

Full wwPDB X-ray Structure Validation Report (i)

Oct 15, 2023 – 05:33 AM EDT

PDB ID : 8ET5

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 (i) 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 (1)) 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 : 2.36

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

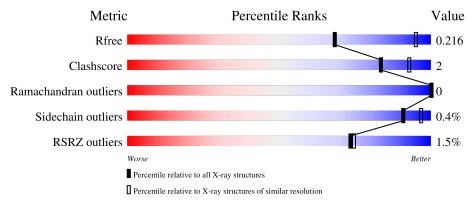
Validation Pipeline (wwPDB-VP) : 2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

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.



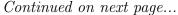
Metric	Whole archive $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\AA)}) \end{array}$
R_{free}	130704	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	708	-	-	-	X





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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	A	710	-	-	-	X
8	SO4	A	711	-	-	-	X
8	SO4	A	712	-	-	-	X



2 Entry composition (i)

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		At	oms			ZeroOcc	AltConf	Trace
1	Λ	582	Total	С	N	О	S	0	1	0
1	Λ	362	4469	2835	770	839	25	0	1	0

There are 9 discrepancies between the modelled and reference sequences:

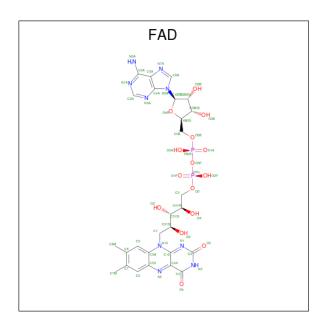
Chain	Residue	Modelled	Actual	Comment	Reference
A	653	THR	SER	engineered mutation	UNP P17597
A	668	LEU	-	expression tag	UNP P17597
A	669	GLU	-	expression tag	UNP P17597
A	670	HIS	-	expression tag	UNP P17597
A	671	HIS	-	expression tag	UNP P17597
A	672	HIS	-	expression tag	UNP P17597
A	673	HIS	-	expression tag	UNP P17597
A	674	HIS	-	expression tag	UNP P17597
A	675	HIS	-	expression tag	UNP P17597

• Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

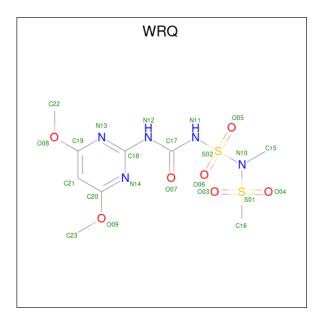
• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





Mo	Chain	Residues		Atoms					AltConf
3	A	1	Total 53	C 27		O 15	P 2	0	0

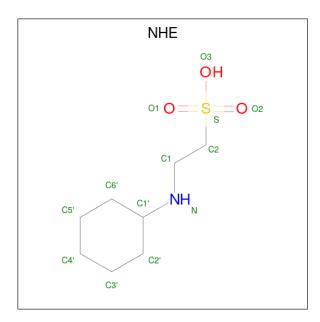
• Molecule 4 is N-{[(4,6-dimethoxypyrimidin-2-yl)carbamoyl]sulfamoyl}-N-methylmethanesul fonamide (three-letter code: WRQ) (formula: $C_9H_{15}N_5O_7S_2$).



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

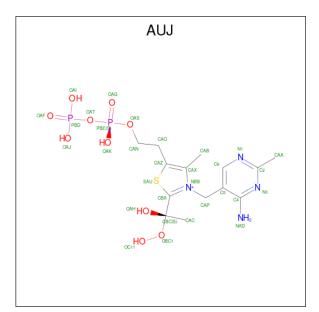
 \bullet Molecule 5 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: C₈H₁₇NO₃S).





