



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 04:12 pm BST

PDB ID : 1YHZ  
Title : Crystal structure of Arabidopsis thaliana Acetohydroxyacid synthase In Complex With A Sulfonylurea Herbicide, Chlorsulfuron  
Authors : McCourt, J.A.; Pang, S.S.; King-Scott, J.; Guddat, L.W.; Duggleby, R.G.  
Deposited on : 2005-01-10  
Resolution : 2.70 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

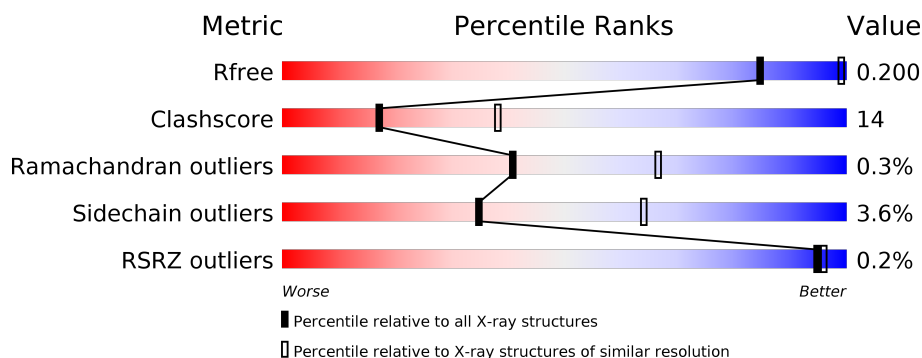
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	<div> <div></div> <div>74%</div> <div>23%</div> <div>..</div> </div>

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
3	1CS	A	695	-	X	-	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4864 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4419	2803	759	833	24			

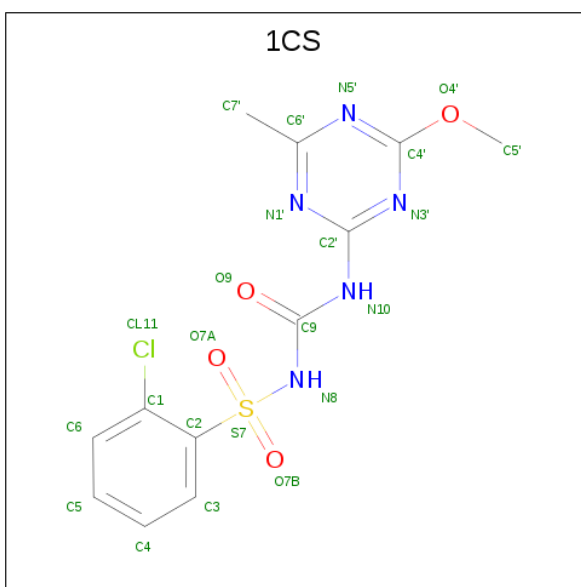
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	340	CSD	CYS	MODIFIED RESIDUE	UNP P17597
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 (three-letter code: MG) (formula: Mg).

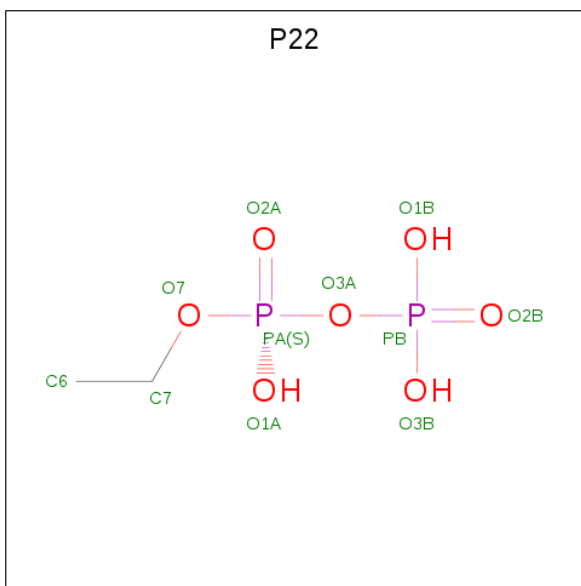
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1-(2-CHLOROPHENYLSULFONYL)-3-(4-METHOXY-6-METHYL-L,3,5-T RIAZIN-2-YL)UREA (three-letter code: 1CS) (formula: C<sub>12</sub>H<sub>12</sub>ClN<sub>5</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			23	12	1	5	4	1		

- Molecule 4 is ETHYL DIHYDROGEN DIPHOSPHATE (three-letter code: P22) (formula:  $C_2H_8O_7P_2$ ).



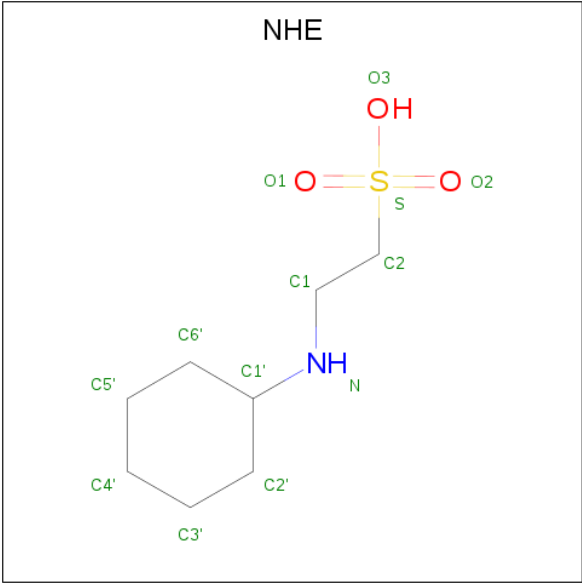
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			11	2	7	2		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



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

- Molecule 6 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C<sub>8</sub>H<sub>17</sub>NO<sub>3</sub>S).



