



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:27 AM UTC

PDB ID : 8ET5 / pdb_00008et5
Title : Crystal structure of arabidopsis thaliana acetohydroxyacid synthase S653T mutant in complex with amidosulfuron
Authors : Guddat, L.W.; Cheng, Y.
Deposited on : 2022-10-16
Resolution : 2.94 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

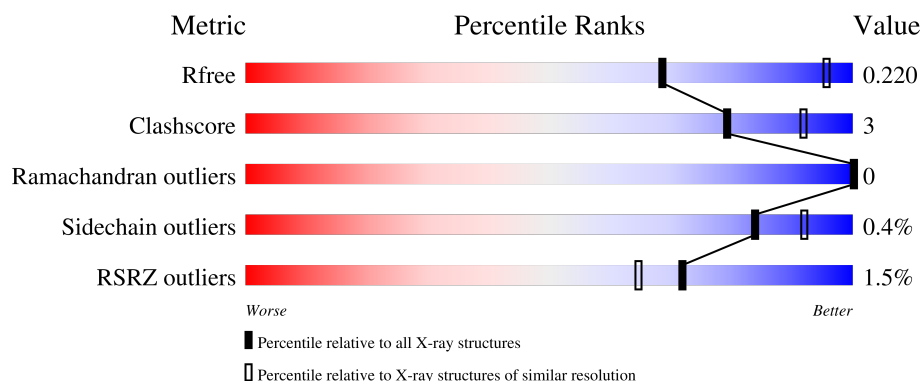
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

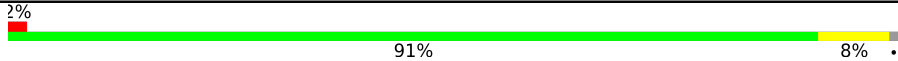
The reported resolution of this entry is 2.94 Å.

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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	

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
8	SO4	A	710	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	A	712	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4623 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
			Total	C	N	O	S			
1	A	582	4469	2835	770	839	25	0	1	0

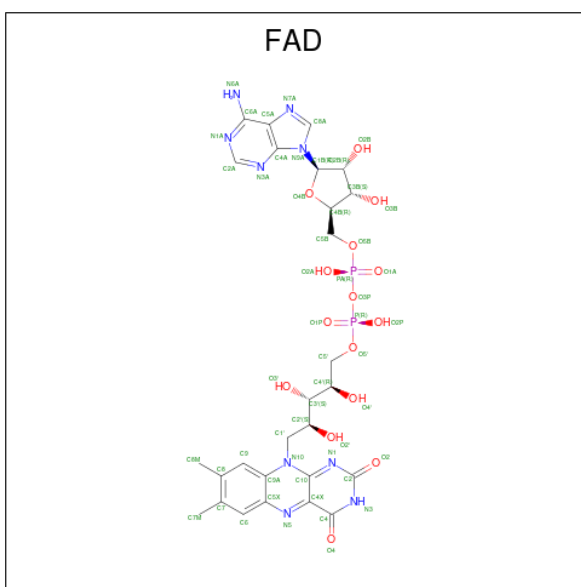
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	653	THR	SER	engineered mutation	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 (CCD ID: MG) (formula: Mg).

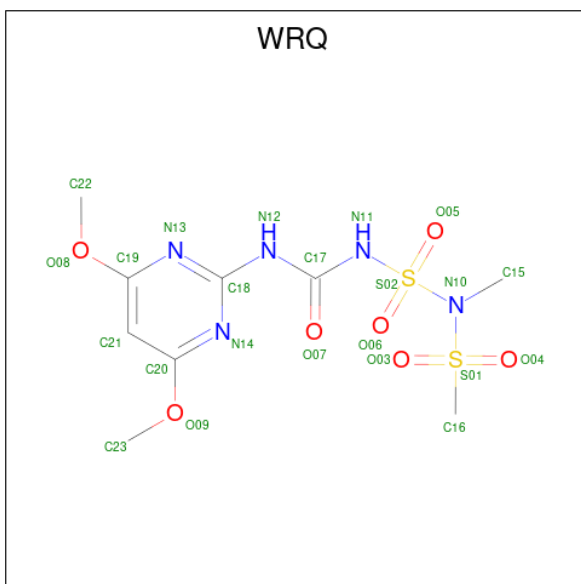
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Mg	0	0
			3	3		

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



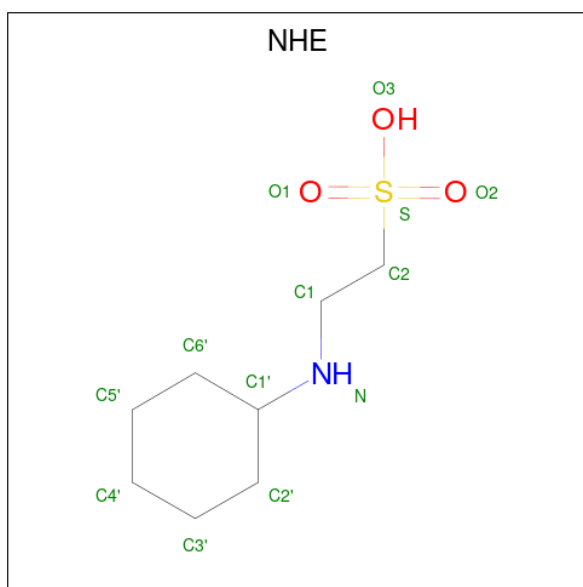
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is N-[[[(4,6-dimethoxypyrimidin-2-yl)carbamoyl]sulfamoyl]-N-methylmethanesulfonamide (CCD ID: WRQ) (formula: $C_9H_{15}N_5O_7S_2$).



