



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2026 – 12:12 PM EDT

PDB ID : 12AL / pdb_000012al
Title : Human Ornithine Aminotransferase soaked with its inhibitor, (S)-3-amino-4-vinylidenecyclopent-1-ene-1-carboxylic acid
Authors : Corrigan, M.C.; Wang, F.; Silverman, R.B.; Liu, D.
Deposited on : 2026-03-23
Resolution : 1.72 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

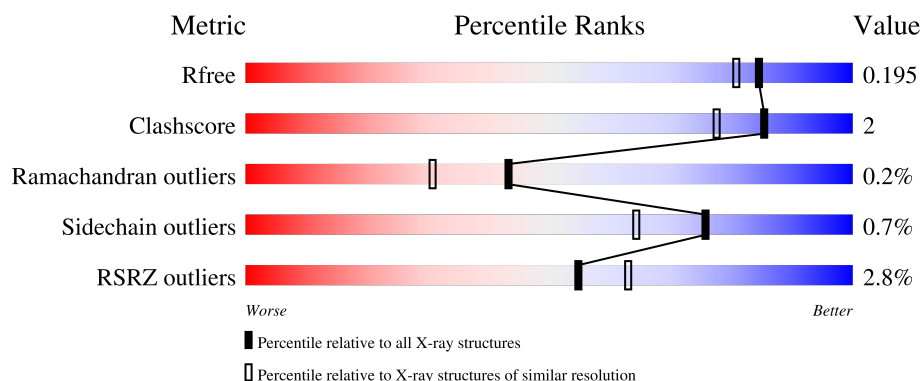
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	439	2% 87% • 8%
1	B	439	3% 87% 5% 8%
1	C	439	2% 86% 6% 8%

2 Entry composition [i](#)

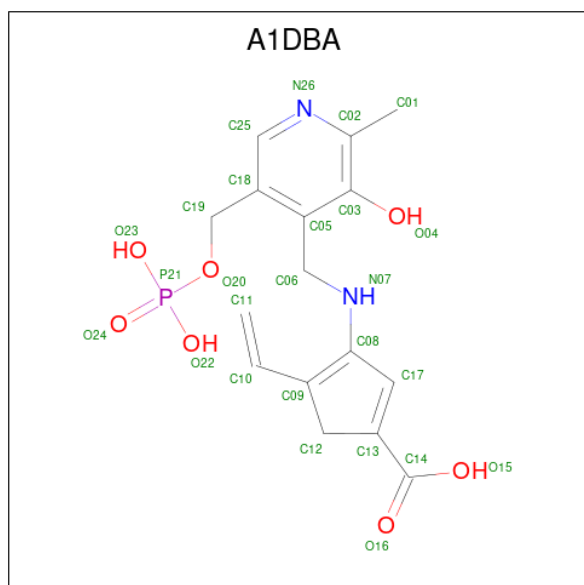
There are 4 unique types of molecules in this entry. The entry contains 10551 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ornithine aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	1	0
			3169	2035	534	587	13			
1	B	403	Total	C	N	O	S	0	0	0
			3157	2028	532	585	12			
1	C	403	Total	C	N	O	S	0	0	0
			3157	2028	532	585	12			

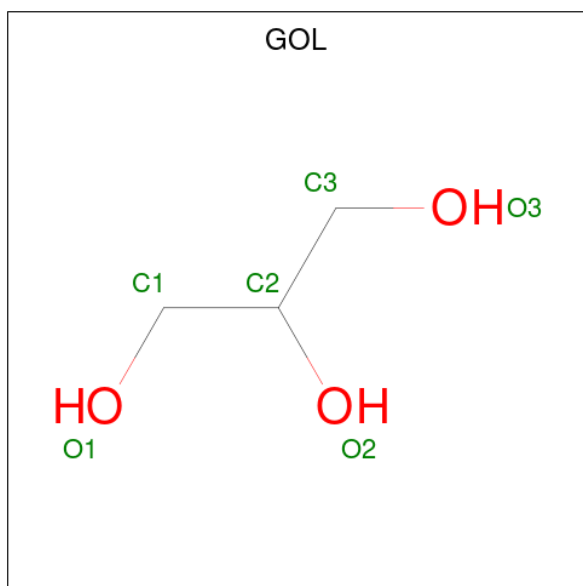
- Molecule 2 is 4-ethenyl-3-[[2-methyl-3-oxidanyl-5-[[oxidanyl-bis(oxidanylidene)- $\text{S}^{\{6\}}$ -phosphanyl]oxymethyl]pyridin-4-yl]methylamino]cyclopenta-1,3-diene-1-carboxylic acid (CCD ID: A1DBA) (formula: $\text{C}_{16}\text{H}_{19}\text{N}_2\text{O}_7\text{P}$) (labeled as "Ligand of Interest" by depositor).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			26	16	2	7	1		

- 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	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	307	Total	O	0	0
			307	307		