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

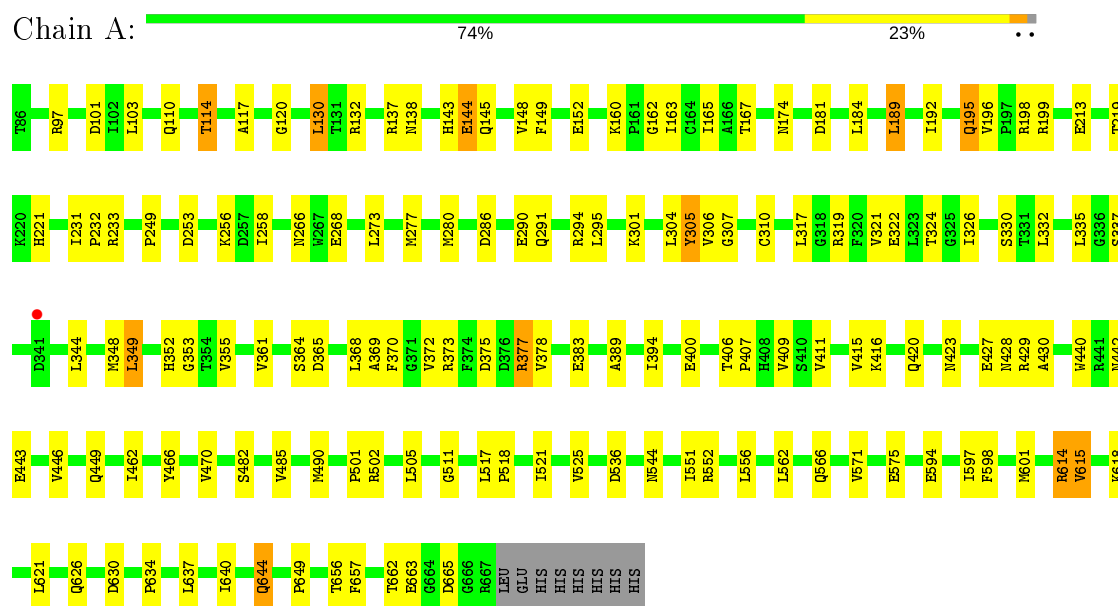
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	344	Total 344	O 344	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.51Å 178.51Å 185.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 89.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.70) 95.2 (89.26-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.16 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.177 , 0.201 0.176 , 0.200	Depositor DCC
$R_{free}$ test set	4867 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4864	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: NHE, 1CS, MG, CSD, P22, 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	0.32	0/4507	0.60	0/6127

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	4419	0	4367	122	0
2	A	1	0	0	0	0
3	A	23	0	12	1	0
4	A	11	0	5	0	0
5	A	53	0	31	4	0
6	A	13	0	17	1	0
7	A	344	0	0	15	0
All	All	4864	0	4432	124	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 14.

