

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 - 01:00 PM EDT

:	7U1U
:	Crystal structure of arabidopsis thaliana acetohydroxyacid synthase W574L
	mutant
:	Guddat, L.W.; Cheng, Y.
	2022-02-22
:	3.22 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:

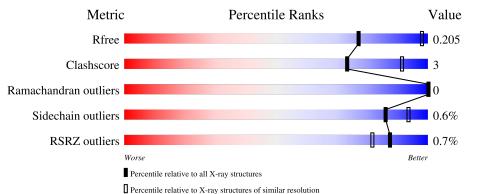
MolProbity	:	4.02b-467 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)		
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.22 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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		
1	٨	500	-% -		
1	А	590	91%	8%	•

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
6	SO4	А	705	-	-	-	Х



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2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4522 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	А	582	Total 4424	C 2804	N 760	O 836	S 24	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

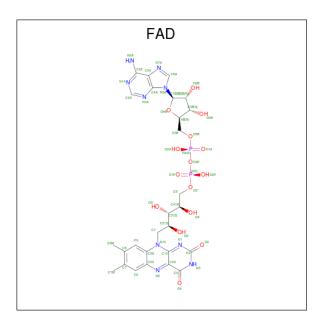
Chain	Residue	Modelled	Actual	Comment	Reference
А	574	LEU	TRP	engineered mutation	UNP P17597
А	668	LEU	-	expression tag	UNP P17597
А	669	GLU	-	expression tag	UNP P17597
А	670	HIS	-	expression tag	UNP P17597
А	671	HIS	-	expression tag	UNP P17597
А	672	HIS	-	expression tag	UNP P17597
А	673	HIS	-	expression tag	UNP P17597
А	674	HIS	-	expression tag	UNP P17597
А	675	HIS	-	expression tag	UNP P17597

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

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

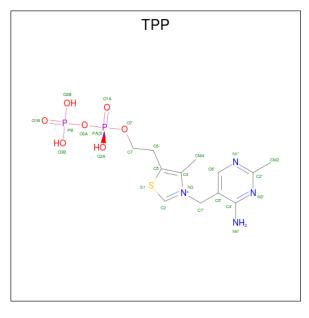
• Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\rm C_{27}H_{33}N_9O_{15}P_2).$





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Λ	1	Total	С	Ν	Ο	Р	0	0
0	A	1	53	27	9	15	2	0	U

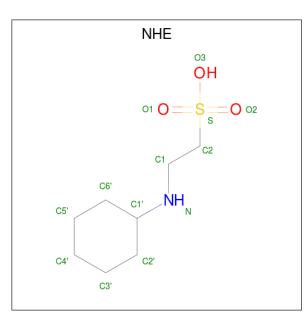
• Molecule 4 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



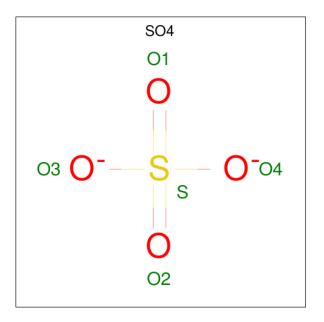
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	А	1	Total 26	C 12	N 4	0 7	Р 2	S 1	0	0

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





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	Δ	1	Total	С	Ν	0	S	0	0
0	A	1	13	8	1	3	1	0	0



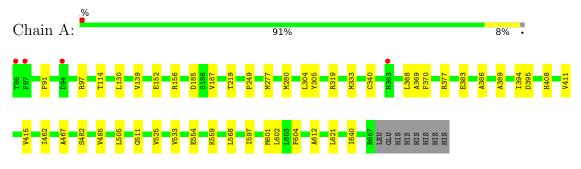
Mol	Chain	Residues	Ato	\mathbf{ms}		ZeroOcc	AltConf
6	А	1	Total 5	0 4	S 1	0	0



