



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 9C4Q / pdb_00009c4q
Title : Crystal structure of wild-type arabidopsis thaliana acetohydroxyacid synthase
in complex with newly designed herbicide FMO
Authors : Cheng, Y.; Guddat, L.W.
Deposited on : 2024-06-05
Resolution : 2.52 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

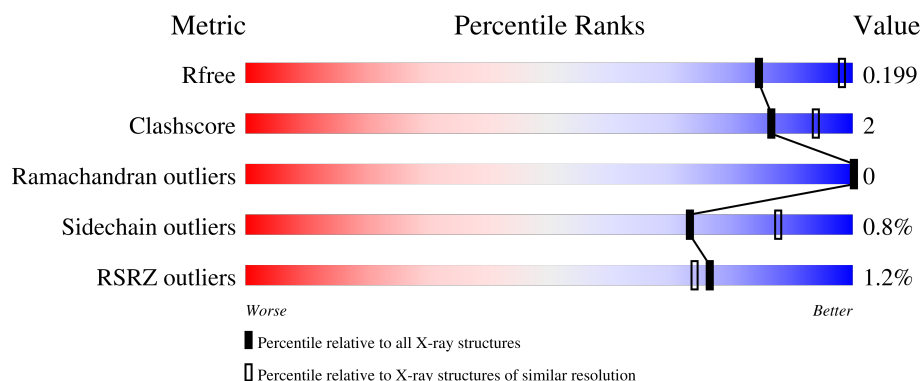
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	590	 93% 6%

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
10	FMT	A	710	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	ACT	A	711	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4789 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
			4456	2828	767	836	25			

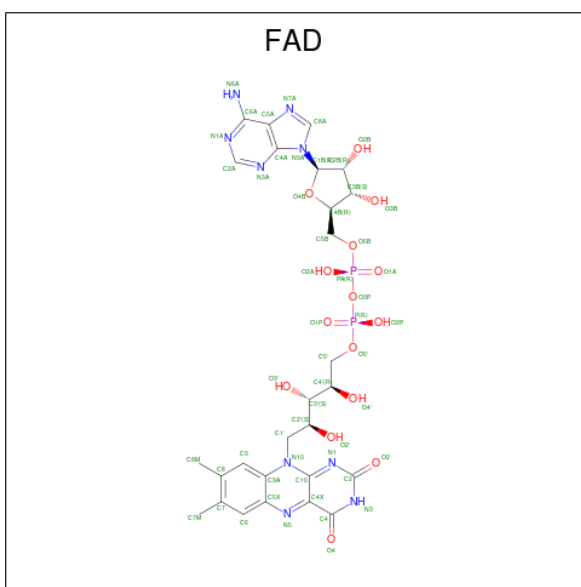
There are 8 discrepancies between the modelled and reference sequences:

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).

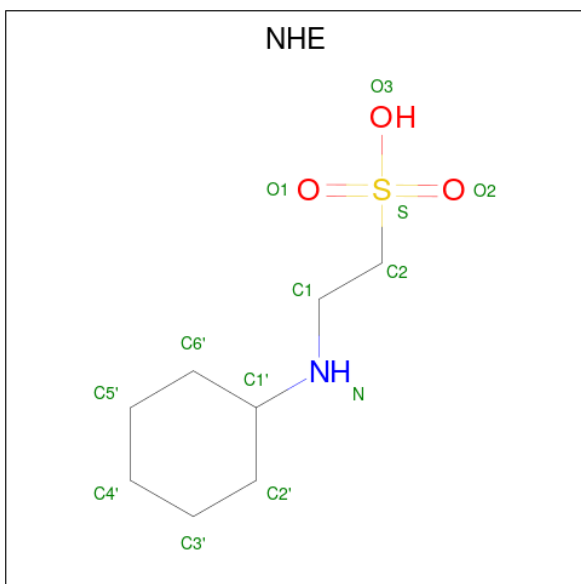
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



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

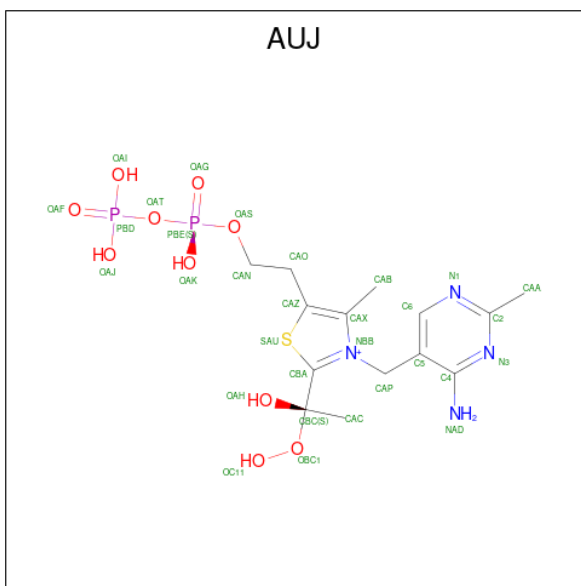
- Molecule 4 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



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

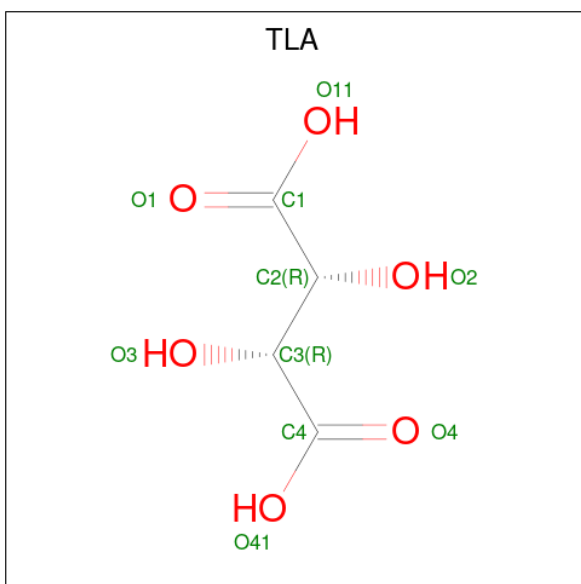
- Molecule 5 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID:

AUJ) (formula: $C_{14}H_{23}N_4O_{10}P_2S$) (labeled as "Ligand of Interest" by depositor).



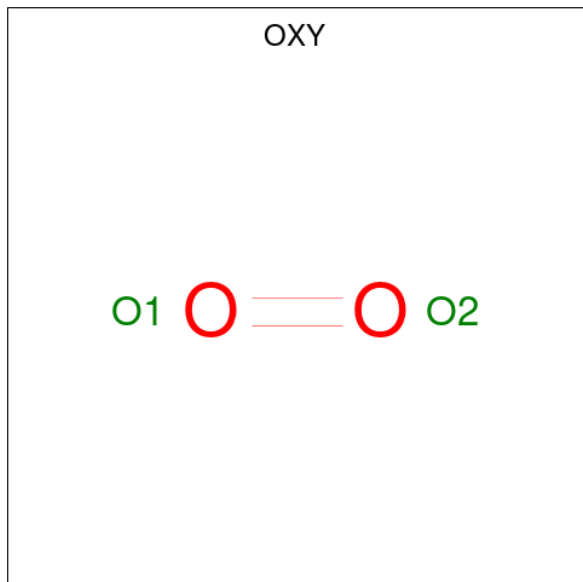
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	14	4	10	2	1		

- Molecule 6 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$) (labeled as "Ligand of Interest" by depositor).



