Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:19 AM UTC

PDB ID	:	9C4R / pdb_00009c4r
Title	:	Crystal structure of wild-type arabidopsis thaliana acetohydroxyacid synthase in complex with newly designed herbicide CMO
Authors	:	Cheng, Y.; Guddat, L.W.
Deposited on	:	2024-06-05
Resolution	:	2.84 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:

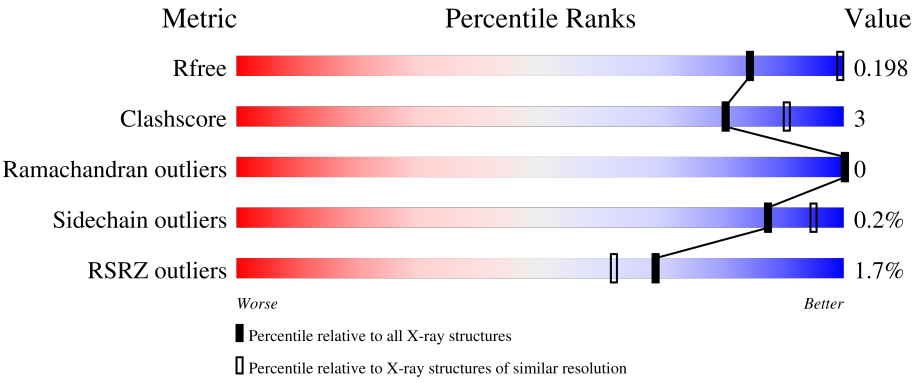
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 2.84 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	590	2% 92% 7%

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
5	A1AUL	A	704[A]	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	A1AUL	A	704[B]	-	X	-	-
6	ACT	A	705	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 4625 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 Acetolactate synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	1	0
			4468	2834	770	839	25			

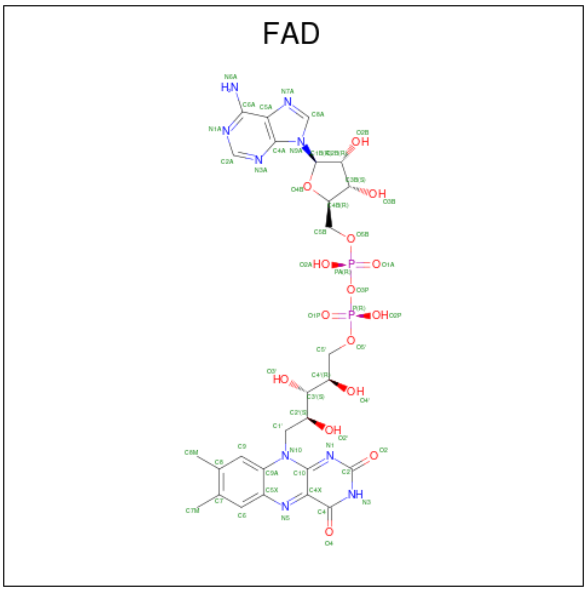
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LEU	-	expression tag	UNP P17597
A	669	GLU	-	expression tag	UNP P17597
A	670	HIS	-	expression tag	UNP P17597
A	671	HIS	-	expression tag	UNP P17597
A	672	HIS	-	expression tag	UNP P17597
A	673	HIS	-	expression tag	UNP P17597
A	674	HIS	-	expression tag	UNP P17597
A	675	HIS	-	expression tag	UNP P17597

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

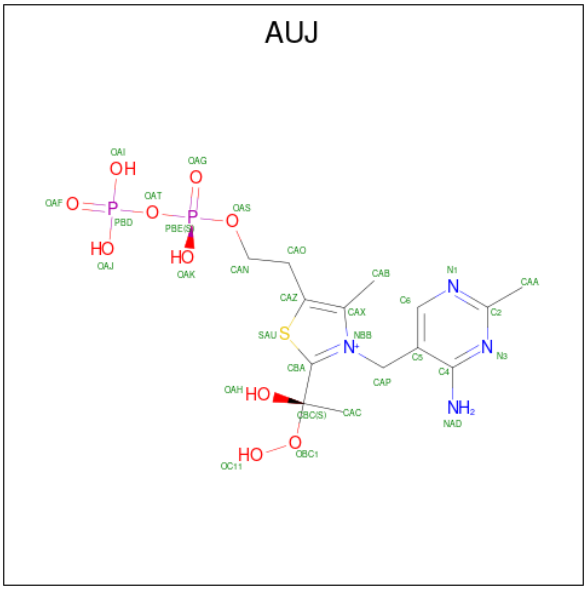
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0

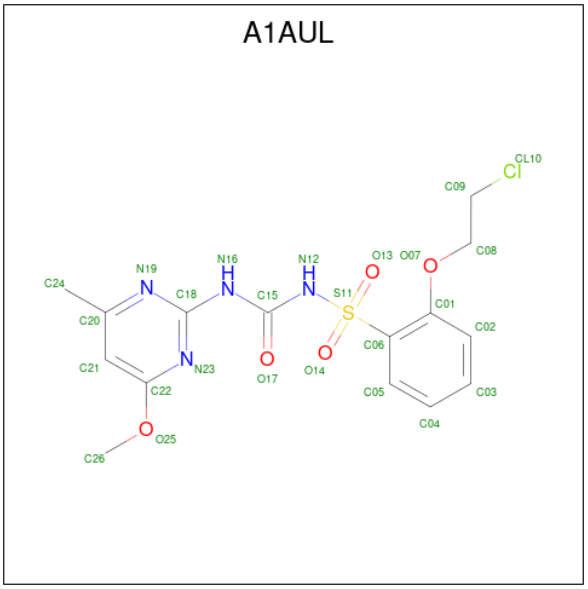
- Molecule 4 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1 -oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID: AUJ) (formula: $C_{14}H_{23}N_4O_{10}P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	A	1	31	14	4	10	2	1	0	0

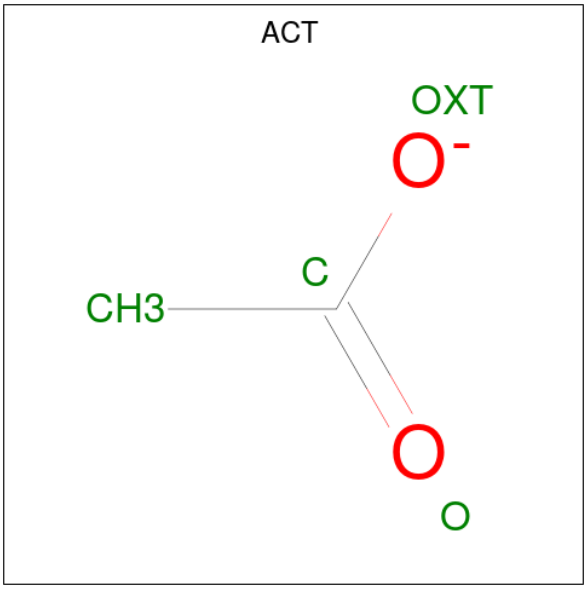
- Molecule 5 is 2-(2-chloroethoxy)-N-[(4-methoxy-6-methylpyrimidin-2-yl)carbamoyl]ben

zene-1-sulfonamide (CCD ID: A1AUL) (formula: $C_{15}H_{17}ClN_4O_5S$) (labeled as "Ligand of Interest" by depositor).