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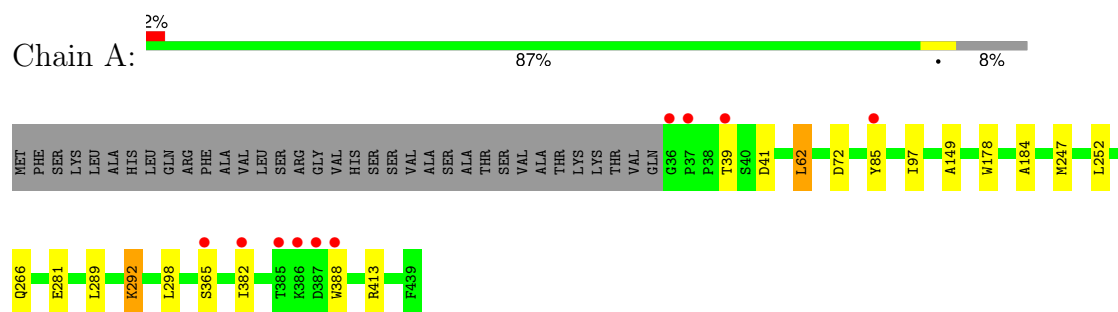
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	299	Total 299	O 299	0	0
4	C	342	Total 342	O 342	0	0

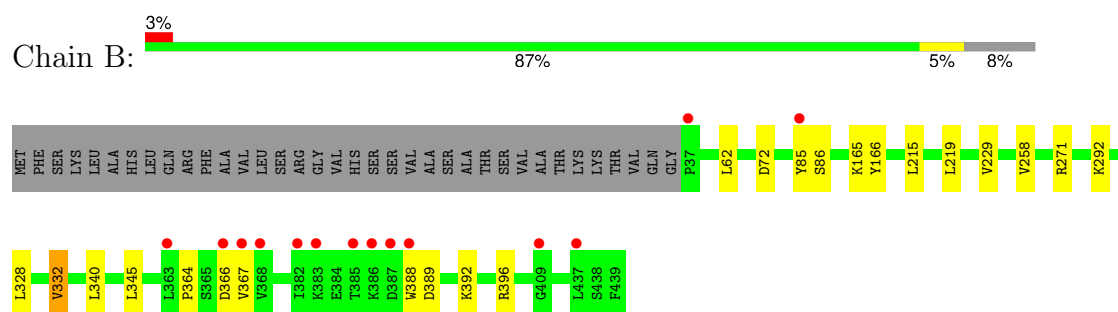
3 Residue-property plots [i](#)

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.

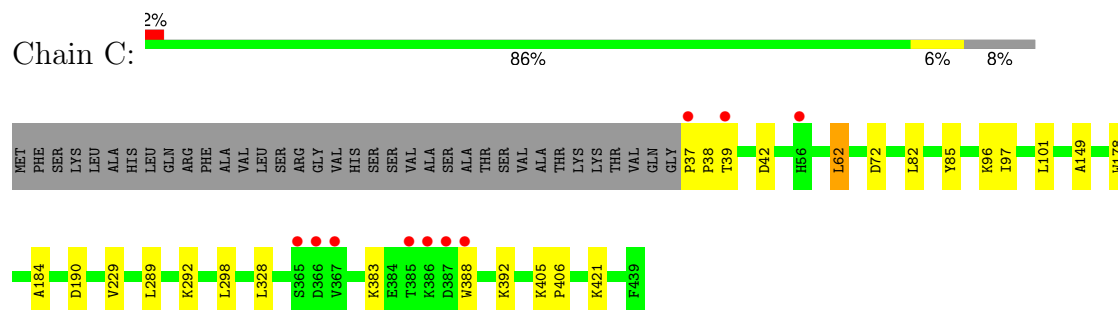
- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial



- Molecule 1: Ornithine aminotransferase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.53Å 115.53Å 186.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.17 – 1.72 55.17 – 1.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (55.17-1.72) 100.0 (55.17-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.166 , 0.195 0.165 , 0.195	Depositor DCC
R_{free} test set	7916 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10551	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: GOL, A1DBA

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	0.26	0/3243	0.48	0/4403
1	B	0.26	0/3231	0.46	0/4387
1	C	0.29	0/3231	0.48	0/4387
All	All	0.27	0/9705	0.47	0/13177

There are no bond length outliers.

There are no bond angle outliers.

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	3169	0	3171	14	0
1	B	3157	0	3161	12	0
1	C	3157	0	3161	15	0
2	A	26	0	0	3	0
2	B	26	0	0	1	0
2	C	26	0	0	2	0
3	A	12	0	16	2	0
3	B	12	0	16	0	0
3	C	18	0	24	2	0
4	A	307	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	299	0	0	0	0
4	C	342	0	0	1	0
All	All	10551	0	9549	43	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 2.

