



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 04:06 PM EDT

PDB ID : 9C85 / pdb\_00009c85  
Title : Crystal structure of arabidopsis thaliana acetohydroxyacid synthase in complex with 2022-LS5  
Authors : Gao, Y.; Guddat, L.W.  
Deposited on : 2024-06-12  
Resolution : 2.72 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

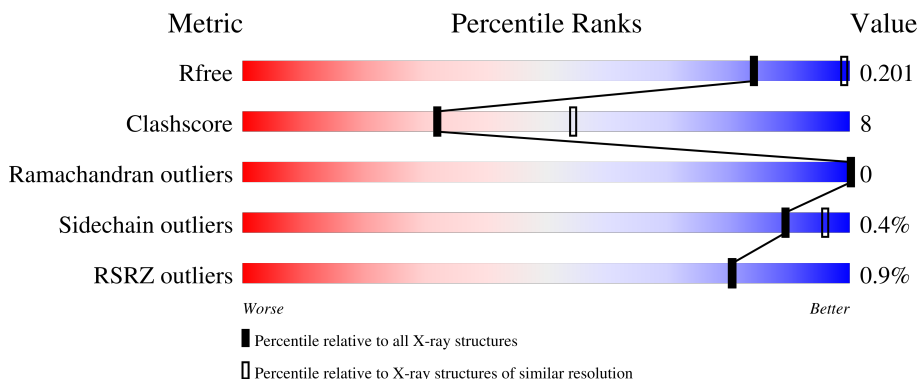
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


The reported resolution of this entry is 2.72 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))
$R_{free}$	164625	4050 (2.74-2.70)
Clashscore	180529	4439 (2.74-2.70)
Ramachandran outliers	177936	4374 (2.74-2.70)
Sidechain outliers	177891	4375 (2.74-2.70)
RSRZ outliers	164620	4050 (2.74-2.70)

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  $\geq 3$ , 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	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4616 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	0	0
			4460	2829	769	838	24			

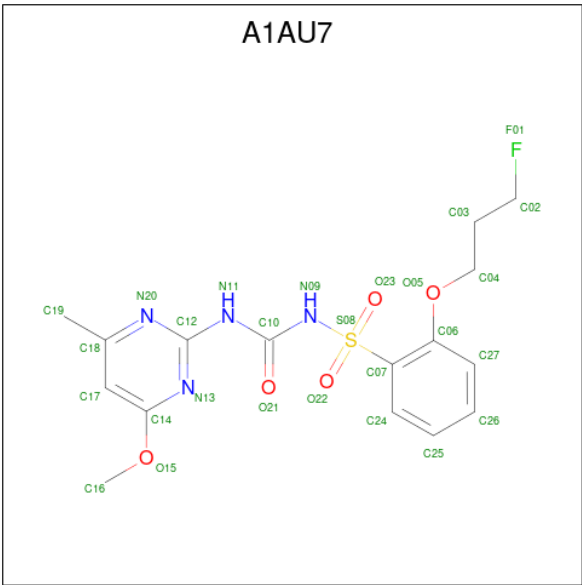
There are 8 discrepancies between the modelled and reference sequences:

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).

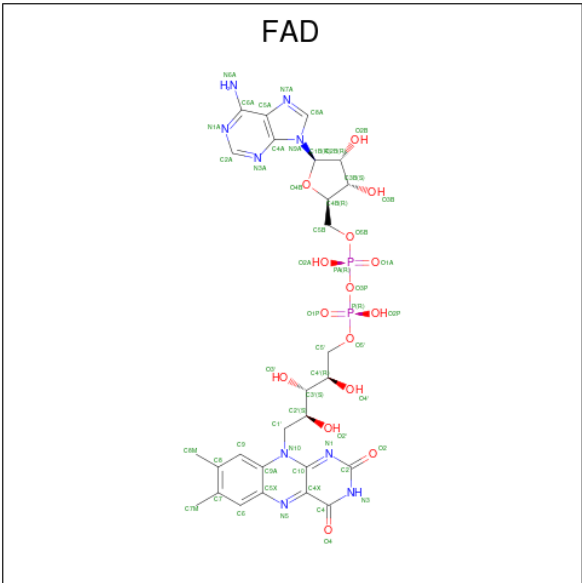
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 2-(3-fluoropropoxy)-N-[(4-methoxy-6-methylpyrimidin-2-yl)carbamoyl]benzene-1-sulfonamide (CCD ID: A1AU7) (formula: C<sub>16</sub>H<sub>19</sub>FN<sub>4</sub>O<sub>5</sub>S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
3	A	1	27	16	1	4	5	0	0

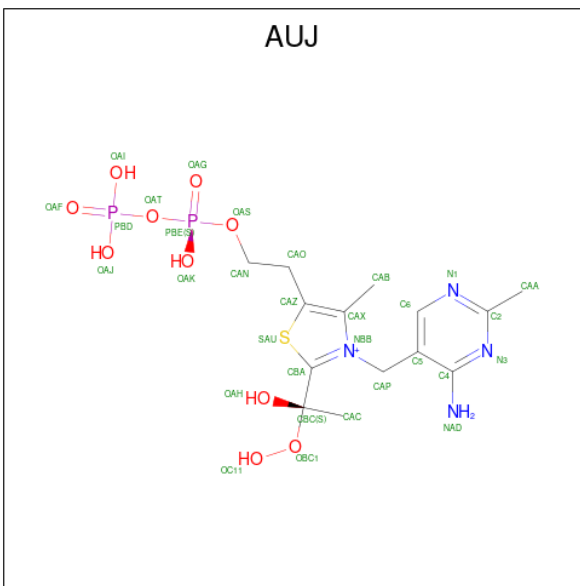
- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