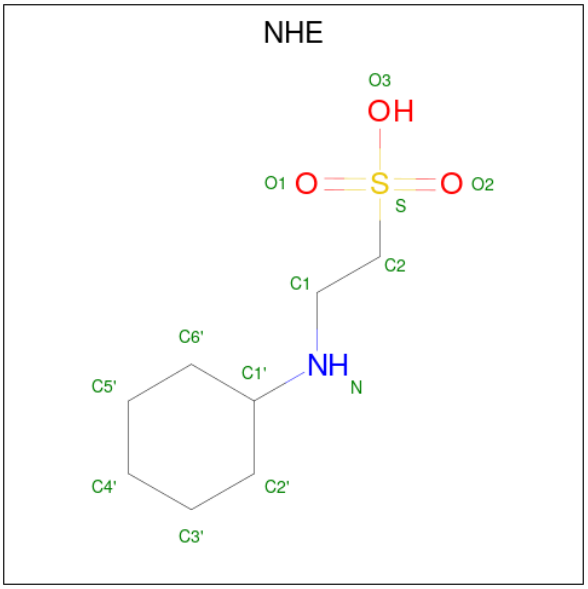
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	S	0	1
			52	30	2	8	10	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



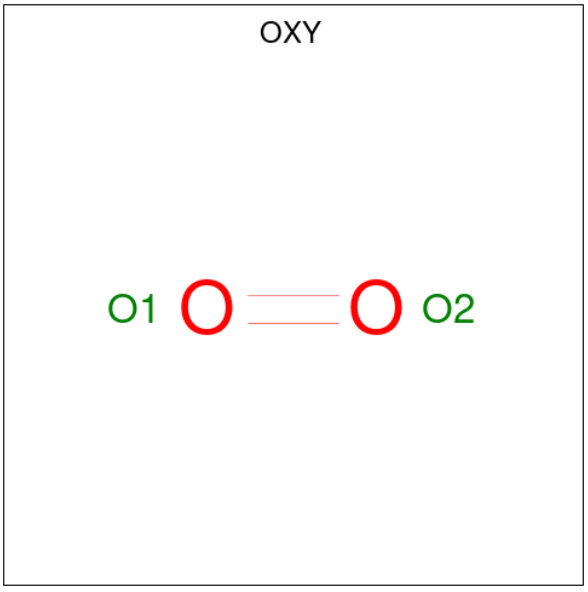
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			2	2		

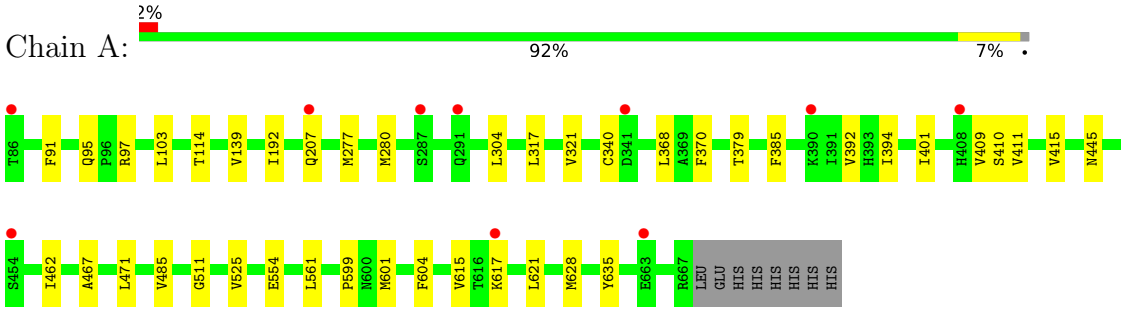
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 1 1	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: Acetolactate synthase, chloroplastic



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α, β, γ	178.41Å 178.41Å 184.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.33 – 2.84 49.33 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.33-2.84) 99.3 (49.33-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.179 , 0.198 0.181 , 0.198	Depositor DCC
R_{free} test set	2000 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å^2)	76.1	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4625	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, AUJ, ACT, A1AUL, MG, OXY, NHE, CSD

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	0.08	0/4556	0.25	0/6184

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

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	4468	0	4464	22	1
2	A	1	0	0	0	0
3	A	53	0	31	1	0
4	A	31	0	0	0	1
5	A	52	0	0	1	0
6	A	4	0	3	0	0
7	A	13	0	17	0	0
8	A	2	0	0	0	0
9	A	1	0	0	0	0
All	All	4625	0	4515	24	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 3.

All (24) 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:394:ILE:HG12	1:A:411:VAL:HB	1.86	0.57
1:A:277:MET:HA	1:A:280:MET:HG3	1.87	0.57
1:A:103:LEU:HD21	1:A:192:ILE:HD13	1.91	0.53
1:A:467:ALA:HA	1:A:621:LEU:HD21	1.94	0.50
1:A:485:VAL:HG21	1:A:511:GLY:C	2.38	0.48
1:A:139:VAL:HG13	1:A:554:GLU:HG3	1.95	0.47
1:A:91:PHE:CG	1:A:97:ARG:HD3	2.50	0.47
1:A:601:MET:HA	1:A:604:PHE:HD2	1.81	0.46
1:A:471:LEU:HD22	1:A:561:LEU:HD22	1.96	0.45
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.99	0.44
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.00	0.44
1:A:304:LEU:HD23	1:A:368:LEU:HB2	1.99	0.44
1:A:379:THR:HA	1:A:385:PHE:CD1	2.53	0.44
1:A:401:ILE:HG21	1:A:410:SER:HB2	2.01	0.43
1:A:462:ILE:HD11	1:A:615:VAL:HG22	2.00	0.42
1:A:617:LYS:HD3	1:A:617:LYS:HA	1.81	0.42
3:A:702:FAD:H9	3:A:702:FAD:H1'1	1.73	0.42
1:A:392:VAL:HG22	1:A:409:VAL:HB	2.02	0.41
1:A:317:LEU:O	1:A:321:VAL:HG23	2.21	0.41
1:A:462:ILE:HG23	1:A:621:LEU:HD22	2.03	0.41
1:A:599:PRO:HD2	1:A:601:MET:HE2	2.02	0.41
5:A:704[B]:A1AUL:O07	5:A:704[B]:A1AUL:N12	2.54	0.41
1:A:628:MET:HG3	1:A:635:TYR:HB3	2.03	0.41
1:A:95:GLN:O	1:A:97:ARG:NH1	2.54	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:A:207:GLN:NE2	4:A:703:AUJ:OAH[12_544]	2.17	0.03

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	580/590 (98%)	570 (98%)	10 (2%)	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	479/486 (99%)	478 (100%)	1 (0%)	87 95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	445	ASN

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	269	GLN
1	A	527	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
1	CSD	A	340	1	4,7,8	1.04	0	1,8,10	7.74	1 (100%)

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
1	CSD	A	340	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	340	CSD	OD1-SG-CB	7.74	119.86	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	340	CSD	CA-CB-SG-OD1
1	A	340	CSD	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	AUJ	A	703	2	27,32,32	2.24	8 (29%)	36,49,49	1.70	13 (36%)
5	A1AUL	A	704[B]	-	27,27,27	4.78	22 (81%)	37,37,37	3.40	13 (35%)
3	FAD	A	702	-	58,58,58	2.99	24 (41%)	85,89,89	1.72	20 (23%)
8	OXY	A	707	-	1,1,1	0.10	0	-		
5	A1AUL	A	704[A]	-	27,27,27	4.79	21 (77%)	37,37,37	3.48	13 (35%)
7	NHE	A	706	-	13,13,13	1.35	3 (23%)	16,17,17	1.79	5 (31%)
6	ACT	A	705	-	3,3,3	0.97	0	3,3,3	0.82	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
4	AUJ	A	703	2	-	7/20/26/26	0/2/2/2
5	A1AUL	A	704[B]	-	-	15/21/21/21	0/2/2/2
3	FAD	A	702	-	-	7/34/50/50	0/6/6/6
5	A1AUL	A	704[A]	-	-	17/21/21/21	0/2/2/2
7	NHE	A	706	-	-	5/7/15/15	0/1/1/1

