



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 02:09 PM JST

PDB ID : 7EHE
Title : Acetolactate Synthase from *Trichoderma harzianum*
Authors : Zang, X.; Tang, Y.; Zhou, J.
Deposited on : 2021-03-29
Resolution : 2.28 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 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 : 2.20
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) : 2.20

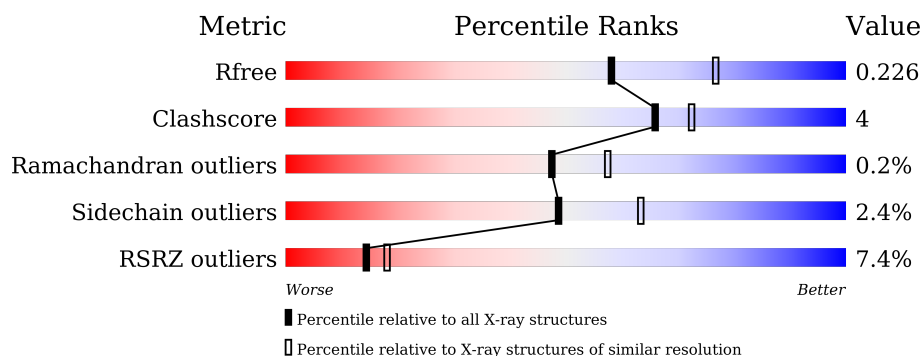
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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	688	<div> <div>2%</div> <div>78%</div> <div>8%</div> <div>14%</div> </div>
1	B	688	<div> <div>10%</div> <div>72%</div> <div>10%</div> <div>16%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9196 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	589	Total	C	N	O	S	0	0	0
			4508	2851	797	833	27			
1	B	581	Total	C	N	O	S	0	0	0
			4447	2815	784	821	27			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP A0A2N1LPC4
A	3	HIS	-	expression tag	UNP A0A2N1LPC4
A	4	HIS	-	expression tag	UNP A0A2N1LPC4
A	5	HIS	-	expression tag	UNP A0A2N1LPC4
A	6	HIS	-	expression tag	UNP A0A2N1LPC4
A	7	HIS	-	expression tag	UNP A0A2N1LPC4
A	8	HIS	-	expression tag	UNP A0A2N1LPC4
A	9	SER	-	expression tag	UNP A0A2N1LPC4
A	10	SER	-	expression tag	UNP A0A2N1LPC4
A	11	GLY	-	expression tag	UNP A0A2N1LPC4
A	12	LEU	-	expression tag	UNP A0A2N1LPC4
A	13	VAL	-	expression tag	UNP A0A2N1LPC4
A	14	PRO	-	expression tag	UNP A0A2N1LPC4
A	15	ARG	-	expression tag	UNP A0A2N1LPC4
A	16	GLY	-	expression tag	UNP A0A2N1LPC4
A	17	SER	-	expression tag	UNP A0A2N1LPC4
A	18	GLY	-	expression tag	UNP A0A2N1LPC4
A	19	MET	-	expression tag	UNP A0A2N1LPC4
A	20	LYS	-	expression tag	UNP A0A2N1LPC4
A	21	GLU	-	expression tag	UNP A0A2N1LPC4
A	22	THR	-	expression tag	UNP A0A2N1LPC4
A	23	ALA	-	expression tag	UNP A0A2N1LPC4
A	24	ALA	-	expression tag	UNP A0A2N1LPC4
A	25	ALA	-	expression tag	UNP A0A2N1LPC4
A	26	LYS	-	expression tag	UNP A0A2N1LPC4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	PHE	-	expression tag	UNP A0A2N1LPC4
A	28	GLU	-	expression tag	UNP A0A2N1LPC4
A	29	ARG	-	expression tag	UNP A0A2N1LPC4
A	30	GLN	-	expression tag	UNP A0A2N1LPC4
A	31	HIS	-	expression tag	UNP A0A2N1LPC4
A	32	MET	-	expression tag	UNP A0A2N1LPC4
A	33	ASP	-	expression tag	UNP A0A2N1LPC4
A	34	SER	-	expression tag	UNP A0A2N1LPC4
A	35	PRO	-	expression tag	UNP A0A2N1LPC4
A	36	ASP	-	expression tag	UNP A0A2N1LPC4
A	37	LEU	-	expression tag	UNP A0A2N1LPC4
A	38	GLY	-	expression tag	UNP A0A2N1LPC4
A	39	THR	-	expression tag	UNP A0A2N1LPC4
A	40	ASP	-	expression tag	UNP A0A2N1LPC4
A	41	ASP	-	expression tag	UNP A0A2N1LPC4
A	42	ASP	-	expression tag	UNP A0A2N1LPC4
A	43	ASP	-	expression tag	UNP A0A2N1LPC4
A	44	LYS	-	expression tag	UNP A0A2N1LPC4
A	45	ALA	-	expression tag	UNP A0A2N1LPC4
A	46	MET	-	expression tag	UNP A0A2N1LPC4
A	47	ALA	-	expression tag	UNP A0A2N1LPC4
A	48	ASP	-	expression tag	UNP A0A2N1LPC4
A	49	ILE	-	expression tag	UNP A0A2N1LPC4
A	50	GLY	-	expression tag	UNP A0A2N1LPC4
A	51	SER	-	expression tag	UNP A0A2N1LPC4
A	52	MET	-	expression tag	UNP A0A2N1LPC4
A	602	ARG	LYS	engineered mutation	UNP A0A2N1LPC4
A	615	ILE	VAL	engineered mutation	UNP A0A2N1LPC4
A	627	VAL	ILE	engineered mutation	UNP A0A2N1LPC4
B	2	MET	-	initiating methionine	UNP A0A2N1LPC4
B	3	HIS	-	expression tag	UNP A0A2N1LPC4
B	4	HIS	-	expression tag	UNP A0A2N1LPC4
B	5	HIS	-	expression tag	UNP A0A2N1LPC4
B	6	HIS	-	expression tag	UNP A0A2N1LPC4
B	7	HIS	-	expression tag	UNP A0A2N1LPC4
B	8	HIS	-	expression tag	UNP A0A2N1LPC4
B	9	SER	-	expression tag	UNP A0A2N1LPC4
B	10	SER	-	expression tag	UNP A0A2N1LPC4
B	11	GLY	-	expression tag	UNP A0A2N1LPC4
B	12	LEU	-	expression tag	UNP A0A2N1LPC4
B	13	VAL	-	expression tag	UNP A0A2N1LPC4
B	14	PRO	-	expression tag	UNP A0A2N1LPC4