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

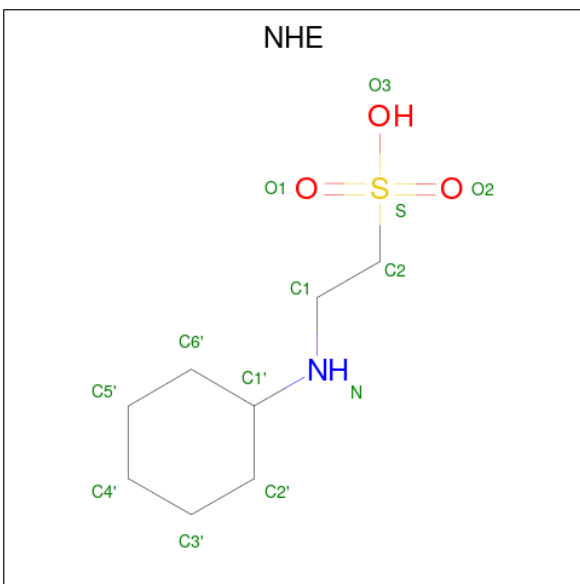
- Molecule 5 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID:

AUJ) (formula: C<sub>14</sub>H<sub>23</sub>N<sub>4</sub>O<sub>10</sub>P<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



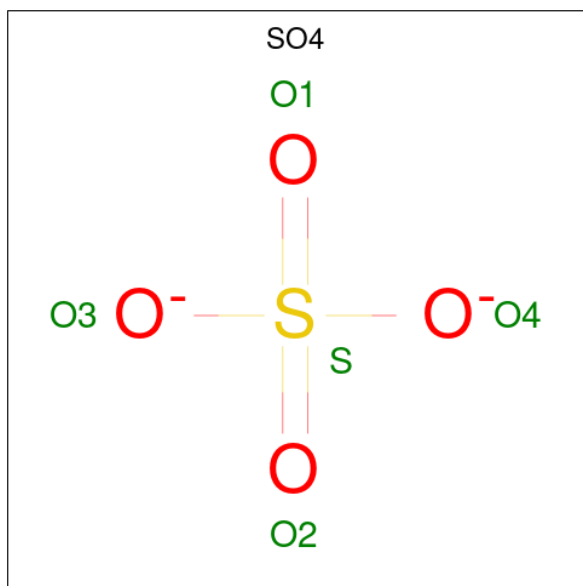
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	14	4	10	2	1		

- Molecule 6 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula:  $\text{C}_8\text{H}_{17}\text{NO}_3\text{S}$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

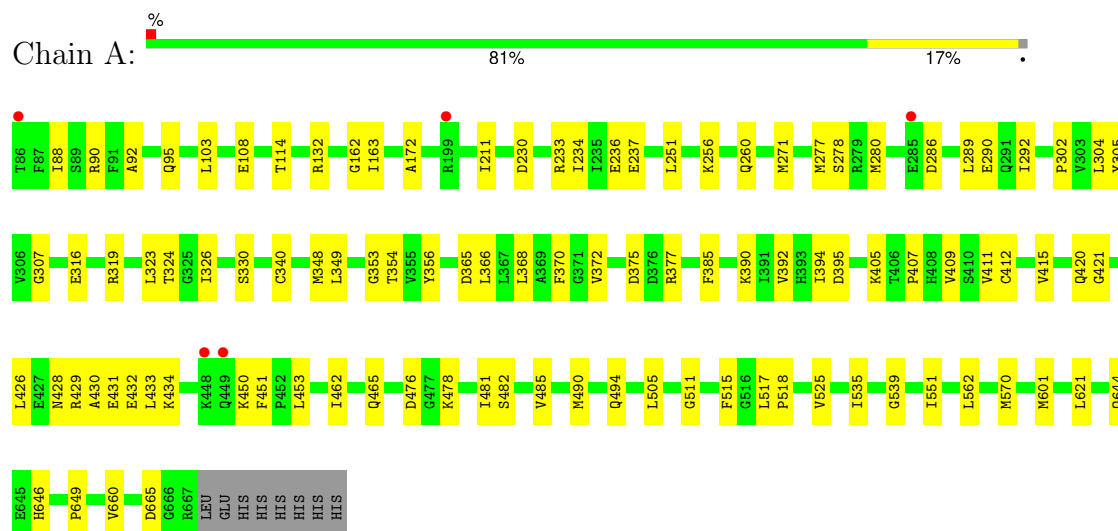
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	21	Total	O	0	0
			21	21		

### 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, $\alpha$ , $\beta$ , $\gamma$	178.74Å 178.74Å 185.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.08 – 2.72 36.08 – 2.72	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.08-2.72) 99.9 (36.08-2.72)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.179 , 0.202 0.178 , 0.201	Depositor DCC
$R_{free}$ test set	2340 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.2	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	4616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AUJ, SO4, NHE, CSD, MG, A1AU7, FAD

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	0.36	0/4548	0.52	0/6174

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	4460	0	4456	72	0
2	A	1	0	0	0	0
3	A	27	0	0	0	0
4	A	53	0	31	0	0
5	A	31	0	0	2	0
6	A	13	0	17	0	0
7	A	10	0	0	0	0
8	A	21	0	0	1	0
All	All	4616	0	4504	72	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 8.