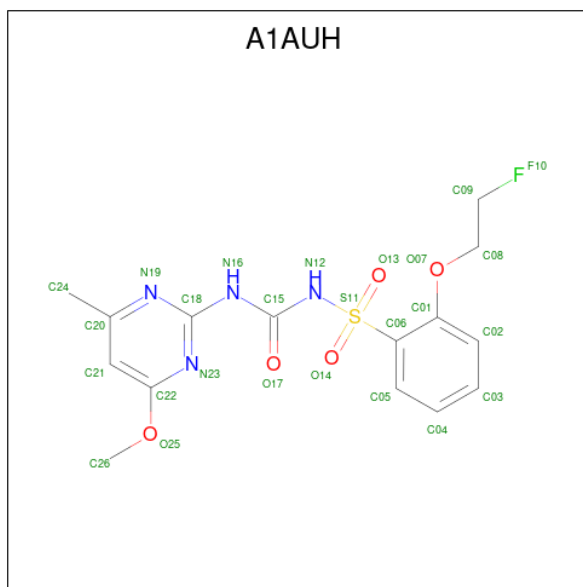
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 7 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂) (labeled as "Ligand of Interest" by depositor).



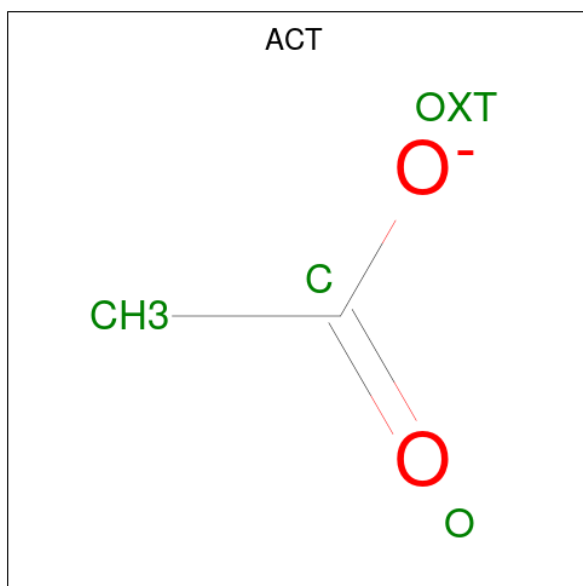
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0

- Molecule 8 is 2-(2-fluoroethoxy)-N-[(4-methoxy-6-methylpyrimidin-2-yl)carbamoyl]benzene-1-sulfonamide (CCD ID: A1AUH) (formula: C₁₅H₁₇FN₄O₅S) (labeled as "Ligand of Interest" by depositor).



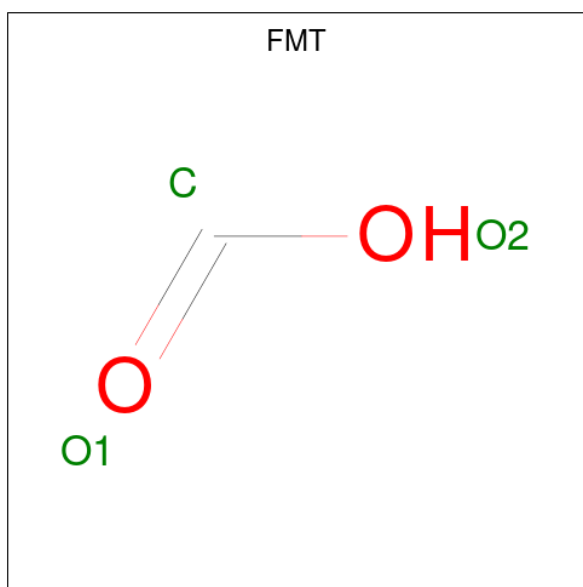
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	F	N	O	S	
			26	15	1	4	5	1	
								0	0

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



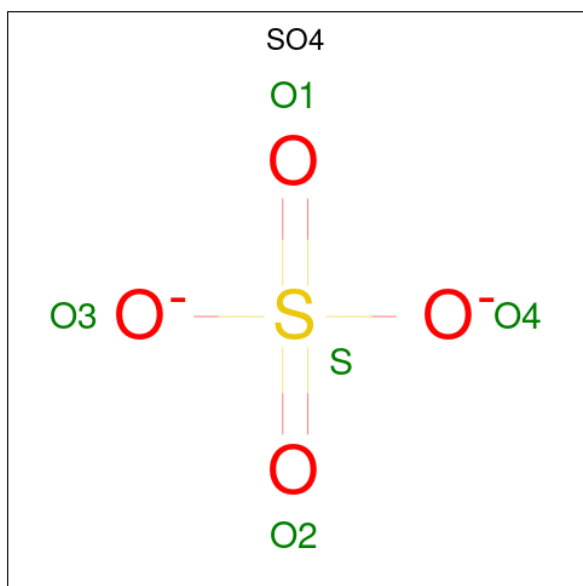
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O		
			4	2	2	0	0
9	A	1	Total	C	O		
			4	2	2	0	0
9	A	1	Total	C	O		
			4	2	2	0	0

- Molecule 10 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			3	1	2		

- Molecule 11 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

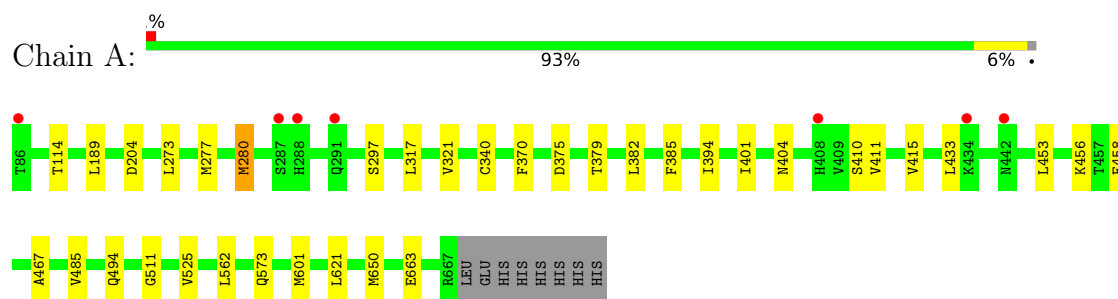
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	175	Total 175	O 175	0	0

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: Acetolactate synthase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	179.66Å 179.66Å 185.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.40 – 2.52 48.40 – 2.52	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.40-2.52) 99.4 (48.40-2.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.173 , 0.198 0.174 , 0.199	Depositor DCC
R_{free} test set	2000 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	61.5	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4789	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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: TLA, MG, NHE, SO4, OXY, AUJ, CSD, FAD, A1AUH, FMT, ACT