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	177.95Å 177.95Å 184.73Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor	
Resolution (Å)	48.10 - 3.22	Depositor	
Resolution (A)	48.10 - 3.22	EDS	
% Data completeness	99.4 (48.10-3.22)	Depositor	
(in resolution range)	99.4 (48.10-3.22)	EDS	
R _{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
$< I/\sigma(I) > 1$	$2.06 (at 3.25 \text{\AA})$	Xtriage	
Refinement program	PHENIX 1.17.1_3660	Depositor	
D D.	0.186 , 0.205	Depositor	
R, R_{free}	0.186 , 0.205	DCC	
R_{free} test set	1998 reflections (7.06%)	wwPDB-VP	
Wilson B-factor $(Å^2)$	80.8	Xtriage	
Anisotropy	0.392	Xtriage	
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.33, 44.2	EDS	
L-test for twinning ²	$ \langle L \rangle = 0.50, \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	4522	wwPDB-VP	
Average B, all atoms $(Å^2)$	76.0	wwPDB-VP	

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.

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.



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: FAD, NHE, CSD, SO4, MG, TPP

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	А	0.24	0/4510	0.41	0/6130	

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	А	4424	0	4387	26	0
2	А	1	0	0	0	0
3	А	53	0	30	2	0
4	А	26	0	16	2	0
5	А	13	0	17	1	0
6	А	5	0	0	0	0
All	All	4522	0	4450	30	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 (30) 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:277:MET:HA	1:A:280:MET:HG3	1.76	0.65
1:A:394:ILE:HG12	1:A:411:VAL:HB	1.83	0.59
1:A:114:THR:HG21	1:A:525:VAL:HG11	1.88	0.56
1:A:597:ILE:HG12	1:A:640:ILE:HD12	1.89	0.54
1:A:386:ALA:HB1	1:A:389:ALA:HB3	1.91	0.53
1:A:152:GLU:OE1	1:A:156:ARG:NH1	2.43	0.51
1:A:304:LEU:HD23	1:A:368:LEU:HB2	1.94	0.49
1:A:156:ARG:NH2	1:A:185:ASP:OD2	2.43	0.49
1:A:602:LEU:HD22	1:A:612:ALA:HB1	1.96	0.48
1:A:139:VAL:HG13	1:A:554:GLU:HG3	1.99	0.45
1:A:482:SER:HA	1:A:505:LEU:O	2.17	0.45
5:A:704:NHE:H6'1	5:A:704:NHE:HC11	1.70	0.44
1:A:383:GLU:OE1	1:A:383:GLU:N	2.48	0.44
1:A:305:TYR:HB3	1:A:369:ALA:HA	1.99	0.44
1:A:533:VAL:HG22	1:A:559:LYS:HB2	1.99	0.44
1:A:333:MET:HG3	3:A:702:FAD:H5'2	2.00	0.43
1:A:601:MET:HA	1:A:604:PHE:HD2	1.82	0.43
1:A:91:PHE:CG	1:A:97:ARG:HD3	2.54	0.43
1:A:467:ALA:HA	1:A:621:LEU:HD21	2.01	0.43
1:A:485:VAL:HG21	1:A:511:GLY:C	2.38	0.42
1:A:130:LEU:HD23	1:A:130:LEU:HA	1.87	0.42
1:A:156:ARG:NH1	1:A:187:VAL:HG21	2.33	0.42
4:A:703:TPP:HN42	4:A:703:TPP:H2	1.85	0.42
1:A:370:PHE:HB3	1:A:415:VAL:HG21	2.02	0.42
1:A:219:THR:HA	1:A:249:PRO:HG2	2.02	0.41
1:A:568:LEU:HD23	1:A:568:LEU:HA	1.92	0.41
4:A:703:TPP:HN42	4:A:703:TPP:C2	2.33	0.41
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.96	0.40
3:A:702:FAD:H9	3:A:702:FAD:H1'1	1.71	0.40
1:A:462:ILE:HG23	1:A:621:LEU:HD22	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	Analysed Favoured Allowed		Outliers	Percentiles		
1	А	579/590~(98%)	562 (97%)	17 (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	А	471/486~(97%)	468 (99%)	3(1%)	86 93		