All (72) 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:319:ARG:HH21	1:A:323:LEU:HD21	1.42	0.85
1:A:450:LYS:HB3	1:A:451:PHE:CD1	2.27	0.70
1:A:319:ARG:NH2	1:A:323:LEU:HD21	2.07	0.69
1:A:450:LYS:HB3	1:A:451:PHE:CE1	2.29	0.67
1:A:431:GLU:O	1:A:434:LYS:HG2	1.99	0.62
1:A:172:ALA:HB1	1:A:211:ILE:HG12	1.82	0.61
1:A:481:ILE:HG23	1:A:535:ILE:HD12	1.84	0.59
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.84	0.59
1:A:307:GLY:HA3	1:A:372:VAL:HG12	1.86	0.58
1:A:305:TYR:CE2	1:A:372:VAL:HG21	2.40	0.57
1:A:515:PHE:O	1:A:518:PRO:HD2	2.05	0.57
1:A:319:ARG:HE	1:A:323:LEU:HD21	1.69	0.56
1:A:429:ARG:O	1:A:433:LEU:HD12	2.05	0.56
1:A:490:MET:HA	1:A:490:MET:HE2	1.87	0.54
1:A:481:ILE:CG2	1:A:535:ILE:HD12	2.36	0.54
1:A:236:GLU:HG2	1:A:271:MET:SD	2.47	0.54
1:A:132:ARG:NH2	8:A:801:HOH:O	2.41	0.54
1:A:462:ILE:HG23	1:A:621:LEU:HD22	1.91	0.52
1:A:256:LYS:O	1:A:260:GLN:HG3	2.10	0.52
1:A:476:ASP:O	1:A:478:LYS:HG2	2.10	0.51
1:A:237:GLU:HG2	1:A:271:MET:HG2	1.92	0.51
1:A:162:GLY:C	1:A:163:ILE:HD12	2.35	0.51
1:A:286:ASP:O	1:A:290:GLU:HG2	2.11	0.50
1:A:375:ASP:OD1	1:A:377:ARG:N	2.44	0.50
1:A:324:THR:OG1	1:A:326:ILE:HD12	2.12	0.50
1:A:562:LEU:CD2	1:A:601:MET:HG3	2.42	0.50
1:A:482:SER:HA	1:A:505:LEU:O	2.11	0.50
1:A:375:ASP:OD1	1:A:377:ARG:HB2	2.11	0.50
1:A:302:PRO:HG2	1:A:326:ILE:HG23	1.94	0.50
1:A:385:PHE:O	1:A:405:LYS:HE2	2.12	0.49
1:A:465:GLN:H	1:A:465:GLN:CD	2.21	0.49
1:A:366:LEU:HD12	1:A:390:LYS:O	2.13	0.48
1:A:453:LEU:HD13	1:A:494:GLN:HB3	1.95	0.48
1:A:292:ILE:HG12	1:A:392:VAL:HG11	1.93	0.48
1:A:485:VAL:HG21	1:A:511:GLY:C	2.37	0.48
1:A:277:MET:HA	1:A:280:MET:HG3	1.95	0.48
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.94	0.48
1:A:365:ASP:O	1:A:390:LYS:N	2.42	0.47
1:A:407:PRO:HB2	1:A:409:VAL:O	2.15	0.47
1:A:539:GLY:N	5:A:704:AUJ:OAK	2.44	0.46
1:A:92:ALA:HB3	1:A:95:GLN:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LEU:HD21	1:A:601:MET:HG3	1.98	0.46
1:A:517:LEU:HD11	1:A:551:ILE:CD1	2.47	0.45
1:A:319:ARG:NE	1:A:323:LEU:HD21	2.31	0.45
1:A:354:THR:HB	1:A:356:TYR:CE1	2.52	0.45
1:A:431:GLU:HA	1:A:431:GLU:OE1	2.16	0.45
1:A:88:ILE:HD13	1:A:88:ILE:HA	1.83	0.45
1:A:103:LEU:C	1:A:103:LEU:HD23	2.41	0.44
1:A:353:GLY:O	1:A:649:PRO:HG2	2.18	0.44
1:A:251:LEU:C	1:A:251:LEU:HD23	2.42	0.44
1:A:280:MET:HE2	1:A:280:MET:HB3	1.65	0.44
1:A:233:ARG:O	1:A:237:GLU:HG3	2.18	0.44
1:A:370:PHE:HB3	1:A:415:VAL:HG21	1.99	0.44
1:A:163:ILE:HD12	1:A:163:ILE:N	2.33	0.43
1:A:646:HIS:CG	1:A:665:ASP:HA	2.53	0.43
1:A:211:ILE:HD12	1:A:211:ILE:HA	1.81	0.43
1:A:644:GLN:O	1:A:665:ASP:HB2	2.19	0.43
1:A:330:SER:O	1:A:348:MET:HA	2.18	0.43
1:A:660:VAL:O	1:A:660:VAL:HG13	2.19	0.42
1:A:304:LEU:HD23	1:A:368:LEU:HB2	2.00	0.42
1:A:90:ARG:NH1	1:A:108:GLU:OE2	2.53	0.42
1:A:289:LEU:CD1	1:A:421:GLY:HA3	2.49	0.42
1:A:307:GLY:CA	1:A:372:VAL:HG12	2.49	0.42
1:A:319:ARG:HA	1:A:319:ARG:HD2	1.73	0.42
1:A:570:MET:HG2	5:A:704:AUJ:CAC	2.49	0.41
1:A:316:GLU:HG2	1:A:420:GLN:HG3	2.01	0.41
1:A:319:ARG:CZ	1:A:323:LEU:HD21	2.51	0.41
1:A:349:LEU:H	1:A:349:LEU:HD23	1.86	0.41
1:A:230:ASP:HB3	1:A:234:ILE:HD12	2.03	0.40
1:A:428:ASN:C	1:A:430:ALA:H	2.29	0.40
1:A:395:ASP:O	1:A:412:CYS:HA	2.22	0.40
1:A:324:THR:CG2	1:A:426:LEU:HD13	2.51	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	579/590 (98%)	563 (97%)	16 (3%)	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	478/486 (98%)	476 (100%)	2 (0%)	89	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	A	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	527	ASN
1	A	593	GLN
1	A	626	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	1.00	0	1,8,10	7.04	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(°)	Ideal(°)
1	A	340	CSD	OD1-SG-CB	7.04	118.56	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