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	0.12	0/4544	0.31	0/6169

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	4456	0	4444	17	0
2	A	3	0	0	0	0
3	A	53	0	31	1	0
4	A	13	0	17	0	0
5	A	31	0	0	1	0
6	A	10	0	4	0	0
7	A	2	0	0	0	0
8	A	26	0	0	0	0
9	A	12	0	9	1	0
10	A	3	0	2	0	0
11	A	5	0	0	0	0
12	A	175	0	0	0	0
All	All	4789	0	4507	19	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 (19) 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:573:GLN:HE21	1:A:650:MET:HE2	1.64	0.62
1:A:467:ALA:HA	1:A:621:LEU:HD21	1.87	0.57
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.89	0.55
1:A:273:LEU:HB2	1:A:277:MET:HE2	1.90	0.53
1:A:485:VAL:HG21	1:A:511:GLY:C	2.39	0.47
1:A:562:LEU:HD21	1:A:601:MET:HG3	1.96	0.46
5:A:704:AUJ:NAD	5:A:704:AUJ:OAH	2.49	0.46
1:A:204:ASP:HA	9:A:708:ACT:H1	1.98	0.45
1:A:401:ILE:HG21	1:A:410:SER:HB2	1.98	0.45
3:A:702:FAD:H1'1	3:A:702:FAD:H9	1.71	0.43
1:A:277:MET:HA	1:A:280:MET:HG3	2.01	0.43
1:A:394:ILE:HG12	1:A:411:VAL:HB	2.01	0.42
1:A:456:LYS:HD3	1:A:458:PHE:CZ	2.54	0.42
1:A:379:THR:HA	1:A:385:PHE:CD1	2.55	0.42
1:A:453:LEU:HD13	1:A:494:GLN:HB3	2.02	0.42
1:A:317:LEU:O	1:A:321:VAL:HG23	2.20	0.41
1:A:382:LEU:HD11	1:A:404:ASN:HB3	2.02	0.41
1:A:297:SER:HB3	1:A:433:LEU:HD22	2.03	0.40
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/590 (98%)	572 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	476/486 (98%)	472 (99%)	4 (1%)	73 88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LEU
1	A	280	MET
1	A	375	ASP
1	A	663	GLU

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	447	GLN
1	A	527	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	7.77	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	-	0/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	CSD	OD1-SG-CB	7.77	119.91	105.60

There are no chirality outliers.

There are no torsion outliers.

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 14 ligands modelled in this entry, 3 are monoatomic - 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	$\# Z > 2$
11	SO4	A	714	-	4,4,4	0.23	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	A1AUH	A	707	-	27,27,27	5.52	10 (37%)	37,37,37	2.61	8 (21%)
7	OXY	A	706	-	1,1,1	0.09	0	-		
5	AUJ	A	704	2	27,32,32	2.26	8 (29%)	36,49,49	1.75	12 (33%)
9	ACT	A	709	-	3,3,3	0.95	0	3,3,3	0.86	0
9	ACT	A	711	-	3,3,3	0.96	0	3,3,3	0.89	0
3	FAD	A	702	-	58,58,58	3.00	24 (41%)	85,89,89	1.69	19 (22%)
10	FMT	A	710	-	2,2,2	2.84	2 (100%)	1,1,1	1.61	0
4	NHE	A	703	-	13,13,13	1.36	3 (23%)	16,17,17	1.90	7 (43%)
6	TLA	A	705	-	9,9,9	1.03	0	12,12,12	1.28	2 (16%)
9	ACT	A	708	-	3,3,3	0.94	0	3,3,3	0.84	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
8	A1AUH	A	707	-	-	7/21/21/21	0/2/2/2
5	AUJ	A	704	2	-	6/20/26/26	0/2/2/2
3	FAD	A	702	-	-	10/34/50/50	0/6/6/6
4	NHE	A	703	-	-	0/7/15/15	0/1/1/1
6	TLA	A	705	-	-	10/12/12/12	-

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	707	A1AUH	O13-S11	19.02	1.65	1.43
8	A	707	A1AUH	O14-S11	18.96	1.65	1.43
3	A	702	FAD	O4-C4	9.30	1.41	1.23
3	A	702	FAD	PA-O3P	9.20	1.69	1.59
3	A	702	FAD	P-O3P	8.84	1.69	1.59
3	A	702	FAD	O2-C2	7.96	1.40	1.24
5	A	704	AUJ	C5-C4	5.43	1.51	1.42
8	A	707	A1AUH	C18-N16	5.07	1.45	1.38
5	A	704	AUJ	CAP-NBB	-4.95	1.42	1.47
5	A	704	AUJ	C2-N3	4.84	1.42	1.34
3	A	702	FAD	C6A-N6A	4.55	1.45	1.34
3	A	702	FAD	O4B-C1B	-4.32	1.32	1.42
3	A	702	FAD	C2B-C1B	4.06	1.66	1.53
5	A	704	AUJ	C6-N1	3.98	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	707	A1AUH	C15-N16	3.84	1.45	1.37
3	A	702	FAD	C5B-C4B	-3.68	1.40	1.51
8	A	707	A1AUH	O25-C22	3.32	1.40	1.35
10	A	710	FMT	O1-C	3.31	1.40	1.22
3	A	702	FAD	C9A-N10	-3.24	1.35	1.41
5	A	704	AUJ	C4-NAD	3.21	1.42	1.34
3	A	702	FAD	C4-N3	-3.18	1.32	1.38
8	A	707	A1AUH	C06-S11	3.18	1.82	1.77
4	A	703	NHE	C2-S	3.16	1.82	1.77
3	A	702	FAD	O4B-C4B	3.07	1.51	1.45
3	A	702	FAD	O3B-C3B	3.06	1.50	1.43
5	A	704	AUJ	C4-N3	-2.99	1.31	1.35
8	A	707	A1AUH	S11-N12	2.93	1.71	1.64
8	A	707	A1AUH	C15-N12	2.85	1.45	1.39
3	A	702	FAD	C3B-C4B	2.81	1.60	1.53
3	A	702	FAD	C8A-N9A	-2.80	1.32	1.37
8	A	707	A1AUH	C09-C08	2.74	1.53	1.49
3	A	702	FAD	C5'-C4'	2.65	1.55	1.51
3	A	702	FAD	C2-N3	-2.59	1.33	1.39
3	A	702	FAD	C1'-C2'	2.47	1.56	1.52
3	A	702	FAD	PA-O5B	2.44	1.68	1.59
3	A	702	FAD	C5A-N7A	-2.37	1.34	1.39
3	A	702	FAD	P-O5'	2.35	1.68	1.59
10	A	710	FMT	O2-C	2.28	1.40	1.28
3	A	702	FAD	C4X-N5	2.26	1.35	1.30
3	A	702	FAD	O4'-C4'	-2.26	1.38	1.43
4	A	703	NHE	O2-S	2.25	1.51	1.45
5	A	704	AUJ	C2-N1	-2.23	1.31	1.34
4	A	703	NHE	O1-S	2.23	1.51	1.45
5	A	704	AUJ	CAX-NBB	2.23	1.43	1.40
3	A	702	FAD	O2B-C2B	2.11	1.48	1.43
3	A	702	FAD	C5X-N5	-2.08	1.35	1.39
8	A	707	A1AUH	O17-C15	-2.04	1.19	1.23