All (124) 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:195:GLN:HE21	1:A:196:VAL:N	1.60	0.97
1:A:195:GLN:NE2	1:A:196:VAL:H	1.62	0.96
1:A:566:GLN:HE22	1:A:598:PHE:H	1.07	0.96
1:A:195:GLN:HE21	1:A:196:VAL:H	0.94	0.93
1:A:117:ALA:H	1:A:138:ASN:HD21	1.18	0.92
1:A:143:HIS:HD2	1:A:145:GLN:H	1.16	0.92
1:A:364:SER:O	1:A:389:ALA:HB2	1.72	0.89
1:A:501:PRO:HA	7:A:4208:HOH:O	1.81	0.80
1:A:145:GLN:HE21	1:A:544:ASN:HD21	1.30	0.79
1:A:614:ARG:HD2	1:A:640:ILE:HD11	1.69	0.75
1:A:332:LEU:HD13	1:A:348:MET:HE1	1.69	0.74
1:A:332:LEU:CD1	1:A:348:MET:HE1	2.20	0.72
1:A:233:ARG:HD3	7:A:4261:HOH:O	1.90	0.71
1:A:375:ASP:OD2	1:A:377:ARG:HB2	1.92	0.69
1:A:352:HIS:HB2	1:A:490:MET:CE	2.23	0.68
1:A:352:HIS:HB2	1:A:490:MET:HE3	1.78	0.65
1:A:273:LEU:O	1:A:277:MET:HG2	1.97	0.65
1:A:332:LEU:HA	1:A:348:MET:HE2	1.77	0.65
1:A:306:VAL:HG13	1:A:310:CYS:SG	2.36	0.65
1:A:365:ASP:C	1:A:389:ALA:HB1	2.18	0.63
1:A:373:ARG:HG2	5:A:701:FAD:O1P	1.99	0.63
1:A:443:GLU:O	1:A:446:VAL:HG22	1.99	0.62
1:A:656:THR:HG22	1:A:657:PHE:N	2.16	0.60
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.84	0.60
1:A:337:SER:HA	1:A:501:PRO:HG3	1.84	0.58
1:A:406:THR:HG22	7:A:4097:HOH:O	2.02	0.58
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.87	0.57
1:A:502:ARG:HG2	1:A:502:ARG:HH11	1.70	0.55
1:A:552:ARG:O	1:A:552:ARG:HD3	2.07	0.55
1:A:597:ILE:HD13	1:A:640:ILE:CD1	2.36	0.55
5:A:701:FAD:H51A	7:A:4055:HOH:O	2.08	0.54
1:A:184:LEU:HD22	7:A:4062:HOH:O	2.09	0.53
1:A:332:LEU:HA	1:A:348:MET:CE	2.38	0.53
1:A:406:THR:HG23	7:A:4301:HOH:O	2.08	0.53
1:A:370:PHE:HB3	1:A:415:VAL:HG21	1.90	0.53
1:A:117:ALA:H	1:A:138:ASN:ND2	1.96	0.53
1:A:144:GLU:HG3	1:A:174:ASN:HB2	1.89	0.53
1:A:352:HIS:CB	1:A:490:MET:HE3	2.39	0.52
1:A:502:ARG:N	7:A:4208:HOH:O	2.43	0.52
1:A:562:LEU:HD21	1:A:601:MET:HG3	1.90	0.52
1:A:485:VAL:HG21	1:A:511:GLY:C	2.30	0.52
1:A:502:ARG:NH1	1:A:502:ARG:HG2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:GLN:NE2	1:A:598:PHE:H	1.92	0.51
1:A:321:VAL:HG12	1:A:344:LEU:HD13	1.91	0.51
1:A:266:ASN:ND2	1:A:268:GLU:H	2.09	0.51
1:A:286:ASP:O	1:A:290:GLU:HG3	2.10	0.51
1:A:416:LYS:O	1:A:420:GLN:HG3	2.11	0.51
1:A:256:LYS:HE3	7:A:4184:HOH:O	2.10	0.51
1:A:277:MET:SD	1:A:280:MET:HE1	2.50	0.51
1:A:571:VAL:O	1:A:575:GLU:HG3	2.11	0.51
1:A:195:GLN:HE21	1:A:195:GLN:CA	2.24	0.50
1:A:305:TYR:CE2	1:A:372:VAL:HG21	2.47	0.50
1:A:304:LEU:HD23	1:A:368:LEU:HB2	1.93	0.50
1:A:120:GLY:HA3	1:A:167:THR:HB	1.93	0.50
1:A:163:ILE:HD12	1:A:163:ILE:N	2.27	0.50
1:A:117:ALA:HB2	1:A:165:ILE:HB	1.94	0.50
1:A:423:ASN:O	1:A:427:GLU:HG3	2.11	0.50
1:A:195:GLN:NE2	1:A:196:VAL:HG22	2.26	0.50
1:A:307:GLY:HA3	1:A:372:VAL:HG12	1.94	0.49
1:A:442:ASN:O	1:A:446:VAL:HG13	2.12	0.49
1:A:556:LEU:O	1:A:634:PRO:HG3	2.12	0.49
1:A:428:ASN:C	1:A:430:ALA:H	2.15	0.49
1:A:552:ARG:C	1:A:552:ARG:HD3	2.33	0.49
1:A:103:LEU:HD21	1:A:192:ILE:HD13	1.93	0.49
1:A:144:GLU:HG3	1:A:174:ASN:CB	2.43	0.49
1:A:349:LEU:HD23	1:A:361:VAL:HG21	1.94	0.48
1:A:517:LEU:HB3	1:A:518:PRO:HD3	1.95	0.48
1:A:466:TYR:O	1:A:470:VAL:HG23	2.14	0.48
1:A:400:GLU:HG3	5:A:701:FAD:O3B	2.13	0.48
1:A:231:ILE:HB	1:A:232:PRO:HD3	1.96	0.48
1:A:317:LEU:O	1:A:321:VAL:HG23	2.13	0.48
1:A:143:HIS:CD2	1:A:145:GLN:H	2.09	0.48
1:A:482:SER:HA	1:A:505:LEU:O	2.14	0.48
1:A:319:ARG:HA	1:A:322:GLU:HG2	1.97	0.47
1:A:462:ILE:HG23	1:A:621:LEU:HD22	1.96	0.47
1:A:615:VAL:HG22	1:A:637:LEU:HD11	1.97	0.47
1:A:364:SER:C	1:A:389:ALA:HB2	2.36	0.46
1:A:101:ASP:OD1	1:A:132:ARG:NH1	2.46	0.46
1:A:353:GLY:O	1:A:649:PRO:HG2	2.16	0.46
1:A:349:LEU:HD13	1:A:378:VAL:HG13	1.97	0.46
1:A:332:LEU:HD12	1:A:348:MET:HE1	1.97	0.46
1:A:321:VAL:CG1	1:A:344:LEU:HD13	2.47	0.46
1:A:656:THR:CG2	1:A:657:PHE:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:GLN:HG3	1:A:630:ASP:OD2	2.16	0.45
1:A:566:GLN:NE2	1:A:597:ILE:HA	2.31	0.45
1:A:198:ARG:HD3	1:A:258:ILE:HD11	1.98	0.44
1:A:162:GLY:C	1:A:163:ILE:HD12	2.38	0.44
1:A:517:LEU:HD11	1:A:551:ILE:CD1	2.47	0.44
1:A:221:HIS:ND1	6:A:696:NHE:H2'2	2.33	0.44
1:A:213:GLU:HG3	7:A:4018:HOH:O	2.17	0.44
1:A:355:VAL:HA	7:A:4084:HOH:O	2.19	0.43
1:A:330:SER:O	1:A:348:MET:HA	2.18	0.43
1:A:132:ARG:NH2	7:A:4149:HOH:O	2.48	0.43
3:A:695:ICS:H5'2	5:A:701:FAD:HM72	2.01	0.43
1:A:130:LEU:HA	1:A:130:LEU:HD12	1.89	0.42
1:A:120:GLY:HA3	1:A:167:THR:CB	2.49	0.42
1:A:466:TYR:CD2	1:A:618:LYS:HE3	2.55	0.42
1:A:501:PRO:O	1:A:502:ARG:HB2	2.19	0.42
1:A:117:ALA:CB	1:A:165:ILE:HB	2.49	0.42
1:A:291:GLN:O	1:A:294:ARG:HB3	2.19	0.42
1:A:195:GLN:HG2	1:A:253:ASP:OD1	2.20	0.42
1:A:406:THR:HA	1:A:407:PRO:HD3	1.86	0.42
1:A:152:GLU:OE2	1:A:181:ASP:OD2	2.37	0.42
1:A:195:GLN:CA	1:A:195:GLN:NE2	2.82	0.42
1:A:295:LEU:HD11	1:A:409:VAL:HG21	2.01	0.42
1:A:266:ASN:HD21	1:A:268:GLU:HB2	1.85	0.41
1:A:369:ALA:HB1	1:A:372:VAL:CG2	2.51	0.41
1:A:335:LEU:HD11	1:A:348:MET:CE	2.51	0.41
1:A:184:LEU:HD13	7:A:4062:HOH:O	2.20	0.41
1:A:521:ILE:HD11	1:A:551:ILE:HG13	2.01	0.41
1:A:117:ALA:N	1:A:138:ASN:HD21	1.99	0.41
1:A:301:LYS:HG2	1:A:440:TRP:CE3	2.56	0.41
1:A:377:ARG:HD2	1:A:377:ARG:HA	1.83	0.41
1:A:324:THR:HB	1:A:326:ILE:HG13	2.03	0.41
1:A:383:GLU:CD	1:A:383:GLU:H	2.24	0.41
1:A:233:ARG:HB2	7:A:4040:HOH:O	2.20	0.41
1:A:349:LEU:H	1:A:349:LEU:HD12	1.86	0.40
1:A:662:THR:O	1:A:663:GLU:HG3	2.21	0.40
1:A:644:GLN:O	1:A:665:ASP:HB2	2.22	0.40
1:A:189:LEU:O	1:A:249:PRO:HA	2.21	0.40
1:A:199:ARG:HG2	7:A:4189:HOH:O	2.22	0.40
1:A:149:PHE:HB3	1:A:518:PRO:HB2	2.04	0.40
1:A:110:GLN:HG2	7:A:4066:HOH:O	2.20	0.40
1:A:219:THR:HA	1:A:249:PRO:HG2	2.04	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	579/590 (98%)	559 (96%)	18 (3%)	2 (0%)	41 66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	429	ARG
1	A	594	GLU