All (78) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704[A]	A1AUL	C05-C06	12.32	1.53	1.39
5	A	704[B]	A1AUL	C05-C06	12.29	1.53	1.39
3	A	702	FAD	O4-C4	9.22	1.41	1.23
3	A	702	FAD	PA-O3P	8.96	1.69	1.59
3	A	702	FAD	P-O3P	8.61	1.68	1.59
3	A	702	FAD	O2-C2	7.93	1.40	1.24
5	A	704[A]	A1AUL	C21-C22	7.31	1.49	1.38
5	A	704[B]	A1AUL	C21-C22	7.30	1.49	1.38
5	A	704[B]	A1AUL	C04-C03	7.05	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704[A]	A1AUL	C04-C03	6.97	1.53	1.38
5	A	704[B]	A1AUL	C02-C01	6.77	1.53	1.39
5	A	704[A]	A1AUL	C02-C01	6.69	1.53	1.39
5	A	704[A]	A1AUL	C18-N16	6.67	1.47	1.38
5	A	704[B]	A1AUL	C18-N16	6.53	1.47	1.38
5	A	704[B]	A1AUL	C20-N19	6.45	1.46	1.34
5	A	704[A]	A1AUL	C20-N19	6.41	1.46	1.34
4	A	703	AUJ	C5-C4	5.31	1.51	1.42
5	A	704[A]	A1AUL	C18-N23	5.28	1.49	1.34
5	A	704[B]	A1AUL	C18-N23	5.23	1.49	1.34
5	A	704[B]	A1AUL	C21-C20	-5.23	1.29	1.38
5	A	704[A]	A1AUL	C21-C20	-5.17	1.29	1.38
4	A	703	AUJ	C2-N3	4.93	1.42	1.34
4	A	703	AUJ	CAP-NBB	-4.86	1.42	1.47
5	A	704[B]	A1AUL	C01-C06	-4.73	1.33	1.40
5	A	704[A]	A1AUL	C01-C06	-4.72	1.33	1.40
5	A	704[A]	A1AUL	C06-S11	4.65	1.84	1.77
3	A	702	FAD	C6A-N6A	4.60	1.46	1.34
5	A	704[B]	A1AUL	C06-S11	4.59	1.84	1.77
5	A	704[B]	A1AUL	C15-N16	4.46	1.47	1.37
5	A	704[A]	A1AUL	C15-N16	4.43	1.47	1.37
3	A	702	FAD	O4B-C1B	-4.36	1.31	1.42
3	A	702	FAD	C2B-C1B	4.07	1.66	1.53
4	A	703	AUJ	C6-N1	3.94	1.42	1.34
5	A	704[A]	A1AUL	C22-N23	-3.90	1.26	1.33
5	A	704[A]	A1AUL	C15-N12	3.88	1.48	1.39
5	A	704[B]	A1AUL	C22-N23	-3.87	1.26	1.33
5	A	704[A]	A1AUL	S11-N12	3.82	1.73	1.64
5	A	704[B]	A1AUL	S11-N12	3.82	1.73	1.64
5	A	704[B]	A1AUL	C15-N12	3.79	1.47	1.39
5	A	704[A]	A1AUL	O25-C22	3.76	1.41	1.35
3	A	702	FAD	C5B-C4B	-3.71	1.40	1.51
5	A	704[B]	A1AUL	O25-C22	3.70	1.41	1.35
5	A	704[A]	A1AUL	C04-C05	-3.62	1.32	1.38
5	A	704[A]	A1AUL	C03-C02	-3.58	1.32	1.38
5	A	704[B]	A1AUL	C04-C05	-3.50	1.32	1.38
5	A	704[B]	A1AUL	C03-C02	-3.49	1.32	1.38
3	A	702	FAD	C4-N3	-3.24	1.32	1.38
7	A	706	NHE	C2-S	3.19	1.82	1.77
4	A	703	AUJ	C4-NAD	3.18	1.42	1.34
3	A	702	FAD	O4B-C4B	3.14	1.52	1.45
3	A	702	FAD	C9A-N10	-3.11	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	O3B-C3B	3.10	1.50	1.43
4	A	703	AUJ	C4-N3	-3.03	1.31	1.35
3	A	702	FAD	C8A-N9A	-2.98	1.32	1.37
3	A	702	FAD	C3B-C4B	2.86	1.60	1.53
3	A	702	FAD	C5'-C4'	2.79	1.55	1.51
5	A	704[B]	A1AUL	O14-S11	2.77	1.46	1.43
5	A	704[A]	A1AUL	O14-S11	2.76	1.46	1.43
5	A	704[B]	A1AUL	O13-S11	2.75	1.46	1.43
5	A	704[A]	A1AUL	O13-S11	2.71	1.46	1.43
3	A	702	FAD	C1'-C2'	2.63	1.56	1.52
3	A	702	FAD	C2-N3	-2.55	1.33	1.39
3	A	702	FAD	P-O5'	2.46	1.69	1.59
3	A	702	FAD	PA-O5B	2.41	1.68	1.59
4	A	703	AUJ	CAX-NBB	2.41	1.43	1.40
3	A	702	FAD	C5A-N7A	-2.38	1.34	1.39
3	A	702	FAD	O4'-C4'	-2.29	1.38	1.43
5	A	704[A]	A1AUL	O17-C15	-2.27	1.18	1.23
3	A	702	FAD	C5X-N5	-2.27	1.35	1.39
7	A	706	NHE	O2-S	2.25	1.51	1.45
5	A	704[B]	A1AUL	O17-C15	-2.24	1.18	1.23
7	A	706	NHE	O1-S	2.21	1.51	1.45
3	A	702	FAD	C4X-N5	2.18	1.35	1.30
5	A	704[A]	A1AUL	C18-N19	-2.11	1.29	1.34
3	A	702	FAD	O2B-C2B	2.10	1.48	1.43
4	A	703	AUJ	C2-N1	-2.09	1.31	1.34
5	A	704[B]	A1AUL	C18-N19	-2.06	1.29	1.34
5	A	704[B]	A1AUL	O07-C01	2.04	1.41	1.37