Mol	Chain	Residues		Atoms					AltConf
5	Λ	1	Total	С	N	О	S	0	0
9	A	1	13	8	1	3	1	0	0

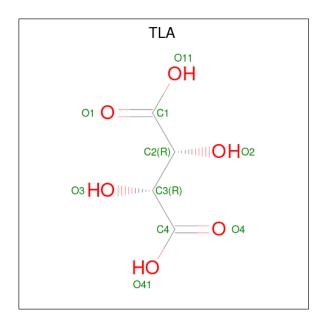
• Molecule 6 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 $\{S\}$)-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (three-letter code: AUJ) (formula: $C_{14}H_{23}N_4O_{10}P_2S$).



Mol	Chain	Residues		A	ton	ıs			ZeroOcc	AltConf
6	A	1	Total	C 14	N 4	O 10	P	S	0	0
			91	14	4	10	2	T		

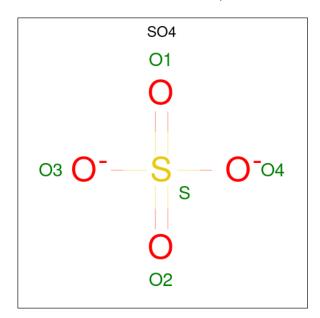
• Molecule 7 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: $C_4H_6O_6$).





Mol	Chain	Residues	Ato	$\overline{\mathbf{m}}$		ZeroOcc	AltConf
7	A	1	Total 10	C 4	O 6	0	0

 \bullet Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



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



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

• Molecule 9 is water.

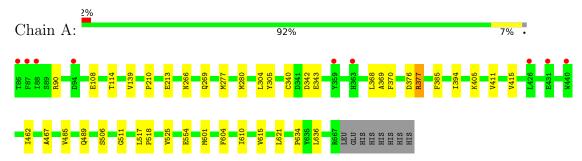
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total O 1 1	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Acetolactate synthase, chloroplastic





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants	179.59Å 179.59Å 184.77Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.28 - 2.94	Depositor
Resolution (A)	48.28 - 2.94	EDS
% Data completeness	99.5 (48.28-2.94)	Depositor
(in resolution range)	99.5 (48.28-2.94)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.68 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.188 , 0.217	Depositor
R, R_{free}	0.188 , 0.216	DCC
R_{free} test set	1998 reflections (5.31%)	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, 38.0	EDS
L-test for twinning ²	$ < L >=0.52, < L^2>=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.

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



¹Intensities estimated from amplitudes.

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: MG, WRQ, CSD, SO4, AUJ, TLA, FAD, NHE

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		
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.24	0/4557	0.46	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	21	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	22	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 (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${f distance}({ m \AA})$	overlap (Å)
6:A:705:AUJ:NAD	6:A:705:AUJ: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: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: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:485:VAL:HG21	1:A:511:GLY:C	2.40	0.41
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 (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	Perce	ntiles
1	A	580/590 (98%)	568 (98%)	12 (2%)	0	100	100



There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	$\begin{array}{c c} \operatorname{Analysed} & \operatorname{Rotameric} & \operatorname{C} \end{array}$		Outliers	Percentiles
1	A	479/486 (99%)	477 (100%)	2 (0%)	91 97

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

Mol	Chain	Res	Type
1	A	377	ARG
1	A	636	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	503	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		e Chain Res		Chain	Pog	Link	В	ond leng	${ m gths}$	F	Bond an	gles
MIOI	туре	nes	Lilik		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2		
1	CSD	A	340	1	3,7,8	1.08	0	1,8,10	7.80	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	$Observed(^o)$	$Ideal(^{o})$
1	A	340	CSD	OD1-SG-CB	7.80	120.38	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 monosaccharides 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).

Mal	Mol Type Chain Res L		Tiple	Bond lengths			Bond angles			
IVIOI	Туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	WRQ	A	703	-	20,23,23	2.57	12 (60%)	29,34,34	2.98	12 (41%)