### 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	468/486 (96%)	451 (96%)	17 (4%)	35 64

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	ARG
1	A	114	THR
1	A	130	LEU
1	A	137	ARG
1	A	144	GLU
1	A	148	VAL

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Mol	Chain	Res	Type
1	A	160	LYS
1	A	189	LEU
1	A	195	GLN
1	A	305	TYR
1	A	349	LEU
1	A	377	ARG
1	A	449	GLN
1	A	536	ASP
1	A	614	ARG
1	A	615	VAL
1	A	644	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	143	HIS
1	A	145	GLN
1	A	174	ASN
1	A	195	GLN
1	A	266	ASN
1	A	288	HIS
1	A	291	GLN
1	A	312	ASN
1	A	363	HIS
1	A	566	GLN
1	A	626	GLN
1	A	643	HIS
1	A	644	GLN

### 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	3,7,8	0.70	0	1,8,10	7.01	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	7.01	118.89	105.54

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\# Z  > 2$
6	NHE	A	696	-	13,13,13	3.26	6 (46%)	16,17,17	2.54	8 (50%)
3	1CS	A	695	-	24,24,24	3.54	16 (66%)	33,34,34	4.33	16 (48%)
5	FAD	A	701	-	51,58,58	3.03	25 (49%)	60,89,89	2.00	10 (16%)
4	P22	A	702	2	8,10,10	1.72	3 (37%)	12,15,15	1.64	2 (16%)