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	319	ARG
1	А	395	ASP
1	А	408	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	Tiple	Bond lengths			Bond angles		
IVI01	Type	Unam	nes	Link	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2	
	1	CSD	А	340	1	3,7,8	1.06	0	$1,\!8,\!10$	7.89	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	А	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	А	340	CSD	OD1-SG-CB	7.89	120.56	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 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		
	Type		nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
3	FAD	А	702	-	53,58,58	1.71	11 (20%)	68,89,89	1.37	14 (20%)



Mol	Turne	e Chain	n Res	Link	B	Bond lengths			Bond angles		
WIOI	Type				Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	TPP	А	703	2	22,27,27	1.86	3 (13%)	29,40,40	2.15	12 (41%)	
6	SO4	А	705	-	4,4,4	0.14	0	6,6,6	0.05	0	
5	NHE	А	704	-	$13,\!13,\!13$	1.30	2 (15%)	16,17,17	1.90	4 (25%)	

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
3	FAD	А	702	-	-	13/30/50/50	0/6/6/6
4	TPP	А	703	2	-	4/16/17/17	0/2/2/2
5	NHE	А	704	-	-	2/7/15/15	0/1/1/1

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	А	703	TPP	C4-N3	-6.68	1.33	1.39
3	А	702	FAD	C10-N1	5.14	1.43	1.33
3	А	702	FAD	C4X-N5	4.66	1.39	1.30
3	А	702	FAD	C2B-C1B	-4.58	1.46	1.53
4	А	703	TPP	C4'-N4'	3.37	1.42	1.34
5	А	704	NHE	C2-S	3.09	1.81	1.77
3	А	702	FAD	O4B-C1B	2.90	1.45	1.41
3	А	702	FAD	O3'-C3'	-2.76	1.36	1.43
3	А	702	FAD	C1'-N10	-2.61	1.41	1.48
3	А	702	FAD	C2-N1	2.59	1.42	1.36
4	А	703	TPP	C6-C5	2.44	1.52	1.50
5	А	704	NHE	O2-S	2.18	1.51	1.45
3	А	702	FAD	C2B-C3B	-2.16	1.47	1.53
3	А	702	FAD	C4X-C4	2.14	1.52	1.44
3	А	702	FAD	C4X-C10	-2.04	1.38	1.44
3	А	702	FAD	C2'-C3'	2.01	1.57	1.53

All (16) bond length outliers are listed below:

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	703	TPP	PA-O3A-PB	-5.23	114.89	132.83
5	А	704	NHE	O3-S-O1	-4.13	101.18	111.27
3	А	702	FAD	N3A-C2A-N1A	-4.10	122.26	128.68
5	А	704	NHE	O2-S-C2	3.70	111.37	106.92