Mol	Tuno	Chain	Res	Link	В	Bond lengths			Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
8	SO4	A	709	-	4,4,4	0.14	0	6,6,6	0.05	0	
8	SO4	A	710	-	4,4,4	0.14	0	6,6,6	0.05	0	
8	SO4	A	711	_	4,4,4	0.14	0	6,6,6	0.05	0	
6	AUJ	A	705	2	25,32,32	2.13	6 (24%)	30,49,49	1.91	11 (36%)	
5	NHE	A	704	-	13,13,13	1.32	3 (23%)	16,17,17	1.97	5 (31%)	
3	FAD	A	702	-	53,58,58	2.82	20 (37%)	68,89,89	1.55	14 (20%)	
8	SO4	A	712	-	4,4,4	0.14	0	6,6,6	0.06	0	
7	TLA	A	706	-	9,9,9	1.00	0	12,12,12	1.29	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
4	WRQ	A	703	-	-	8/23/25/25	0/1/1/1
6	AUJ	A	705	2	-	9/17/26/26	0/2/2/2
5	NHE	A	704	-	-	4/7/15/15	0/1/1/1
3	FAD	A	702	-	-	7/30/50/50	0/6/6/6
7	TLA	A	706	-	-	6/12/12/12	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$Ideal(\AA)$
3	A	702	FAD	O4-C4	9.18	1.41	1.23
3	A	702	FAD	O2-C2	8.61	1.40	1.24
3	A	702	FAD	C2B-C1B	8.28	1.66	1.53
3	A	702	FAD	O4B-C1B	-6.60	1.31	1.41
4	A	703	WRQ	C18-N12	5.16	1.45	1.38
6	A	705	AUJ	C5-C4	5.06	1.51	1.42
6	A	705	AUJ	C2-N3	4.80	1.42	1.34
4	A	703	WRQ	C17-N12	3.85	1.45	1.37
6	A	705	AUJ	C6-N1	3.80	1.42	1.34
4	A	703	WRQ	O06-S02	3.65	1.46	1.43
4	A	703	WRQ	O05-S02	3.60	1.46	1.43
3	A	702	FAD	C5B-C4B	-3.59	1.40	1.51
3	A	702	FAD	C6A-N6A	3.28	1.46	1.34
3	A	702	FAD	O3B-C3B	3.26	1.50	1.43
6	A	705	AUJ	CBA-NBB	3.24	1.42	1.35
6	A	705	AUJ	C4-NAD	3.21	1.42	1.34



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	Observed(A)	$Ideal(\AA)$
4	A	703	WRQ	O08-C19	3.18	1.40	1.35
3	A	702	FAD	C4-N3	-3.17	1.33	1.38
3	A	702	FAD	O4B-C4B	3.13	1.52	1.45
4	A	703	WRQ	S01-N10	3.11	1.71	1.68
5	A	704	NHE	C2-S	3.10	1.81	1.77
4	A	703	WRQ	O09-C20	3.06	1.40	1.35
6	A	705	AUJ	C4-N3	-2.90	1.30	1.35
3	A	702	FAD	C9A-N10	-2.89	1.36	1.41
3	A	702	FAD	C3B-C4B	2.85	1.60	1.53
3	A	702	FAD	C5'-C4'	2.66	1.55	1.51
4	A	703	WRQ	C17-N11	2.65	1.45	1.39
3	A	702	FAD	C1'-C2'	2.62	1.56	1.52
4	A	703	WRQ	C16-S01	2.57	1.81	1.75
3	A	702	FAD	C4X-N5	2.45	1.35	1.30
3	A	702	FAD	P-O5'	2.41	1.69	1.59
3	A	702	FAD	C2-N3	-2.39	1.33	1.39
3	A	702	FAD	PA-O5B	2.32	1.68	1.59
3	A	702	FAD	O4'-C4'	-2.25	1.38	1.43
4	A	703	WRQ	O03-S01	2.23	1.46	1.43
3	A	702	FAD	O2B-C2B	2.20	1.48	1.43
5	A	704	NHE	O2-S	2.18	1.51	1.45
5	A	704	NHE	O1-S	2.18	1.51	1.45
4	A	703	WRQ	O04-S01	2.13	1.46	1.43
4	A	703	WRQ	O07-C17	-2.11	1.19	1.23
3	A	702	FAD	C5X-N5	-2.11	1.35	1.39