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
6	NHE	A	696	-	-	1/7/15/15	0/1/1/1
3	1CS	A	695	-	-	5/17/17/17	0/2/2/2
5	FAD	A	701	-	-	1/30/50/50	0/6/6/6
4	P22	A	702	2	-	3/10/10/10	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	701	FAD	C4A-N3A	8.93	1.48	1.35
5	A	701	FAD	C4X-C10	7.92	1.46	1.38
3	A	695	1CS	C1-C2	7.21	1.50	1.40
6	A	696	NHE	O1-S	6.47	1.64	1.45
5	A	701	FAD	C2A-N1A	6.42	1.45	1.33
3	A	695	1CS	C3-C2	6.05	1.46	1.39
6	A	696	NHE	O2-S	5.95	1.62	1.45
3	A	695	1CS	C6'-N5'	5.81	1.44	1.34
5	A	701	FAD	C4-N3	5.69	1.42	1.33
3	A	695	1CS	C6'-N1'	5.32	1.43	1.34
6	A	696	NHE	O3-S	5.16	1.65	1.47
3	A	695	1CS	C4-C3	5.11	1.49	1.38
5	A	701	FAD	C2A-N3A	5.05	1.40	1.32
3	A	695	1CS	C4'-N5'	4.75	1.42	1.33
5	A	701	FAD	C10-N1	4.65	1.39	1.33
5	A	701	FAD	O4'-C4'	4.58	1.53	1.43
3	A	695	1CS	C5-C4	4.53	1.50	1.38
3	A	695	1CS	O4'-C4'	4.47	1.44	1.33
5	A	701	FAD	O3'-C3'	4.29	1.53	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	695	1CS	C6-C1	3.61	1.46	1.38
5	A	701	FAD	C6A-C5A	3.56	1.56	1.43
5	A	701	FAD	C4-C4X	3.51	1.47	1.41
5	A	701	FAD	C4X-N5	3.50	1.38	1.33
5	A	701	FAD	C1'-N10	3.49	1.51	1.48
3	A	695	1CS	C2'-N1'	3.33	1.44	1.34
6	A	696	NHE	C6'-C1'	3.31	1.59	1.52
5	A	701	FAD	C9A-N10	3.31	1.43	1.38
5	A	701	FAD	C5A-C4A	3.14	1.49	1.40
5	A	701	FAD	C5'-C4'	-3.11	1.47	1.51
5	A	701	FAD	C3B-C4B	2.82	1.60	1.53
5	A	701	FAD	P-O2P	-2.79	1.42	1.55
5	A	701	FAD	C8-C7	2.72	1.47	1.40
5	A	701	FAD	C9A-C5X	2.63	1.47	1.42
5	A	701	FAD	PA-O2A	-2.47	1.43	1.55
3	A	695	1CS	C2'-N3'	2.43	1.42	1.34
3	A	695	1CS	O7B-S7	2.41	1.46	1.43
4	A	702	P22	PA-O1A	-2.36	1.44	1.55
6	A	696	NHE	C5'-C6'	-2.31	1.47	1.53
3	A	695	1CS	C2'-N10	-2.29	1.35	1.38
3	A	695	1CS	C7'-C6'	-2.25	1.43	1.49
4	A	702	P22	PA-O2A	-2.21	1.43	1.50
5	A	701	FAD	C6-C7	2.15	1.43	1.37
5	A	701	FAD	O2B-C2B	-2.13	1.38	1.43
4	A	702	P22	PB-O1B	-2.11	1.46	1.54
5	A	701	FAD	C6A-N1A	2.05	1.46	1.37
5	A	701	FAD	C8A-N7A	-2.04	1.31	1.34
3	A	695	1CS	C4'-N3'	2.04	1.37	1.33
5	A	701	FAD	PA-O5B	-2.03	1.51	1.59
6	A	696	NHE	C4'-C3'	2.02	1.59	1.51
3	A	695	1CS	C5-C6	2.02	1.43	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	695	1CS	C4'-N3'-C2'	12.49	122.87	112.86
3	A	695	1CS	C1-C2-S7	11.88	131.02	123.25
5	A	701	FAD	C4-N3-C2	8.17	122.04	115.14
3	A	695	1CS	O7A-S7-C2	6.92	119.05	107.66
3	A	695	1CS	O7B-S7-N8	-6.87	87.42	106.74
3	A	695	1CS	O7B-S7-C2	-6.57	96.86	107.66
6	A	696	NHE	O1-S-C2	6.11	114.27	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	FAD	C1B-N9A-C4A	5.79	136.81	126.64
3	A	695	1CS	O7A-S7-N8	5.76	122.93	106.74
3	A	695	1CS	C3-C2-S7	-5.28	110.25	117.42
5	A	701	FAD	C4X-C4-N3	-5.13	116.42	123.43
3	A	695	1CS	C2'-N10-C9	-5.05	125.01	130.40
3	A	695	1CS	N8-C9-N10	-4.77	108.60	114.93
3	A	695	1CS	N3'-C2'-N1'	-4.70	118.80	126.23
6	A	696	NHE	C1-N-C1'	-4.51	105.27	114.14
4	A	702	P22	O7-C7-C6	4.29	137.41	110.97
3	A	695	1CS	N3'-C4'-N5'	-3.53	120.83	127.63
6	A	696	NHE	C2-C1-N	3.38	120.84	111.25
5	A	701	FAD	C4-C4X-C10	-3.24	117.81	119.95
5	A	701	FAD	N3A-C2A-N1A	-3.13	123.79	128.68
3	A	695	1CS	O9-C9-N10	3.12	128.91	123.62
5	A	701	FAD	O2B-C2B-C3B	2.86	121.06	111.82
5	A	701	FAD	O2B-C2B-C1B	2.67	120.71	110.85
6	A	696	NHE	O3-S-O1	-2.56	105.01	111.27
6	A	696	NHE	C3'-C2'-C1'	-2.55	106.30	111.11
5	A	701	FAD	C5B-C4B-C3B	2.54	124.69	115.18
6	A	696	NHE	O2-S-C2	2.46	109.88	106.92
3	A	695	1CS	C7'-C6'-N1'	2.35	120.81	117.15
5	A	701	FAD	C1'-N10-C9A	2.15	119.99	118.29
3	A	695	1CS	N1'-C6'-N5'	-2.11	121.84	125.72
5	A	701	FAD	C1'-C2'-C3'	2.07	115.58	109.79
6	A	696	NHE	O2-S-O1	-2.07	106.79	113.95
3	A	695	1CS	C5'-O4'-C4'	2.06	120.88	117.58
6	A	696	NHE	C6'-C1'-C2'	-2.05	107.26	110.82
3	A	695	1CS	C2'-N1'-C6'	2.05	117.84	114.61
4	A	702	P22	O3B-PB-O1B	2.01	115.31	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	695	1CS	N8-C9-N10-C2'
4	A	702	P22	C7-O7-PA-O2A
3	A	695	1CS	C9-N8-S7-O7A
3	A	695	1CS	C1-C2-S7-N8
4	A	702	P22	PB-O3A-PA-O7
4	A	702	P22	C7-O7-PA-O3A
3	A	695	1CS	O9-C9-N10-C2'
3	A	695	1CS	C3-C2-S7-N8