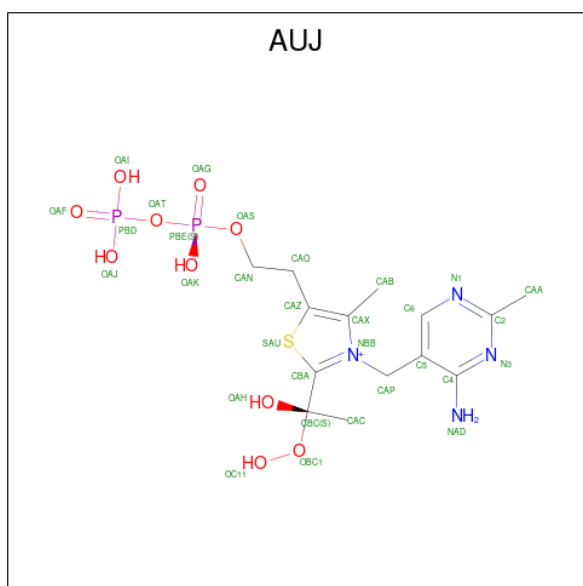
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	9	5	7	2		

- Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: $C_8H_{17}NO_3S$).



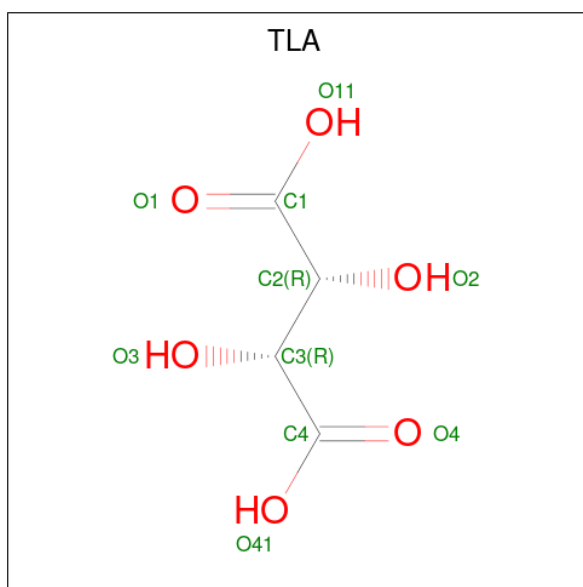
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 6 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: $C_{14}H_{23}N_4O_{10}P_2S$).



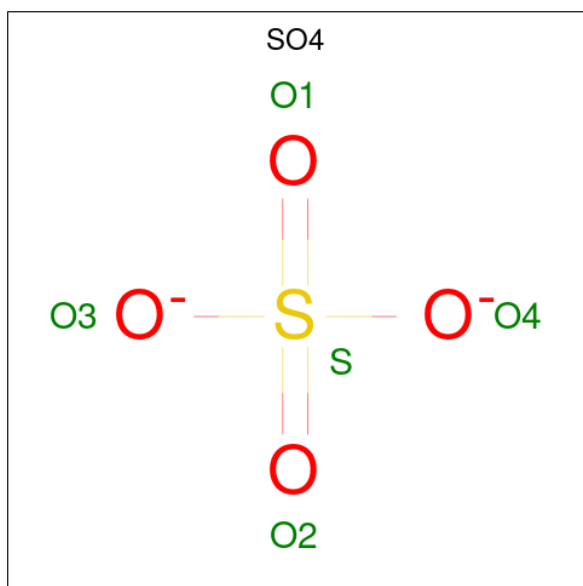
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			31	14	4	10	2	1		

- Molecule 7 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: $C_4H_6O_6$).



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

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

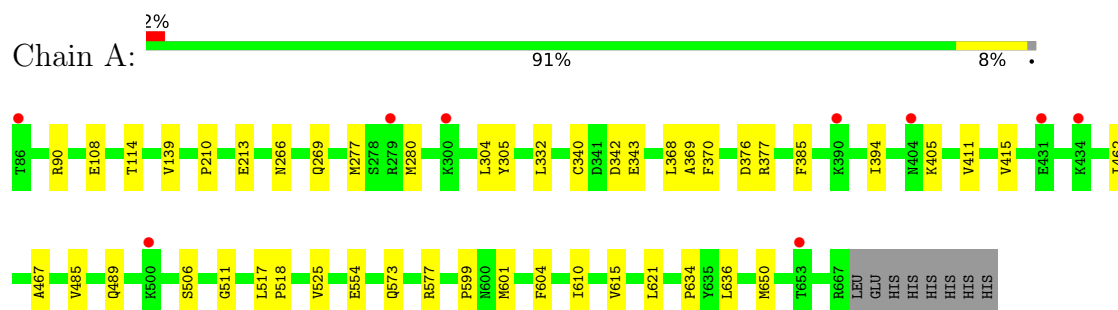
- Molecule 9 is water.