All (43) 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:C:190:ASP:HB2	3:C:504:GOL:H11	1.61	0.83
1:C:39:THR:HG23	1:C:42:ASP:H	1.51	0.74
1:C:101:LEU:HD12	1:C:328:LEU:HD11	1.77	0.67
1:B:86:SER:OG	1:B:271:ARG:HD3	1.95	0.67
1:B:367:VAL:HG13	1:B:388:TRP:HH2	1.63	0.64
1:A:39:THR:HG22	1:A:41:ASP:H	1.64	0.60
3:A:503:GOL:H32	4:A:604:HOH:O	2.02	0.59
1:B:389:ASP:OD1	1:B:392:LYS:HG2	2.05	0.56
1:C:388:TRP:HA	1:C:392:LYS:HD2	1.89	0.55
1:A:39:THR:HG22	1:A:41:ASP:N	2.23	0.54
1:A:97:ILE:HG22	1:A:298:LEU:HD22	1.88	0.54
1:A:85:TYR:HB3	2:A:501:A1DBA:C10	2.38	0.53
1:C:39:THR:HG22	1:C:42:ASP:CG	2.36	0.51
3:C:504:GOL:H12	4:C:728:HOH:O	2.10	0.51
1:B:396:ARG:HH11	1:B:396:ARG:HG3	1.77	0.49
1:A:382:ILE:HG23	1:A:388:TRP:CZ3	2.46	0.49
1:B:367:VAL:HG13	1:B:388:TRP:CH2	2.46	0.48
1:C:97:ILE:HG22	1:C:298:LEU:HD22	1.95	0.47
1:B:85:TYR:HB3	2:B:501:A1DBA:C10	2.45	0.47
1:C:62:LEU:HA	1:C:72:ASP:HA	1.97	0.47
1:C:37:PRO:HA	1:C:38:PRO:HD3	1.87	0.46
1:C:405:LYS:HG3	1:C:406:PRO:HD2	1.98	0.46
1:C:178:TRP:CZ2	1:C:184:ALA:HA	2.51	0.45
1:A:247[A]:MET:HG3	1:A:281:GLU:HB3	1.99	0.45
1:B:165:LYS:HA	1:B:166:TYR:HA	1.77	0.45
1:A:149:ALA:HB2	1:A:289:LEU:HD21	1.99	0.44
1:C:85:TYR:HB3	2:C:501:A1DBA:C10	2.48	0.43
1:A:266:GLN:HE22	1:A:413:ARG:NH1	2.16	0.43
1:B:62:LEU:HA	1:B:72:ASP:HA	1.99	0.43
1:B:364:PRO:HB2	1:B:366:ASP:OD1	2.20	0.42
1:A:365:SER:HB3	1:C:383:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:LEU:O	1:B:332:VAL:HG13	2.20	0.42
1:C:149:ALA:HB2	1:C:289:LEU:HD21	2.03	0.41
1:C:96:LYS:HD2	1:C:96:LYS:HA	1.79	0.41
1:A:292:LYS:HE3	2:A:501:A1DBA:N07	2.35	0.41
1:B:219:LEU:HD22	1:B:258:VAL:HG21	2.03	0.41
1:A:252:LEU:HD11	3:A:502:GOL:H2	2.03	0.41
1:A:178:TRP:CZ2	1:A:184:ALA:HA	2.55	0.41
2:C:501:A1DBA:O04	2:C:501:A1DBA:N07	2.54	0.41
1:A:62:LEU:HA	1:A:72:ASP:HA	2.03	0.41
1:B:340:LEU:HD23	1:B:345:LEU:HD12	2.03	0.40
1:C:421:LYS:HB3	1:C:421:LYS:HE2	1.94	0.40
1:A:85:TYR:HB3	2:A:501:A1DBA:C11	2.52	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	403/439 (92%)	388 (96%)	14 (4%)	1 (0%)	43	31
1	B	401/439 (91%)	386 (96%)	14 (4%)	1 (0%)	43	31
1	C	401/439 (91%)	387 (96%)	13 (3%)	1 (0%)	43	31
All	All	1205/1317 (92%)	1161 (96%)	41 (3%)	3 (0%)	43	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	LYS
1	B	292	LYS
1	C	292	LYS

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	338/366 (92%)	337 (100%)	1 (0%)	86	79
1	B	337/366 (92%)	334 (99%)	3 (1%)	70	57
1	C	337/366 (92%)	334 (99%)	3 (1%)	70	57
All	All	1012/1098 (92%)	1005 (99%)	7 (1%)	76	64

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

Mol	Chain	Res	Type
1	A	62	LEU
1	B	215	LEU
1	B	229	VAL
1	B	332	VAL
1	C	62	LEU
1	C	82	LEU
1	C	229	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	266	GLN
1	A	348	ASN
1	B	176	ASN
1	B	358	ASN
1	B	433	ASN
1	C	56	HIS
1	C	176	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	A1DBA	A	501	1	27,27,27	3.00	7 (25%)	34,39,39	2.81	10 (29%)
3	GOL	B	502	-	5,5,5	0.31	0	5,5,5	0.62	0
3	GOL	A	502	-	5,5,5	0.25	0	5,5,5	0.64	0
2	A1DBA	C	501	1	27,27,27	2.84	6 (22%)	34,39,39	2.88	14 (41%)
2	A1DBA	B	501	1	27,27,27	3.06	8 (29%)	34,39,39	2.71	6 (17%)
3	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.59	0
3	GOL	C	503	-	5,5,5	0.41	0	5,5,5	0.38	0
3	GOL	A	503	-	5,5,5	0.54	0	5,5,5	0.99	0
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.64	0
3	GOL	C	502	-	5,5,5	0.45	0	5,5,5	0.48	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
2	A1DBA	A	501	1	-	4/16/29/29	0/2/2/2
3	GOL	B	502	-	-	0/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
2	A1DBA	C	501	1	-	6/16/29/29	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1DBA	B	501	1	-	5/16/29/29	0/2/2/2
3	GOL	C	504	-	-	1/4/4/4	-
3	GOL	C	503	-	-	2/4/4/4	-
3	GOL	A	503	-	-	3/4/4/4	-
3	GOL	B	503	-	-	3/4/4/4	-
3	GOL	C	502	-	-	0/4/4/4	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1DBA	C10-C09	9.80	1.55	1.46
2	B	501	A1DBA	C10-C09	9.42	1.55	1.46
2	C	501	A1DBA	C10-C09	9.14	1.54	1.46
2	B	501	A1DBA	C08-N07	6.72	1.46	1.34
2	A	501	A1DBA	C08-N07	6.61	1.45	1.34
2	B	501	A1DBA	C17-C13	6.05	1.53	1.36
2	C	501	A1DBA	C08-N07	6.03	1.44	1.34
2	A	501	A1DBA	C17-C13	5.61	1.52	1.36
2	C	501	A1DBA	C17-C13	5.57	1.52	1.36
2	B	501	A1DBA	C17-C08	4.61	1.52	1.42
2	A	501	A1DBA	C17-C08	4.45	1.51	1.42
2	C	501	A1DBA	C17-C08	4.03	1.51	1.42
2	B	501	A1DBA	C01-C02	3.22	1.55	1.50
2	A	501	A1DBA	C01-C02	3.12	1.55	1.50
2	C	501	A1DBA	C06-C05	2.75	1.56	1.52
2	B	501	A1DBA	C06-C05	2.62	1.55	1.52
2	C	501	A1DBA	C01-C02	2.59	1.54	1.50
2	B	501	A1DBA	P21-O23	2.26	1.63	1.54
2	B	501	A1DBA	C12-C13	2.20	1.55	1.50
2	A	501	A1DBA	C12-C13	2.06	1.54	1.50
2	A	501	A1DBA	P21-O23	2.02	1.62	1.54

