



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:38 AM UTC

PDB ID : 7EGV / pdb_00007egv
Title : Acetolactate Synthase from *Trichoderma harzianum* with inhibitor harzianic acid
Authors : Zang, X.; Xie, L.; Chen, M.; Tang, Y.; Zhou, J.
Deposited on : 2021-03-26
Resolution : 2.54 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

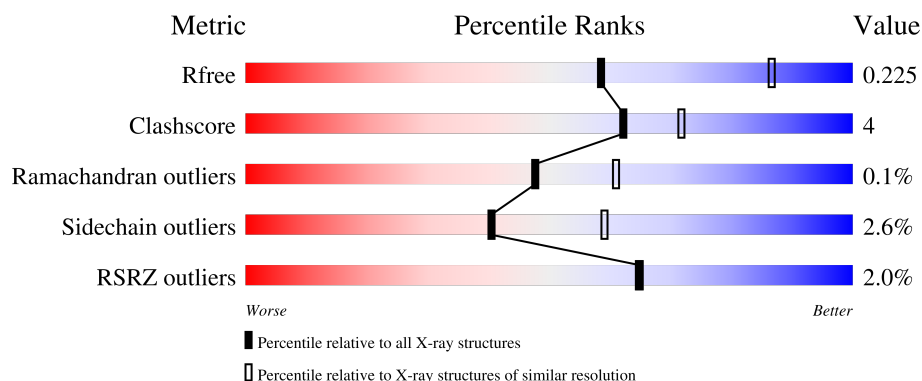
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	% 75% 11% 14%
1	B	688	2% 74% 9% 16%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9206 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	590	Total	C	N	O	S	0	0	0
			4520	2859	799	836	26			
1	B	576	Total	C	N	O	S	0	0	0
			4383	2778	767	812	26			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

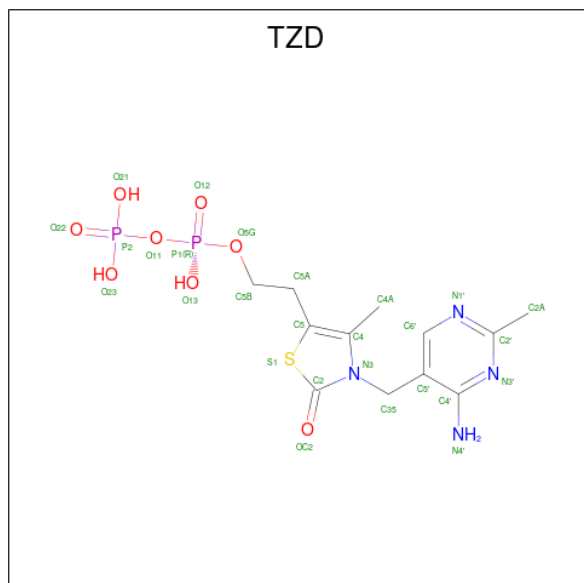
Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

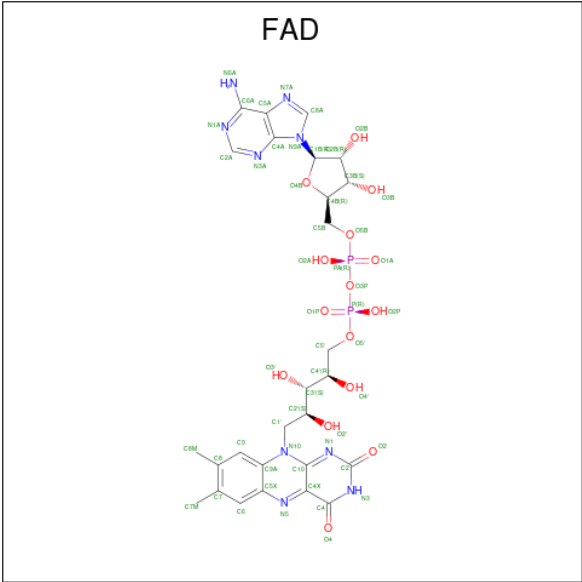
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is 2-{3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-4-METHYL-2-OXO-2,3-DIHYDRO-1,3-THIAZOL-5-YL}ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TZD) (formula: $C_{12}H_{18}N_4O_8P_2S$) (labeled as "Ligand of Interest" by depositor).