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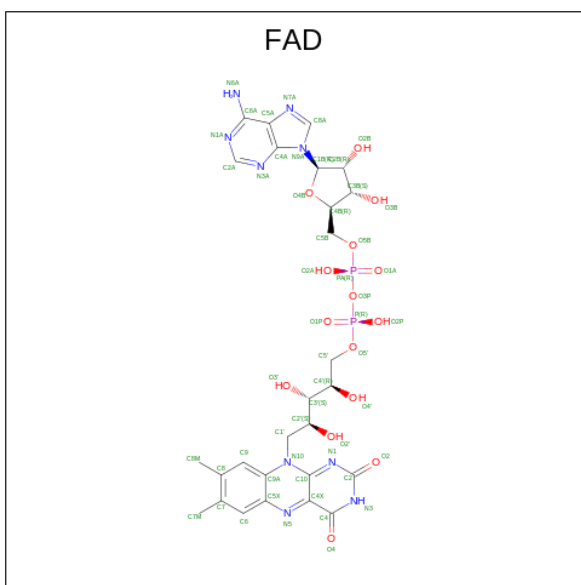
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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ARG	-	expression tag	UNP A0A2N1LPC4
B	16	GLY	-	expression tag	UNP A0A2N1LPC4
B	17	SER	-	expression tag	UNP A0A2N1LPC4
B	18	GLY	-	expression tag	UNP A0A2N1LPC4
B	19	MET	-	expression tag	UNP A0A2N1LPC4
B	20	LYS	-	expression tag	UNP A0A2N1LPC4
B	21	GLU	-	expression tag	UNP A0A2N1LPC4
B	22	THR	-	expression tag	UNP A0A2N1LPC4
B	23	ALA	-	expression tag	UNP A0A2N1LPC4
B	24	ALA	-	expression tag	UNP A0A2N1LPC4
B	25	ALA	-	expression tag	UNP A0A2N1LPC4
B	26	LYS	-	expression tag	UNP A0A2N1LPC4
B	27	PHE	-	expression tag	UNP A0A2N1LPC4
B	28	GLU	-	expression tag	UNP A0A2N1LPC4
B	29	ARG	-	expression tag	UNP A0A2N1LPC4
B	30	GLN	-	expression tag	UNP A0A2N1LPC4
B	31	HIS	-	expression tag	UNP A0A2N1LPC4
B	32	MET	-	expression tag	UNP A0A2N1LPC4
B	33	ASP	-	expression tag	UNP A0A2N1LPC4
B	34	SER	-	expression tag	UNP A0A2N1LPC4
B	35	PRO	-	expression tag	UNP A0A2N1LPC4
B	36	ASP	-	expression tag	UNP A0A2N1LPC4
B	37	LEU	-	expression tag	UNP A0A2N1LPC4
B	38	GLY	-	expression tag	UNP A0A2N1LPC4
B	39	THR	-	expression tag	UNP A0A2N1LPC4
B	40	ASP	-	expression tag	UNP A0A2N1LPC4
B	41	ASP	-	expression tag	UNP A0A2N1LPC4
B	42	ASP	-	expression tag	UNP A0A2N1LPC4
B	43	ASP	-	expression tag	UNP A0A2N1LPC4
B	44	LYS	-	expression tag	UNP A0A2N1LPC4
B	45	ALA	-	expression tag	UNP A0A2N1LPC4
B	46	MET	-	expression tag	UNP A0A2N1LPC4
B	47	ALA	-	expression tag	UNP A0A2N1LPC4
B	48	ASP	-	expression tag	UNP A0A2N1LPC4
B	49	ILE	-	expression tag	UNP A0A2N1LPC4
B	50	GLY	-	expression tag	UNP A0A2N1LPC4
B	51	SER	-	expression tag	UNP A0A2N1LPC4
B	52	MET	-	expression tag	UNP A0A2N1LPC4
B	602	ARG	LYS	engineered mutation	UNP A0A2N1LPC4
B	615	ILE	VAL	engineered mutation	UNP A0A2N1LPC4
B	627	VAL	ILE	engineered mutation	UNP A0A2N1LPC4

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

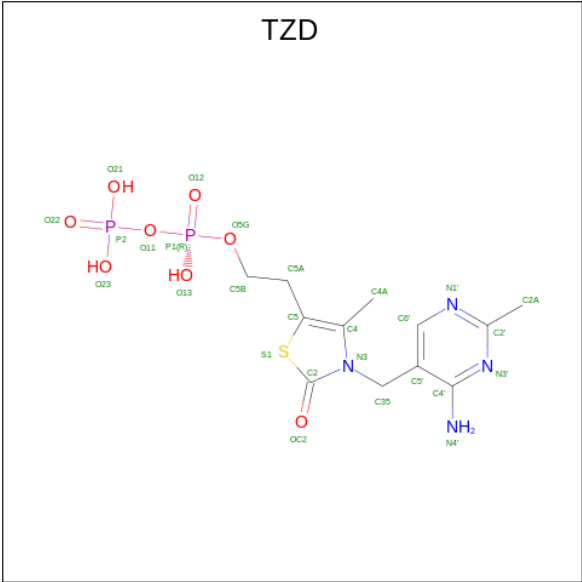
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: TZD) (formula: C₁₂H₁₈N₄O₈P₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

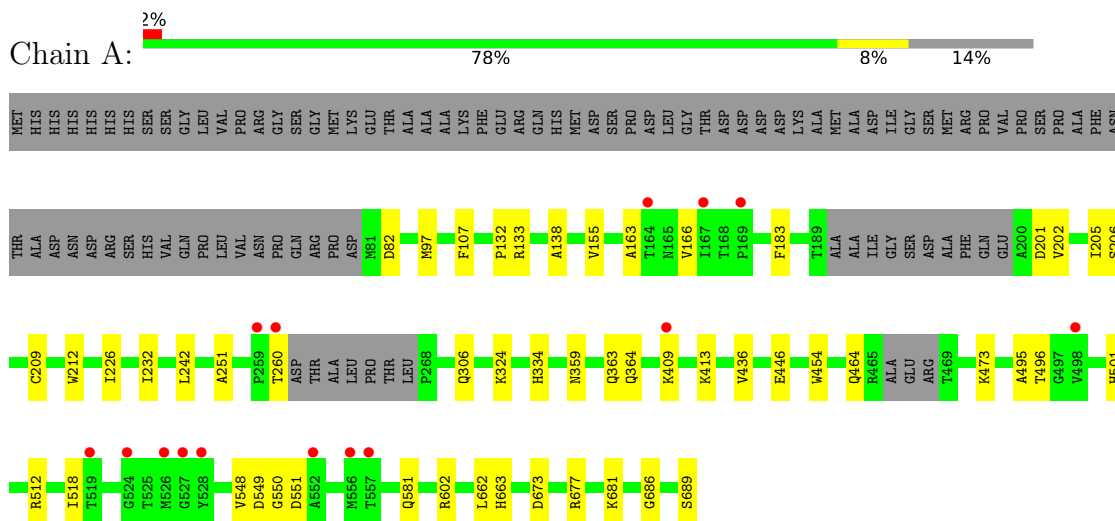
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	65	Total	O	0	0
			65	65		
5	B	14	Total	O	0	0
			14	14		