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	703	WRQ	C18-N12-C17	-9.68	120.08	130.40
6	A	705	AUJ	CAO-CAZ-CAX	-5.07	123.36	127.43
4	A	703	WRQ	C20-C21-C19	5.04	119.79	115.21
3	A	702	FAD	N3A-C2A-N1A	-4.87	121.06	128.68
4	A	703	WRQ	C18-N13-C19	4.56	120.35	114.99
4	A	703	WRQ	C18-N14-C20	4.32	120.08	114.99
5	A	704	NHE	O3-S-O2	-4.16	101.11	111.27
3	A	702	FAD	O2'-C2'-C3'	4.02	118.88	109.10
4	A	703	WRQ	N14-C18-N13	-3.94	119.99	126.23
3	A	702	FAD	O2'-C2'-C1'	3.88	119.19	109.80
5	A	704	NHE	O2-S-C2	3.81	111.50	106.92
4	A	703	WRQ	N11-C17-N12	3.72	119.86	114.93
4	A	703	WRQ	C21-C19-N13	-3.72	119.74	124.08



 $Continued\ from\ previous\ page...$

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
4	A	703	WRQ	C21-C20-N14	-3.46	120.05	124.08
3	A	702	FAD	C1'-C2'-C3'	3.31	119.05	109.79
6	A	705	AUJ	C6-N1-C2	3.21	121.42	115.96
5	A	704	NHE	O3-S-C2	3.16	110.87	105.77
6	A	705	AUJ	CAZ-CAX-NBB	2.95	113.84	107.66
3	A	702	FAD	C4A-C5A-N7A	-2.85	106.43	109.40
3	A	702	FAD	C4X-C10-N10	2.79	120.55	116.48
5	A	704	NHE	O1-S-C2	2.77	110.25	106.92
3	A	702	FAD	C4-N3-C2	-2.76	120.55	125.64
6	A	705	AUJ	C5-C6-N1	-2.58	119.53	123.82
3	A	702	FAD	P-O3P-PA	-2.57	124.01	132.83
6	A	705	AUJ	N1-C2-N3	-2.56	121.13	125.54
3	A	702	FAD	C4X-C4-N3	2.55	119.67	113.19
3	A	702	FAD	C4-C4X-N5	2.54	121.85	118.23
4	A	703	WRQ	C16-S01-N10	2.49	107.57	105.39
7	A	706	TLA	O41-C4-C3	2.46	119.93	113.27
7	A	706	TLA	O11-C1-C2	2.46	119.91	113.27
6	A	705	AUJ	OAI-PBD-OAF	-2.45	101.11	110.68
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
3	A	702	FAD	O4-C4-C4X	-2.38	120.30	126.60
6	A	705	AUJ	OAK-PBE-OAG	-2.31	100.84	112.24
5	A	704	NHE	C1-N-C1'	-2.29	109.64	114.14
6	A	705	AUJ	CAB-CAX-CAZ	-2.24	122.70	127.60
4	A	703	WRQ	C23-O09-C20	-2.24	113.85	117.36
4	A	703	WRQ	O06-S02-O05	-2.18	116.53	119.72
3	A	702	FAD	C4X-C10-N1	-2.14	119.77	124.73
3	A	702	FAD	C10-C4X-N5	-2.09	120.43	124.86
6	A	705	AUJ	CAA-C2-N1	2.07	119.42	117.14
3	A	702	FAD	C9A-N10-C10	-2.02	117.61	120.77
6	A	705	AUJ	NAD-C4-N3	2.02	119.89	117.03

There are no chirality outliers.

All (34) 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	N11-C17-N12-C18



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Mol	Chain	Res	Type	Atoms
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	OAS-CAN-CAO-CAZ
6	A	705	AUJ	CAN-CAO-CAZ-CAX
6	A	705	AUJ	CAN-OAS-PBE-OAT
6	A	705	AUJ	PBE-OAT-PBD-OAI
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
6	A	705	AUJ	CAN-OAS-PBE-OAG
6	A	705	AUJ	CAN-OAS-PBE-OAK
5	A	704	NHE	C1-C2-S-O2
4	A	703	WRQ	O07-C17-N12-C18
3	A	702	FAD	C4B-C5B-O5B-PA
6	A	705	AUJ	PBE-OAT-PBD-OAF
5	A	704	NHE	N-C1-C2-S
3	A	702	FAD	O4B-C4B-C5B-O5B
5	A	704	NHE	C1-C2-S-O1

There are no ring outliers.