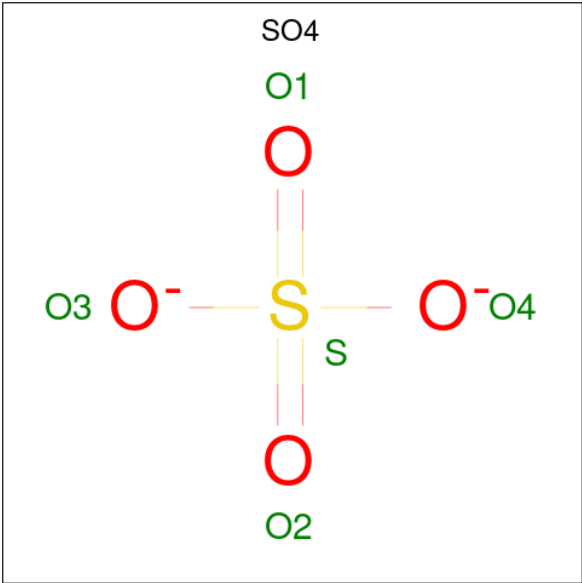
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



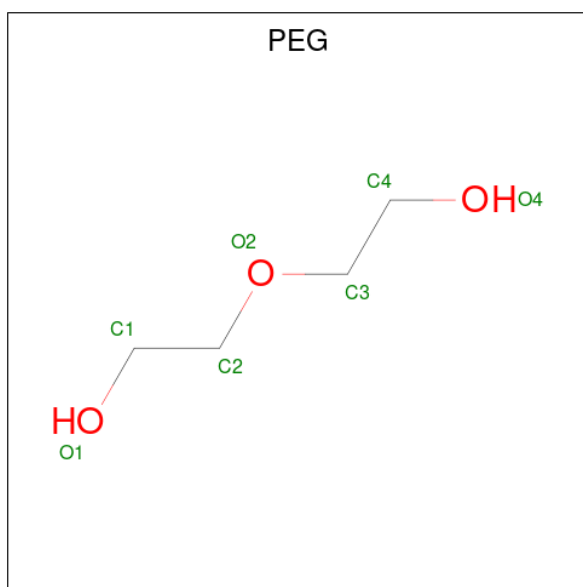
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



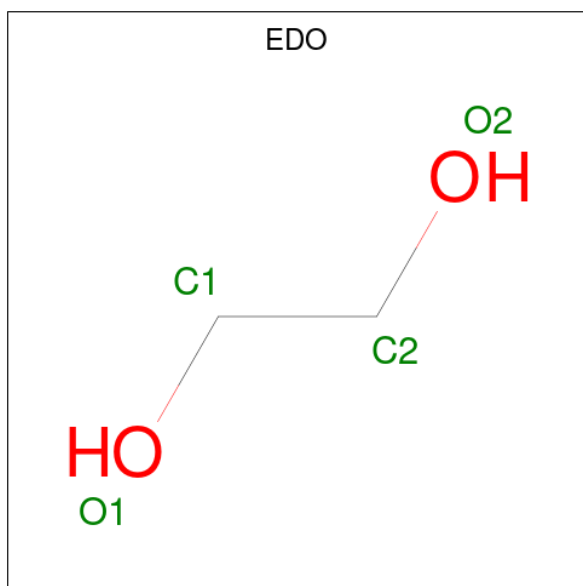
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O S	0	0
			5	4 1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



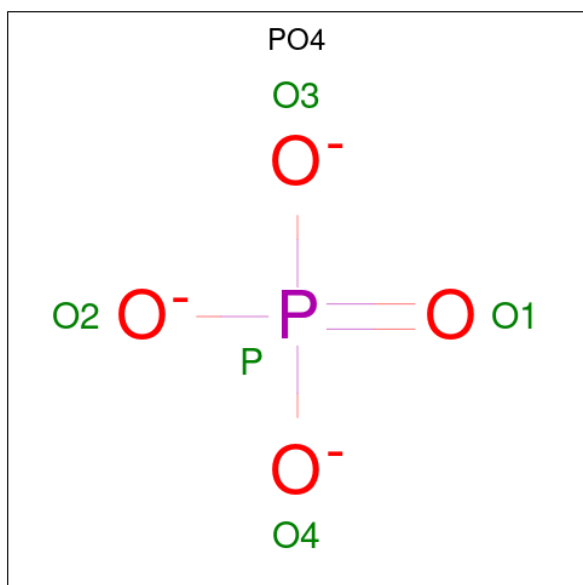
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