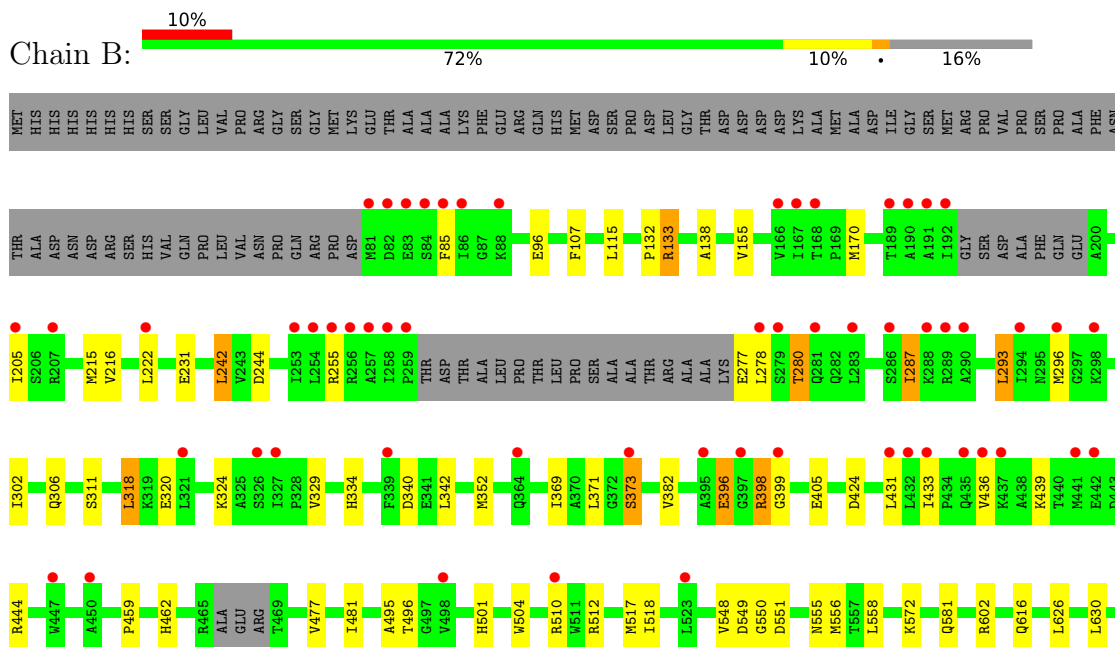
3 Residue-property plots [i](#)

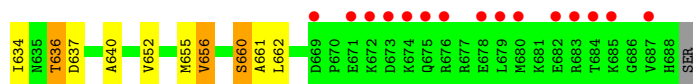
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Acetolactate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.10Å 88.53Å 188.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.26 – 2.28 47.03 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.26-2.28) 100.0 (47.03-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.230 0.192 , 0.226	Depositor DCC
R_{free} test set	3045 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	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	0.96	EDS
Total number of atoms	9196	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: TZD, FAD, MG

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	0.44	0/4599	0.59	3/6218 (0.0%)
1	B	0.39	0/4537	0.57	0/6136
All	All	0.42	0/9136	0.58	3/12354 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	551	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	551	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	512	ARG	NE-CZ-NH1	5.49	123.04	120.30

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	4508	0	4541	26	0
1	B	4447	0	4466	48	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	15	1	0
4	B	27	0	15	2	0
5	A	65	0	0	1	0
5	B	14	0	0	0	0
All	All	9196	0	9099	73	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 4.

All (73) 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:B:352:MET:HA	1:B:656:VAL:HG13	1.71	0.71
1:B:382:VAL:HG22	1:B:661:ALA:HA	1.79	0.66
1:B:132:PRO:HG3	1:B:138:ALA:HB2	1.78	0.64
1:B:215:MET:HA	1:B:244:ASP:HB2	1.80	0.62
1:B:396:GLU:HB3	1:B:398:ARG:HG2	1.82	0.62
1:B:656:VAL:HG23	1:B:660:SER:HB3	1.82	0.60
1:B:342:LEU:HD21	1:B:510:ARG:HD3	1.83	0.60
1:B:340:ASP:OD2	1:B:512:ARG:NH1	2.33	0.59
1:A:132:PRO:HG3	1:A:138:ALA:HB2	1.85	0.59
4:B:703:TZD:C2	4:B:703:TZD:H4'2	2.15	0.59
1:A:581:GLN:HB3	4:A:703:TZD:H5A1	1.84	0.59
1:B:572:LYS:NZ	1:B:636:THR:HG22	2.18	0.59
1:B:302:ILE:HD13	1:B:369:ILE:HB	1.85	0.58
1:B:636:THR:HG21	1:B:640:ALA:CB	2.35	0.56
1:B:495:ALA:HA	1:B:518:ILE:O	2.05	0.55
1:B:636:THR:HG21	1:B:640:ALA:HB2	1.89	0.54
1:A:209:CYS:HB3	1:B:205:ILE:HD11	1.90	0.54
1:A:97:MET:HB3	1:A:226:ILE:HG21	1.88	0.54
1:A:82:ASP:HB2	1:A:260:THR:HG22	1.91	0.53
1:B:630:LEU:O	1:B:634:ILE:HG13	2.08	0.53
1:A:673:ASP:O	1:A:677:ARG:HG3	2.09	0.52
1:A:201:ASP:O	1:A:205:ILE:HG13	2.10	0.52
1:B:170:MET:SD	1:B:242:LEU:HD23	2.50	0.52
1:A:206:SER:HA	1:A:209:CYS:SG	2.50	0.51
1:B:504:TRP:CE2	1:B:652:VAL:HG22	2.45	0.51
1:B:302:ILE:HB	1:B:329:VAL:HG22	1.94	0.50
1:B:85:PHE:HE1	1:B:96:GLU:HG2	1.77	0.50
1:B:302:ILE:HG23	1:B:371:LEU:HD12	1.94	0.50
1:A:202:VAL:HG12	1:A:242:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:306:GLN:HB2	1:B:334:HIS:HB3	1.94	0.48
1:B:277:GLU:HB3	1:B:280:THR:HG22	1.95	0.48
1:A:681:LYS:HG2	1:A:686:GLY:HA2	1.95	0.48
1:A:464:GLN:O	1:A:473:LYS:HD2	2.14	0.47
1:B:311:SER:OG	1:B:424:ASP:OD1	2.21	0.47
1:B:302:ILE:HG21	1:B:318:LEU:HD21	1.96	0.47
1:B:459:PRO:HG2	1:B:462:HIS:HB2	1.96	0.47
1:A:364:GLN:HG3	1:A:454:TRP:CH2	2.50	0.47
1:B:572:LYS:HZ1	1:B:636:THR:HG22	1.79	0.47
1:B:405:GLU:OE2	3:B:702:FAD:O3B	2.28	0.46
1:A:212:TRP:CE3	1:A:232:ILE:HD12	2.50	0.46
1:B:107:PHE:O	1:B:155:VAL:HA	2.16	0.46
1:B:296:MET:SD	1:B:398:ARG:HA	2.56	0.46
1:A:496:THR:HA	1:A:548:VAL:O	2.16	0.45
1:B:496:THR:HA	1:B:548:VAL:O	2.16	0.45
1:A:495:ALA:HA	1:A:518:ILE:O	2.16	0.45
1:B:439:LYS:HG3	1:B:444:ARG:NH2	2.31	0.45
1:B:293:LEU:HD21	1:B:399:GLY:C	2.37	0.45
1:B:616:GLN:NE2	1:B:637:ASP:O	2.49	0.45
1:B:581:GLN:HB3	4:B:703:TZD:H5A1	1.99	0.45
1:A:107:PHE:O	1:A:155:VAL:HA	2.17	0.45
1:A:306:GLN:HB2	1:A:334:HIS:HB3	1.99	0.44
1:B:287:ILE:HD12	1:B:431:LEU:HB2	1.98	0.44
1:B:324:LYS:NZ	1:B:436:VAL:O	2.42	0.44
1:A:251:ALA:O	5:A:801:HOH:O	2.21	0.44
1:A:409:LYS:HE2	1:A:409:LYS:HB2	1.81	0.44
1:A:363:GLN:HG3	1:A:663:HIS:HB3	2.00	0.44
1:A:183:PHE:HE1	1:A:226:ILE:HD12	1.83	0.44
1:B:133:ARG:HA	1:B:133:ARG:HD2	1.84	0.43
1:A:324:LYS:HE2	1:A:436:VAL:O	2.18	0.43
1:A:359:ASN:HB3	1:A:662:LEU:HG	2.00	0.43
1:A:602:ARG:O	1:B:133:ARG:NH2	2.30	0.43
1:B:216:VAL:HG11	1:B:222:LEU:HD13	2.01	0.43
1:B:501:HIS:CE1	1:B:550:GLY:H	2.36	0.43
1:A:501:HIS:CE1	1:A:550:GLY:H	2.37	0.42
1:B:115:LEU:HD12	1:B:115:LEU:HA	1.86	0.41
1:B:555:ASN:HA	1:B:558:LEU:HD23	2.02	0.41
1:B:255:ARG:HD3	1:B:255:ARG:HA	1.78	0.41
1:B:352:MET:O	1:B:655:MET:HA	2.21	0.41
1:B:477:VAL:O	1:B:481:ILE:HG13	2.21	0.41
1:B:551:ASP:OD1	1:B:551:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:O	1:A:166:VAL:HG22	2.21	0.40
1:B:278:LEU:H	1:B:278:LEU:HD23	1.86	0.40
1:B:320:GLU:OE2	1:B:433:ILE:HG21	2.21	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	581/688 (84%)	574 (99%)	7 (1%)	0	100	100
1	B	573/688 (83%)	551 (96%)	20 (4%)	2 (0%)	41	49
All	All	1154/1376 (84%)	1125 (98%)	27 (2%)	2 (0%)	47	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	373	SER
1	B	662	LEU