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	707	A1AUH	O13-S11-O14	-9.88	107.52	119.52
8	A	707	A1AUH	C18-N23-C22	5.78	121.60	115.00
8	A	707	A1AUH	C18-N16-C15	-5.37	124.81	130.34
3	A	702	FAD	N3A-C2A-N1A	-5.08	120.89	128.58
8	A	707	A1AUH	C06-S11-N12	5.04	112.22	105.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C5A-C4A-N3A	-4.89	119.99	126.72
8	A	707	A1AUH	C21-C22-N23	-4.40	119.02	124.16
4	A	703	NHE	O2-S-O1	-3.92	101.07	113.82
3	A	702	FAD	C2A-N3A-C4A	3.70	120.88	111.83
3	A	702	FAD	C4A-C5A-N7A	-3.70	106.36	110.58
3	A	702	FAD	N9A-C8A-N7A	-3.66	108.74	113.94
5	A	704	AUJ	C6-N1-C2	3.57	121.94	116.07
3	A	702	FAD	C5A-N7A-C8A	3.53	108.99	103.45
3	A	702	FAD	O2'-C2'-C3'	3.45	117.32	109.25
3	A	702	FAD	N3A-C4A-N9A	3.27	132.74	127.17
5	A	704	AUJ	SAU-CBA-NBB	-3.22	109.08	112.24
8	A	707	A1AUH	N23-C18-N19	-3.04	121.27	126.26
4	A	703	NHE	O1-S-C2	3.02	111.29	106.73
4	A	703	NHE	O2-S-C2	2.99	111.24	106.73
3	A	702	FAD	C4-C4X-N5	2.98	122.32	118.21
3	A	702	FAD	C4X-C10-N10	2.88	120.60	116.48
5	A	704	AUJ	C5-C6-N1	-2.84	119.22	123.83
5	A	704	AUJ	N1-C2-N3	-2.83	120.82	125.53
3	A	702	FAD	C1'-C2'-C3'	2.77	117.18	109.66
3	A	702	FAD	C4A-N9A-C8A	2.76	108.64	105.74
5	A	704	AUJ	CAO-CAZ-SAU	2.71	125.10	119.29
3	A	702	FAD	C4-N3-C2	-2.68	120.88	125.64
5	A	704	AUJ	OAI-PBD-OAF	-2.66	100.46	110.83
3	A	702	FAD	C5'-C4'-C3'	-2.66	107.20	112.22
5	A	704	AUJ	OAK-PBE-OAG	-2.48	100.91	112.44
6	A	705	TLA	O41-C4-C3	2.47	120.16	113.31
3	A	702	FAD	C4X-C4-N3	2.46	119.52	113.25
8	A	707	A1AUH	O07-C01-C06	2.42	120.45	116.70
5	A	704	AUJ	OAI-PBD-OAT	2.42	112.74	104.64
4	A	703	NHE	C1-N-C1'	-2.32	109.71	114.18
6	A	705	TLA	O11-C1-C2	2.31	119.73	113.31
4	A	703	NHE	O3-S-C2	2.30	110.51	106.00
5	A	704	AUJ	NAD-C4-N3	2.25	120.06	117.03
3	A	702	FAD	O4-C4-C4X	-2.23	120.64	126.53
8	A	707	A1AUH	C18-N19-C20	2.22	120.28	115.98
4	A	703	NHE	C3'-C2'-C1'	2.19	115.02	111.09
3	A	702	FAD	C10-C4X-N5	-2.17	120.37	124.81
3	A	702	FAD	C9A-N10-C10	-2.14	117.48	120.75
5	A	704	AUJ	C6-C5-C4	2.10	118.13	115.55
3	A	702	FAD	C6A-C5A-N7A	2.09	136.12	132.09
5	A	704	AUJ	CAO-CAZ-CAX	-2.07	122.99	128.17
5	A	704	AUJ	CAB-CAX-CAZ	-2.04	122.53	127.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	NHE	C6'-C1'-C2'	2.04	114.32	110.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

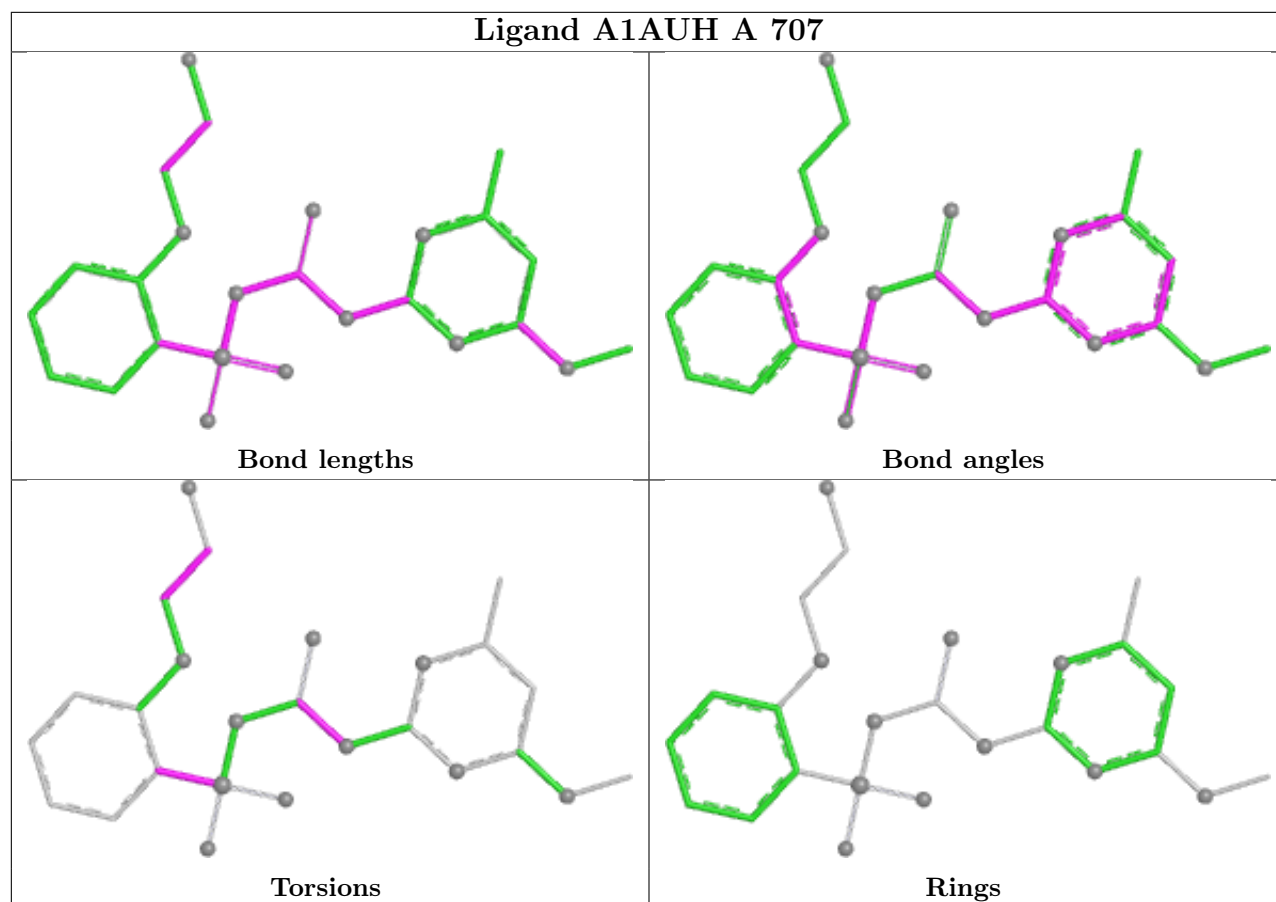
Mol	Chain	Res	Type	Atoms
3	A	702	FAD	C3'-C4'-C5'-O5'
3	A	702	FAD	O4'-C4'-C5'-O5'
3	A	702	FAD	PA-O3P-P-O5'
5	A	704	AUJ	CAN-OAS-PBE-OAG
5	A	704	AUJ	SAU-CBA-CBC-CAC
5	A	704	AUJ	CAC-CBC-OBC1-OC11
6	A	705	TLA	C2-C3-C4-O4
6	A	705	TLA	C2-C3-C4-O41
8	A	707	A1AUH	C01-C06-S11-O14
6	A	705	TLA	O3-C3-C4-O4
6	A	705	TLA	O3-C3-C4-O41
6	A	705	TLA	O1-C1-C2-C3
6	A	705	TLA	O11-C1-C2-C3
6	A	705	TLA	O1-C1-C2-O2
6	A	705	TLA	O11-C1-C2-O2
3	A	702	FAD	O2'-C2'-C3'-O3'
3	A	702	FAD	O2'-C2'-C3'-C4'
8	A	707	A1AUH	C05-C06-S11-O14
8	A	707	A1AUH	C01-C06-S11-N12
6	A	705	TLA	C1-C2-C3-C4
8	A	707	A1AUH	C05-C06-S11-N12
6	A	705	TLA	O2-C2-C3-O3
5	A	704	AUJ	OAS-CAN-CAO-CAZ
3	A	702	FAD	O3'-C3'-C4'-C5'
5	A	704	AUJ	CAN-OAS-PBE-OAT
5	A	704	AUJ	PBE-OAT-PBD-OAF
8	A	707	A1AUH	O07-C08-C09-F10
3	A	702	FAD	C2'-C3'-C4'-O4'
3	A	702	FAD	O3'-C3'-C4'-O4'
3	A	702	FAD	C4B-C5B-O5B-PA
8	A	707	A1AUH	O17-C15-N16-C18
8	A	707	A1AUH	N12-C15-N16-C18
3	A	702	FAD	C2'-C3'-C4'-C5'