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704[B]	A1AUL	O13-S11-O14	-15.22	101.03	119.52
5	A	704[A]	A1AUL	O13-S11-O14	-15.15	101.12	119.52
5	A	704[A]	A1AUL	C18-N16-C15	-9.18	120.89	130.34
5	A	704[B]	A1AUL	C18-N16-C15	-8.61	121.47	130.34
3	A	702	FAD	C5A-C4A-N3A	-5.09	119.71	126.72
3	A	702	FAD	N3A-C2A-N1A	-5.00	121.01	128.58
5	A	704[A]	A1AUL	C18-N23-C22	4.62	120.28	115.00
5	A	704[B]	A1AUL	C18-N23-C22	4.34	119.96	115.00
3	A	702	FAD	O2'-C2'-C3'	4.05	118.72	109.25
5	A	704[A]	A1AUL	N23-C18-N19	-3.95	119.79	126.26
7	A	706	NHE	O2-S-O1	-3.82	101.39	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	704[B]	A1AUL	N23-C18-N19	-3.80	120.03	126.26
5	A	704[A]	A1AUL	C21-C22-N23	-3.73	119.80	124.16
3	A	702	FAD	C2A-N3A-C4A	3.70	120.88	111.83
3	A	702	FAD	C4A-C5A-N7A	-3.60	106.46	110.58
3	A	702	FAD	N3A-C4A-N9A	3.60	133.29	127.17
3	A	702	FAD	N9A-C8A-N7A	-3.60	108.83	113.94
5	A	704[B]	A1AUL	C21-C22-N23	-3.56	120.00	124.16
5	A	704[A]	A1AUL	O13-S11-C06	3.54	113.52	107.68
3	A	702	FAD	C5A-N7A-C8A	3.51	108.96	103.45
5	A	704[A]	A1AUL	N12-C15-N16	3.38	120.24	114.87
3	A	702	FAD	C1'-C2'-C3'	3.32	118.66	109.66
4	A	703	AUJ	C6-N1-C2	3.24	121.40	116.07
5	A	704[B]	A1AUL	C06-S11-N12	3.22	109.96	105.96
7	A	706	NHE	O1-S-C2	3.16	111.51	106.73
7	A	706	NHE	O2-S-C2	3.11	111.42	106.73
3	A	702	FAD	C4A-N9A-C8A	2.86	108.75	105.74
4	A	703	AUJ	CAO-CAZ-SAU	2.86	125.43	119.29
3	A	702	FAD	C4-N3-C2	-2.80	120.67	125.64
4	A	703	AUJ	SAU-CBA-NBB	-2.71	109.58	112.24
5	A	704[B]	A1AUL	N12-C15-N16	2.70	119.17	114.87
3	A	702	FAD	C4X-C10-N10	2.69	120.33	116.48
4	A	703	AUJ	C5-C6-N1	-2.65	119.53	123.83
5	A	704[A]	A1AUL	O07-C01-C06	2.64	120.80	116.70
4	A	703	AUJ	N1-C2-N3	-2.61	121.18	125.53
4	A	703	AUJ	OAI-PBD-OAF	-2.53	100.98	110.83
4	A	703	AUJ	OAK-PBE-OAG	-2.51	100.75	112.44
3	A	702	FAD	C4-C4X-N5	2.50	121.66	118.21
3	A	702	FAD	C4X-C4-N3	2.46	119.52	113.25
5	A	704[B]	A1AUL	O13-S11-C06	2.42	111.67	107.68
4	A	703	AUJ	CAB-CAX-CAZ	-2.37	121.69	127.75
3	A	702	FAD	O4-C4-C4X	-2.34	120.36	126.53
5	A	704[B]	A1AUL	O07-C01-C06	2.29	120.25	116.70
5	A	704[A]	A1AUL	O17-C15-N16	-2.28	119.59	123.64
7	A	706	NHE	C1-N-C1'	-2.28	109.80	114.18
4	A	703	AUJ	NAD-C4-N3	2.27	120.09	117.03
3	A	702	FAD	C4'-C3'-C2'	-2.26	109.81	113.57
5	A	704[A]	A1AUL	O14-S11-C06	2.26	111.41	107.68
4	A	703	AUJ	OAI-PBD-OAT	2.24	112.16	104.64
5	A	704[B]	A1AUL	C24-C20-N19	2.22	119.91	116.56
5	A	704[A]	A1AUL	C18-N19-C20	2.19	120.23	115.98
3	A	702	FAD	C9A-N10-C10	-2.19	117.41	120.75
4	A	703	AUJ	CAO-CAZ-CAX	-2.18	122.70	128.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	FAD	O2'-C2'-C1'	2.17	119.12	110.20
5	A	704[B]	A1AUL	C18-N19-C20	2.16	120.17	115.98
4	A	703	AUJ	C6-C5-C4	2.15	118.19	115.55
5	A	704[B]	A1AUL	C26-O25-C22	-2.14	114.14	117.33
5	A	704[A]	A1AUL	C26-O25-C22	-2.10	114.21	117.33
7	A	706	NHE	O3-S-C2	2.09	110.09	106.00
5	A	704[A]	A1AUL	O07-C01-C02	-2.08	119.40	123.95
4	A	703	AUJ	CAA-C2-N1	2.08	119.41	117.20
3	A	702	FAD	C10-C4X-N5	-2.08	120.57	124.81
5	A	704[B]	A1AUL	O14-S11-C06	2.02	111.02	107.68
3	A	702	FAD	C5X-C9A-N10	2.01	119.78	117.97

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	FAD	O2'-C2'-C3'-O3'
3	A	702	FAD	C3'-C4'-C5'-O5'
3	A	702	FAD	O4'-C4'-C5'-O5'
4	A	703	AUJ	PBE-OAT-PBD-OAI
4	A	703	AUJ	SAU-CBA-CBC-CAC
5	A	704[A]	A1AUL	N19-C18-N16-C15
5	A	704[A]	A1AUL	C06-C01-O07-C08
5	A	704[A]	A1AUL	C01-C06-S11-O14
5	A	704[A]	A1AUL	C01-C06-S11-N12
5	A	704[A]	A1AUL	C01-C06-S11-O13
5	A	704[A]	A1AUL	O07-C08-C09-CL10
5	A	704[B]	A1AUL	N19-C18-N16-C15
5	A	704[B]	A1AUL	N23-C18-N16-C15
5	A	704[B]	A1AUL	N23-C22-O25-C26
5	A	704[B]	A1AUL	C01-C06-S11-O14
5	A	704[B]	A1AUL	C01-C06-S11-N12
5	A	704[B]	A1AUL	C01-C06-S11-O13
5	A	704[B]	A1AUL	C05-C06-S11-N12
7	A	706	NHE	N-C1-C2-S
7	A	706	NHE	C1-C2-S-O1
7	A	706	NHE	C1-C2-S-O3
5	A	704[B]	A1AUL	C05-C06-S11-O14
5	A	704[B]	A1AUL	C21-C22-O25-C26
5	A	704[A]	A1AUL	N23-C22-O25-C26
5	A	704[A]	A1AUL	C15-N12-S11-O13
5	A	704[A]	A1AUL	C21-C22-O25-C26

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Mol	Chain	Res	Type	Atoms
5	A	704[A]	A1AUL	C05-C06-S11-O14
5	A	704[A]	A1AUL	C05-C06-S11-N12
3	A	702	FAD	O2'-C2'-C3'-C4'
5	A	704[A]	A1AUL	N23-C18-N16-C15
7	A	706	NHE	C2-C1-N-C1'
5	A	704[B]	A1AUL	C05-C06-S11-O13
5	A	704[A]	A1AUL	C02-C01-O07-C08
5	A	704[A]	A1AUL	C05-C06-S11-O13
5	A	704[A]	A1AUL	C15-N12-S11-C06
7	A	706	NHE	C1-C2-S-O2
5	A	704[B]	A1AUL	C06-C01-O07-C08
4	A	703	AUJ	OAS-CAN-CAO-CAZ
5	A	704[B]	A1AUL	C02-C01-O07-C08
3	A	702	FAD	N10-C1'-C2'-C3'
4	A	703	AUJ	CAN-OAS-PBE-OAG
4	A	703	AUJ	CAN-OAS-PBE-OAT
4	A	703	AUJ	PBD-OAT-PBE-OAG
5	A	704[B]	A1AUL	C15-N12-S11-O14
3	A	702	FAD	C4B-C5B-O5B-PA
4	A	703	AUJ	PBE-OAT-PBD-OAF
5	A	704[A]	A1AUL	O17-C15-N16-C18
5	A	704[B]	A1AUL	O17-C15-N16-C18
5	A	704[A]	A1AUL	N12-C15-N16-C18
5	A	704[B]	A1AUL	N12-C15-N16-C18
3	A	702	FAD	C2B-C1B-N9A-C8A

There are no ring outliers.