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

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	179.59Å 179.59Å 184.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 – 2.94 48.28 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.28-2.94) 99.4 (48.28-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.188 , 0.217 0.194 , 0.220	Depositor DCC
R_{free} test set	2000 reflections (5.28%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4623	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: CSD, SO4, AUJ, MG, WRQ, FAD, NHE, TLA

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	0.07	0/4557	0.22	0/6186

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	4469	0	4466	24	0
2	A	3	0	0	0	0
3	A	53	0	31	0	0
4	A	23	0	0	1	0
5	A	13	0	17	0	0
6	A	31	0	0	1	0
7	A	10	0	4	0	0
8	A	20	0	0	0	0
9	A	1	0	0	0	0
All	All	4623	0	4518	25	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 3.

All (25) 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)
6:A:705:AUI:NAD	6:A:705:AUI:OAH	2.33	0.61
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.84	0.60
1:A:305:TYR:HB3	1:A:369:ALA:HA	1.84	0.59
1:A:573:GLN:HE21	1:A:650:MET:HE2	1.70	0.55
1:A:577:ARG:HG3	1:A:650:MET:HE1	1.90	0.53
1:A:599:PRO:HD2	1:A:601:MET:HE2	1.91	0.53
1:A:489:GLN:NE2	1:A:506:SER:OG	2.40	0.52
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.92	0.51
1:A:377:ARG:NH2	4:A:703:WRQ:O07	2.42	0.51
1:A:266:ASN:HB3	1:A:269:GLN:HE21	1.76	0.50
1:A:304:LEU:HD23	1:A:368:LEU:HB2	1.94	0.48
1:A:277:MET:HA	1:A:280:MET:HG3	1.95	0.48
1:A:139:VAL:HG13	1:A:554:GLU:HG3	1.95	0.48
1:A:467:ALA:HA	1:A:621:LEU:HD21	1.96	0.46
1:A:376:ASP:OD2	1:A:377:ARG:NH1	2.48	0.46
1:A:601:MET:HA	1:A:604:PHE:HD2	1.81	0.46
1:A:485:VAL:HG21	1:A:511:GLY:C	2.40	0.45
1:A:462:ILE:HD11	1:A:615:VAL:HG22	1.98	0.44
1:A:385:PHE:O	1:A:405:LYS:HE2	2.17	0.44
1:A:342:ASP:OD1	1:A:343:GLU:N	2.52	0.43
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.01	0.43
1:A:610:ILE:HG23	1:A:634:PRO:HB2	2.00	0.42
1:A:210:PRO:HB2	1:A:213:GLU:HB2	2.01	0.42
1:A:517:LEU:HB3	1:A:518:PRO:HD3	2.03	0.40
1:A:90:ARG:NH1	1:A:108:GLU:OE2	2.54	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	580/590 (98%)	568 (98%)	12 (2%)	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	479/486 (99%)	477 (100%)	2 (0%)	84	92

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

Mol	Chain	Res	Type
1	A	332	LEU
1	A	636	LEU

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	221	HIS
1	A	428	ASN
1	A	503	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	4,7,8	1.04	0	1,8,10	8.02	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	8.02	120.38	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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	AUJ	A	705	2	27,32,32	2.25	8 (29%)	36,49,49	1.65	12 (33%)
3	FAD	A	702	-	58,58,58	2.98	24 (41%)	85,89,89	1.73	19 (22%)
8	SO4	A	709	-	4,4,4	0.23	0	6,6,6	0.08	0
8	SO4	A	710	-	4,4,4	0.24	0	6,6,6	0.07	0
8	SO4	A	712	-	4,4,4	0.23	0	6,6,6	0.09	0
7	TLA	A	706	-	9,9,9	1.04	0	12,12,12	1.27	2 (16%)
5	NHE	A	704	-	13,13,13	1.34	3 (23%)	16,17,17	1.80	5 (31%)
8	SO4	A	711	-	4,4,4	0.24	0	6,6,6	0.08	0
4	WRQ	A	703	-	20,23,23	2.54	12 (60%)	28,34,34	3.04	11 (39%)