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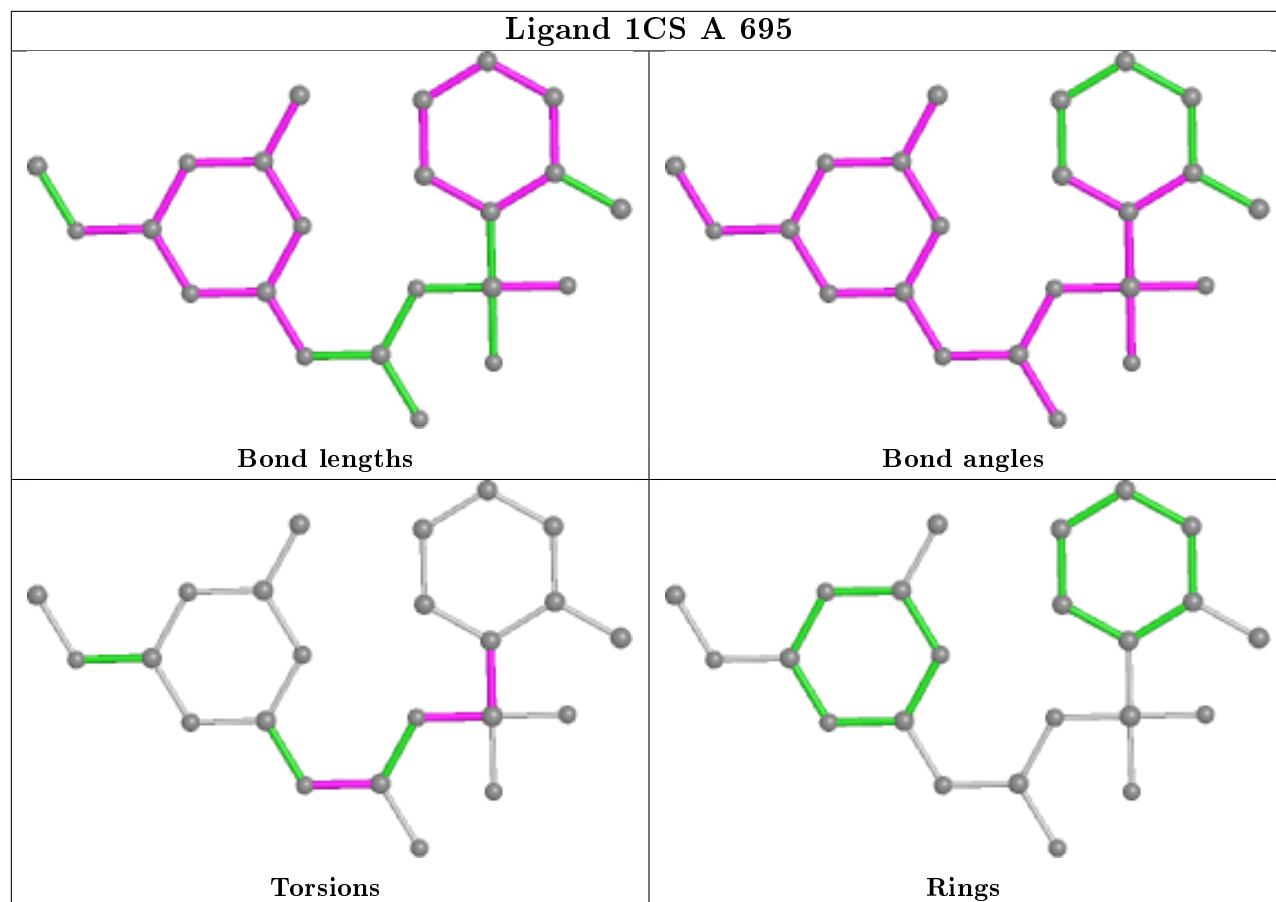
Mol	Chain	Res	Type	Atoms
6	A	696	NHE	C2'-C1'-N-C1
5	A	701	FAD	O4B-C4B-C5B-O5B