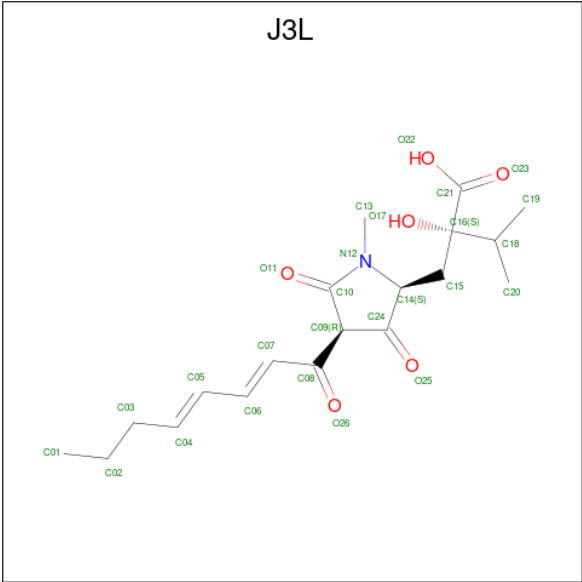
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 9 is (2S)-3-methyl-2-[[[(2S,4R)-1-methyl-4-[(2E,4E)-octa-2,4-dienoyl]-3,5-bis(oxidanylidene)pyrrolidin-2-yl]methyl]-2-oxidanyl-butanoic acid (CCD ID: J3L) (formula: C₁₉H₂₇NO₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	N	O	0	0
			26	19	1	6		

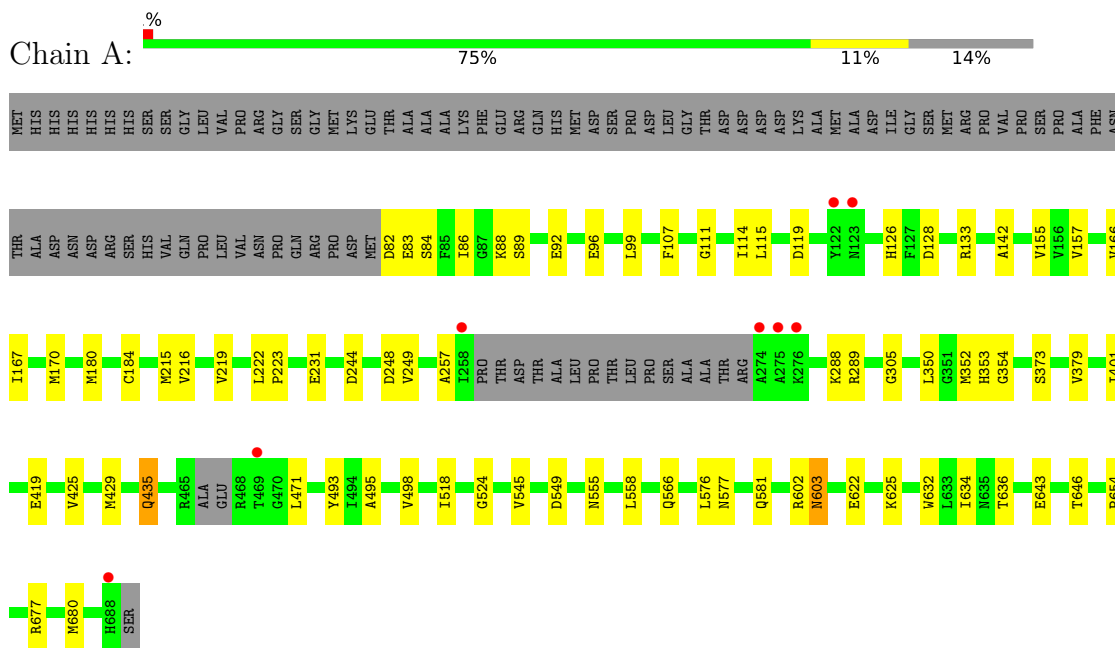
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	45	Total	O	0	0
			45	45		
10	B	33	Total	O	0	0
			33	33		