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

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
5	AUJ	A	704	2	27,32,32	2.62	10 (37%)	31,49,49	2.39	16 (51%)
4	FAD	A	703	-	54,58,58	2.67	16 (29%)	71,89,89	1.74	16 (22%)
3	A1AU7	A	702	-	28,28,28	1.98	8 (28%)	38,38,38	2.96	8 (21%)
6	NHE	A	705	-	13,13,13	1.86	3 (23%)	16,17,17	2.72	4 (25%)
7	SO4	A	707	-	4,4,4	0.25	0	6,6,6	0.18	0
7	SO4	A	706	-	4,4,4	0.30	0	6,6,6	0.06	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
5	AUJ	A	704	2	-	5/17/26/26	0/2/2/2
4	FAD	A	703	-	-	7/30/50/50	0/6/6/6
6	NHE	A	705	-	-	6/7/15/15	0/1/1/1
3	A1AU7	A	702	-	-	6/22/22/22	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	FAD	O4-C4	9.22	1.41	1.23
4	A	703	FAD	O4B-C1B	-7.86	1.30	1.40
4	A	703	FAD	PA-O3P	7.53	1.67	1.59
4	A	703	FAD	O2-C2	6.59	1.37	1.24
5	A	704	AUJ	C6-N1	6.23	1.47	1.34
5	A	704	AUJ	C5-C4	6.10	1.52	1.42
5	A	704	AUJ	C2-N3	5.75	1.43	1.34
3	A	702	A1AU7	C12-N11	5.13	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	705	NHE	C2-S	4.84	1.84	1.77
5	A	704	AUJ	CBA-NBB	4.01	1.44	1.35
3	A	702	A1AU7	C10-N11	3.72	1.45	1.37
5	A	704	AUJ	CAO-CAZ	3.56	1.53	1.51
4	A	703	FAD	P-O3P	3.56	1.63	1.59
4	A	703	FAD	C5B-C4B	-3.43	1.41	1.51
3	A	702	A1AU7	O23-S08	3.35	1.47	1.43
4	A	703	FAD	O3B-C3B	3.27	1.51	1.43
4	A	703	FAD	C6A-N6A	3.21	1.45	1.34
3	A	702	A1AU7	C10-N09	3.19	1.46	1.39
3	A	702	A1AU7	C07-S08	3.10	1.81	1.77
5	A	704	AUJ	C4-NAD	2.99	1.41	1.34
3	A	702	A1AU7	S08-N09	2.93	1.71	1.64
6	A	705	NHE	O1-S	2.92	1.53	1.45
4	A	703	FAD	C4-N3	-2.79	1.33	1.38
3	A	702	A1AU7	O15-C14	2.76	1.39	1.35
4	A	703	FAD	C4X-N5	2.70	1.36	1.30
4	A	703	FAD	C1'-C2'	2.66	1.56	1.52
4	A	703	FAD	PA-O5B	2.54	1.69	1.59
4	A	703	FAD	C3B-C4B	2.51	1.59	1.53
6	A	705	NHE	O2-S	2.50	1.52	1.45
4	A	703	FAD	O4B-C4B	2.43	1.50	1.45
5	A	704	AUJ	PBE-OAT	-2.41	1.56	1.59
5	A	704	AUJ	CAP-NBB	-2.40	1.44	1.49
4	A	703	FAD	C2-N3	-2.27	1.34	1.39
5	A	704	AUJ	CAX-NBB	2.20	1.44	1.39
4	A	703	FAD	C1B-N9A	-2.18	1.44	1.49
5	A	704	AUJ	C4-N3	-2.05	1.32	1.35
3	A	702	A1AU7	C18-N20	-2.02	1.31	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	A1AU7	O23-S08-O22	-13.70	102.88	119.52
6	A	705	NHE	O1-S-C2	8.11	118.98	106.73
3	A	702	A1AU7	C07-S08-N09	7.18	114.88	105.96
5	A	704	AUJ	CAA-C2-N1	6.70	124.33	117.20
4	A	703	FAD	N3A-C2A-N1A	-6.02	120.50	128.67
3	A	702	A1AU7	C12-N11-C10	-5.68	124.49	130.34
4	A	703	FAD	C5'-C4'-C3'	-4.77	103.22	112.22
4	A	703	FAD	C4B-O4B-C1B	4.48	114.03	109.92
6	A	705	NHE	C3'-C2'-C1'	4.38	118.95	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	705	NHE	C4'-C3'-C2'	4.02	119.69	111.42
5	A	704	AUJ	OAI-PBD-OAT	3.78	117.32	104.64
3	A	702	A1AU7	C12-N13-C14	3.59	119.11	115.00
5	A	704	AUJ	OAJ-PBD-OAT	3.49	116.35	104.64
4	A	703	FAD	C4A-C5A-N7A	-3.47	105.67	109.34
5	A	704	AUJ	CAZ-CAX-NBB	3.33	114.61	107.66
4	A	703	FAD	O2'-C2'-C3'	3.11	116.54	109.25
5	A	704	AUJ	C5-C6-N1	-3.07	118.84	123.83
5	A	704	AUJ	OAK-PBE-OAG	-2.94	98.76	112.44
4	A	703	FAD	C4-N3-C2	-2.91	120.47	125.64
3	A	702	A1AU7	C12-N20-C18	2.90	121.60	115.98
5	A	704	AUJ	C5-C4-NAD	-2.88	118.26	122.14
5	A	704	AUJ	C6-N1-C2	2.83	120.71	116.07
3	A	702	A1AU7	C17-C14-N13	-2.75	120.95	124.16
5	A	704	AUJ	OAI-PBD-OAF	-2.66	100.48	110.83
5	A	704	AUJ	OAT-PBE-OAG	2.65	118.67	110.70
4	A	703	FAD	O2-C2-N1	-2.64	117.41	121.80
3	A	702	A1AU7	N20-C12-N13	-2.54	122.10	126.26
5	A	704	AUJ	NAD-C4-N3	2.49	120.39	117.03
4	A	703	FAD	O4-C4-C4X	-2.47	120.00	126.53
4	A	703	FAD	C4-C4X-N5	2.47	121.62	118.21
5	A	704	AUJ	OAT-PBD-OAF	-2.47	98.05	111.04
4	A	703	FAD	C9A-C5X-N5	-2.45	119.85	122.45
5	A	704	AUJ	CAB-CAX-CAZ	-2.44	122.26	127.60
5	A	704	AUJ	N1-C2-N3	-2.34	121.64	125.53
6	A	705	NHE	O3-S-O2	-2.32	105.58	111.40
4	A	703	FAD	C9A-N10-C10	-2.28	117.27	120.75
4	A	703	FAD	C4X-C4-N3	2.28	119.05	113.25
4	A	703	FAD	C4X-C10-N10	2.27	119.73	116.48
4	A	703	FAD	O3B-C3B-C4B	-2.19	104.78	111.08
5	A	704	AUJ	CAP-C5-C6	2.16	124.75	120.69
3	A	702	A1AU7	O05-C06-C07	2.09	119.94	116.70
5	A	704	AUJ	CAA-C2-N3	-2.07	114.02	117.13
4	A	703	FAD	C4'-C3'-C2'	-2.03	110.18	113.57
4	A	703	FAD	O2'-C2'-C1'	2.01	118.48	110.20