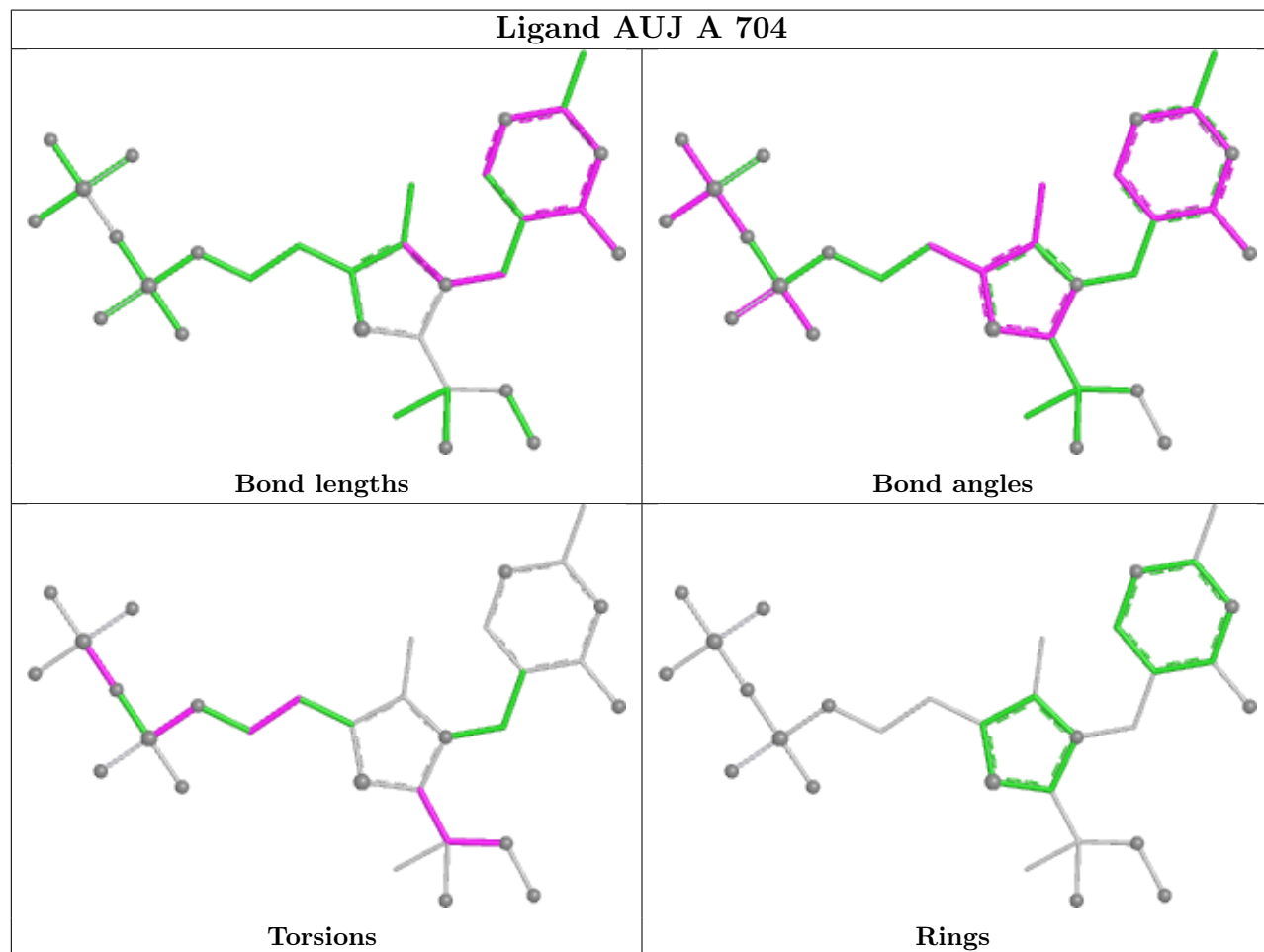
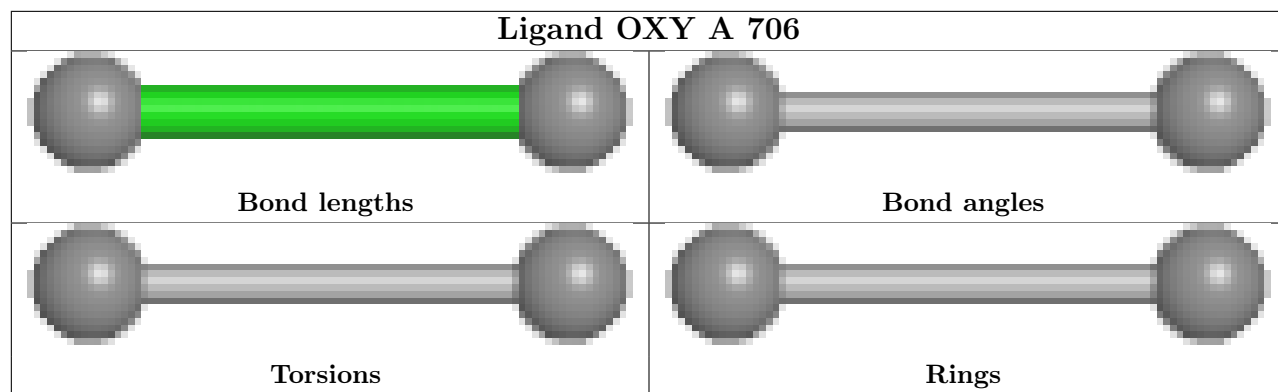
There are no ring outliers.