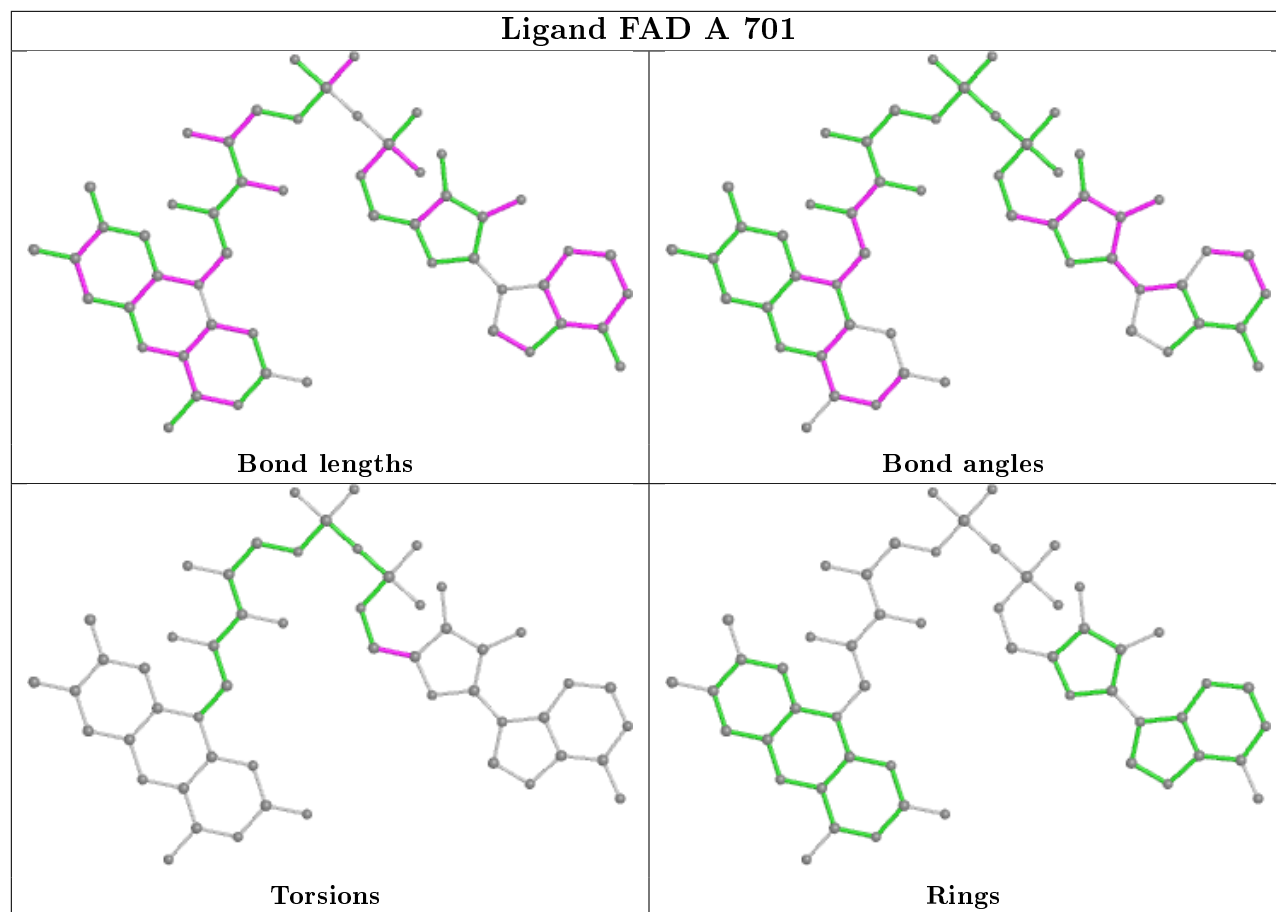
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	696	NHE	1	0
3	A	695	1CS	1	0
5	A	701	FAD	4	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, 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%)	-0.38	1 (0%) 95 96	22, 38, 63, 82	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	341	ASP	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	0.90	0.26	63,66,69,69	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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(Å <sup>2</sup> )	Q<0.9
4	P22	A	702	11/11	0.92	0.16	55,59,63,63	0