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	A1DBA	C11-C10-C09	-11.83	110.86	126.08
2	B	501	A1DBA	C11-C10-C09	-11.72	111.00	126.08
2	A	501	A1DBA	C11-C10-C09	-10.83	112.15	126.08
2	A	501	A1DBA	C06-N07-C08	-7.48	110.24	123.44
2	C	501	A1DBA	C06-N07-C08	-6.51	111.96	123.44
2	B	501	A1DBA	C06-N07-C08	-5.62	113.52	123.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1DBA	C10-C09-C08	-4.55	119.13	126.63
2	B	501	A1DBA	C10-C09-C08	-3.70	120.53	126.63
2	B	501	A1DBA	C06-C05-C03	3.45	124.57	119.98
2	C	501	A1DBA	C05-C06-N07	-3.23	104.62	111.26
2	A	501	A1DBA	C06-C05-C18	-3.04	116.44	119.75
2	C	501	A1DBA	C06-C05-C03	3.03	124.02	119.98
2	A	501	A1DBA	C06-C05-C03	3.03	124.01	119.98
2	A	501	A1DBA	C05-C06-N07	-2.97	105.16	111.26
2	C	501	A1DBA	O16-C14-C13	-2.90	116.55	121.64
2	C	501	A1DBA	C06-C05-C18	-2.67	116.84	119.75
2	C	501	A1DBA	C10-C09-C08	-2.60	122.34	126.63
2	C	501	A1DBA	C12-C13-C17	2.57	109.38	108.05
2	B	501	A1DBA	O20-C19-C18	-2.56	104.55	109.36
2	C	501	A1DBA	C17-C13-C14	-2.46	119.20	126.31
2	B	501	A1DBA	C06-C05-C18	-2.44	117.09	119.75
2	A	501	A1DBA	C19-C18-C25	2.31	123.13	119.36
2	C	501	A1DBA	C18-C25-N26	-2.28	120.13	123.83
2	C	501	A1DBA	C25-N26-C02	2.26	123.30	119.20
2	C	501	A1DBA	O04-C03-C05	2.23	124.64	118.18
2	C	501	A1DBA	O20-C19-C18	-2.16	105.30	109.36
2	A	501	A1DBA	O20-C19-C18	-2.13	105.36	109.36
2	A	501	A1DBA	C12-C09-C10	2.11	127.23	122.63
2	A	501	A1DBA	C19-C18-C05	-2.04	118.38	122.67
2	C	501	A1DBA	O15-C14-C13	2.00	119.67	115.43

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1DBA	C12-C13-C14-O15
2	A	501	A1DBA	C12-C13-C14-O16
2	B	501	A1DBA	C18-C05-C06-N07
2	C	501	A1DBA	C18-C05-C06-N07
2	C	501	A1DBA	C12-C13-C14-O15
2	C	501	A1DBA	C12-C13-C14-O16
3	A	503	GOL	C1-C2-C3-O3
2	A	501	A1DBA	C18-C05-C06-N07
3	B	503	GOL	O2-C2-C3-O3
3	B	503	GOL	C1-C2-C3-O3
2	B	501	A1DBA	C03-C05-C06-N07
2	C	501	A1DBA	C03-C05-C06-N07
3	A	503	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	501	A1DBA	C03-C05-C06-N07
2	C	501	A1DBA	C17-C08-N07-C06
3	C	503	GOL	O1-C1-C2-C3
2	B	501	A1DBA	C12-C13-C14-O16
3	C	504	GOL	C1-C2-C3-O3
2	B	501	A1DBA	C12-C13-C14-O15
3	A	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-O2
3	C	503	GOL	O1-C1-C2-O2
2	B	501	A1DBA	C17-C08-N07-C06
2	C	501	A1DBA	C19-O20-P21-O22