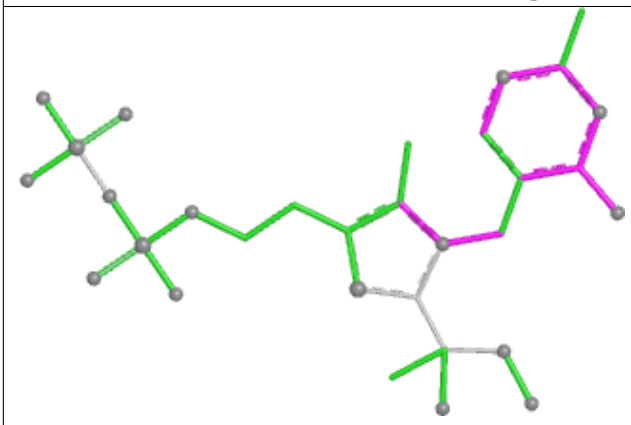
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	AUJ	0	1
5	A	704[B]	A1AUL	1	0
3	A	702	FAD	1	0

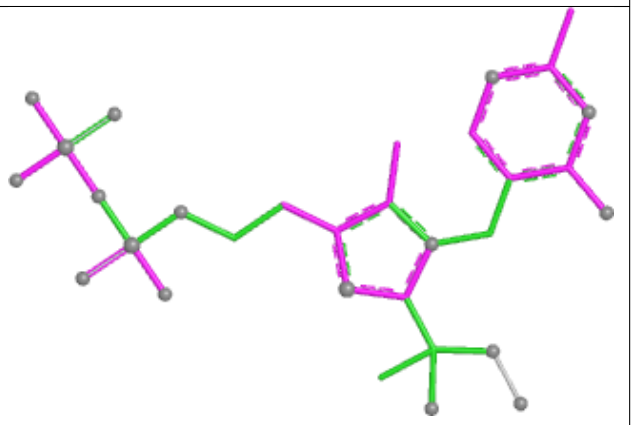
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

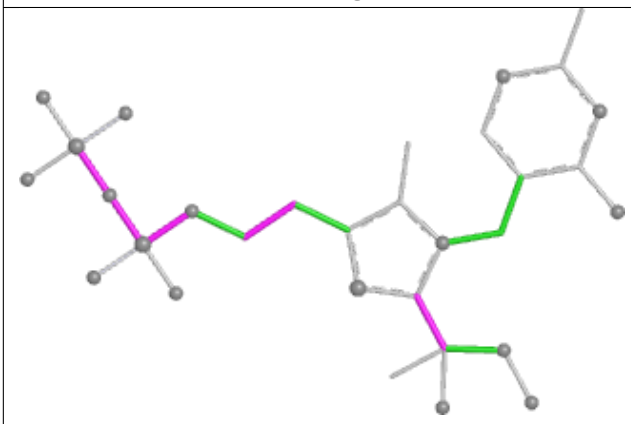
Ligand AUJ A 703



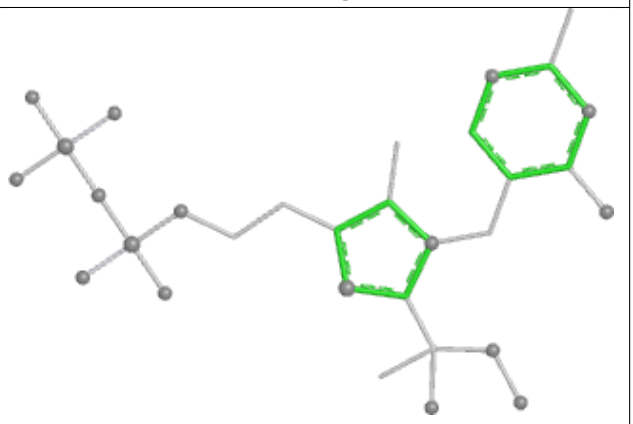
Bond lengths



Bond angles

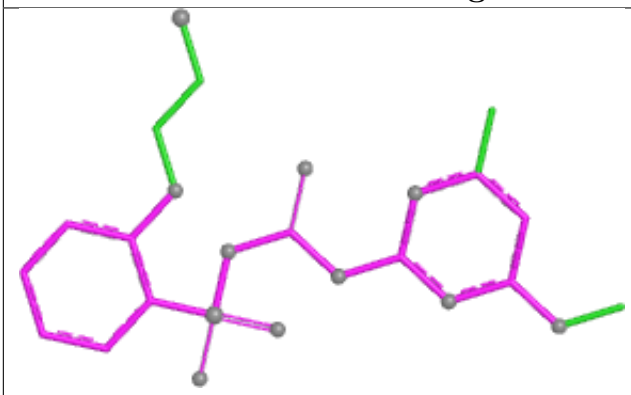


Torsions

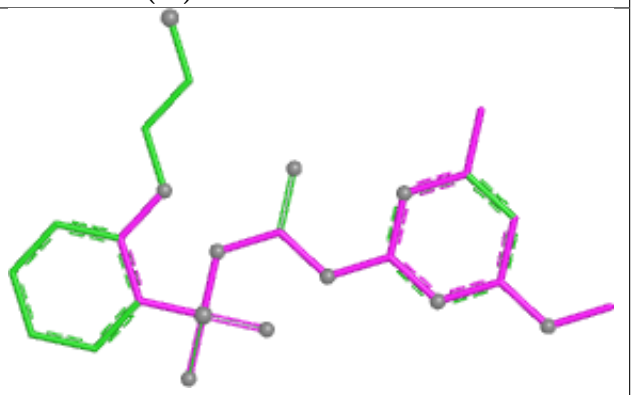


Rings

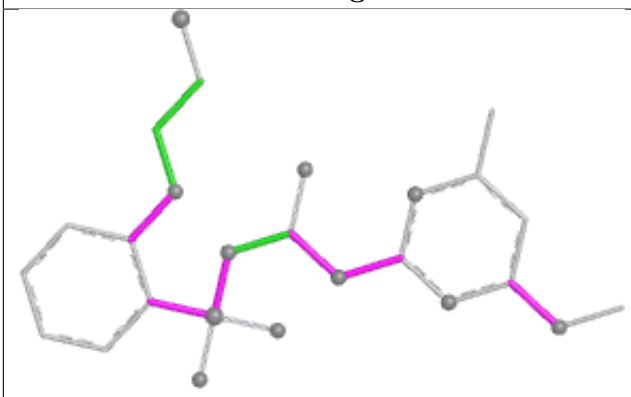
Ligand A1AUL A 704 (B)