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	475/556 (85%)	470 (99%)	5 (1%)	73	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	467/556 (84%)	449 (96%)	18 (4%)	32	43
All	All	942/1112 (85%)	919 (98%)	23 (2%)	49	63

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	413	LYS
1	A	446	GLU
1	A	549	ASP
1	A	689	SER
1	B	133	ARG
1	B	231	GLU
1	B	242	LEU
1	B	280	THR
1	B	287	ILE
1	B	293	LEU
1	B	318	LEU
1	B	373	SER
1	B	396	GLU
1	B	398	ARG
1	B	517	MET
1	B	549	ASP
1	B	556	MET
1	B	602	ARG
1	B	626	LEU
1	B	636	THR
1	B	656	VAL
1	B	660	SER

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

Mol	Chain	Res	Type
1	B	101	GLN
1	B	227	ASN
1	B	364	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are 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
3	FAD	B	702	-	51,58,58	1.21	5 (9%)	60,89,89	2.22	7 (11%)
4	TZD	B	703	2	23,28,28	3.16	6 (26%)	28,42,42	2.04	8 (28%)
4	TZD	A	703	2	23,28,28	3.07	4 (17%)	28,42,42	2.10	8 (28%)
3	FAD	A	702	-	51,58,58	1.42	6 (11%)	60,89,89	2.14	7 (11%)

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	B	702	-	-	11/30/50/50	0/6/6/6
4	TZD	B	703	2	-	2/16/17/17	0/2/2/2
4	TZD	A	703	2	-	1/16/17/17	0/2/2/2
3	FAD	A	702	-	-	2/30/50/50	0/6/6/6

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	TZD	C4-N3	11.04	1.63	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	703	TZD	C4-N3	10.42	1.62	1.39
4	B	703	TZD	C5-S1	-6.39	1.62	1.74
4	A	703	TZD	C5-S1	-6.23	1.62	1.74
3	A	702	FAD	C4X-C10	6.07	1.44	1.38
3	B	702	FAD	C4X-C10	5.56	1.44	1.38
4	A	703	TZD	C5A-C5	4.84	1.53	1.50
4	A	703	TZD	C4'-N4'	4.58	1.45	1.34
4	B	703	TZD	C4'-N4'	4.43	1.45	1.34
3	A	702	FAD	C10-N1	-3.84	1.28	1.33
4	B	703	TZD	C5A-C5	3.84	1.52	1.50
3	A	702	FAD	C4-C4X	2.98	1.46	1.41
3	A	702	FAD	C4-N3	2.83	1.38	1.33
3	A	702	FAD	C5X-N5	2.68	1.39	1.35
4	B	703	TZD	C35-N3	-2.49	1.44	1.48
3	B	702	FAD	C4-C4X	2.43	1.45	1.41
3	A	702	FAD	C9A-N10	2.25	1.41	1.38
3	B	702	FAD	C5X-N5	2.14	1.38	1.35
3	B	702	FAD	C4X-N5	-2.08	1.30	1.33
4	B	703	TZD	C5'-C4'	-2.03	1.39	1.42
3	B	702	FAD	C9A-N10	2.03	1.41	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	FAD	C4-N3-C2	13.01	126.13	115.14
3	A	702	FAD	C4-N3-C2	12.30	125.53	115.14
3	A	702	FAD	C4X-C4-N3	-7.67	112.94	123.43
3	B	702	FAD	C4X-C4-N3	-7.13	113.68	123.43
4	A	703	TZD	C5A-C5-C4	-6.33	122.35	127.43
4	B	703	TZD	C5A-C5-C4	-5.43	123.07	127.43
3	B	702	FAD	C10-C4X-N5	4.52	124.38	121.26
3	A	702	FAD	C10-C4X-N5	3.81	123.89	121.26
4	B	703	TZD	C6'-N1'-C2'	3.75	122.35	115.96
3	B	702	FAD	C4-C4X-C10	-3.68	117.52	119.95
4	A	703	TZD	C6'-N1'-C2'	3.55	122.00	115.96
4	B	703	TZD	N1'-C2'-N3'	-3.53	119.47	125.54
4	A	703	TZD	C5'-C35-N3	-3.37	107.70	113.26
3	A	702	FAD	C4-C4X-C10	-3.34	117.74	119.95
4	A	703	TZD	N1'-C2'-N3'	-3.30	119.86	125.54
3	B	702	FAD	C1'-N10-C9A	3.27	120.87	118.29
3	B	702	FAD	C4X-C10-N10	-3.26	116.96	120.30
3	A	702	FAD	C1'-N10-C9A	3.18	120.80	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	TZD	C2A-C2'-N1'	3.06	120.51	117.14
4	B	703	TZD	C5'-C35-N3	-3.02	108.26	113.26
4	A	703	TZD	C2'-N3'-C4'	3.01	122.77	118.08
3	A	702	FAD	C4X-C10-N10	-2.97	117.25	120.30
4	A	703	TZD	P1-O11-P2	-2.92	122.79	132.83
4	B	703	TZD	C2'-N3'-C4'	2.82	122.48	118.08
4	B	703	TZD	C2A-C2'-N3'	2.79	121.51	117.15
4	B	703	TZD	C5'-C6'-N1'	-2.58	119.53	123.82
4	B	703	TZD	P1-O11-P2	-2.57	124.01	132.83
3	A	702	FAD	C5A-C6A-N6A	2.45	124.07	120.35
3	B	702	FAD	C5A-C6A-N6A	2.36	123.93	120.35
4	A	703	TZD	C5'-C6'-N1'	-2.28	120.01	123.82

There are no chirality outliers.