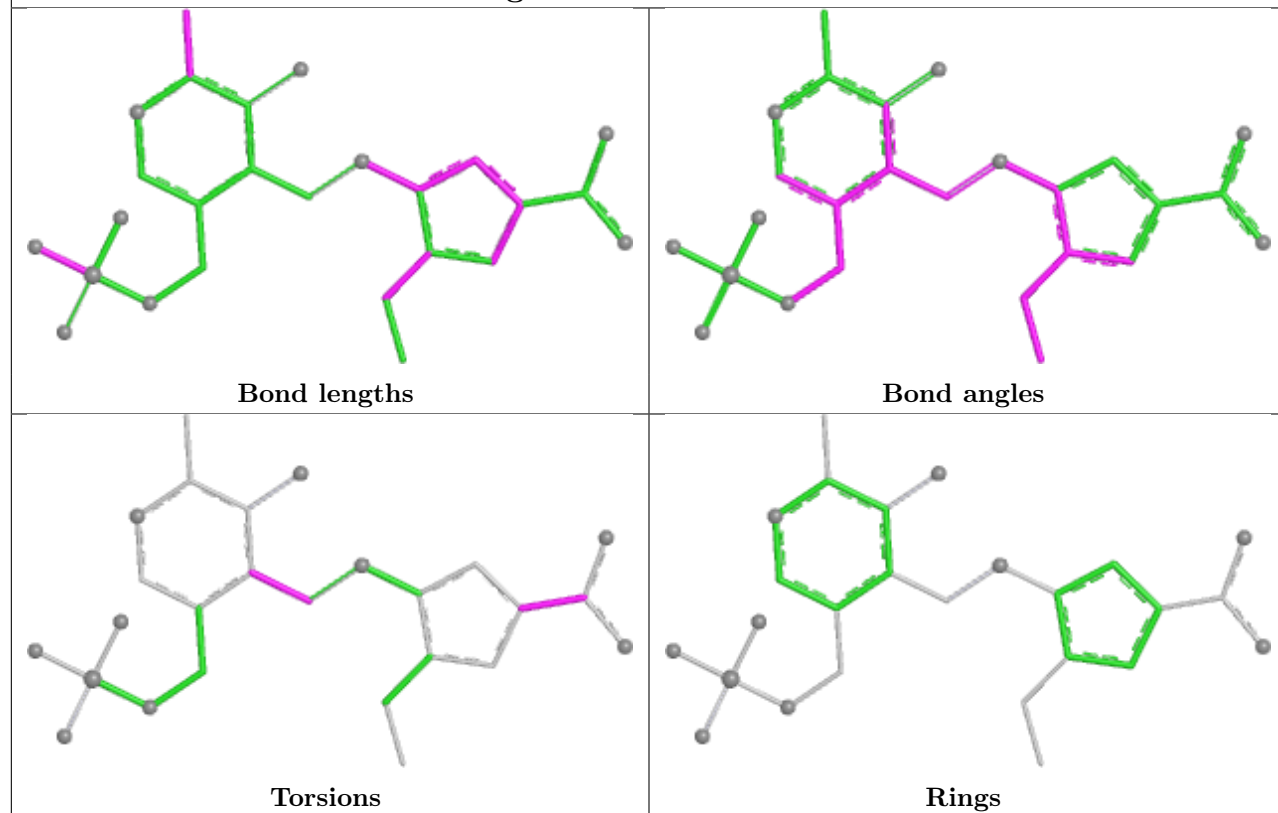
There are no ring outliers.

6 monomers are involved in 10 short contacts:

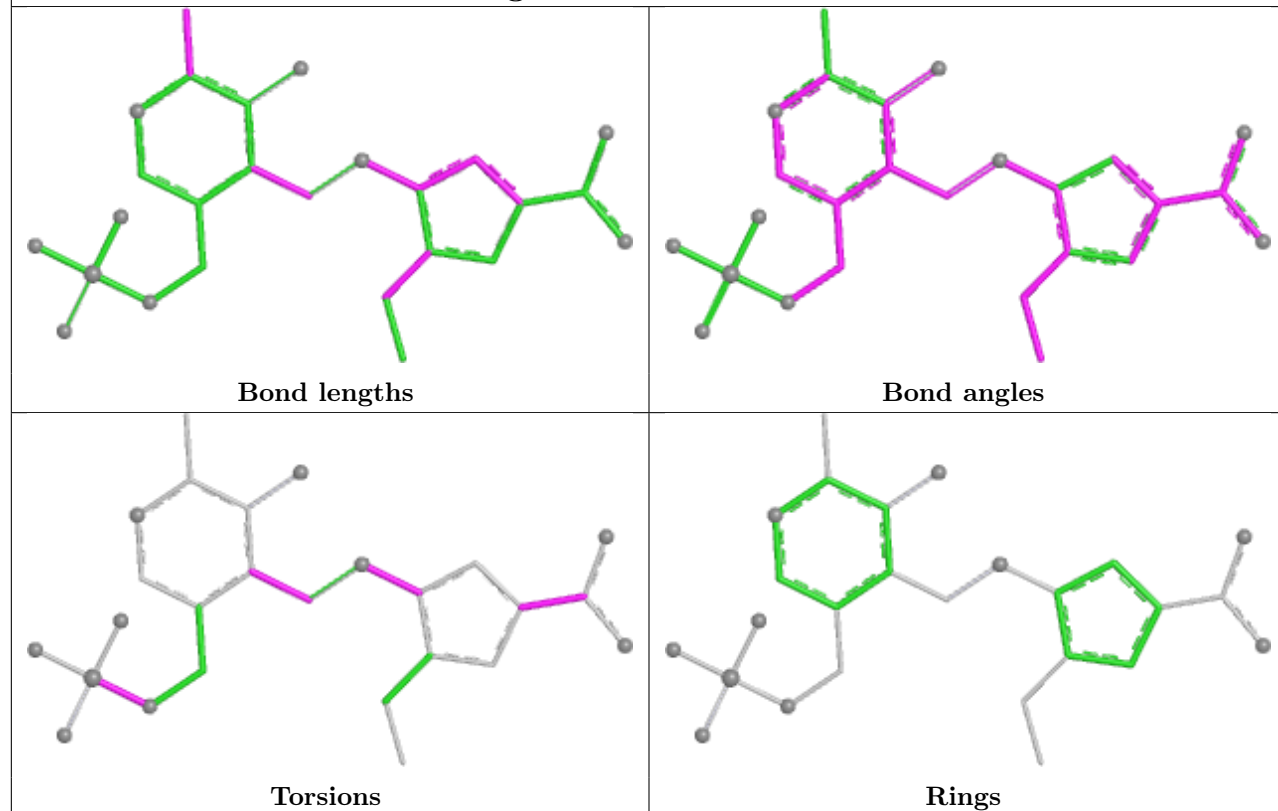
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	A1DBA	3	0
3	A	502	GOL	1	0
2	C	501	A1DBA	2	0
2	B	501	A1DBA	1	0
3	C	504	GOL	2	0
3	A	503	GOL	1	0