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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	703	TPP	C7'-N3-C2	-3.59	118.86	125.35
4	А	703	TPP	N1'-C2'-N3'	-3.42	119.66	125.54
5	А	704	NHE	O3-S-C2	3.38	111.23	105.77
4	А	703	TPP	C5-C4-N3	3.17	113.91	107.57
4	А	703	TPP	CM4-C4-C5	-3.04	120.96	127.60
4	А	703	TPP	C5'-C7'-N3	-3.03	108.24	113.28
3	А	702	FAD	C4A-C5A-N7A	-2.95	106.33	109.40
3	А	702	FAD	C4-N3-C2	-2.94	120.21	125.64
3	А	702	FAD	C4-C4X-N5	2.91	122.38	118.23
3	А	702	FAD	C4X-C4-N3	2.88	120.49	113.19
4	А	703	TPP	C6'-N1'-C2'	2.81	120.75	115.96
5	А	704	NHE	O1-S-C2	2.67	110.14	106.92
3	А	702	FAD	C10-C4X-N5	-2.61	119.31	124.86
4	А	703	TPP	CM2-C2'-N1'	2.51	119.90	117.14
3	А	702	FAD	C4X-C10-N1	-2.50	118.94	124.73
3	А	702	FAD	C5'-C4'-C3'	-2.44	107.48	112.20
3	А	702	FAD	C9A-C5X-N5	-2.38	119.84	122.43
3	А	702	FAD	C10-N1-C2	2.37	121.64	116.90
3	А	702	FAD	C1B-N9A-C4A	-2.32	122.56	126.64
3	А	702	FAD	O4-C4-C4X	-2.32	120.44	126.60
3	А	702	FAD	P-O3P-PA	-2.21	125.23	132.83
4	А	703	TPP	C6'-C5'-C4'	2.21	118.73	115.72
4	А	703	TPP	CM2-C2'-N3'	2.11	120.45	117.15
4	А	703	TPP	C5'-C6'-N1'	-2.08	120.35	123.82
4	А	703	TPP	CM4-C4-N3	2.04	125.13	122.53
3	А	702	FAD	C4'-C3'-C2'	-2.02	109.17	113.36

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There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	702	FAD	C5B-O5B-PA-O1A
3	А	702	FAD	C3'-C4'-C5'-O5'
3	А	702	FAD	O4'-C4'-C5'-O5'
3	А	702	FAD	C5'-O5'-P-O1P
3	А	702	FAD	C5'-O5'-P-O2P
3	А	702	FAD	C5'-O5'-P-O3P
5	А	704	NHE	C6'-C1'-N-C1
4	А	703	TPP	PA-O3A-PB-O1B
5	А	704	NHE	C2-C1-N-C1'
3	А	702	FAD	O2'-C2'-C3'-C4'
3	А	702	FAD	P-O3P-PA-O5B

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Mol	Chain	\mathbf{Res}	Type	Atoms
4	А	703	TPP	PB-O3A-PA-O7
3	А	702	FAD	O2'-C2'-C3'-O3'
4	А	703	TPP	C7-O7-PA-O3A
4	А	703	TPP	C7-O7-PA-O1A
3	А	702	FAD	C3B-C4B-C5B-O5B
3	А	702	FAD	N10-C1'-C2'-O2'
3	А	702	FAD	C1'-C2'-C3'-C4'
3	А	702	FAD	C1'-C2'-C3'-O3'

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There are no ring outliers.

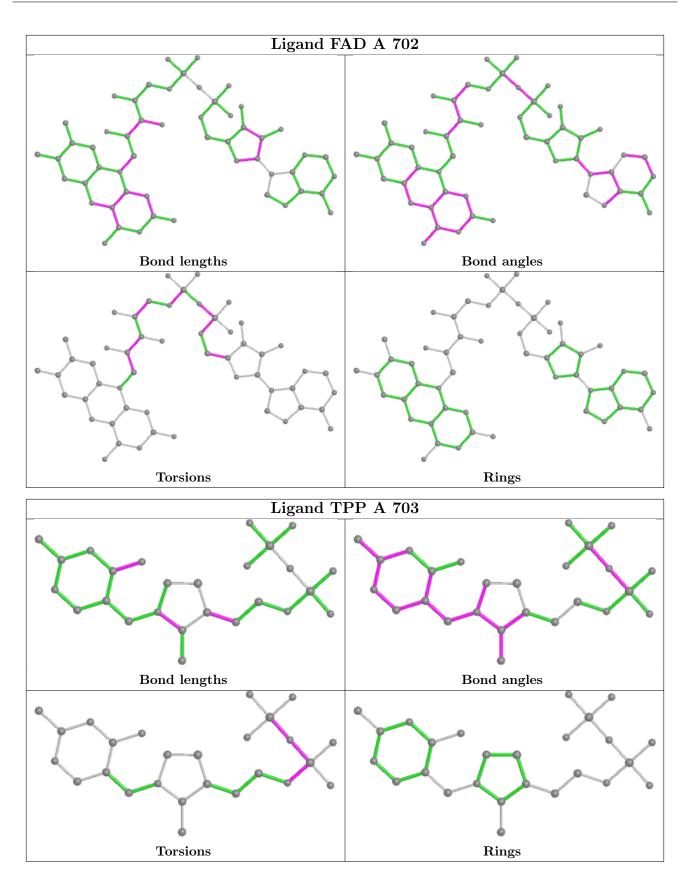
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	А	702	FAD	2	0
4	А	703	TPP	2	0
5	А	704	NHE	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 sufficient 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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	581/590~(98%)	-0.15	4 (0%) 87 82	50, 73, 105, 123	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	86	THR	3.4
1	А	363	HIS	2.9
1	А	94	ASP	2.4
1	А	87	PHE	2.2