All (16) torsion outliers are listed below:

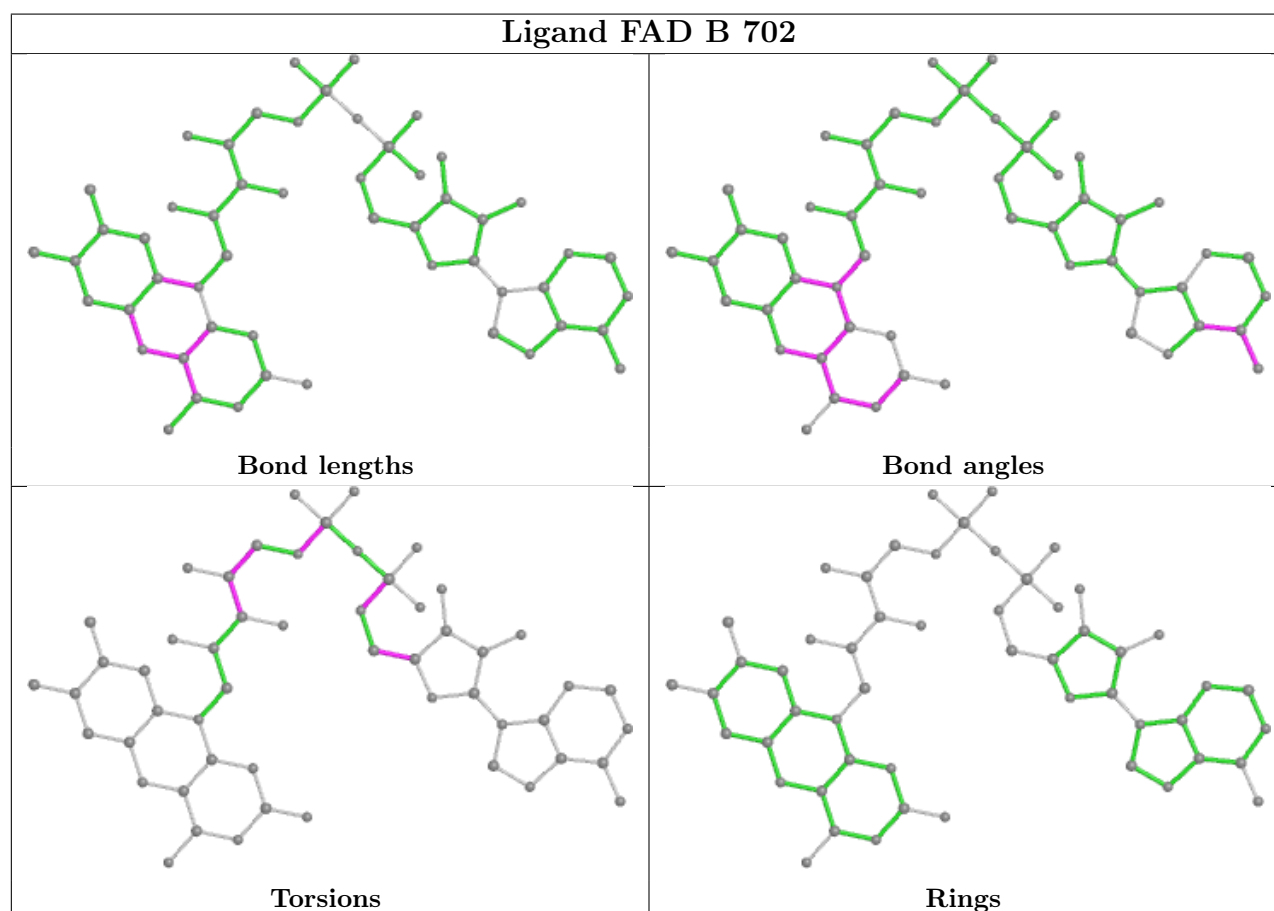
Mol	Chain	Res	Type	Atoms
3	B	702	FAD	C5'-O5'-P-O1P
4	B	703	TZD	N3-C35-C5'-C4'
3	B	702	FAD	O4B-C4B-C5B-O5B
3	B	702	FAD	O4'-C4'-C5'-O5'
3	B	702	FAD	C2'-C3'-C4'-O4'
3	B	702	FAD	C3'-C4'-C5'-O5'
3	A	702	FAD	P-O3P-PA-O5B
3	B	702	FAD	C5B-O5B-PA-O3P
3	B	702	FAD	C5'-O5'-P-O3P
3	B	702	FAD	C5'-O5'-P-O2P
3	B	702	FAD	O3'-C3'-C4'-O4'
3	B	702	FAD	C2'-C3'-C4'-C5'
4	A	703	TZD	P2-O11-P1-O5G
4	B	703	TZD	C5-C5A-C5B-O5G
3	B	702	FAD	O3'-C3'-C4'-C5'
3	A	702	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

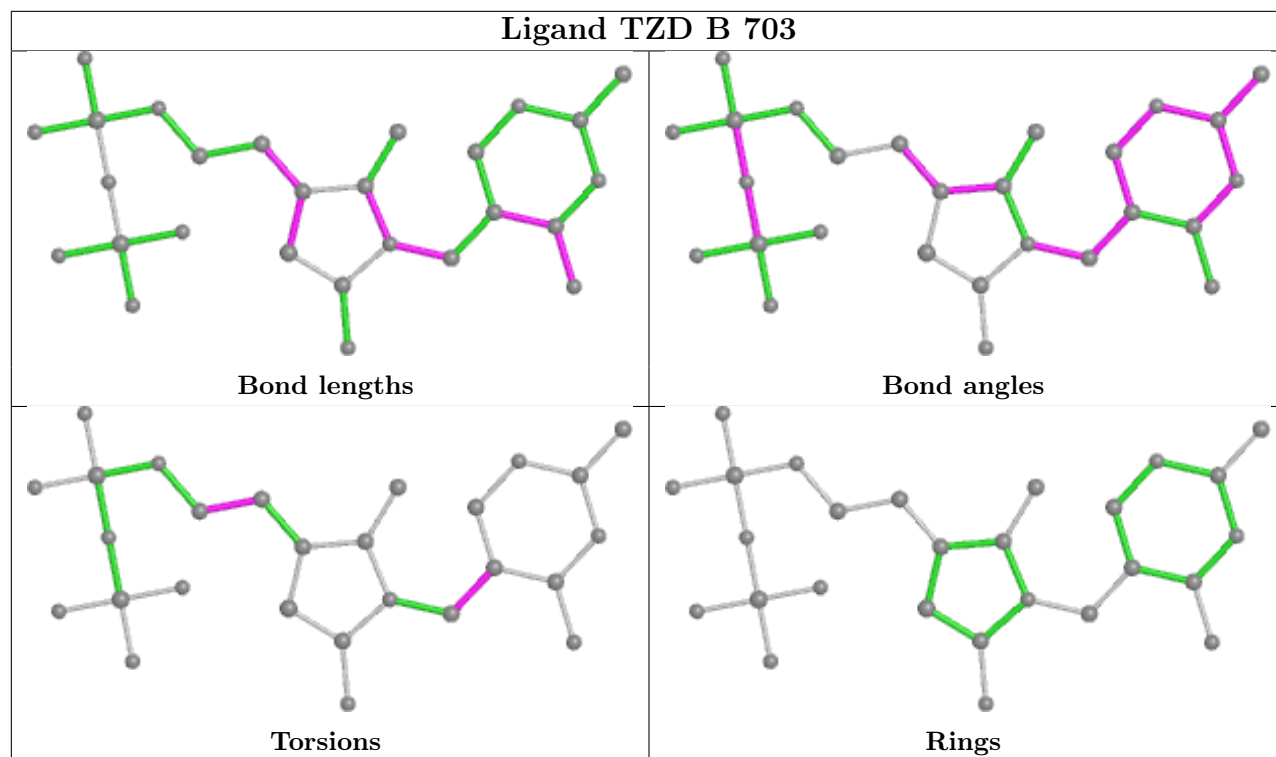
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	FAD	1	0
4	B	703	TZD	2	0
4	A	703	TZD	1	0