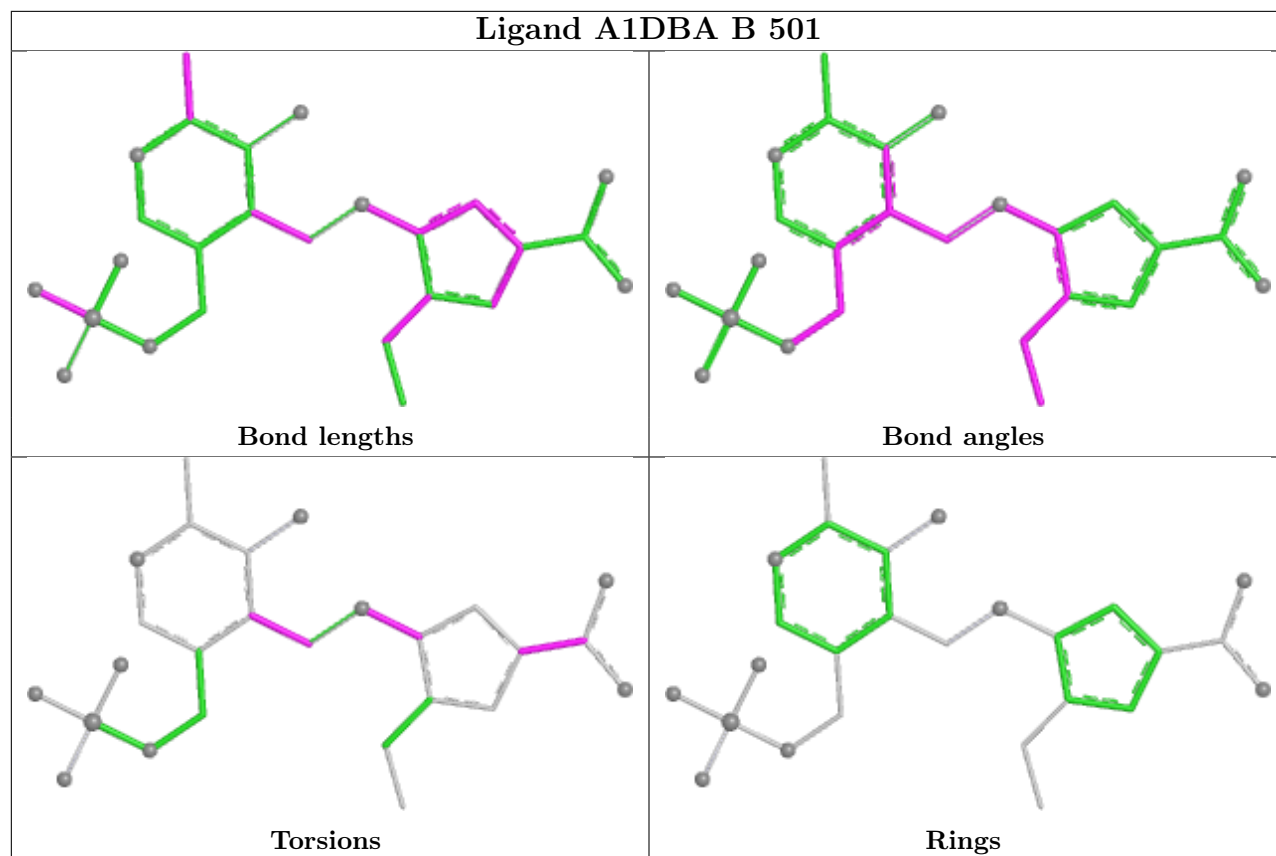
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 A1DBA A 501



Ligand A1DBA C 501





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	404/439 (92%)	-0.23	10 (2%) 58 66	13, 26, 45, 84	1 (0%)
1	B	403/439 (91%)	-0.09	14 (3%) 47 55	15, 26, 58, 111	0
1	C	403/439 (91%)	-0.35	10 (2%) 58 66	14, 23, 41, 99	0
All	All	1210/1317 (91%)	-0.23	34 (2%) 55 63	13, 25, 48, 111	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	388	TRP	5.9
1	B	37	PRO	4.7
1	B	388	TRP	4.7
1	A	36	GLY	4.5
1	C	37	PRO	4.4
1	A	382	ILE	4.1
1	B	382	ILE	4.1
1	C	386	LYS	3.9
1	B	367	VAL	3.8
1	C	387	ASP	3.8
1	B	386	LYS	3.4
1	B	385	THR	3.3
1	A	386	LYS	3.3
1	A	388	TRP	3.0
1	B	387	ASP	3.0
1	C	366	ASP	3.0
1	B	85	TYR	2.9
1	A	37	PRO	2.8
1	A	39	THR	2.6
1	C	365	SER	2.6
1	C	385	THR	2.6
1	B	363	LEU	2.5
1	A	387	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	85	TYR	2.5
1	B	437	LEU	2.4
1	A	385	THR	2.4
1	C	39	THR	2.2
1	B	383	LYS	2.2
1	B	409	GLY	2.0
1	B	366	ASP	2.0
1	C	367	VAL	2.0
1	C	56	HIS	2.0
1	A	365	SER	2.0
1	B	368	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.