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	A1AU7	C06-C07-S08-O23
4	A	703	FAD	C3'-C4'-C5'-O5'

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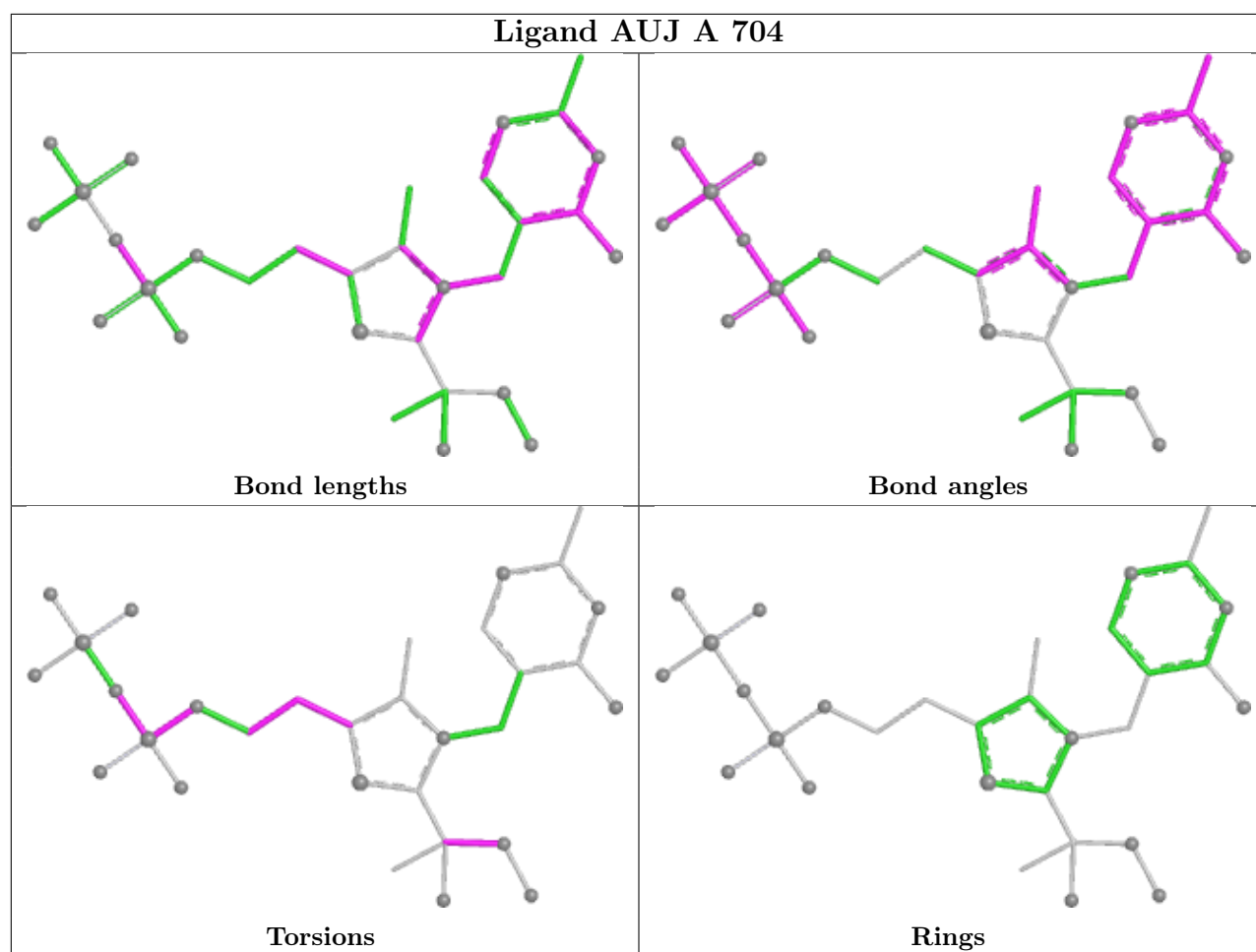
Mol	Chain	Res	Type	Atoms
4	A	703	FAD	O4'-C4'-C5'-O5'
5	A	704	AUJ	OAS-CAN-CAO-CAZ
5	A	704	AUJ	CAN-CAO-CAZ-CAX
5	A	704	AUJ	CAC-CBC-OBC1-OC11
6	A	705	NHE	N-C1-C2-S
3	A	702	A1AU7	C02-C03-C04-O05
3	A	702	A1AU7	C10-N09-S08-O22
6	A	705	NHE	C1-C2-S-O3
6	A	705	NHE	C6'-C1'-N-C1
4	A	703	FAD	O2'-C2'-C3'-C4'
3	A	702	A1AU7	C24-C07-S08-O23
4	A	703	FAD	O2'-C2'-C3'-O3'
6	A	705	NHE	C1-C2-S-O1
5	A	704	AUJ	CAN-OAS-PBE-OAG
4	A	703	FAD	O3'-C3'-C4'-C5'
6	A	705	NHE	C2'-C1'-N-C1
3	A	702	A1AU7	C03-C04-O05-C06
4	A	703	FAD	PA-O3P-P-O5'
6	A	705	NHE	C1-C2-S-O2
4	A	703	FAD	O4B-C4B-C5B-O5B
3	A	702	A1AU7	N09-C10-N11-C12
5	A	704	AUJ	PBD-OAT-PBE-OAK

There are no ring outliers.