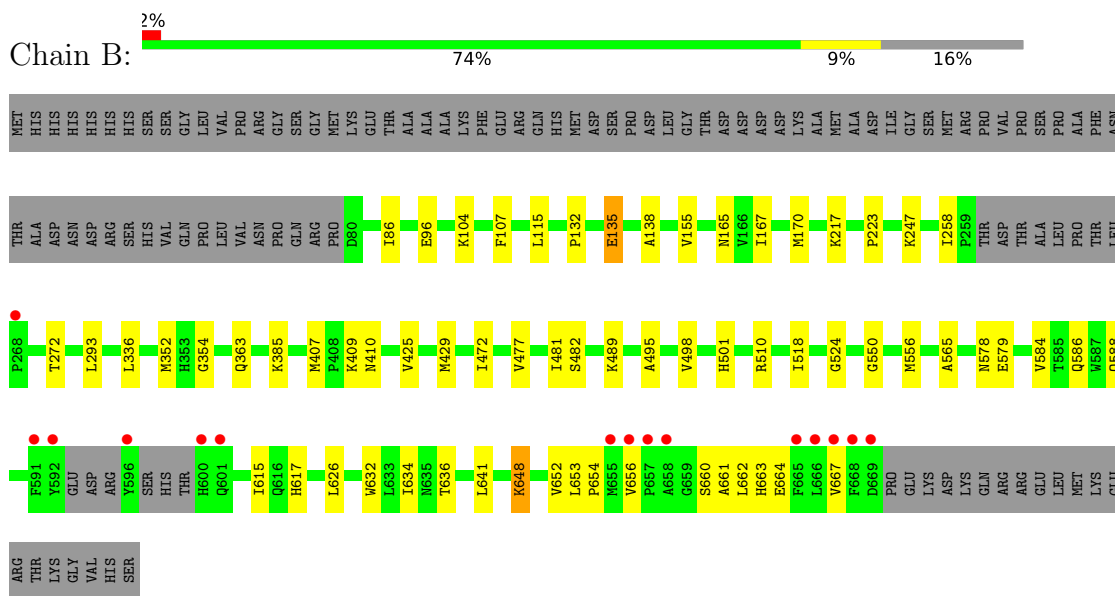
3 Residue-property plots

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



- Molecule 1: Acetolactate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.04Å 79.91Å 111.86Å 90.00° 103.10° 90.00°	Depositor
Resolution (Å)	45.62 – 2.54 45.62 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.62-2.54) 99.9 (45.62-2.54)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.175 , 0.222 0.184 , 0.225	Depositor DCC
R_{free} test set	2404 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.456	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9206	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MG, TZD, PO4, J3L, EDO, SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.35	0/4611	0.54	0/6234
1	B	0.35	0/4472	0.57	0/6052
All	All	0.35	0/9083	0.55	0/12286