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	AUJ	A	705	2	-	9/20/26/26	0/2/2/2
3	FAD	A	702	-	-	6/34/50/50	0/6/6/6
7	TLA	A	706	-	-	6/12/12/12	-
5	NHE	A	704	-	-	4/7/15/15	0/1/1/1
4	WRQ	A	703	-	-	8/23/25/25	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	O4-C4	9.21	1.41	1.23
3	A	702	FAD	PA-O3P	8.88	1.69	1.59
3	A	702	FAD	P-O3P	8.66	1.68	1.59
3	A	702	FAD	O2-C2	8.00	1.40	1.24
6	A	705	AUJ	C5-C4	5.29	1.51	1.42
4	A	703	WRQ	C18-N12	5.11	1.45	1.38
6	A	705	AUJ	CAP-NBB	-4.96	1.42	1.47
6	A	705	AUJ	C2-N3	4.96	1.42	1.34
3	A	702	FAD	C6A-N6A	4.63	1.46	1.34
3	A	702	FAD	O4B-C1B	-4.38	1.31	1.42
3	A	702	FAD	C2B-C1B	4.08	1.66	1.53
6	A	705	AUJ	C6-N1	3.94	1.42	1.34
3	A	702	FAD	C5B-C4B	-3.72	1.40	1.51
4	A	703	WRQ	C17-N12	3.65	1.45	1.37
4	A	703	WRQ	O06-S02	3.48	1.46	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	WRQ	O05-S02	3.44	1.46	1.43
4	A	703	WRQ	O08-C19	3.23	1.40	1.35
3	A	702	FAD	O4B-C4B	3.16	1.52	1.45
3	A	702	FAD	C4-N3	-3.15	1.33	1.38
6	A	705	AUJ	C4-NAD	3.13	1.42	1.34
4	A	703	WRQ	S01-N10	3.11	1.71	1.68
3	A	702	FAD	O3B-C3B	3.11	1.50	1.43
4	A	703	WRQ	O09-C20	3.11	1.40	1.35
5	A	704	NHE	C2-S	3.09	1.81	1.77
6	A	705	AUJ	C4-N3	-3.09	1.30	1.35
3	A	702	FAD	C8A-N9A	-3.00	1.32	1.37
3	A	702	FAD	C9A-N10	-2.95	1.36	1.41
3	A	702	FAD	C3B-C4B	2.88	1.60	1.53
3	A	702	FAD	C5'-C4'	2.76	1.55	1.51
4	A	703	WRQ	C17-N11	2.71	1.45	1.39
4	A	703	WRQ	C16-S01	2.66	1.81	1.75
3	A	702	FAD	C1'-C2'	2.65	1.56	1.52
3	A	702	FAD	C2-N3	-2.51	1.33	1.39
3	A	702	FAD	P-O5'	2.47	1.69	1.59
3	A	702	FAD	C5A-N7A	-2.38	1.34	1.39
3	A	702	FAD	PA-O5B	2.37	1.68	1.59
6	A	705	AUJ	CAX-NBB	2.29	1.43	1.40
3	A	702	FAD	O4'-C4'	-2.27	1.38	1.43
5	A	704	NHE	O2-S	2.25	1.51	1.45
5	A	704	NHE	O1-S	2.25	1.51	1.45
3	A	702	FAD	C5X-N5	-2.20	1.35	1.39
4	A	703	WRQ	O03-S01	2.20	1.46	1.43
3	A	702	FAD	C4X-N5	2.20	1.35	1.30
3	A	702	FAD	O2B-C2B	2.10	1.48	1.43
4	A	703	WRQ	O04-S01	2.10	1.46	1.43
4	A	703	WRQ	O07-C17	-2.07	1.19	1.23
6	A	705	AUJ	C2-N1	-2.06	1.31	1.34

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	WRQ	C18-N12-C17	-9.97	120.08	130.34
4	A	703	WRQ	C20-C21-C19	5.30	119.79	115.20
3	A	702	FAD	C5A-C4A-N3A	-5.22	119.53	126.72
3	A	702	FAD	N3A-C2A-N1A	-4.97	121.06	128.58
4	A	703	WRQ	C18-N13-C19	4.68	120.35	115.00
4	A	703	WRQ	C18-N14-C20	4.44	120.07	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	O2'-C2'-C3'	4.11	118.88	109.25
5	A	704	NHE	O3-S-O2	-4.11	101.12	111.40
4	A	703	WRQ	N14-C18-N13	-3.82	120.00	126.26
4	A	703	WRQ	C21-C19-N13	-3.78	119.74	124.16
3	A	702	FAD	C2A-N3A-C4A	3.73	120.94	111.83
3	A	702	FAD	N3A-C4A-N9A	3.71	133.48	127.17
3	A	702	FAD	C4A-C5A-N7A	-3.63	106.43	110.58
3	A	702	FAD	N9A-C8A-N7A	-3.55	108.90	113.94
3	A	702	FAD	C5A-N7A-C8A	3.53	109.00	103.45
4	A	703	WRQ	C21-C20-N14	-3.52	120.05	124.16
3	A	702	FAD	C1'-C2'-C3'	3.46	119.05	109.66
6	A	705	AUJ	C6-N1-C2	3.26	121.42	116.07
5	A	704	NHE	O2-S-C2	3.16	111.50	106.73
4	A	703	WRQ	N11-C17-N12	3.14	119.86	114.87
6	A	705	AUJ	SAU-CBA-NBB	-2.90	109.40	112.24
3	A	702	FAD	C4-N3-C2	-2.87	120.55	125.64
3	A	702	FAD	C4X-C10-N10	2.84	120.55	116.48
3	A	702	FAD	C4A-N9A-C8A	2.82	108.69	105.74
6	A	705	AUJ	C5-C6-N1	-2.65	119.53	123.83
6	A	705	AUJ	N1-C2-N3	-2.64	121.13	125.53
3	A	702	FAD	C4-C4X-N5	2.64	121.85	118.21
6	A	705	AUJ	CAO-CAZ-SAU	2.56	124.79	119.29
3	A	702	FAD	C4X-C4-N3	2.52	119.67	113.25
6	A	705	AUJ	OAI-PBD-OAF	-2.50	101.11	110.83
6	A	705	AUJ	OAK-PBE-OAG	-2.49	100.84	112.44
4	A	703	WRQ	C16-S01-N10	2.49	107.57	105.39
5	A	704	NHE	O3-S-C2	2.49	110.87	106.00
4	A	703	WRQ	O04-S01-N10	2.41	110.12	106.28
6	A	705	AUJ	OAI-PBD-OAT	2.39	112.65	104.64
7	A	706	TLA	O41-C4-C3	2.38	119.93	113.31
7	A	706	TLA	O11-C1-C2	2.37	119.91	113.31
3	A	702	FAD	O4-C4-C4X	-2.36	120.30	126.53
5	A	704	NHE	C1-N-C1'	-2.36	109.64	114.18
4	A	703	WRQ	C23-O09-C20	-2.34	113.85	117.33
5	A	704	NHE	O1-S-C2	2.33	110.25	106.73
3	A	702	FAD	C4'-C3'-C2'	-2.30	109.75	113.57
3	A	702	FAD	O2'-C2'-C1'	2.19	119.19	110.20
6	A	705	AUJ	C6-C5-C4	2.14	118.18	115.55
3	A	702	FAD	C10-C4X-N5	-2.14	120.43	124.81
6	A	705	AUJ	NAD-C4-N3	2.12	119.89	117.03
6	A	705	AUJ	CAA-C2-N1	2.08	119.42	117.20
3	A	702	FAD	C9A-N10-C10	-2.06	117.61	120.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	705	AUJ	OAK-PBE-OAT	2.02	112.72	107.27