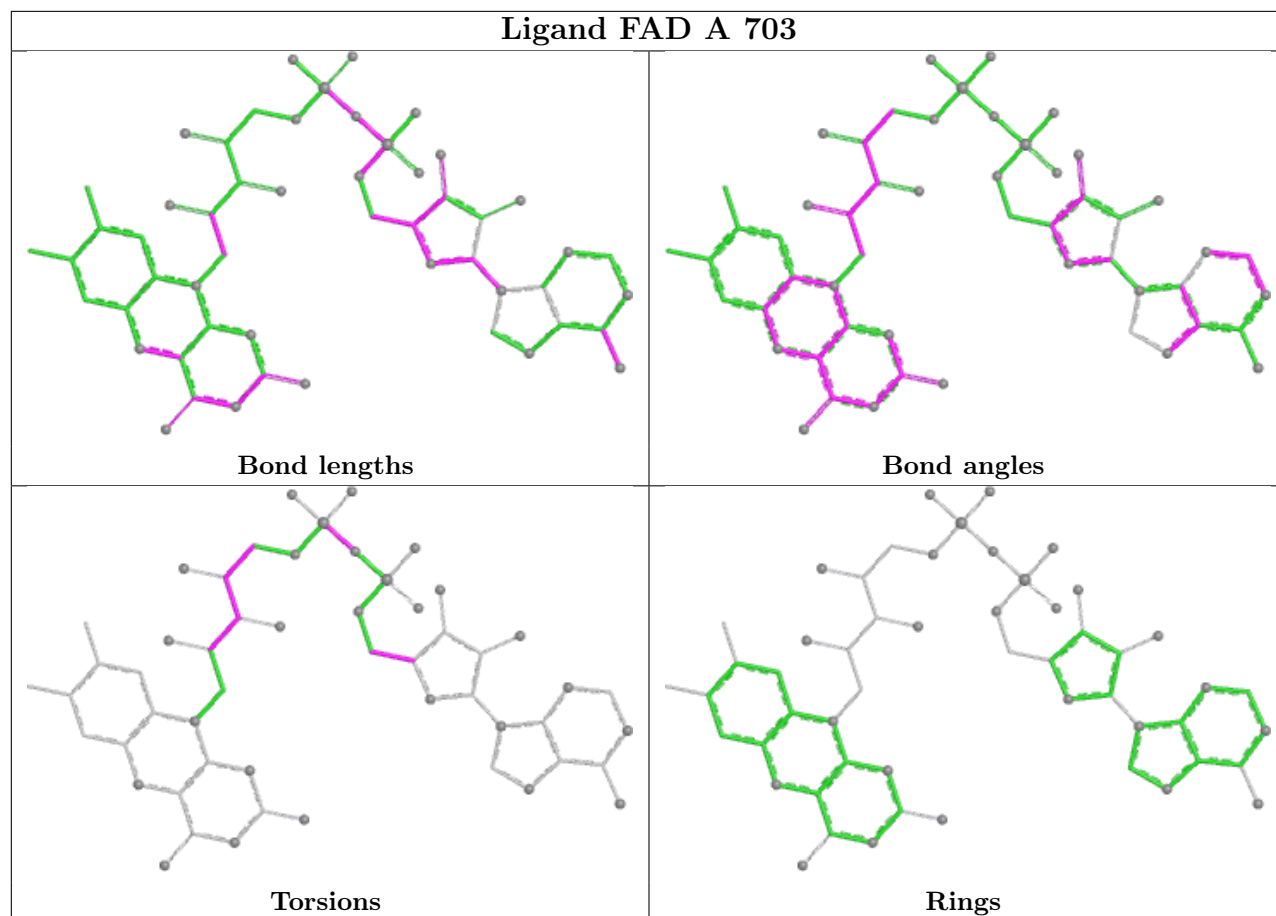
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	704	AUJ	2	0

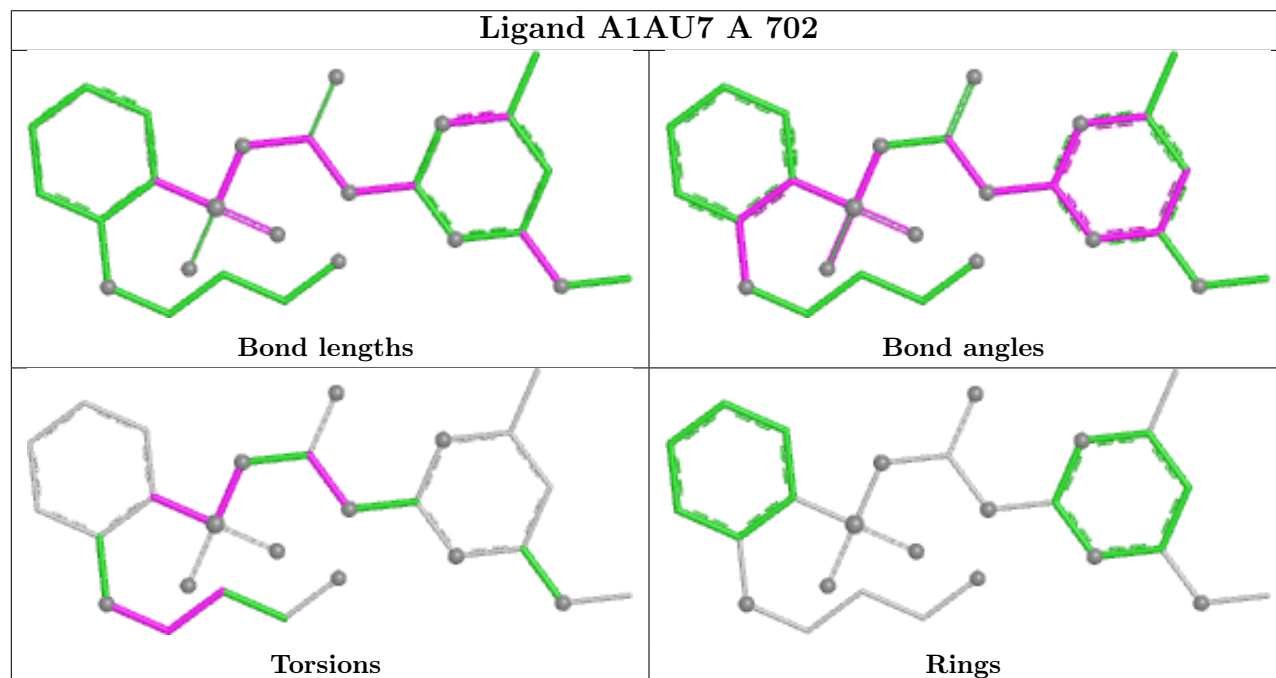
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

