C	288	LEU	3.7
1	A	331	SER	3.7
1	C	295	ILE	3.7
1	C	312	ILE	3.6
1	C	344	ASP	3.6
1	C	39	GLU	3.5
1	C	285	ARG	3.5
1	D	343	LEU	3.5
1	C	296	VAL	3.5
1	D	21	PRO	3.5
1	D	326	VAL	3.4
1	A	23	GLY	3.4
1	D	84	TRP	3.3
1	B	178	VAL	3.2
1	D	346	SER	3.2
1	D	18	ILE	3.2
1	D	270	GLY	3.2
1	D	335	LEU	3.2
1	C	348	ASP	3.1
1	A	334	HIS	3.1
1	D	164	LEU	3.1
1	D	375	PHE	3.1
1	C	291	ASN	3.1
1	C	313	ALA	3.1
1	D	169	VAL	3.1
1	D	165	LEU	3.1
1	C	309	ILE	3.1
1	C	259	ALA	3.0
1	A	232	THR	3.0
1	D	86	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	85	SER	3.0
1	D	360	VAL	3.0
1	D	380	CYS	3.0
1	D	170	ARG	2.9
1	C	36	VAL	2.9
1	A	272	ARG	2.9
1	C	286	ASP	2.9
1	D	288	LEU	2.9
1	D	450	GLN	2.8
1	D	290	SER	2.8
1	B	37	VAL	2.8
1	D	163	ARG	2.8
1	B	322	ASP	2.8
1	C	15[A]	SER	2.7
1	C	347	SER	2.7
1	C	321	ILE	2.7
1	D	158[A]	ARG	2.7
1	C	292	SER	2.7
1	A	285	ARG	2.7
1	C	270	GLY	2.7
1	D	231	ASN	2.7
1	C	287	ASP	2.7
1	C	267	PRO	2.7
1	A	288	LEU	2.6
1	D	351	ALA	2.6
1	B	450	GLN	2.6
1	A	326	VAL	2.6
1	A	16	SER	2.6
1	D	289	GLU	2.6
1	D	296	VAL	2.6
1	A	322	ASP	2.6
1	B	182	ASP	2.6
1	C	200	ALA	2.5
1	C	77	GLY	2.5
1	B	332	VAL	2.5
1	C	232	THR	2.5
1	A	333	GLN	2.5
1	D	17	SER	2.5
1	C	37	VAL	2.5
1	C	346	SER	2.5
1	C	25	ASN	2.5
1	D	80	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	286	ASP	2.4
1	D	284	ALA	2.4
1	B	321	ILE	2.4
1	C	264	ILE	2.4
1	C	102	GLU	2.4
1	D	285	ARG	2.4
1	C	38	THR	2.4
1	D	99	LEU	2.4
1	C	272	ARG	2.3
1	D	348[A]	ASP	2.3
1	D	160	ALA	2.3
1	B	23	GLY	2.3
1	B	280	ILE	2.3
1	D	292	SER	2.3
1	D	83	GLN	2.3
1	D	430	ARG	2.3
1	C	290	SER	2.3
1	B	380	CYS	2.2
1	B	15	SER	2.2
1	D	309	ILE	2.2
1	D	321	ILE	2.2
1	B	273	ALA	2.2
1	D	196	ASP	2.2
1	C	307	GLU	2.2
1	D	167	THR	2.2
1	C	40	SER	2.2
1	D	295	ILE	2.2
1	C	23	GLY	2.2
1	C	310	THR	2.2
1	C	449	ARG	2.2
1	B	193	VAL	2.2
1	C	33	LEU	2.1
1	B	200	ALA	2.1
1	D	415	TRP	2.1
1	C	257	VAL	2.1
1	C	300	ILE	2.1
1	A	327	ARG	2.1
1	B	123	GLN	2.1
1	B	275	GLY	2.1
1	C	412	GLY	2.1
1	D	19	PRO	2.1
1	D	88	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	361	THR	2.1
1	A	335	LEU	2.1
1	D	345	PRO	2.1
1	D	259	ALA	2.0
1	D	334	HIS	2.0
1	D	82	GLN	2.0
1	D	411	GLY	2.0
1	B	98	ARG	2.0
1	A	450	GLN	2.0
1	D	333	GLN	2.0
1	C	24	VAL	2.0
1	C	302	VAL	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 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
3	GOL	B	802	6/6	0.79	0.16	44,45,47,47	0
3	GOL	D	802	6/6	0.82	0.13	48,48,49,49	0
3	GOL	A	802	6/6	0.84	0.14	34,38,41,43	0
3	GOL	A	804	6/6	0.84	0.14	31,38,40,41	0
3	GOL	C	802	6/6	0.85	0.13	40,42,43,44	0
4	FLC	D	803	13/13	0.88	0.11	37,43,46,46	0
4	FLC	A	803	13/13	0.92	0.09	29,34,38,38	0
5	NH4	B	803	1/1	0.93	0.10	25,25,25,25	0
5	NH4	C	804	1/1	0.93	0.11	21,21,21,21	0
2	0GA	D	801	17/17	0.95	0.08	28,32,43,43	0
2	0GA	B	801	17/17	0.96	0.07	25,28,33,33	0