There are no chirality outliers.

All (33) torsion outliers are listed below:

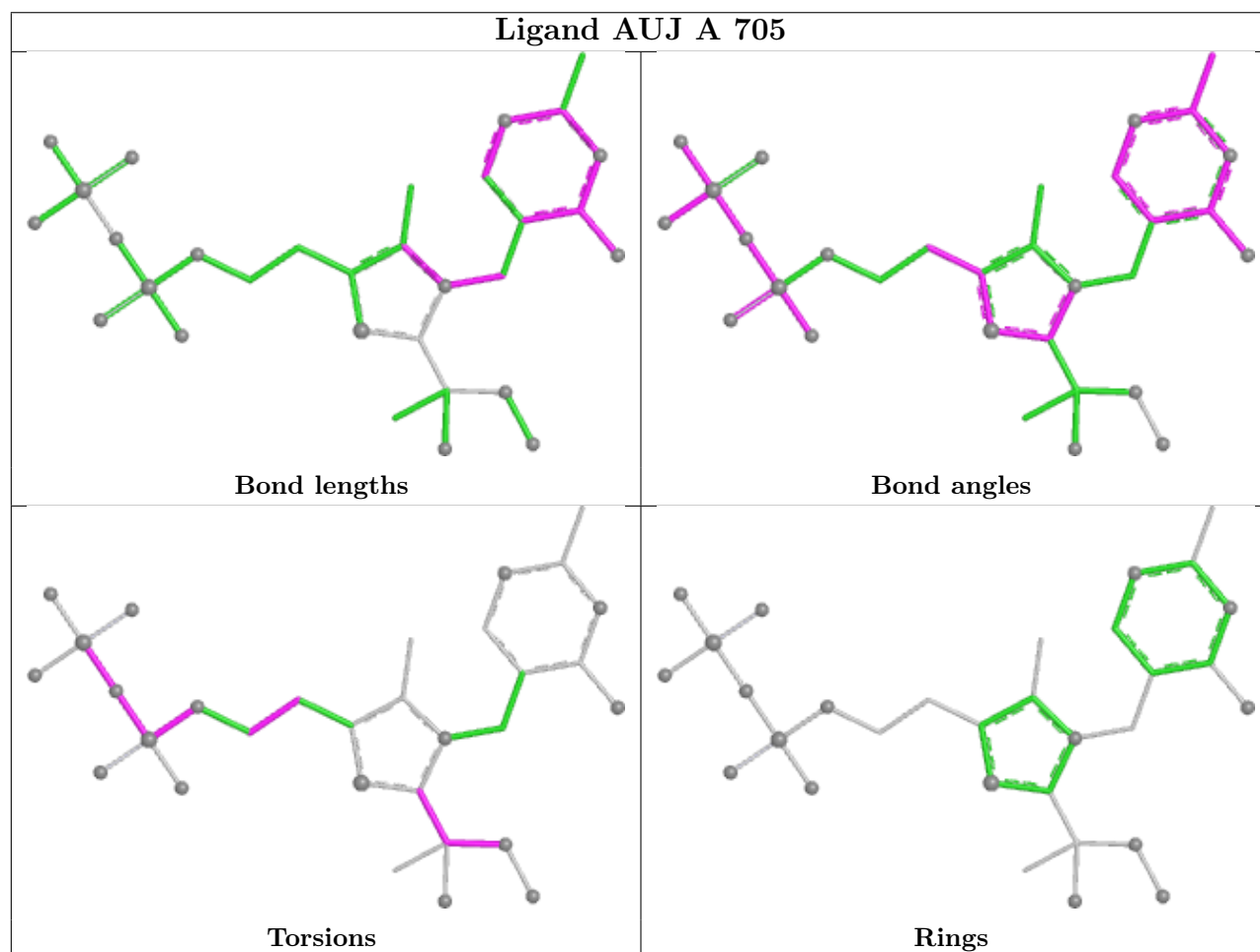
Mol	Chain	Res	Type	Atoms
3	A	702	FAD	N10-C1'-C2'-C3'
3	A	702	FAD	O2'-C2'-C3'-O3'
3	A	702	FAD	O2'-C2'-C3'-C4'
3	A	702	FAD	C3'-C4'-C5'-O5'
3	A	702	FAD	O4'-C4'-C5'-O5'
4	A	703	WRQ	N13-C18-N12-C17
4	A	703	WRQ	N14-C18-N12-C17
4	A	703	WRQ	C15-N10-S02-O06
4	A	703	WRQ	S01-N10-S02-O06
5	A	704	NHE	C2-C1-N-C1'
6	A	705	AUJ	PBE-OAT-PBD-OAI
6	A	705	AUJ	SAU-CBA-CBC-CAC
6	A	705	AUJ	CAC-CBC-OBC1-OC11
7	A	706	TLA	O1-C1-C2-O2
7	A	706	TLA	O11-C1-C2-O2
4	A	703	WRQ	N13-C19-O08-C22
7	A	706	TLA	O2-C2-C3-O3
7	A	706	TLA	O3-C3-C4-O4
7	A	706	TLA	O3-C3-C4-O41
4	A	703	WRQ	C21-C19-O08-C22
7	A	706	TLA	C1-C2-C3-C4
6	A	705	AUJ	PBD-OAT-PBE-OAG
5	A	704	NHE	C1-C2-S-O2
6	A	705	AUJ	OAS-CAN-CAO-CAZ
6	A	705	AUJ	CAN-OAS-PBE-OAG
6	A	705	AUJ	CAN-OAS-PBE-OAK
6	A	705	AUJ	CAN-OAS-PBE-OAT
5	A	704	NHE	C1-C2-S-O1
3	A	702	FAD	C4B-C5B-O5B-PA
6	A	705	AUJ	PBE-OAT-PBD-OAF
4	A	703	WRQ	N11-C17-N12-C18
5	A	704	NHE	N-C1-C2-S
4	A	703	WRQ	O07-C17-N12-C18