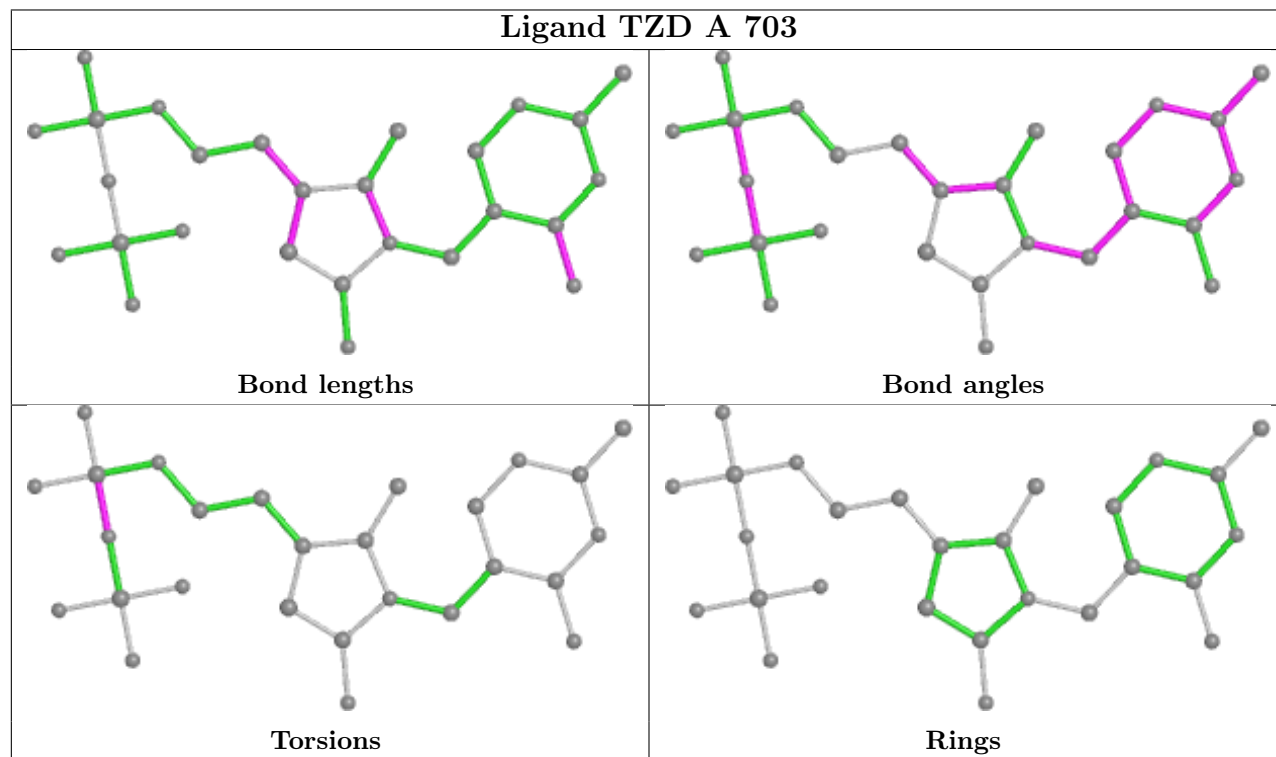
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