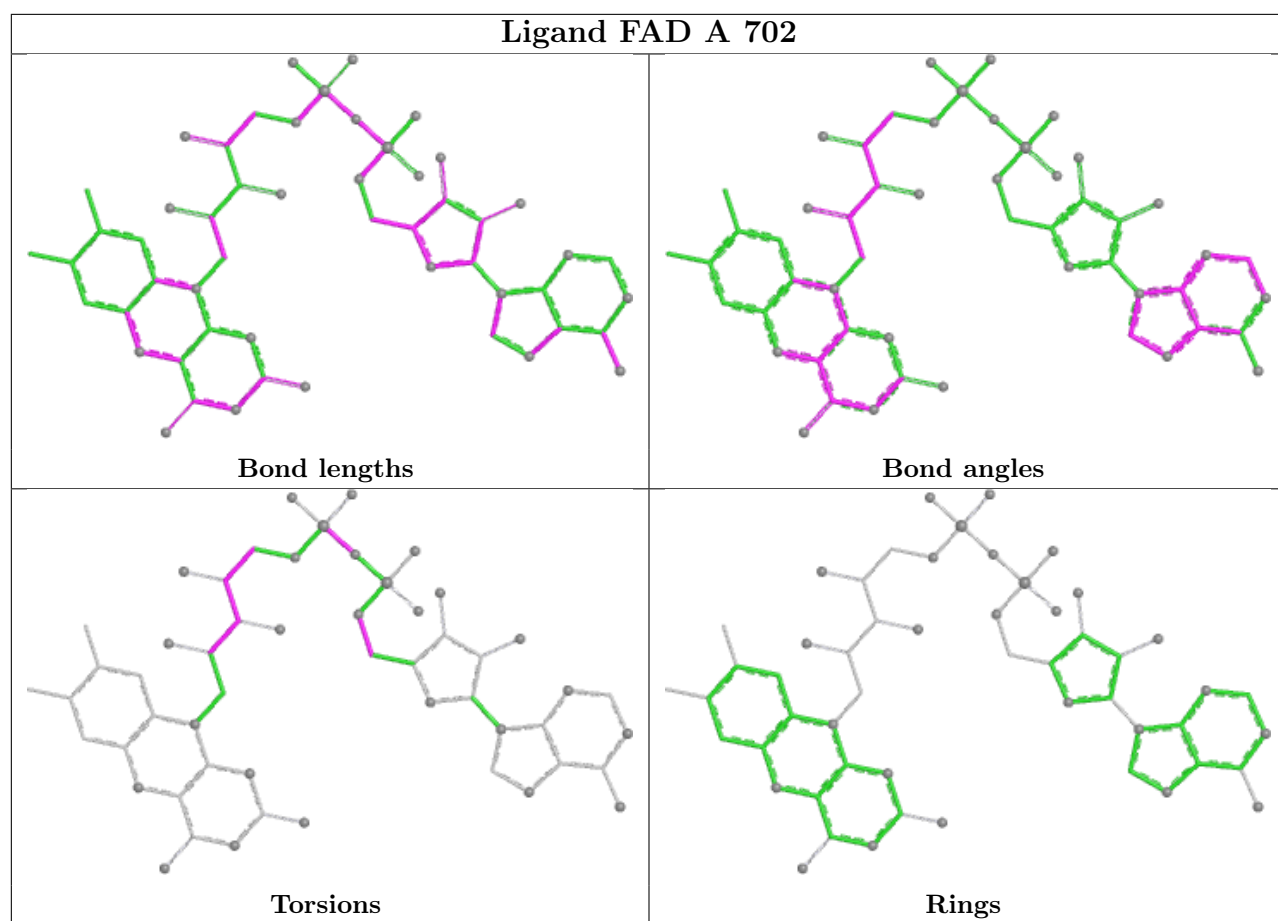
3 monomers are involved in 3 short contacts:

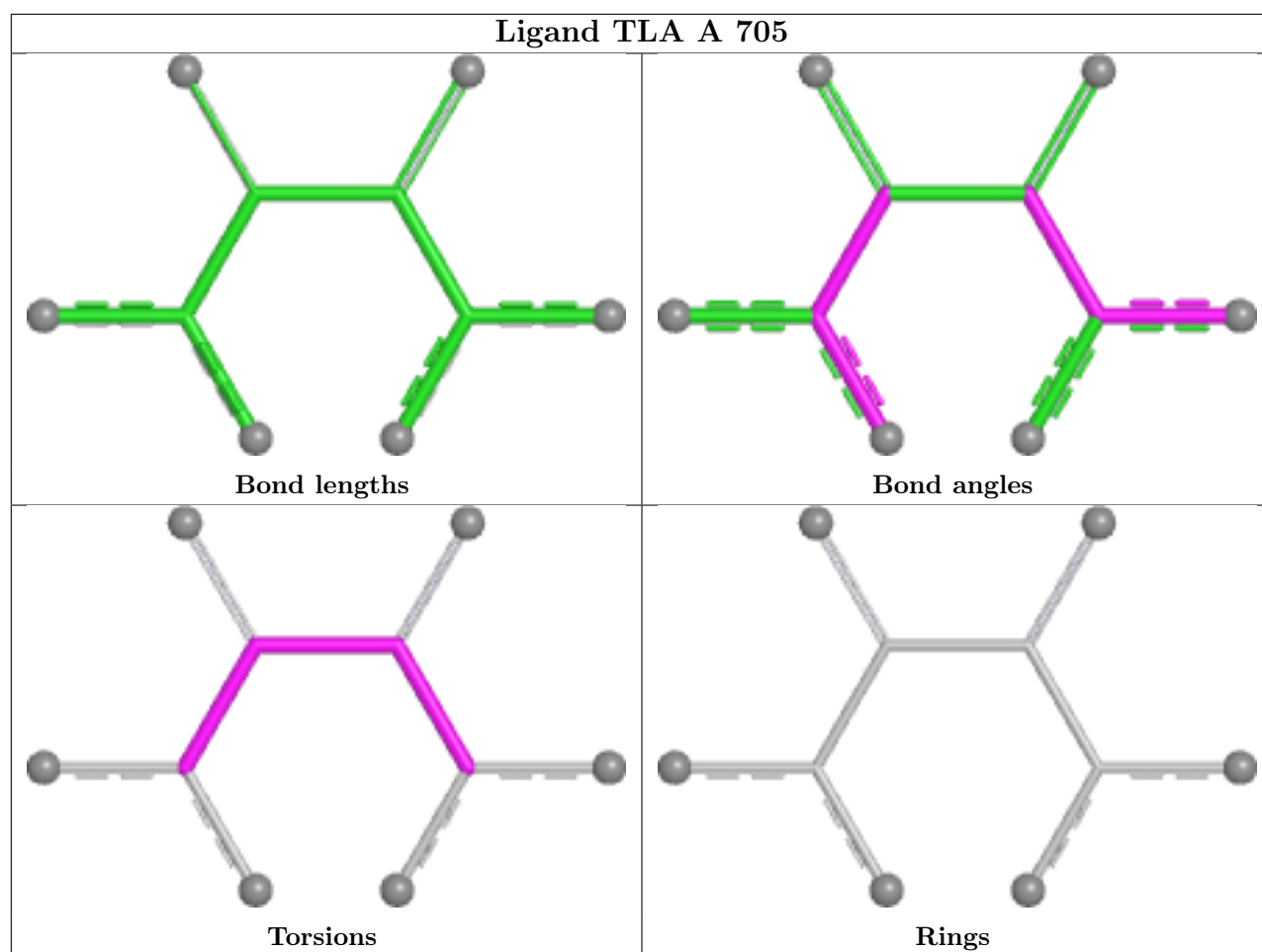
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	AUJ	1	0
3	A	702	FAD	1	0
9	A	708	ACT	1	0

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.