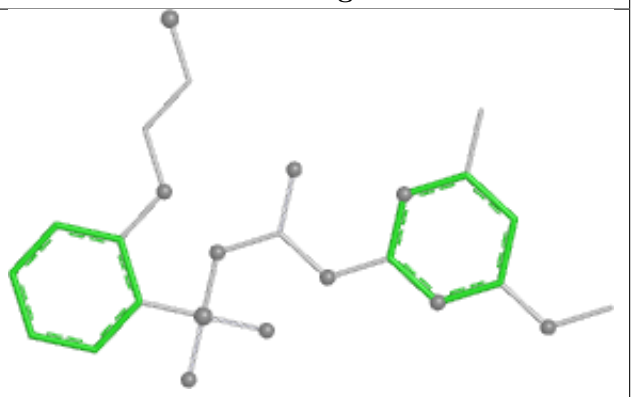
Bond lengths



Bond angles

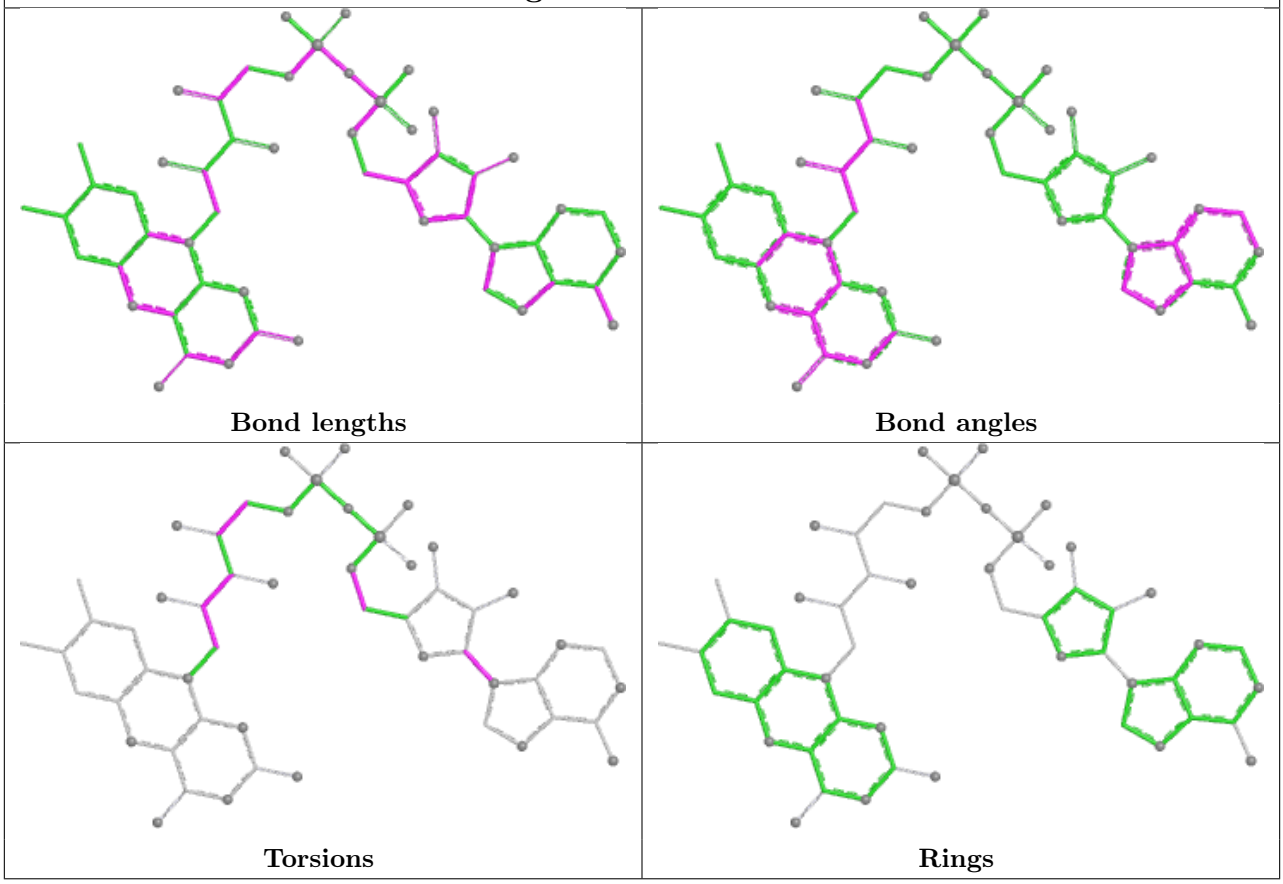


Torsions

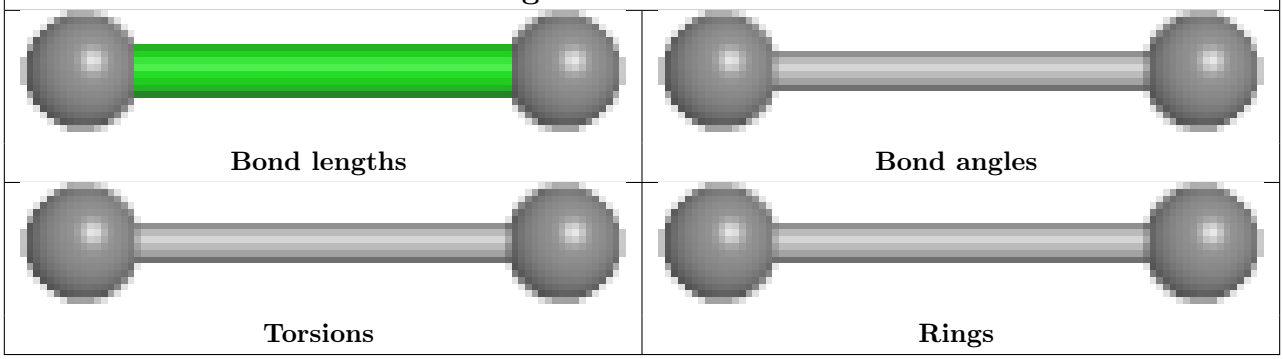


Rings

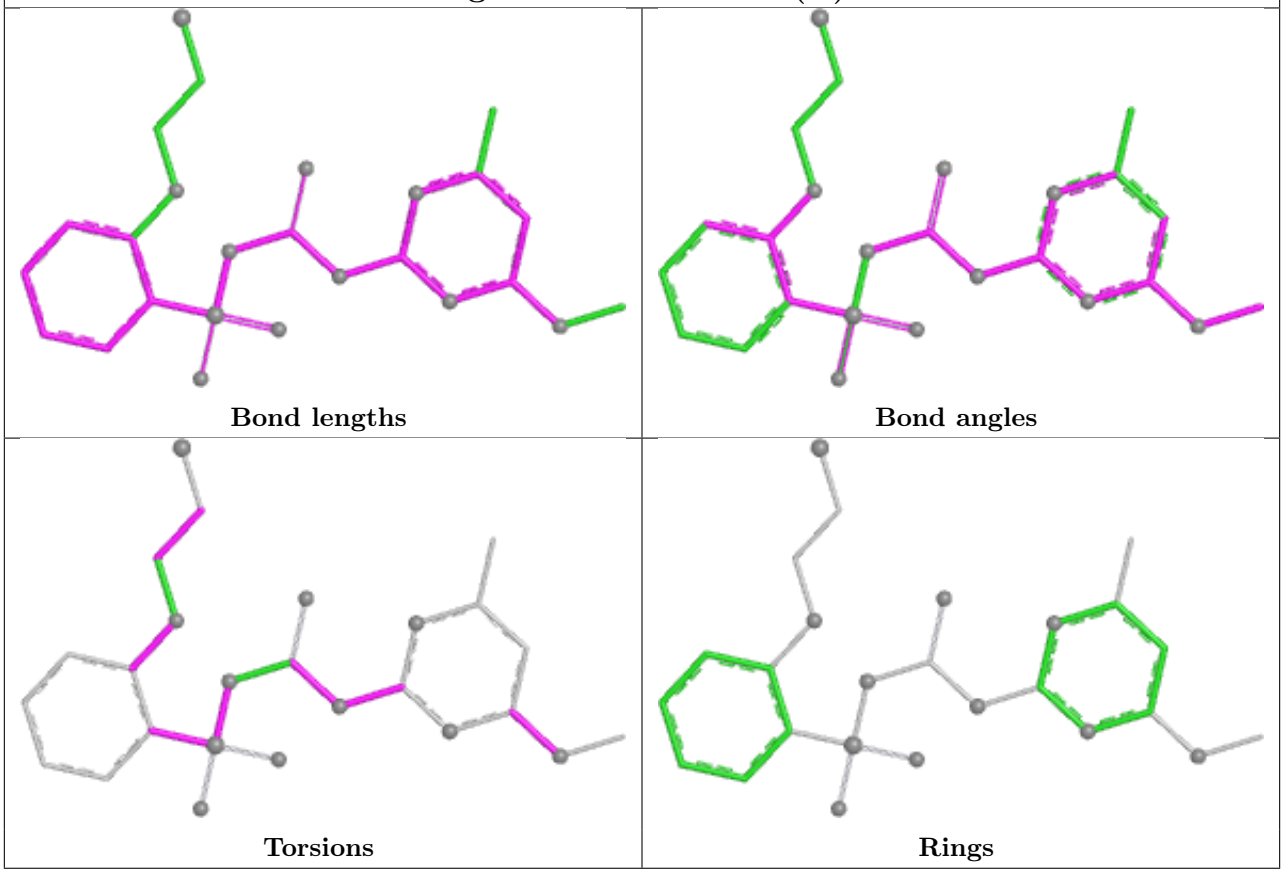
Ligand FAD A 702



Ligand OXY A 707



Ligand A1AUL A 704 (A)