There are no ring outliers.

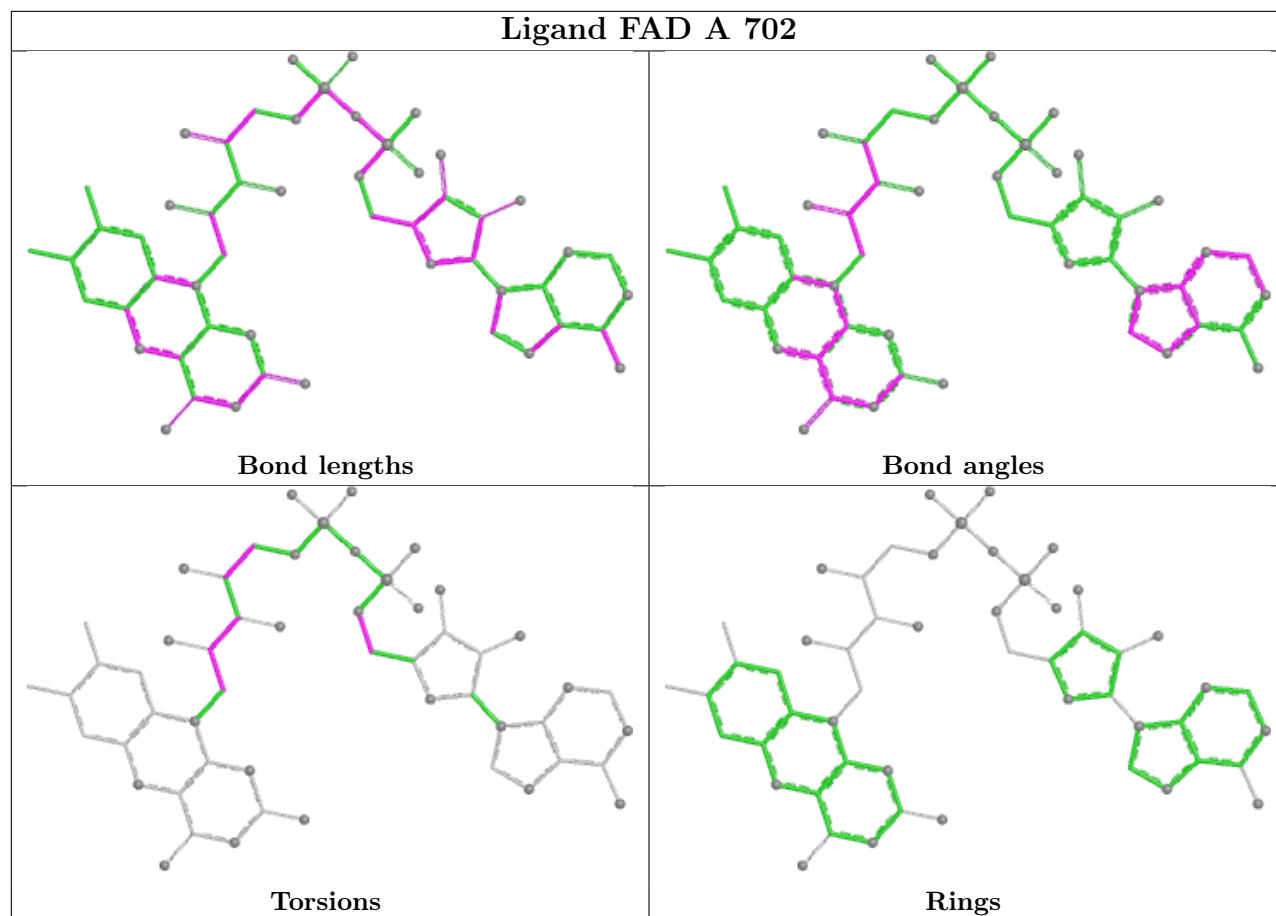
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	705	AUJ	1	0
4	A	703	WRQ	1	0