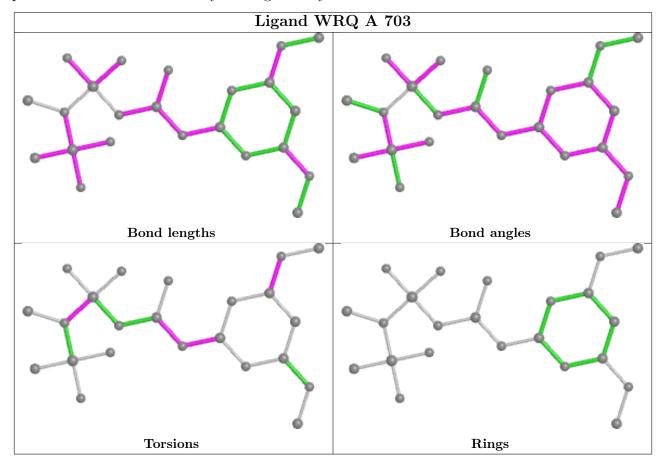
2 monomers are involved in 2 short contacts:

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

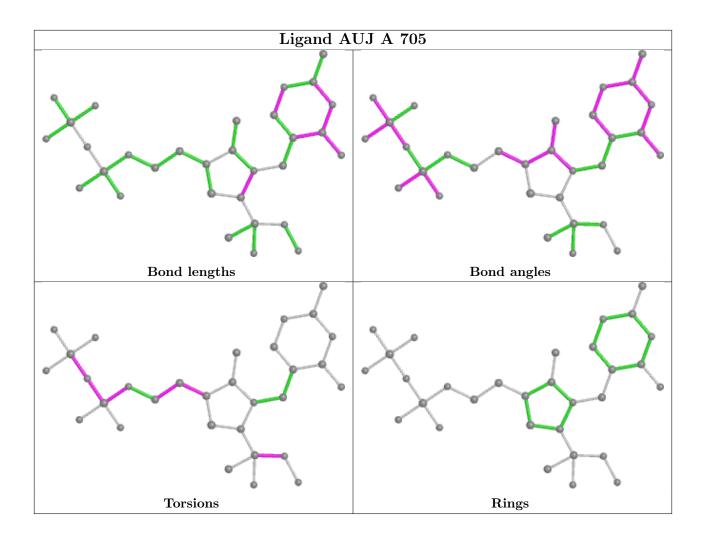
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



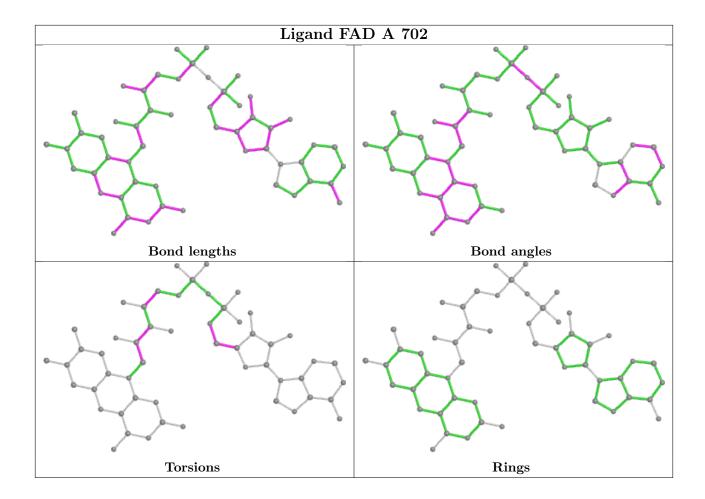
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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^{th} 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>	$\# \mathrm{RSRZ} {>} 2$	$OWAB(A^2)$	Q<0.9
1	A	581/590 (98%)	-0.11	9 (1%) 73 75	40, 57, 86, 111	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	86	THR	4.7
1	A	431	GLU	2.8
1	A	87	PHE	2.6
1	A	88	ILE	2.4
1	A	440	TRP	2.3
1	A	94	ASP	2.3
1	A	363	HIS	2.3
1	A	426	LEU	2.1
1	A	359	TYR	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^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	CSD	A	340	8/9	0.89	0.18	49,78,87,103	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^{th} 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.