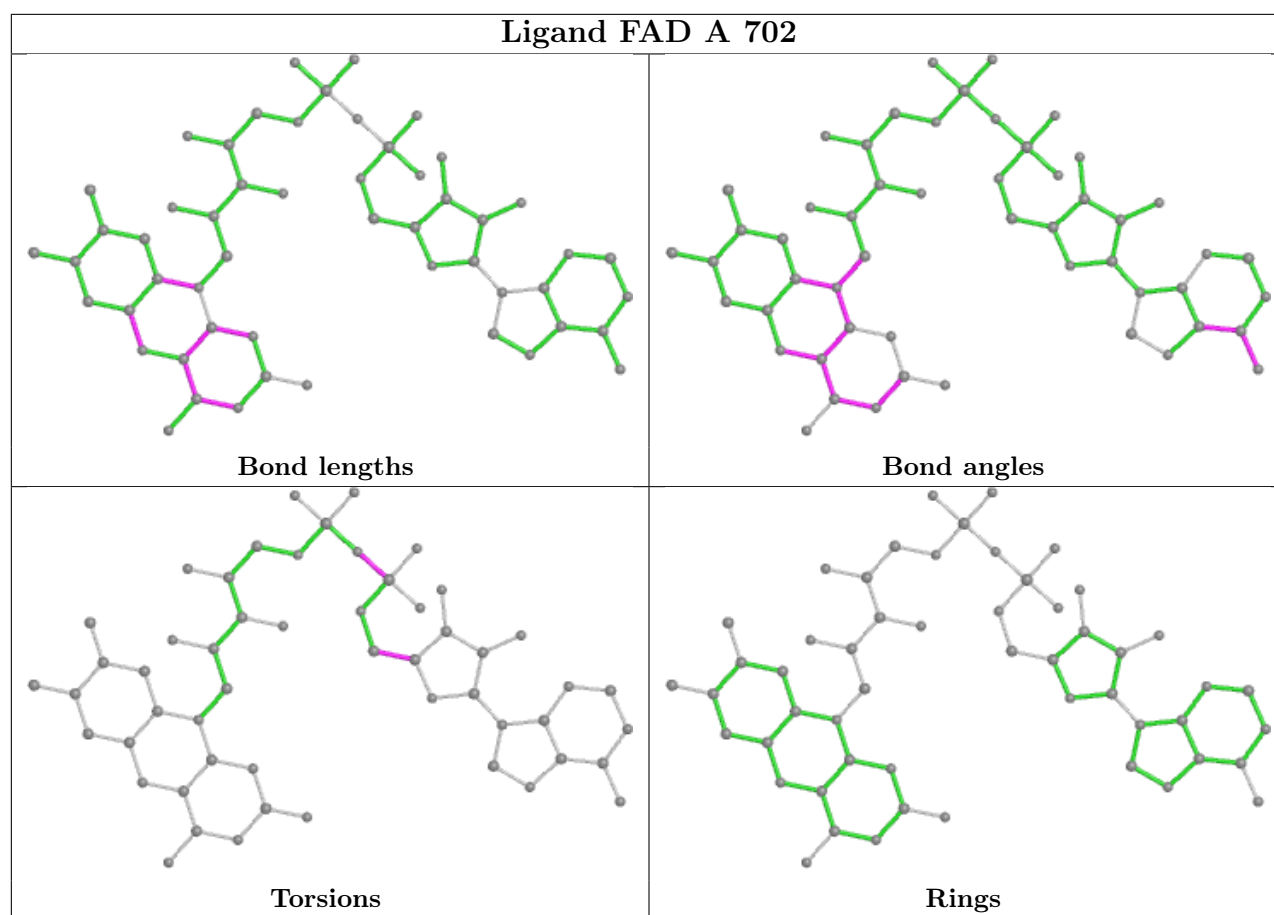


Ligand TZD B 703



Ligand TZD 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

6.1 Protein, DNA and RNA chains

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	589/688 (85%)	0.01	15 (2%) 57 63	29, 42, 61, 89	0
1	B	581/688 (84%)	0.63	72 (12%) 4 5	35, 61, 91, 106	0
All	All	1170/1376 (85%)	0.32	87 (7%) 14 18	29, 49, 87, 106	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ILE	5.8
1	B	192	ILE	5.0
1	B	436	VAL	5.0
1	B	672	LYS	4.8
1	B	83	GLU	4.8
1	B	675	GLN	4.8
1	B	256	ARG	4.5
1	B	294	ILE	4.5
1	B	447	TRP	4.5
1	B	326	SER	4.1
1	B	395	ALA	4.0
1	B	85	PHE	4.0
1	B	364	GLN	4.0
1	B	84	SER	3.9
1	B	442	GLU	3.7
1	B	290	ALA	3.6
1	B	432	LEU	3.5
1	B	279	SER	3.5
1	B	437	LYS	3.5
1	B	673	ASP	3.4
1	B	81	MET	3.3
1	B	296	MET	3.3
1	B	510	ARG	3.3
1	B	682	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	441	MET	3.2
1	B	86	ILE	3.2
1	B	676	ARG	3.2
1	A	557	THR	3.2
1	B	684	THR	3.1
1	B	190	ALA	3.1
1	B	207	ARG	3.0
1	B	298	LYS	3.0
1	B	82	ASP	2.9
1	B	433	ILE	2.9
1	B	683	ARG	2.9
1	B	257	ALA	2.8
1	B	339	PHE	2.8
1	B	687	VAL	2.8
1	B	327	ILE	2.8
1	A	527	GLY	2.8
1	B	281	GLN	2.8
1	A	526	MET	2.7
1	B	205	ILE	2.7
1	B	523	LEU	2.7
1	B	259	PRO	2.7
1	B	399	GLY	2.7
1	B	678	GLU	2.6
1	B	255	ARG	2.6
1	B	288	LYS	2.6
1	B	253	ILE	2.6
1	B	679	LEU	2.5
1	A	498	VAL	2.5
1	A	552	ALA	2.5
1	B	680	MET	2.5
1	B	289	ARG	2.4
1	B	321	LEU	2.4
1	B	168	THR	2.4
1	B	222	LEU	2.4
1	A	260	THR	2.3
1	B	397	GLY	2.3
1	B	278	LEU	2.3
1	A	524	GLY	2.3
1	B	88	LYS	2.3
1	B	191	ALA	2.3
1	A	259	PRO	2.3
1	B	283	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	373	SER	2.3
1	B	166	VAL	2.2
1	B	498	VAL	2.2
1	B	671	GLU	2.2
1	B	674	LYS	2.2
1	B	685	LYS	2.2
1	A	167	ILE	2.2
1	A	169	PRO	2.2
1	B	286	SER	2.2
1	B	669	ASP	2.2
1	A	556	MET	2.2
1	B	189	THR	2.1
1	B	435	GLN	2.1
1	A	409	LYS	2.1
1	A	519	THR	2.1
1	A	164	THR	2.1
1	B	167	ILE	2.0
1	B	254	LEU	2.0
1	B	450	ALA	2.0
1	A	528	TYR	2.0
1	B	431	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 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.

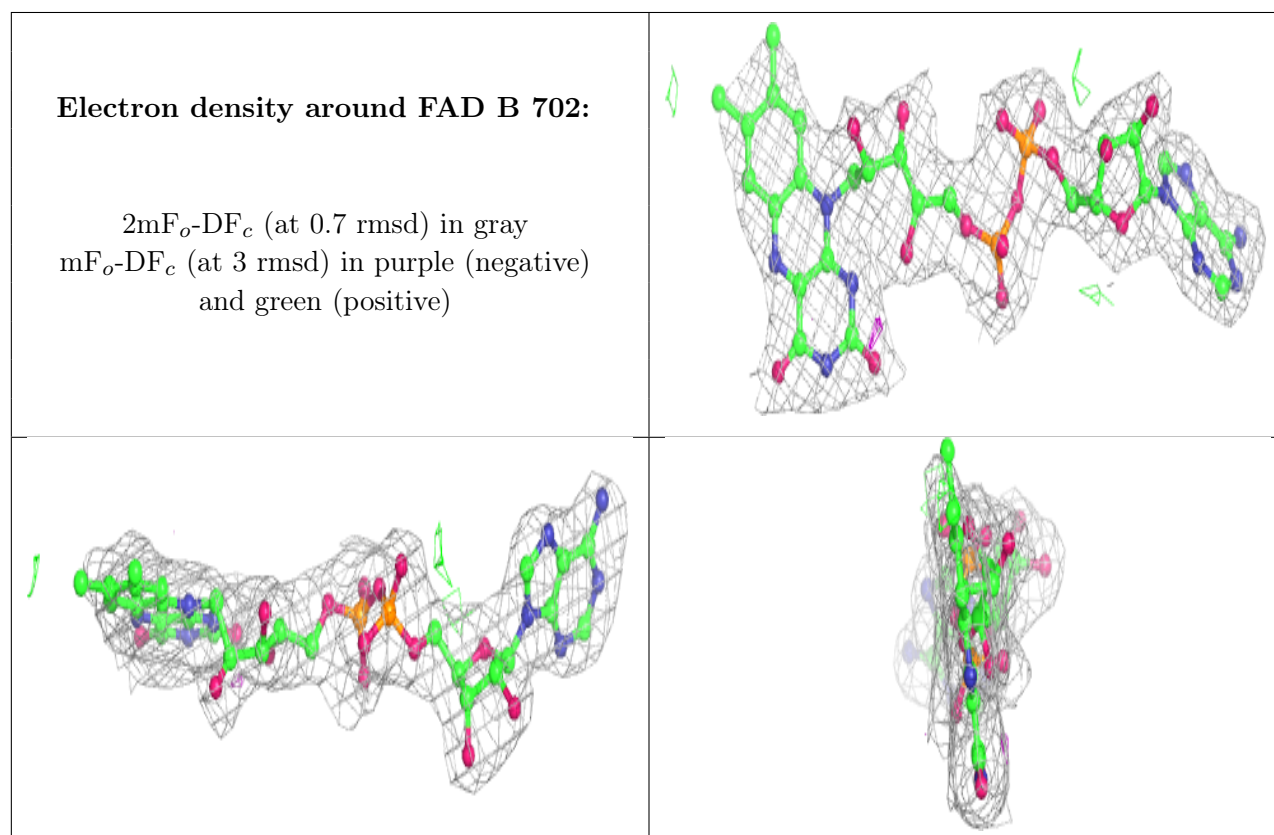
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FAD	B	702	53/53	0.95	0.17	46,57,67,70	0
3	FAD	A	702	53/53	0.98	0.16	29,34,42,48	0