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	581/590 (98%)	-0.11	7 (1%) 76 74	33, 62, 91, 135	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	5.1
1	A	434	LYS	3.0
1	A	408	HIS	2.6
1	A	288	HIS	2.5
1	A	287	SER	2.3
1	A	442	ASN	2.1
1	A	291	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSD	A	340	8/9	0.92	0.17	72,82,98,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

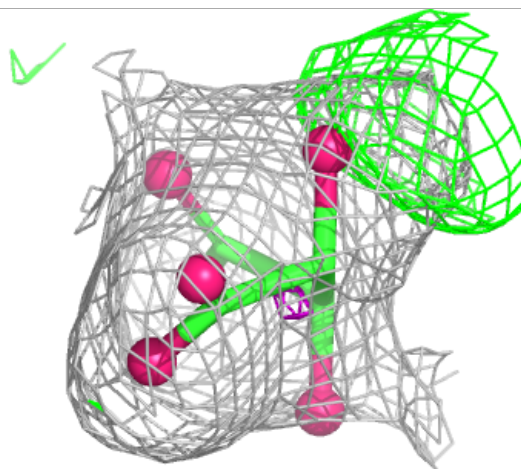
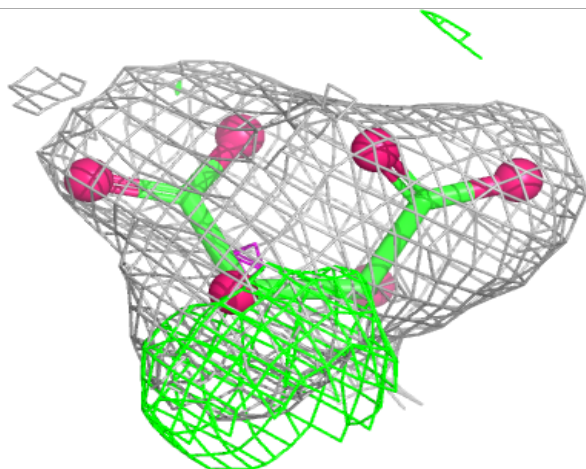
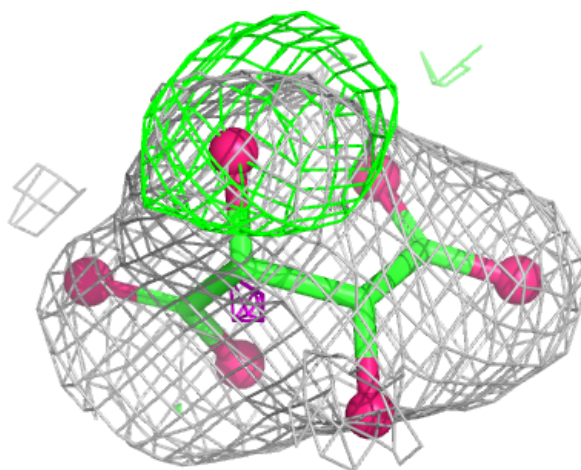
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	ACT	A	709	4/4	0.73	0.38	87,98,102,111	0
10	FMT	A	710	3/3	0.74	0.31	80,80,87,107	0
9	ACT	A	711	4/4	0.75	0.40	81,91,101,102	0
11	SO4	A	714	5/5	0.75	0.21	114,119,127,150	0
9	ACT	A	708	4/4	0.81	0.25	72,86,90,107	0
6	TLA	A	705	10/10	0.82	0.17	77,97,112,114	0
2	MG	A	713	1/1	0.88	0.36	101,101,101,101	1
7	OXY	A	706	2/2	0.95	0.27	42,42,42,77	2
8	A1AUH	A	707	26/26	0.97	0.08	46,62,66,68	4
4	NHE	A	703	13/13	0.97	0.10	57,68,78,84	0
3	FAD	A	702	53/53	0.98	0.07	39,58,67,70	0
5	AUJ	A	704	31/31	0.98	0.09	45,59,81,87	5
2	MG	A	712	1/1	0.99	0.10	84,84,84,84	1
2	MG	A	701	1/1	1.00	0.03	58,58,58,58	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.

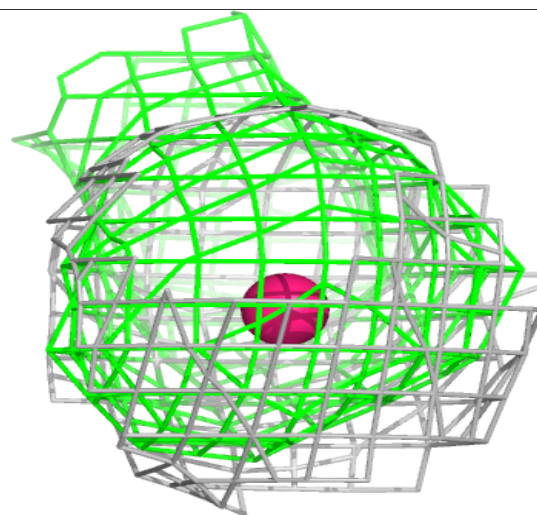
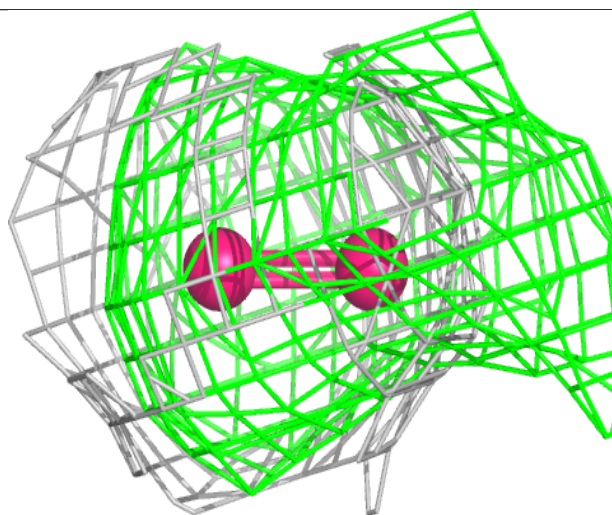
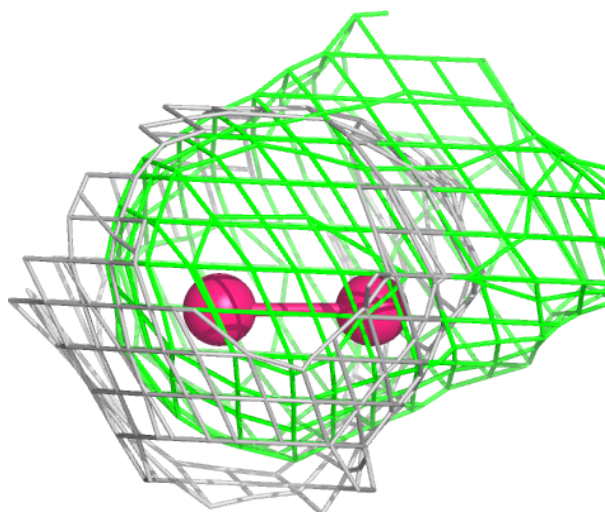
Electron density around TLA A 705:

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



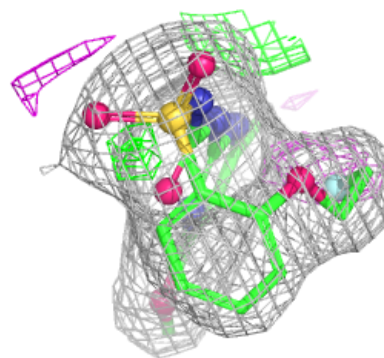
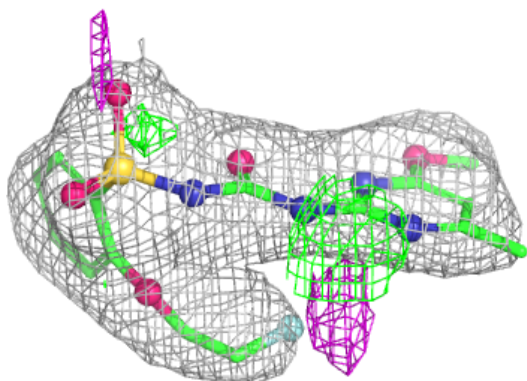
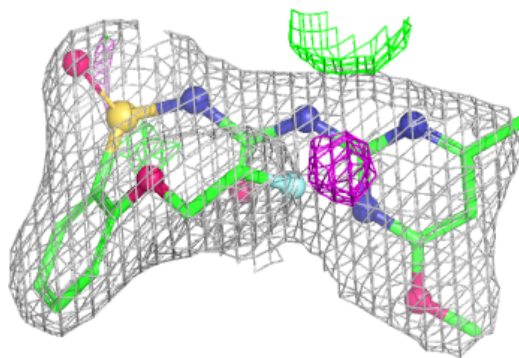
Electron density around OXY A 706:

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

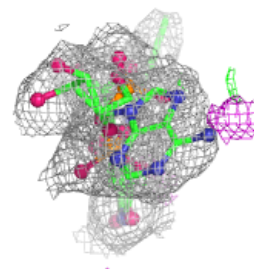
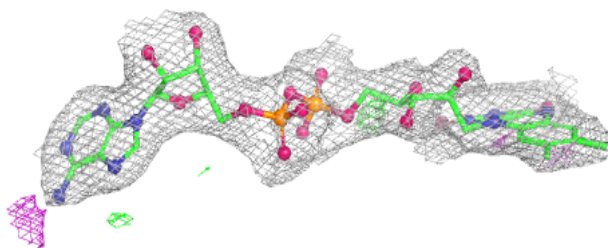
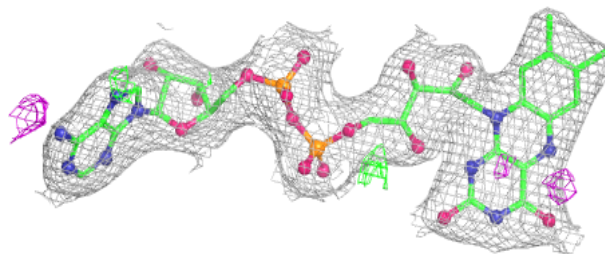


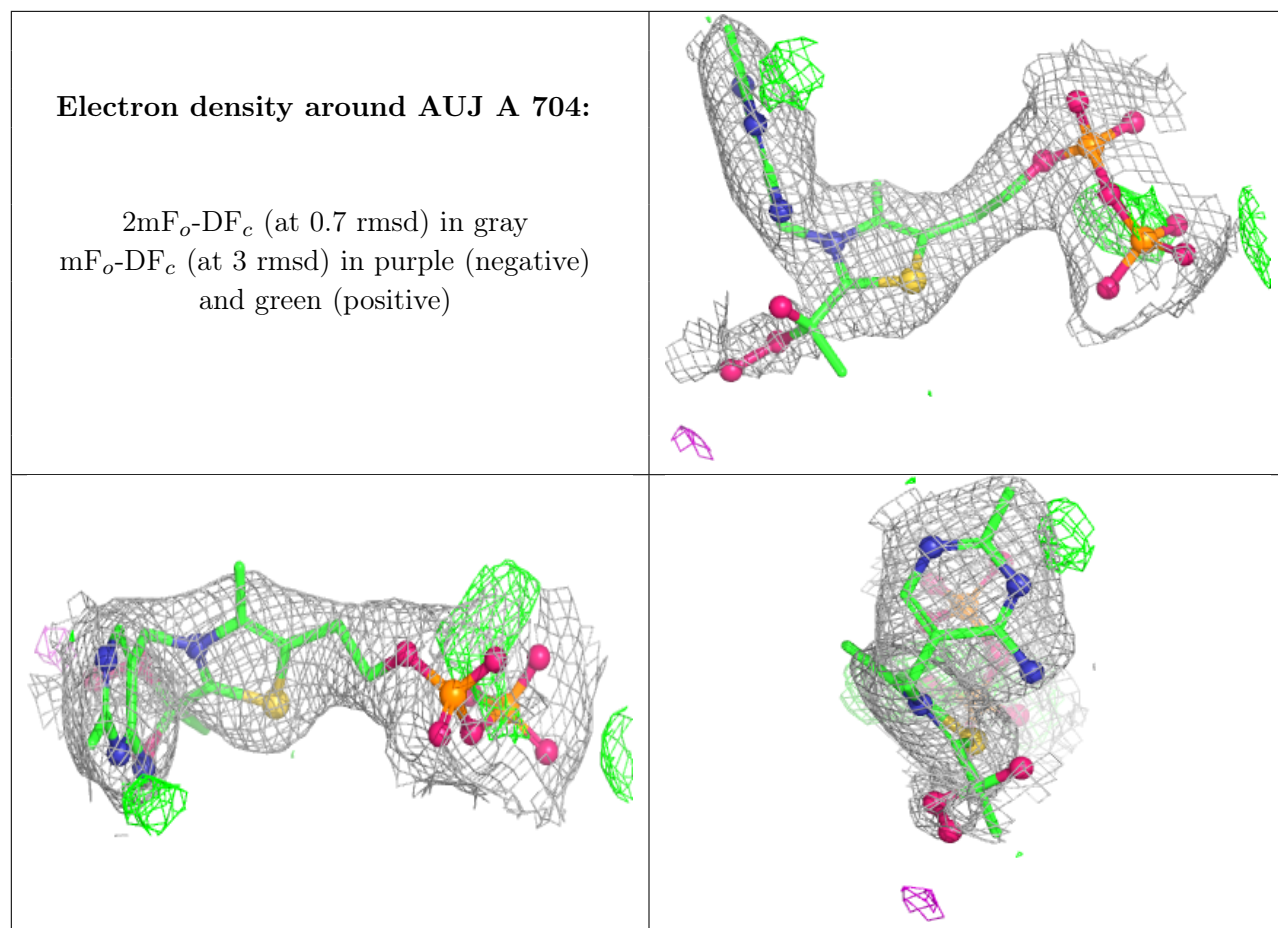
Electron density around A1AUH A 707:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.