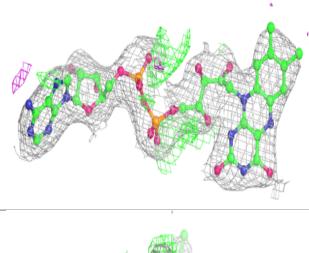
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
2	MG	A	708	1/1	0.42	0.43	82,82,82,82	1
8	SO4	A	710	5/5	0.59	0.79	101,110,117,152	5
8	SO4	A	712	5/5	0.59	0.47	79,85,106,158	5
8	SO4	A	711	5/5	0.79	0.41	87,88,109,129	5
7	TLA	A	706	10/10	0.83	0.26	91,104,127,135	0
8	SO4	A	709	5/5	0.89	0.63	85,92,111,121	5
2	MG	A	701	1/1	0.96	0.20	51,51,51,51	0
6	AUJ	A	705	31/31	0.97	0.25	36,48,61,72	4
3	FAD	A	702	53/53	0.97	0.15	35,51,66,70	0
5	NHE	A	704	13/13	0.97	0.17	48,60,83,86	0
4	WRQ	A	703	23/23	0.98	0.16	43,60,69,73	1
2	MG	A	707	1/1	0.99	0.36	36,36,36,36	1

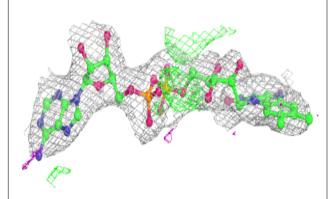
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

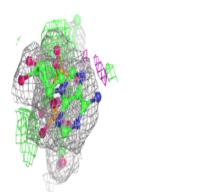


Electron density around AUJ A 705: $2 \mathrm{mF}_o\text{-}\mathrm{DF}_c$ (at 0.7 rmsd) in gray ${ m mF}_o{ m -DF}_c$ (at 3 rmsd) in purple (negative) and green (positive) Electron density around FAD A 702:

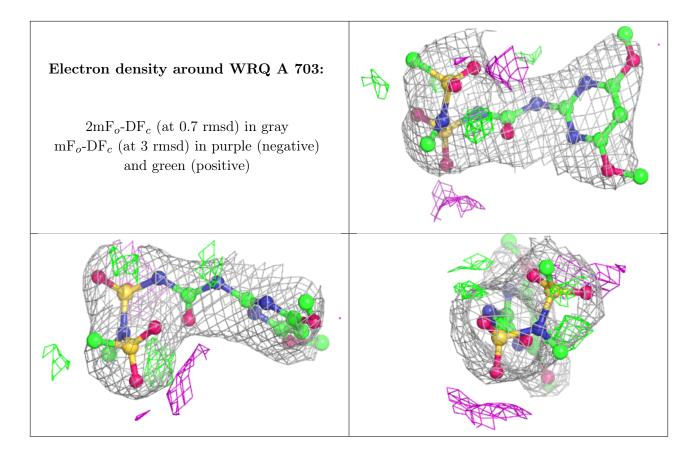
 $2 {\rm mF}_o\text{-}{\rm DF}_c$ (at 0.7 rmsd) in gray ${\rm mF}_o\text{-}{\rm DF}_c$ (at 3 rmsd) in purple (negative) and green (positive)











6.5 Other polymers (i)

There are no such residues in this entry.