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

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	4520	0	4545	40	0
1	B	4383	0	4402	31	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	15	2	0
3	B	27	0	15	1	0
4	A	53	0	31	1	0
4	B	53	0	31	0	0
5	A	5	0	0	0	0
6	A	7	0	10	0	0
7	A	12	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	0	12	0	0
8	A	5	0	0	0	0
9	B	26	0	0	0	0
10	A	45	0	0	0	0
10	B	33	0	0	0	0
All	All	9206	0	9079	74	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 (74) 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:289:ARG:NH2	1:A:419:GLU:OE2	2.25	0.70
3:B:703:TZD:C2	3:B:703:TZD:H4'2	2.09	0.66
1:A:581:GLN:HB3	3:A:702:TZD:H5A1	1.76	0.66
1:B:132:PRO:HG3	1:B:138:ALA:HB2	1.78	0.63
1:B:167:ILE:HD13	1:B:170:MET:HE3	1.83	0.60
1:B:407:MET:HE3	1:B:409:LYS:HD3	1.84	0.59
1:A:425:VAL:HG22	1:A:429:MET:HE2	1.84	0.59
1:B:661:ALA:HB3	1:B:664:GLU:HG3	1.86	0.58
1:A:215:MET:HG3	1:A:244:ASP:HB3	1.86	0.57
1:A:167:ILE:HA	1:A:170:MET:HE3	1.87	0.57
1:A:577:ASN:ND2	1:A:643:GLU:OE1	2.35	0.56
1:B:425:VAL:HG22	1:B:429:MET:HE2	1.89	0.55
1:A:495:ALA:HA	1:A:518:ILE:O	2.08	0.54
1:A:602:ARG:O	1:A:603:ASN:HB2	2.08	0.54
1:B:385:LYS:HD3	1:B:661:ALA:HB2	1.89	0.54
1:A:82:ASP:OD1	1:A:257:ALA:HB1	2.08	0.53
1:A:89:SER:OG	1:A:92:GLU:HG3	2.08	0.53
1:B:107:PHE:O	1:B:155:VAL:HA	2.08	0.53
1:A:555:ASN:HA	1:A:558:LEU:HD23	1.92	0.52
1:B:498:VAL:HG21	1:B:524:GLY:C	2.35	0.52
1:A:576:LEU:HD12	1:A:646:THR:HG21	1.92	0.50
1:A:99:LEU:HD21	1:A:126:HIS:CG	2.46	0.50
1:B:352:MET:HA	1:B:656:VAL:HB	1.92	0.49
1:B:407:MET:HE2	1:B:410:ASN:ND2	2.27	0.49
1:B:495:ALA:HA	1:B:518:ILE:O	2.13	0.49
1:A:222:LEU:HB3	1:A:223:PRO:HD3	1.94	0.49
1:A:493:TYR:HB2	1:A:545:VAL:HG22	1.96	0.47
1:A:88:LYS:HE2	1:A:96:GLU:OE2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:VAL:HG22	1:A:249:VAL:O	2.15	0.46
1:A:632:TRP:O	1:A:636:THR:HG23	2.15	0.46
1:A:350:LEU:HD11	1:A:379:VAL:HG13	1.96	0.46
1:A:142:ALA:HB3	1:A:180:MET:HE2	1.98	0.45
1:B:482:SER:OG	1:B:489:LYS:NZ	2.40	0.45
1:B:501:HIS:CE1	1:B:550:GLY:H	2.33	0.45
1:A:107:PHE:O	1:A:155:VAL:HA	2.17	0.45
1:B:578:ASN:O	1:B:648:LYS:HE3	2.17	0.45
3:A:702:TZD:H4'2	3:A:702:TZD:C2	2.30	0.44
1:A:114:ILE:O	1:A:114:ILE:HG13	2.17	0.44
1:B:363:GLN:HG3	1:B:663:HIS:HB3	1.99	0.44
1:B:472:ILE:HD13	1:B:626:LEU:HD13	1.99	0.44
1:A:167:ILE:HD13	1:A:170:MET:HE3	2.00	0.44
1:B:223:PRO:HG2	1:B:258:ILE:HD13	1.98	0.43
1:A:288:LYS:HG2	1:A:435:GLN:OE1	2.18	0.43
1:A:133:ARG:NH1	1:A:566:GLN:OE1	2.52	0.43
1:A:166:VAL:HG12	1:A:166:VAL:O	2.18	0.43
1:B:632:TRP:O	1:B:636:THR:HG23	2.19	0.43
1:A:111:GLY:O	1:A:115:LEU:HG	2.18	0.43
1:B:660:SER:HB3	1:B:664:GLU:HB2	2.01	0.43
1:B:510:ARG:NE	1:B:510:ARG:HA	2.34	0.43
1:A:498:VAL:HG21	1:A:524:GLY:C	2.44	0.43
1:A:83:GLU:O	1:A:86:ILE:HG13	2.19	0.42
1:B:354:GLY:O	1:B:654:PRO:HG2	2.18	0.42
1:A:216:VAL:HG11	1:A:222:LEU:HD13	2.01	0.42
1:A:354:GLY:O	1:A:654:PRO:HG2	2.19	0.42
1:B:586:GLN:HE22	1:B:652:VAL:H	1.65	0.42
1:A:83:GLU:HA	1:A:86:ILE:HD11	2.02	0.42
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.78	0.42
1:A:248:ASP:OD1	1:A:248:ASP:N	2.48	0.41
1:B:167:ILE:HA	1:B:170:MET:HE3	2.02	0.41
1:B:336:LEU:HA	1:B:336:LEU:HD23	1.84	0.41
1:B:653:LEU:HA	1:B:654:PRO:C	2.44	0.41
1:A:115:LEU:HA	1:A:115:LEU:HD23	1.82	0.41
1:A:305:GLY:HA3	1:A:373:SER:HB3	2.02	0.41
1:A:622:GLU:OE2	1:A:625:LYS:NZ	2.54	0.41
4:A:703:FAD:HM81	4:A:703:FAD:HM73	1.88	0.41
1:A:157:VAL:O	1:A:184:CYS:HA	2.21	0.41
1:A:677:ARG:HA	1:A:680:MET:HE2	2.03	0.41
1:B:617:HIS:HA	1:B:641:LEU:O	2.21	0.41
1:B:135:GLU:HG2	1:B:165:ASN:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LYS:O	1:B:409:LYS:HG2	2.20	0.41
1:B:565:ALA:HB2	1:B:615:ILE:HD11	2.03	0.40
1:A:352:MET:HG2	1:A:353:HIS:ND1	2.35	0.40
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.78	0.40
1:B:477:VAL:O	1:B:481:ILE:HG13	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	584/688 (85%)	563 (96%)	20 (3%)	1 (0%)	43	56
1	B	569/688 (83%)	556 (98%)	13 (2%)	0	100	100
All	All	1153/1376 (84%)	1119 (97%)	33 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	ASN