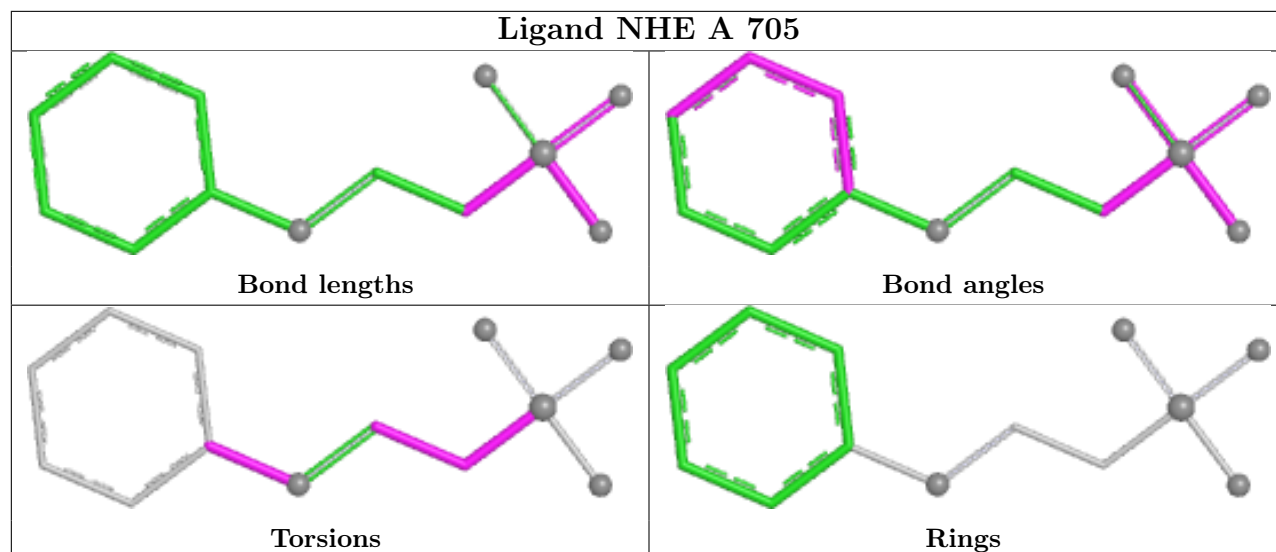


## Ligand FAD A 703



## Ligand A1AU7 A 702





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	581/590 (98%)	-0.42	5 (0%) 81 80	55, 72, 99, 130	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	GLN	2.4
1	A	199	ARG	2.3
1	A	285	GLU	2.1
1	A	86	THR	2.0
1	A	448	LYS	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSD	A	340	8/9	0.94	0.12	77,86,99,110	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

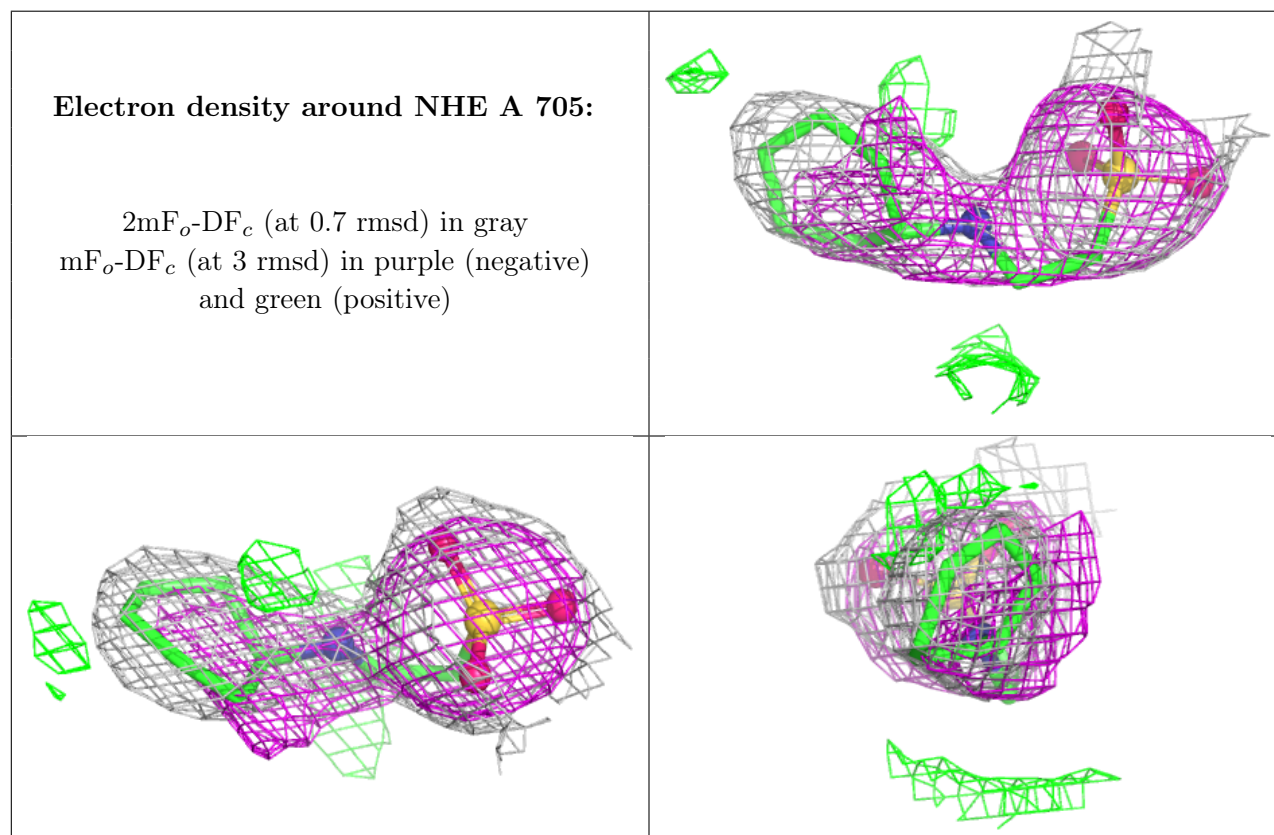
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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.