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	581/590 (98%)	-0.13	10 (1%) 69 62	37, 69, 98, 127	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	LYS	2.9
1	A	86	THR	2.8
1	A	291	GLN	2.7
1	A	408	HIS	2.5
1	A	663	GLU	2.4
1	A	341	ASP	2.1
1	A	287	SER	2.1
1	A	207	GLN	2.1
1	A	617	LYS	2.1
1	A	454	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	CSD	A	340	8/9	0.83	0.20	88,98,118,119	0

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

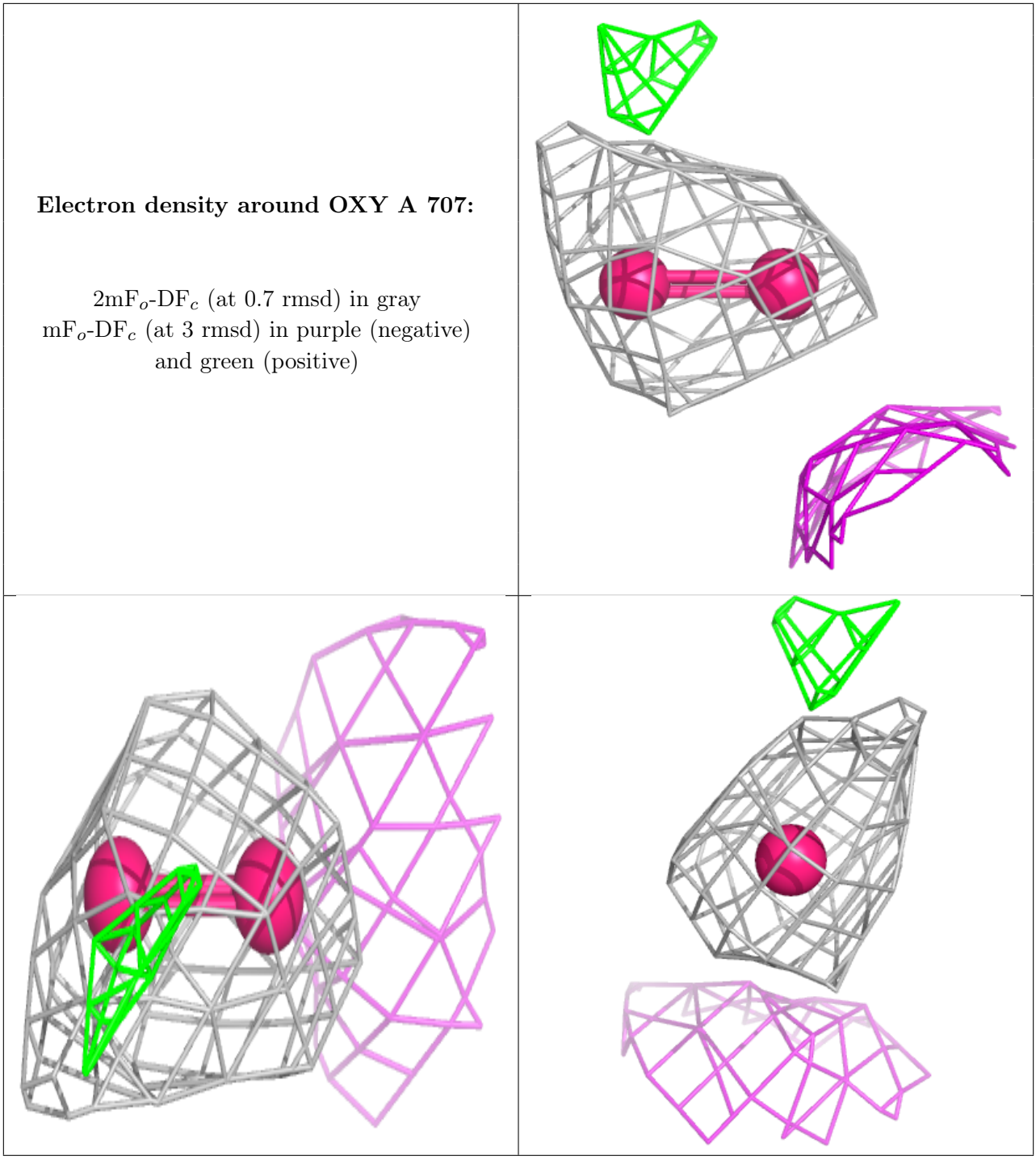
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ACT	A	705	4/4	0.44	0.62	60,75,108,113	0
8	OXY	A	707	2/2	0.65	0.30	105,105,105,107	0
5	A1AUL	A	704[A]	26/26	0.94	0.15	82,94,100,103	26
5	A1AUL	A	704[B]	26/26	0.94	0.15	73,94,100,102	26
7	NHE	A	706	13/13	0.96	0.10	57,70,96,103	0
3	FAD	A	702	53/53	0.96	0.08	48,62,75,80	0
4	AUJ	A	703	31/31	0.98	0.07	52,69,78,110	8
2	MG	A	701	1/1	0.99	0.02	67,67,67,67	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.

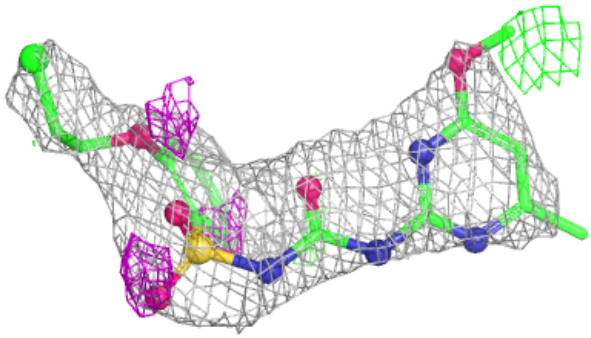
Electron density around OXY A 707:

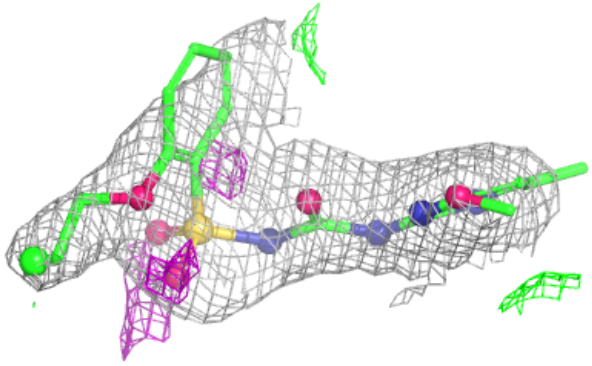
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