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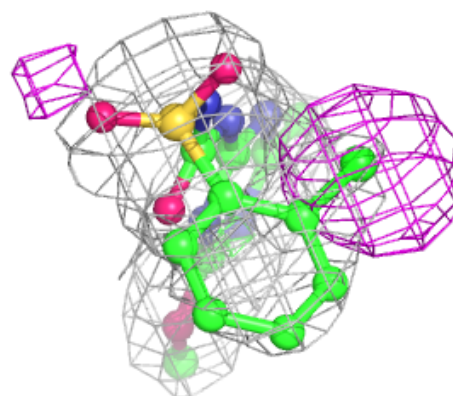
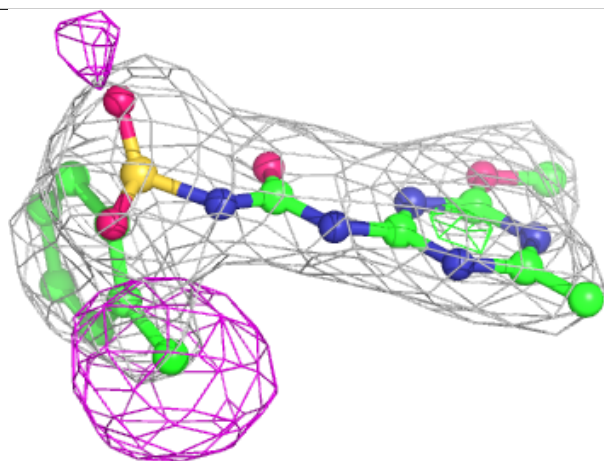
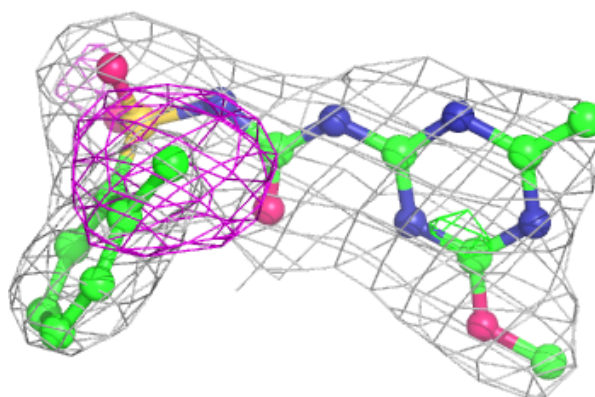
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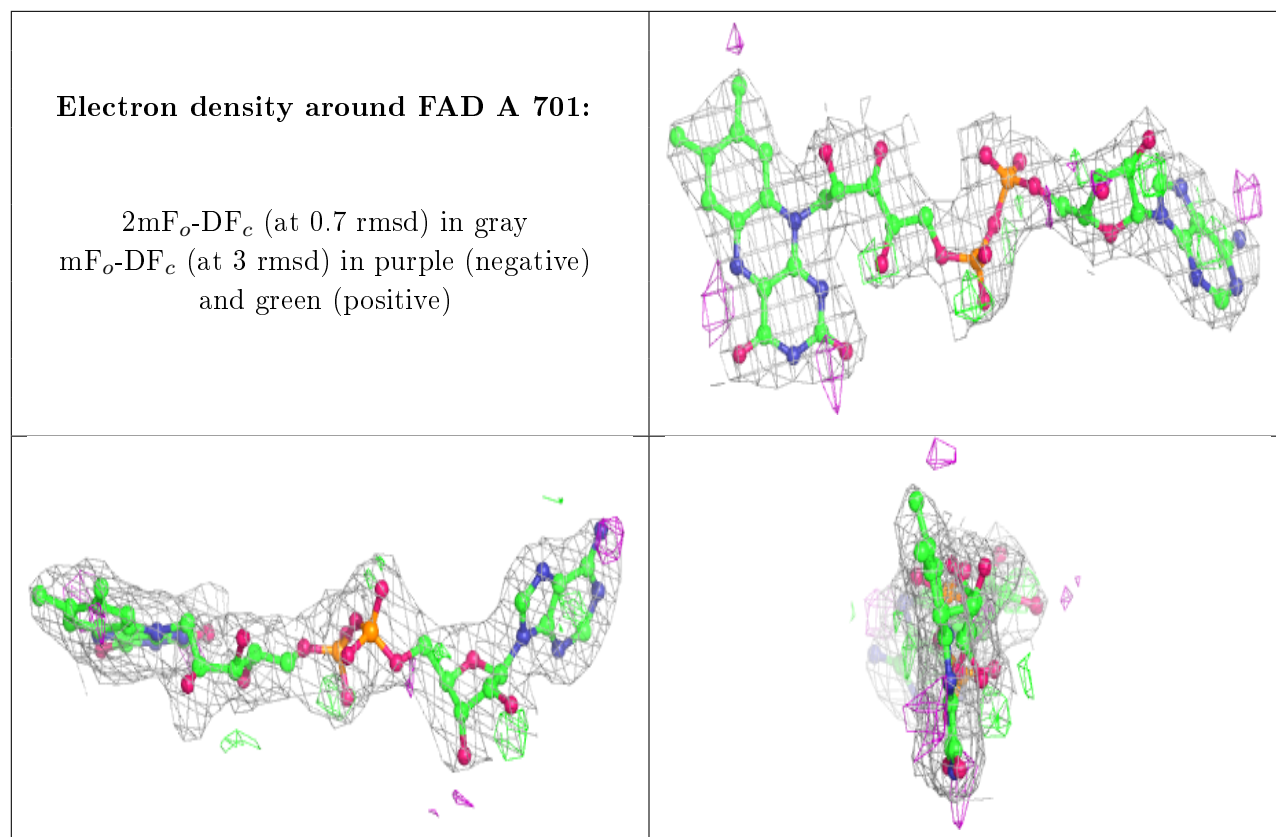
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	1CS	A	695	23/23	0.93	0.21	35,39,42,44	0
6	NHE	A	696	13/13	0.97	0.22	34,36,39,42	0
5	FAD	A	701	53/53	0.98	0.16	21,30,35,37	0
2	MG	A	699	1/1	0.98	0.05	52,52,52,52	0

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 1CS A 695:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.