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	$B-factors(Å^2)$	Q < 0.9
1	CSD	А	340	8/9	0.93	0.16	83,103,112,117	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

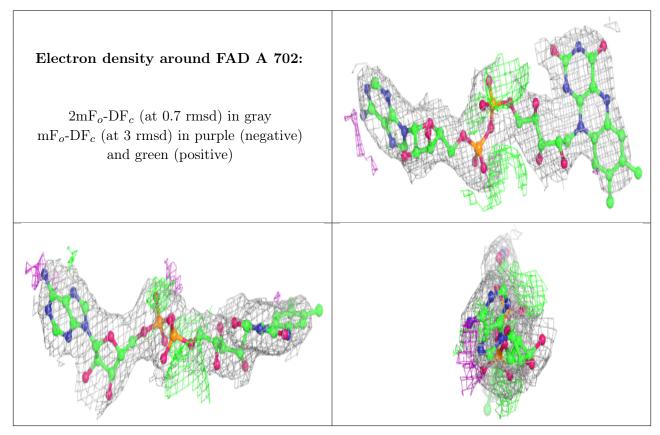
6.4 Ligands (i)

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.

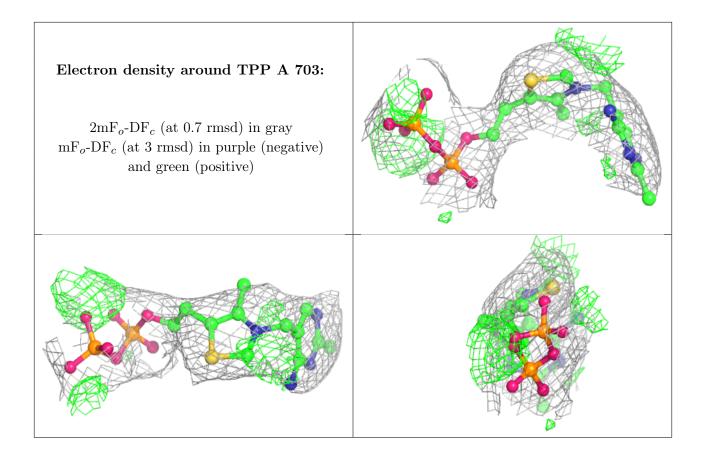


Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
6	SO4	А	705	5/5	0.75	0.54	125,139,143,188	0
2	MG	А	701	1/1	0.95	0.24	59, 59, 59, 59, 59	0
5	NHE	А	704	13/13	0.96	0.27	64,85,113,123	0
3	FAD	А	702	53/53	0.96	0.18	53,70,80,91	0
4	TPP	А	703	26/26	0.98	0.22	47,66,81,86	0

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.







6.5 Other polymers (i)

There are no such residues in this entry.