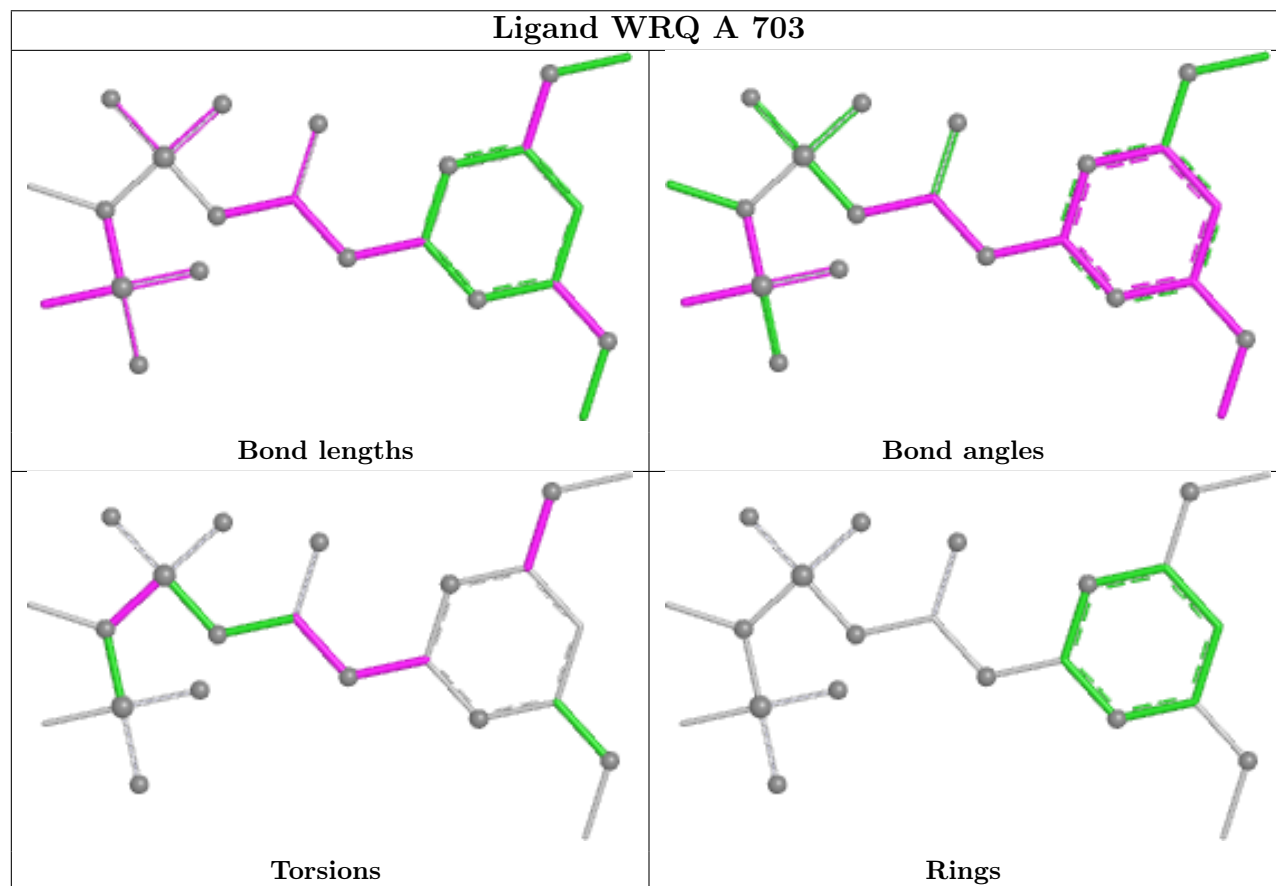
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand FAD A 702



Ligand WRQ A 703



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%)	-0.02	9 (1%) 72 65	29, 57, 86, 111	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	3.5
1	A	653	THR	3.1
1	A	431	GLU	3.0
1	A	300	LYS	2.4
1	A	500	LYS	2.2
1	A	434	LYS	2.1
1	A	404	ASN	2.0
1	A	279	ARG	2.0
1	A	390	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, 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	0.90	0.15	49,78,87,103	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