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	474/556 (85%)	466 (98%)	8 (2%)	53 72
1	B	458/556 (82%)	442 (96%)	16 (4%)	32 48
All	All	932/1112 (84%)	908 (97%)	24 (3%)	40 59

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	SER
1	A	119	ASP
1	A	128	ASP
1	A	231	GLU
1	A	401	ILE
1	A	435	GLN
1	A	549	ASP
1	A	634	ILE
1	B	86	ILE
1	B	96	GLU
1	B	104	LYS
1	B	115	LEU
1	B	135	GLU
1	B	217	LYS
1	B	247	LYS
1	B	272	THR
1	B	556	MET
1	B	579	GLU
1	B	584	VAL
1	B	588	GLN
1	B	634	ILE
1	B	648	LYS
1	B	662	LEU
1	B	667	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	284	ASN
1	A	306	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	675	GLN
1	B	171	GLN
1	B	334	HIS
1	B	464	GLN
1	B	508	HIS
1	B	513	HIS
1	B	600	HIS

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\# Z > 2$
4	FAD	A	703	-	58,58,58	0.54	0	85,89,89	0.63	1 (1%)
9	J3L	B	701	-	21,26,26	3.16	5 (23%)	22,37,37	1.67	6 (27%)
7	EDO	A	706	-	3,3,3	0.08	0	2,2,2	0.20	0
5	SO4	A	704	-	4,4,4	0.24	0	6,6,6	0.17	0
7	EDO	B	706	-	3,3,3	0.06	0	2,2,2	0.11	0
8	PO4	A	709	-	4,4,4	0.97	0	6,6,6	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	EDO	A	708	-	3,3,3	0.13	0	2,2,2	0.27	0
6	PEG	A	705	-	6,6,6	0.15	0	5,5,5	0.08	0
7	EDO	B	705	-	3,3,3	0.19	0	2,2,2	0.18	0
7	EDO	A	707	-	3,3,3	0.09	0	2,2,2	0.04	0
3	TZD	A	702	2	27,28,28	4.89	8 (29%)	37,42,42	4.48	9 (24%)
3	TZD	B	703	2	27,28,28	4.85	10 (37%)	37,42,42	4.25	11 (29%)
4	FAD	B	704	-	58,58,58	0.54	0	85,89,89	0.62	1 (1%)

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	FAD	A	703	-	-	2/34/50/50	0/6/6/6
9	J3L	B	701	-	-	17/26/48/48	0/1/1/1
7	EDO	A	706	-	-	0/1/1/1	-
7	EDO	B	706	-	-	0/1/1/1	-
7	EDO	A	708	-	-	0/1/1/1	-
6	PEG	A	705	-	-	1/4/4/4	-
7	EDO	B	705	-	-	0/1/1/1	-
7	EDO	A	707	-	-	0/1/1/1	-
3	TZD	A	702	2	-	1/17/17/17	0/2/2/2
3	TZD	B	703	2	-	1/17/17/17	0/2/2/2
4	FAD	B	704	-	-	3/34/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	TZD	C4-N3	15.81	1.64	1.39
3	B	703	TZD	C4-N3	15.74	1.64	1.39
9	B	701	J3L	C10-N12	13.05	1.51	1.34
3	A	702	TZD	C2-N3	12.95	1.58	1.38
3	B	703	TZD	C2-N3	12.51	1.57	1.38
3	B	703	TZD	C5-C4	9.40	1.54	1.35
3	A	702	TZD	C5-C4	8.12	1.52	1.35
3	B	703	TZD	C2-S1	-6.73	1.69	1.77
3	A	702	TZD	C2-S1	-6.55	1.69	1.77
3	A	702	TZD	C5-S1	-6.40	1.61	1.74
3	B	703	TZD	C5-S1	-5.81	1.62	1.74
3	A	702	TZD	P1-O11	5.61	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	TZD	C4'-N4'	4.44	1.45	1.34
3	B	703	TZD	P1-O11	4.12	1.63	1.59
3	B	703	TZD	C4'-N4'	3.71	1.43	1.34
9	B	701	J3L	C06-C05	2.58	1.52	1.44
9	B	701	J3L	C15-C14	-2.49	1.50	1.54
3	B	703	TZD	C4A-C4	2.24	1.53	1.49
3	A	702	TZD	C4A-C4	2.19	1.52	1.49
9	B	701	J3L	O26-C08	-2.17	1.19	1.22
3	B	703	TZD	OC2-C2	-2.15	1.18	1.21
3	B	703	TZD	C4'-N3'	-2.13	1.32	1.35
9	B	701	J3L	C14-N12	2.13	1.50	1.44