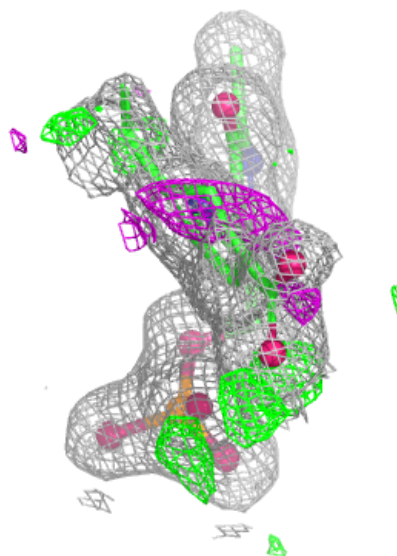
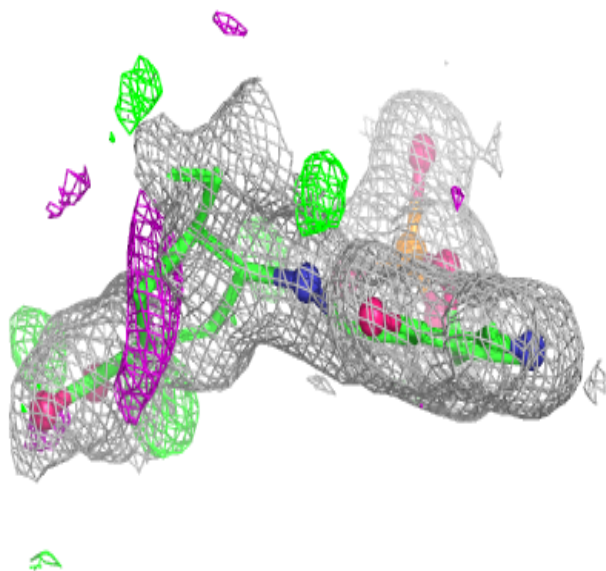
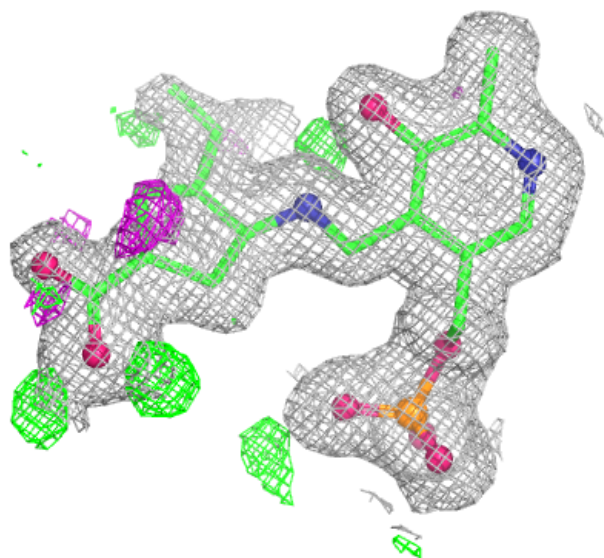
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	C	502	6/6	0.67	0.21	33,38,45,47	0
3	GOL	A	503	6/6	0.76	0.18	22,34,40,44	0
3	GOL	A	502	6/6	0.82	0.14	31,36,42,43	0
3	GOL	B	503	6/6	0.86	0.12	30,33,37,46	0
3	GOL	B	502	6/6	0.86	0.11	30,34,38,41	0
3	GOL	C	504	6/6	0.90	0.10	21,28,33,34	0
3	GOL	C	503	6/6	0.91	0.11	19,27,35,41	0
2	A1DBA	B	501	26/26	0.97	0.08	17,23,39,41	2
2	A1DBA	A	501	26/26	0.97	0.08	15,23,35,43	2
2	A1DBA	C	501	26/26	0.98	0.06	15,20,31,36	2

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.