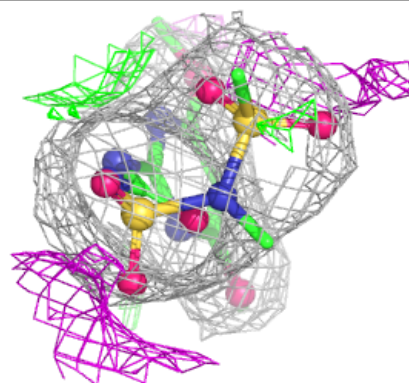
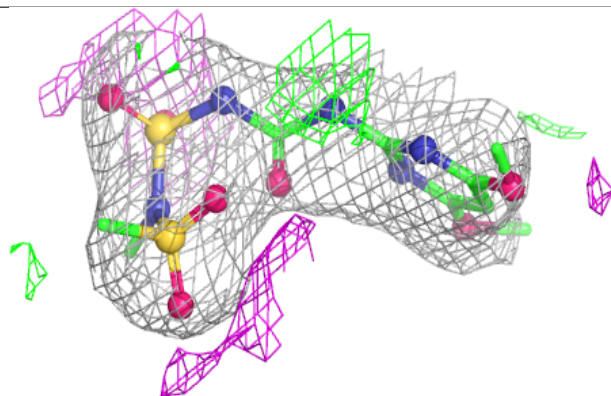
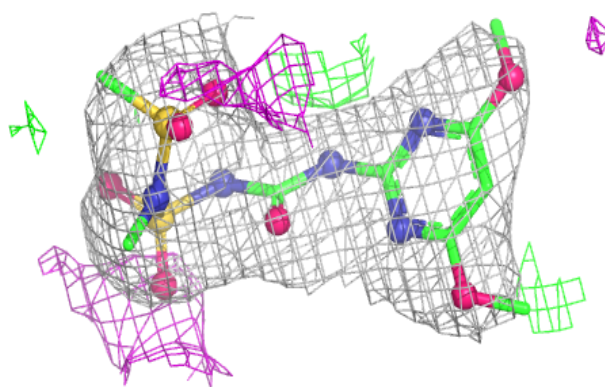
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	SO4	A	712	5/5	0.55	0.46	79,85,106,158	5
8	SO4	A	710	5/5	0.56	0.48	101,110,117,152	5
7	TLA	A	706	10/10	0.76	0.26	91,104,127,135	0
8	SO4	A	711	5/5	0.79	0.23	87,88,109,129	5
2	MG	A	708	1/1	0.79	0.24	82,82,82,82	1
8	SO4	A	709	5/5	0.93	0.28	85,92,111,121	5
4	WRQ	A	703	23/23	0.95	0.11	43,60,69,73	1
5	NHE	A	704	13/13	0.96	0.11	48,60,83,86	0
3	FAD	A	702	53/53	0.96	0.08	35,51,66,70	0
6	AUJ	A	705	31/31	0.97	0.10	36,48,61,72	4
2	MG	A	707	1/1	0.97	0.10	36,36,36,36	1
2	MG	A	701	1/1	1.00	0.03	51,51,51,51	0

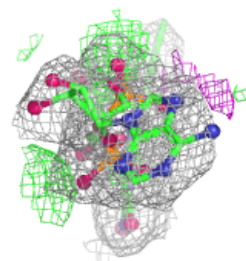
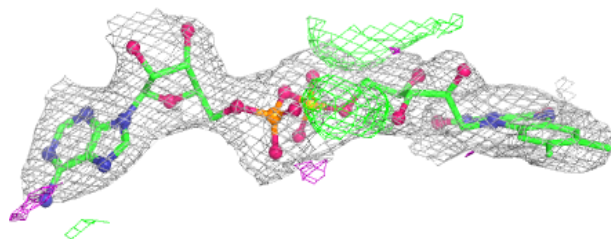
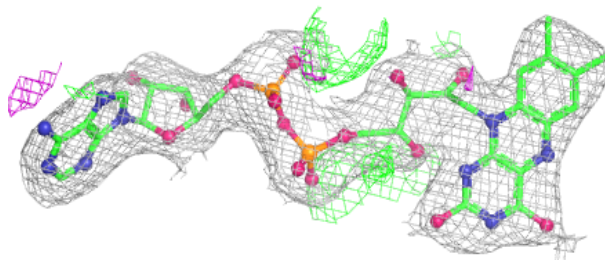
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WRQ 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)

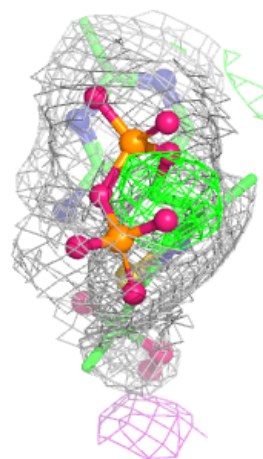
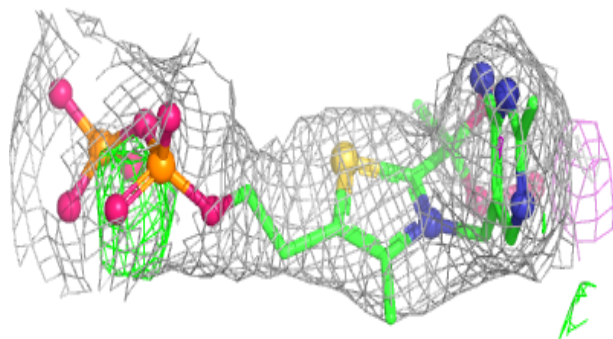
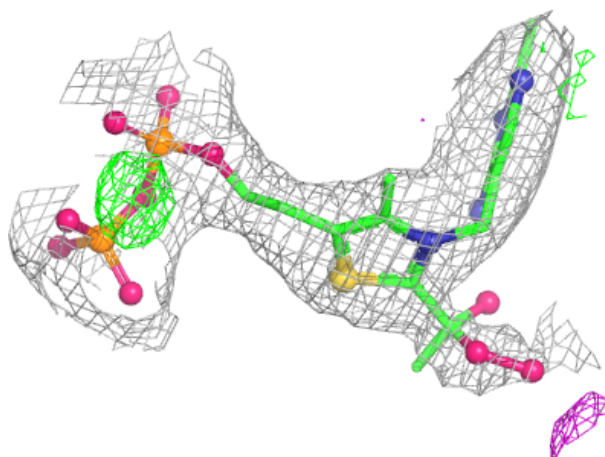
**Electron density around FAD A 702:**

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



Electron density around AUJ A 705:

$2mF_o-DF_c$ (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.