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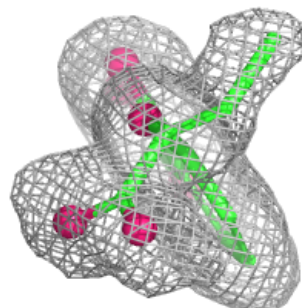
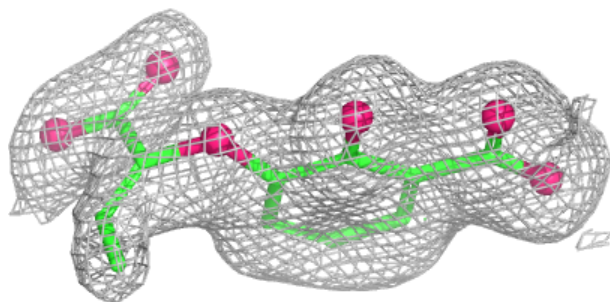
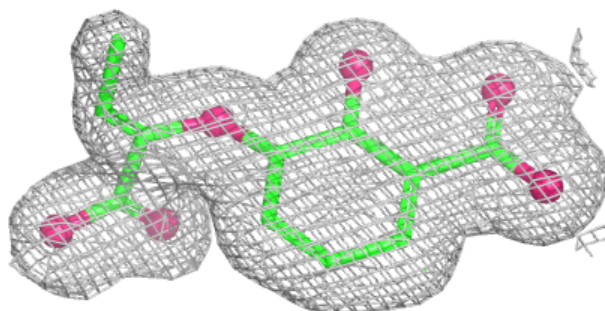
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	0GA	A	801	17/17	0.97	0.07	18,23,38,38	0
2	0GA	C	801	17/17	0.97	0.06	26,31,43,44	0
5	NH4	C	803	1/1	0.98	0.04	14,14,14,14	0

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.

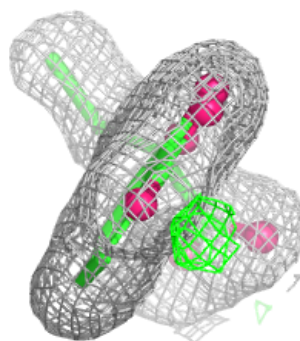
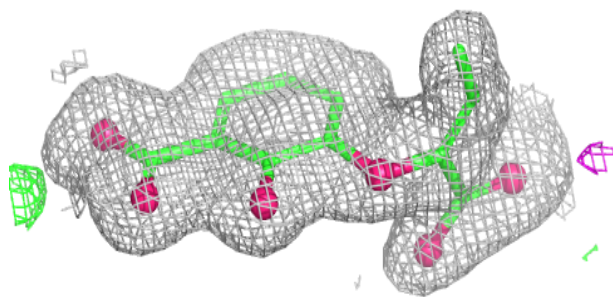
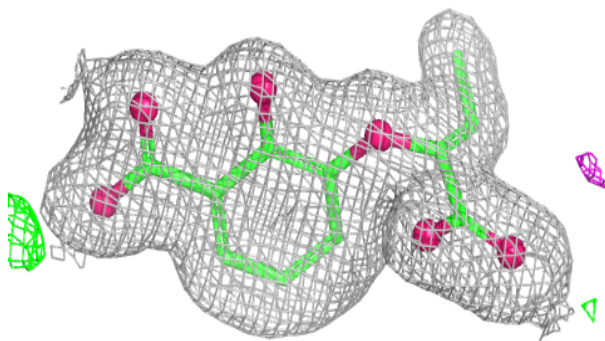
Electron density around 0GA D 801:

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

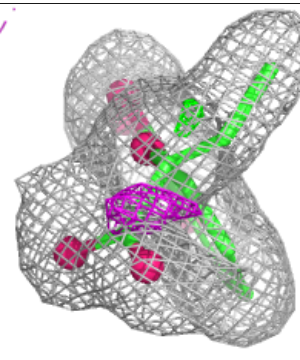
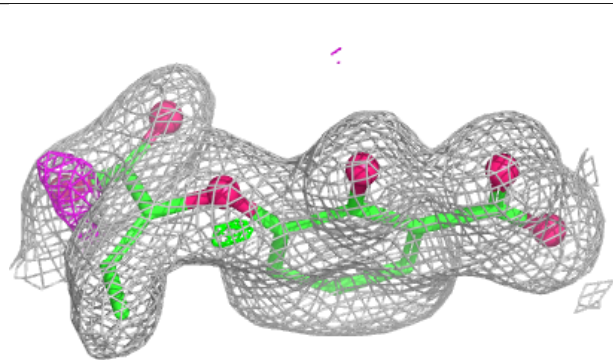
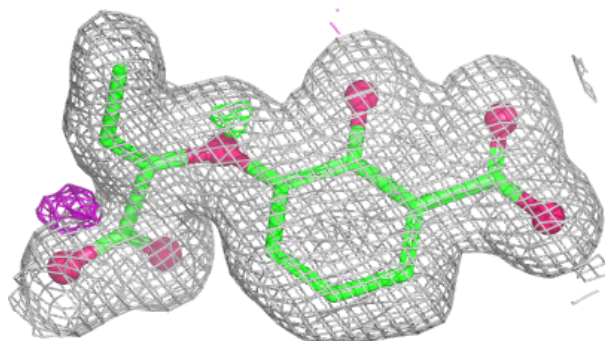


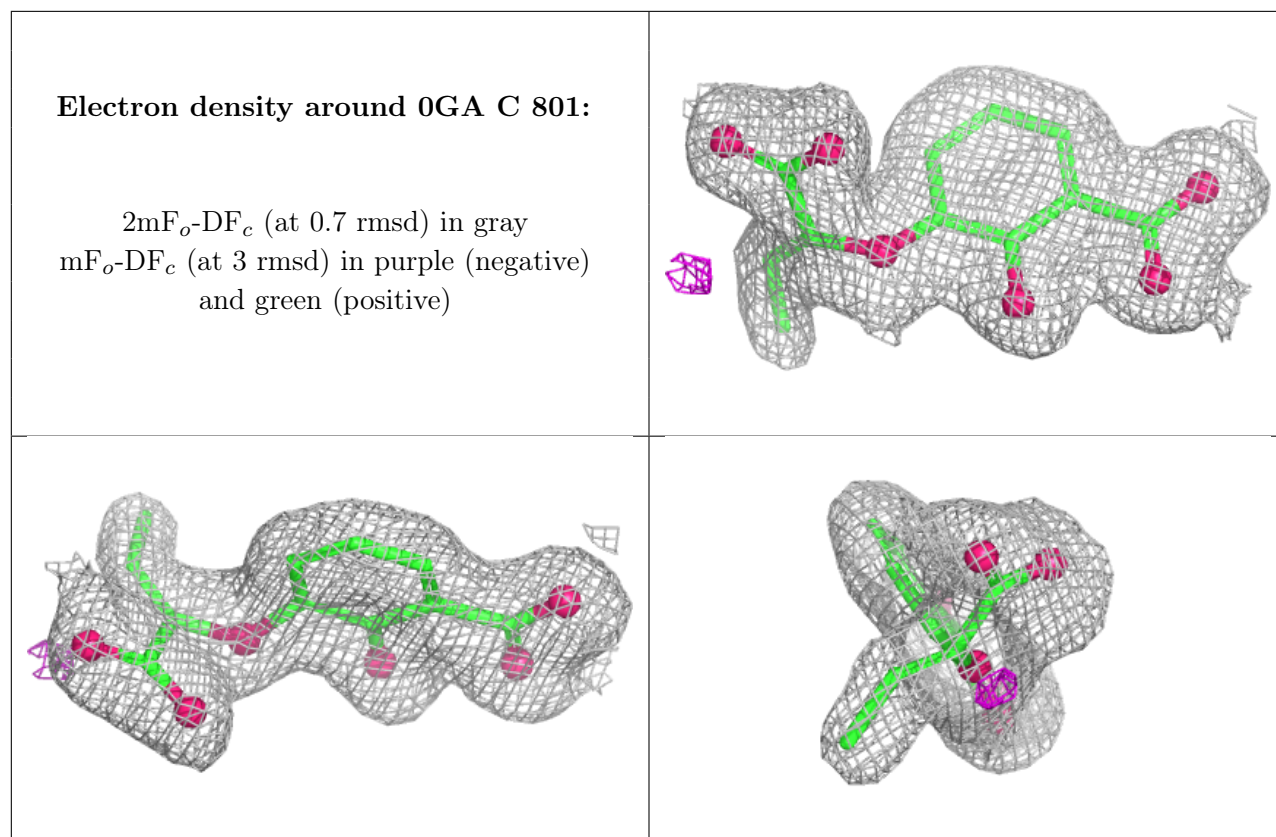
Electron density around 0GA B 801:

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

**Electron density around 0GA A 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.