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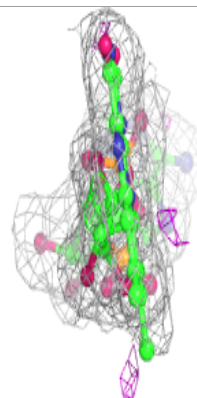
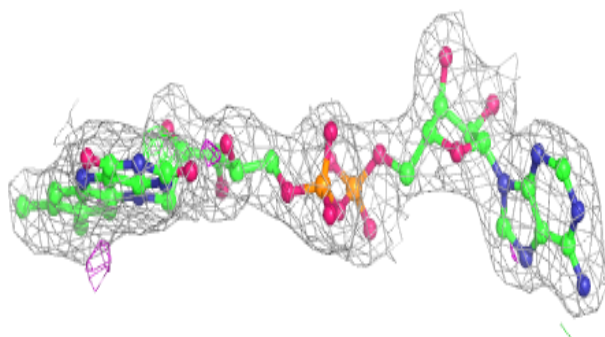
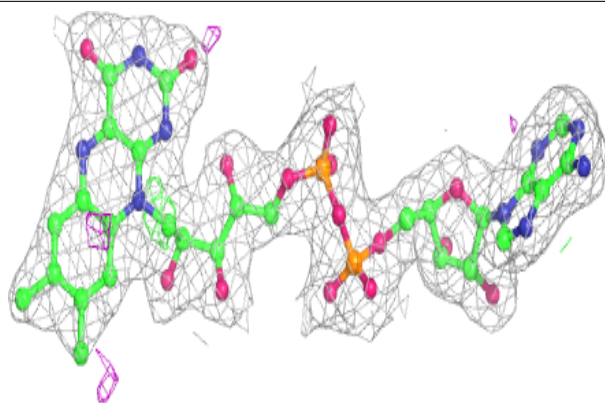
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	701	1/1	0.98	0.22	31,31,31,31	0
4	TZD	A	703	27/27	0.98	0.20	28,33,36,39	0
4	TZD	B	703	27/27	0.98	0.17	38,43,48,50	0
2	MG	A	701	1/1	0.99	0.31	18,18,18,18	0

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.

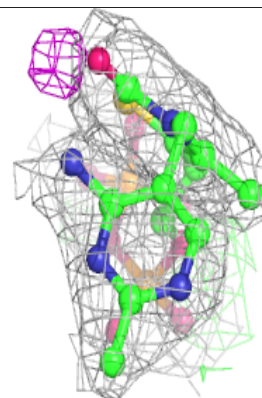
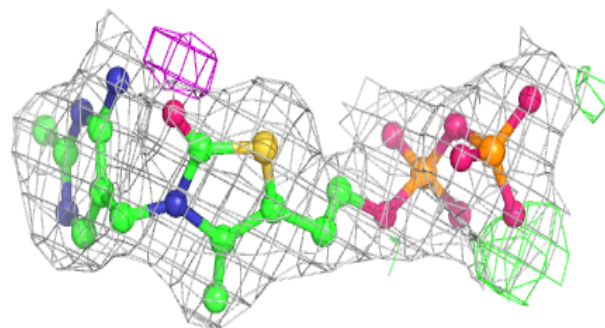
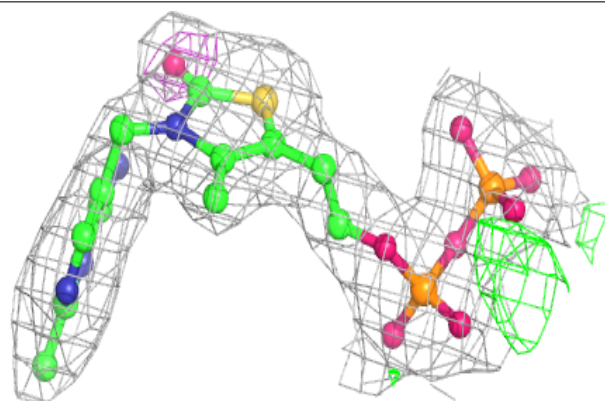


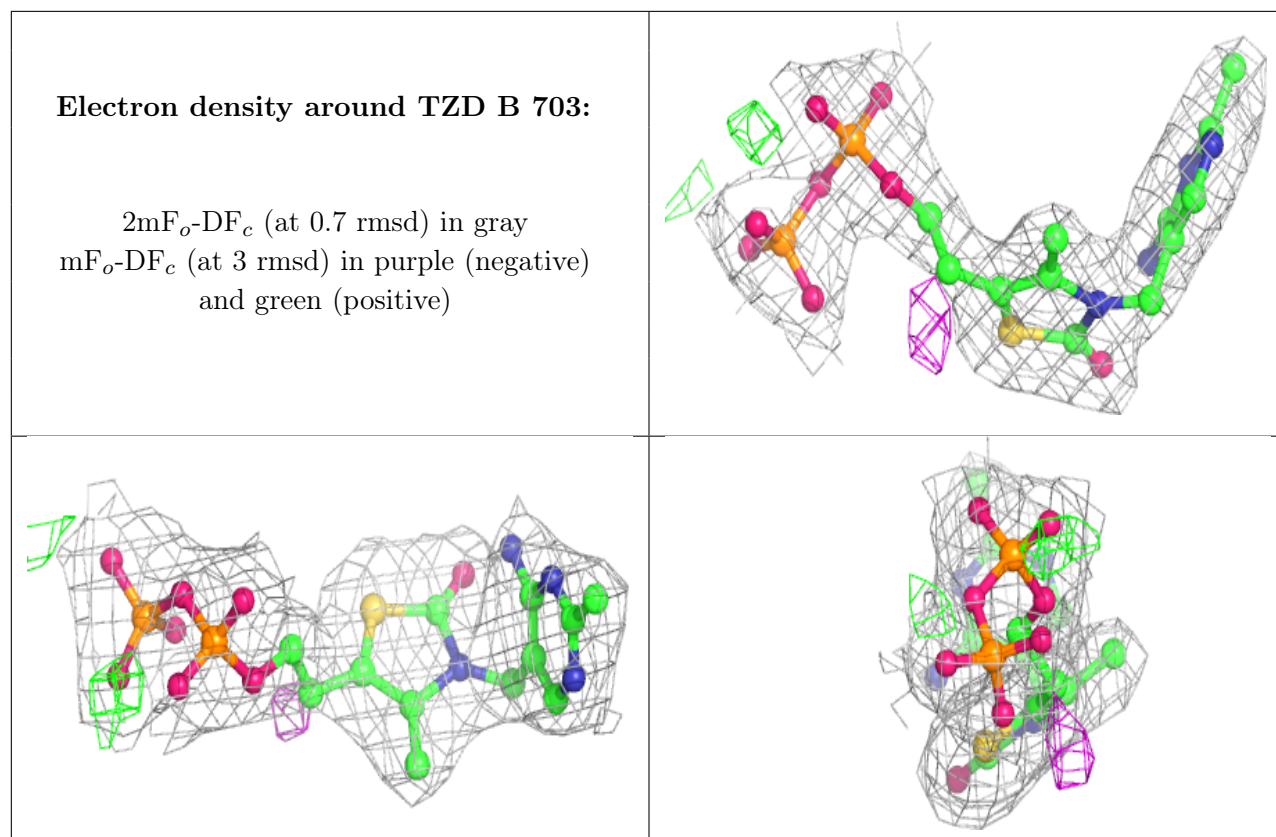
Electron density around FAD A 702:

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

**Electron density around TZD 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.