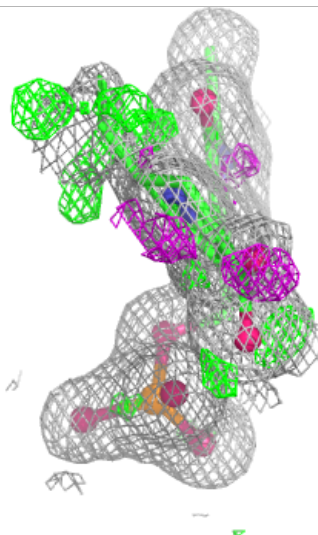
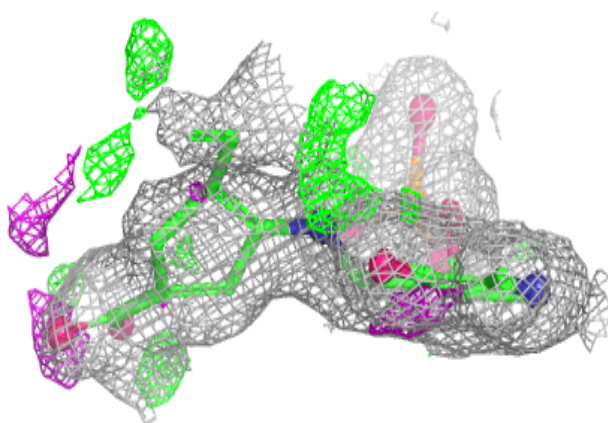
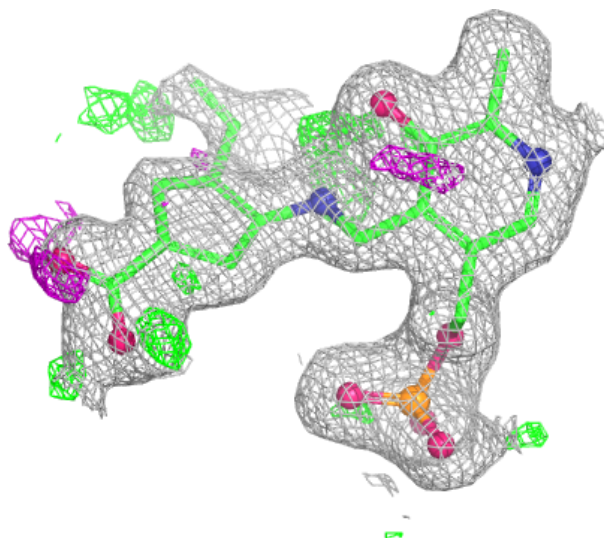
Electron density around A1DBA B 501:

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



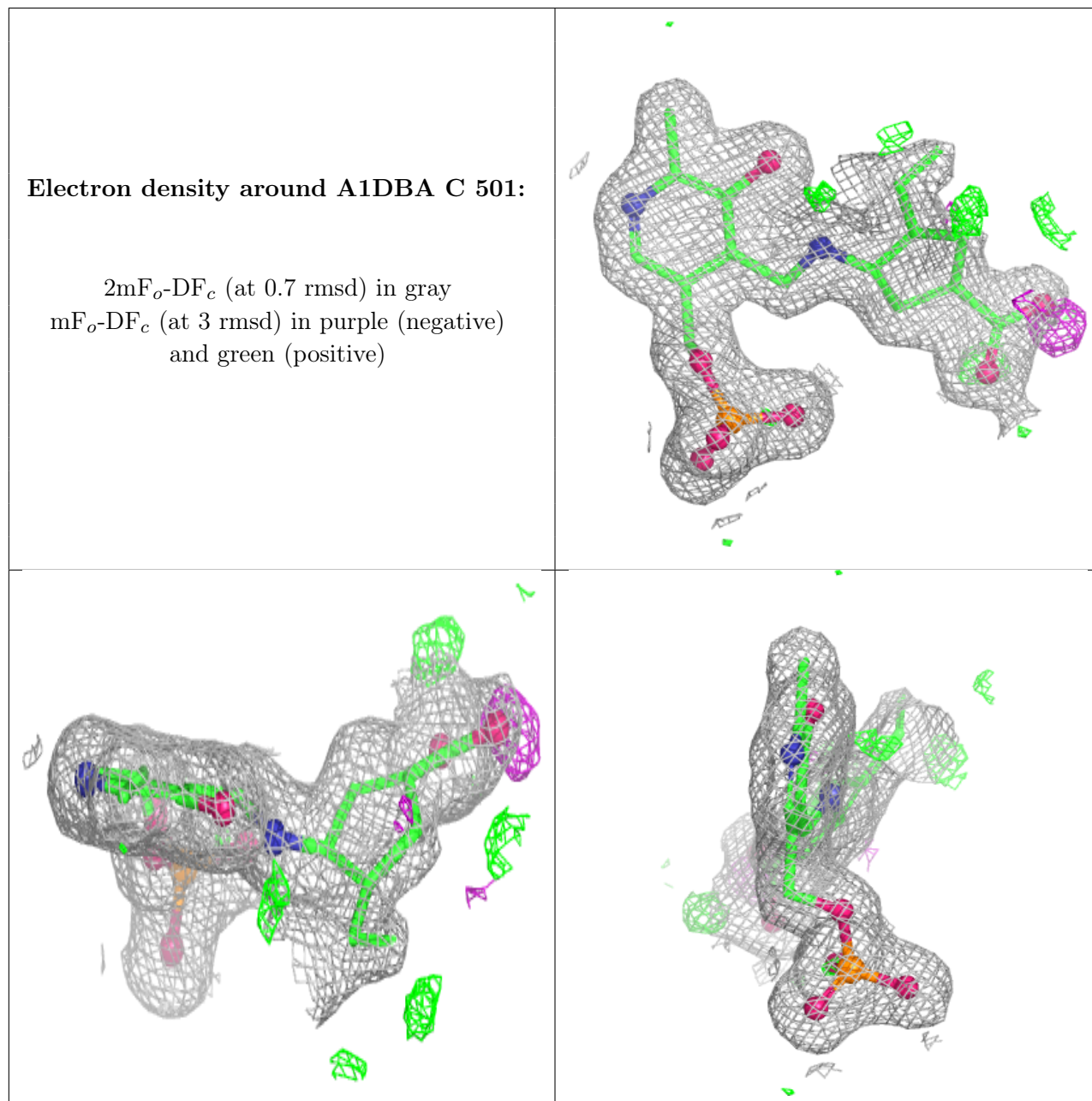
Electron density around A1DBA A 501:

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



Electron density around A1DBA C 501:

$2mF_o-DF_c$ (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.