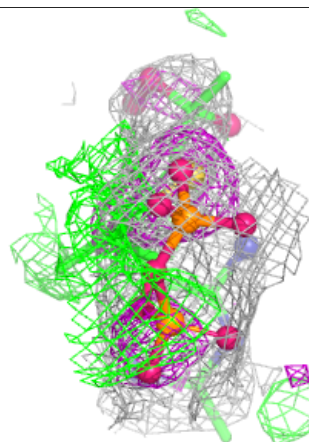
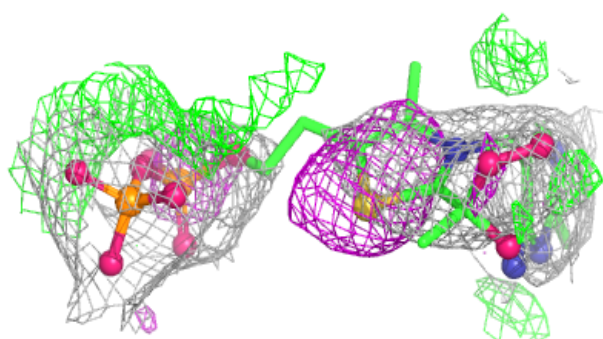
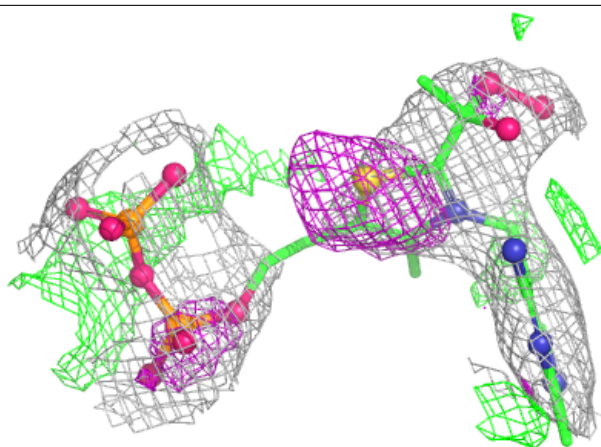
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	A	706	5/5	0.67	0.18	143,144,151,168	0
7	SO4	A	707	5/5	0.78	0.15	115,125,151,172	0
2	MG	A	701	1/1	0.89	0.21	72,72,72,72	0
6	NHE	A	705	13/13	0.90	0.19	49,64,71,72	0
5	AUJ	A	704	31/31	0.92	0.16	49,63,73,89	31
4	FAD	A	703	53/53	0.96	0.08	45,54,58,60	0
3	A1AU7	A	702	27/27	0.97	0.09	74,83,94,101	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.

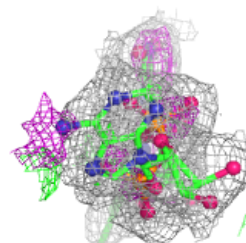
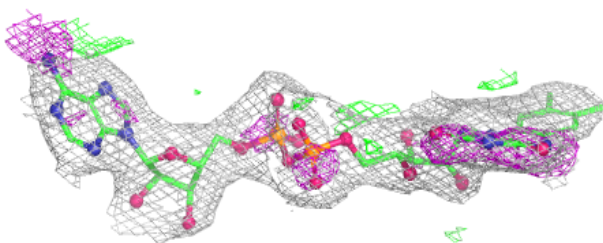
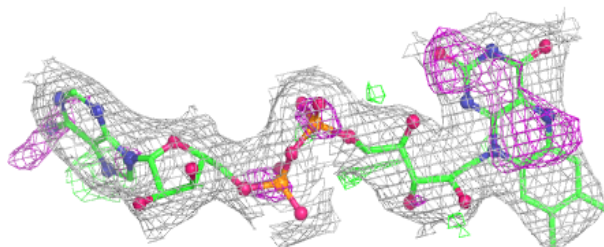


**Electron density around AUJ A 704:**

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

**Electron density around FAD A 703:**

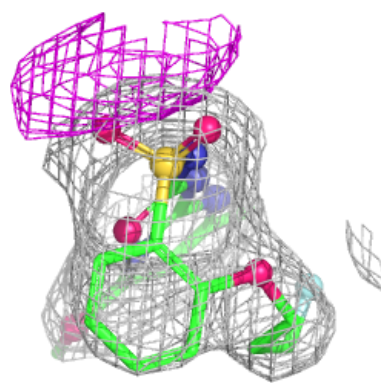
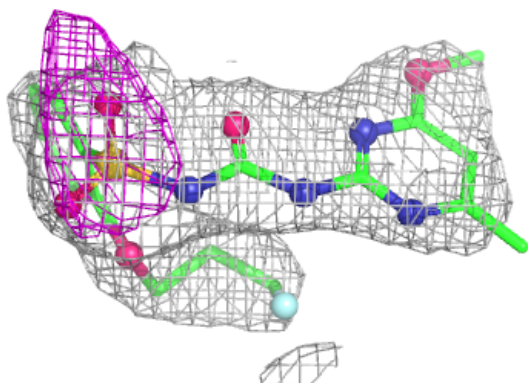
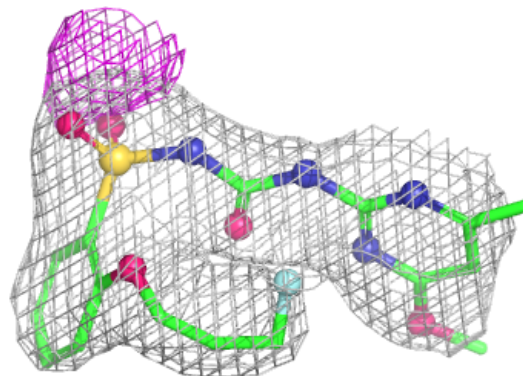
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around A1AU7 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 ⓘ

There are no such residues in this entry.