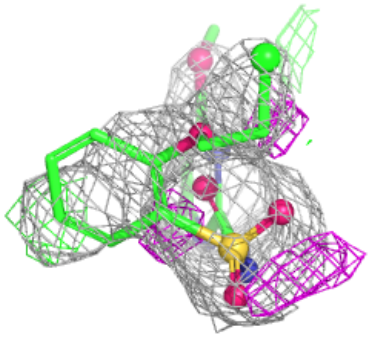


Electron density around A1AUL A 704 (A):

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

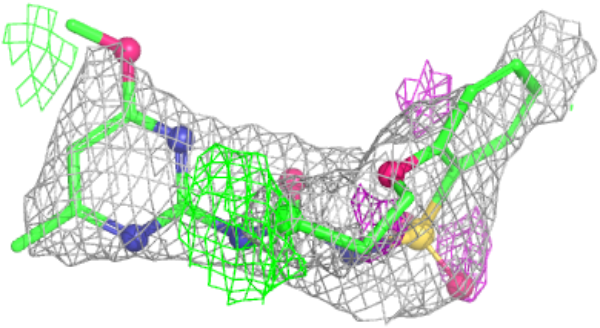


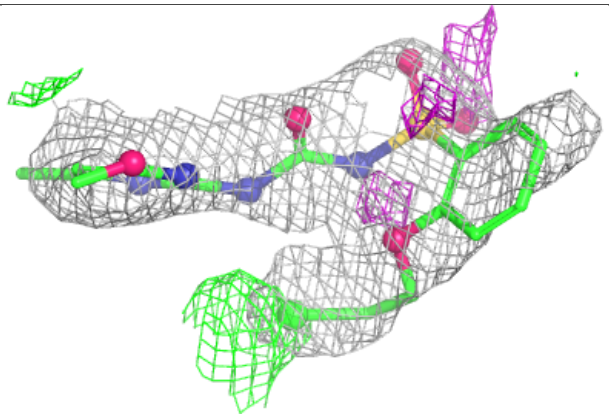


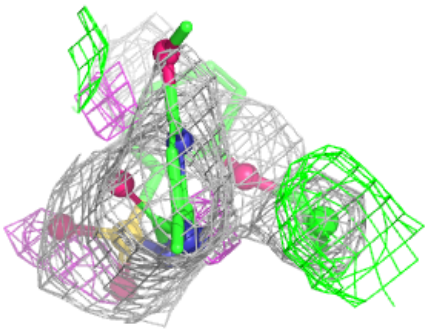


Electron density around A1AUL A 704 (B):

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

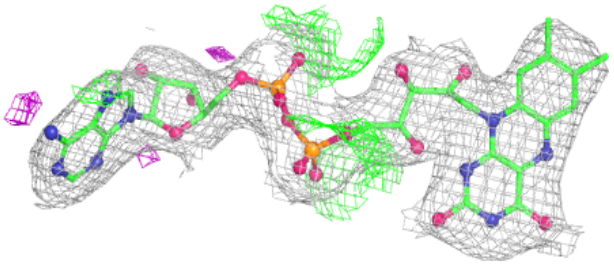


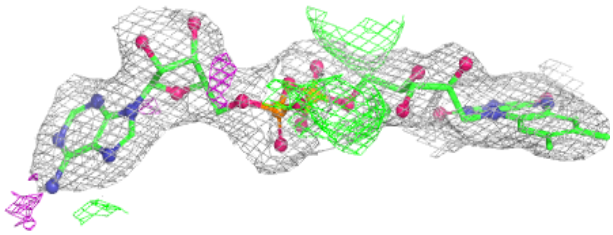


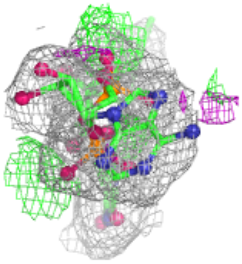


Electron density around FAD A 702:

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

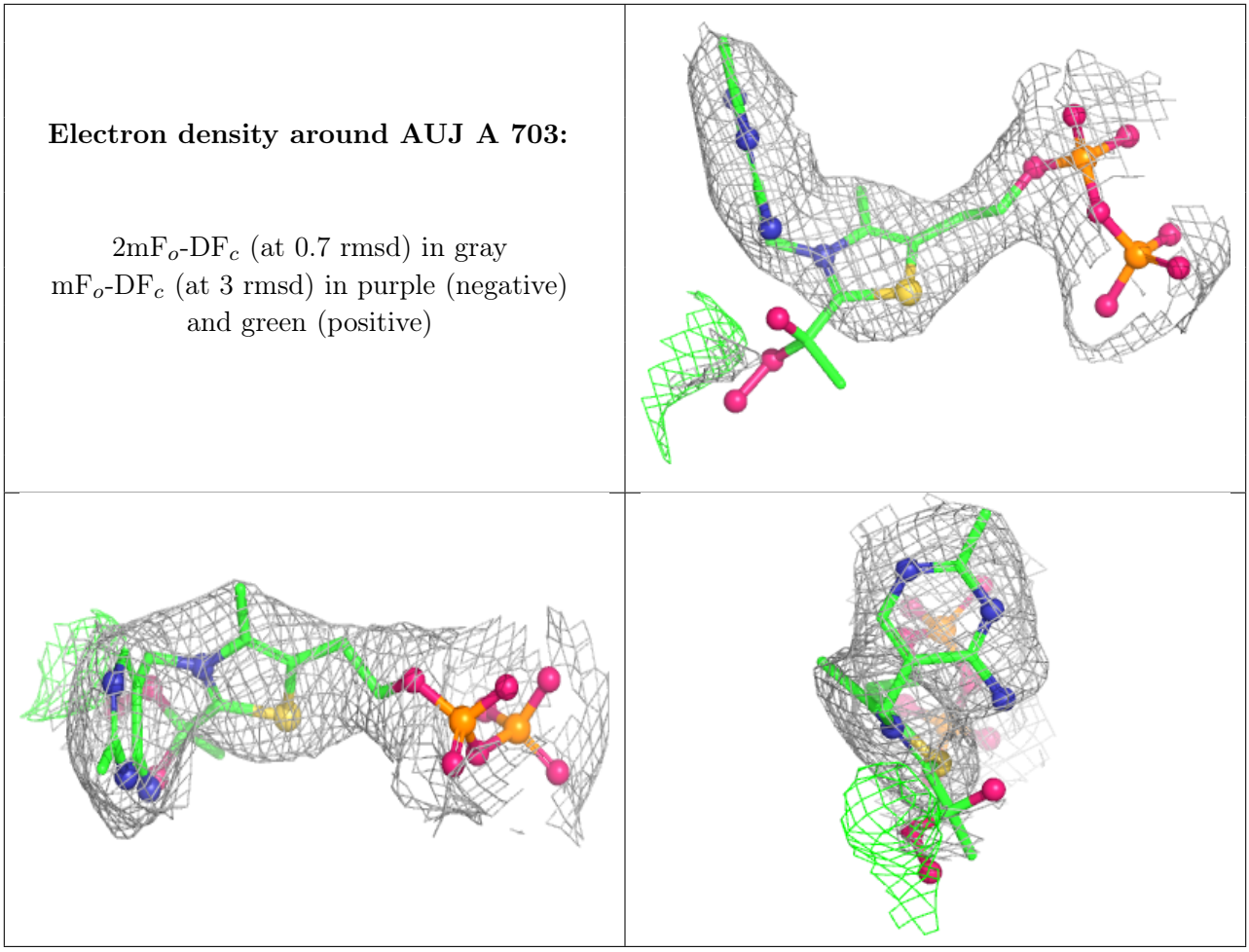






Electron density around AUJ A 703:

$2mF_o$-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.