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	TZD	C5-S1-C2	25.32	103.80	91.64
3	B	703	TZD	C5-S1-C2	23.58	102.97	91.64
3	B	703	TZD	C5'-C35-N3	-5.07	107.01	113.14
9	B	701	J3L	O22-C21-C16	4.13	120.97	114.06
3	A	702	TZD	C2A-C2'-N1'	3.82	121.27	117.20
3	A	702	TZD	C5'-C35-N3	-3.64	108.74	113.14
3	B	703	TZD	C6'-N1'-C2'	3.58	121.95	116.07
3	B	703	TZD	C5'-C6'-N1'	-3.19	118.64	123.83
3	B	703	TZD	N1'-C2'-N3'	-3.01	120.53	125.53
9	B	701	J3L	C13-N12-C10	3.00	125.96	122.07
3	A	702	TZD	C2'-N3'-C4'	2.75	122.32	118.10
3	A	702	TZD	C6'-N1'-C2'	2.72	120.54	116.07
3	B	703	TZD	C2A-C2'-N1'	2.72	120.09	117.20
3	A	702	TZD	N1'-C2'-N3'	-2.62	121.17	125.53
3	B	703	TZD	OC2-C2-N3	-2.59	122.33	125.37
3	A	702	TZD	C5'-C6'-N1'	-2.38	119.96	123.83
9	B	701	J3L	C06-C05-C04	-2.29	112.77	125.30
3	A	702	TZD	C5A-C5-S1	2.28	124.19	119.29
3	B	703	TZD	C4-N3-C2	-2.24	105.76	112.39
9	B	701	J3L	O23-C21-C16	-2.21	118.20	122.32
9	B	701	J3L	C15-C14-N12	-2.15	110.89	114.84
3	B	703	TZD	C6'-C5'-C4'	2.13	118.16	115.55
3	B	703	TZD	C5A-C5-S1	2.12	123.83	119.29
3	B	703	TZD	O21-P2-O11	2.09	111.65	104.64
4	A	703	FAD	C4-N3-C2	-2.07	121.97	125.64
3	A	702	TZD	C5'-C4'-N3'	-2.06	118.29	121.31
4	B	704	FAD	C4-N3-C2	-2.05	122.01	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	701	J3L	C05-C06-C07	-2.03	119.84	124.65

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	TZD	P2-O11-P1-O5G
4	B	704	FAD	P-O3P-PA-O5B
9	B	701	J3L	N12-C14-C15-C16
9	B	701	J3L	C14-C15-C16-C18
9	B	701	J3L	C14-C15-C16-C21
9	B	701	J3L	C14-C15-C16-O17
9	B	701	J3L	C15-C16-C18-C20
9	B	701	J3L	C21-C16-C18-C19
9	B	701	J3L	C21-C16-C18-C20
9	B	701	J3L	O17-C16-C18-C19
9	B	701	J3L	O17-C16-C18-C20
9	B	701	J3L	C15-C16-C21-O22
9	B	701	J3L	C15-C16-C21-O23
9	B	701	J3L	O17-C16-C21-O22
9	B	701	J3L	O17-C16-C21-O23
9	B	701	J3L	C04-C05-C06-C07
9	B	701	J3L	C15-C16-C18-C19
3	B	703	TZD	P2-O11-P1-O5G
4	A	703	FAD	P-O3P-PA-O5B
9	B	701	J3L	O26-C08-C09-C24
4	B	704	FAD	C2B-C1B-N9A-C8A
6	A	705	PEG	C1-C2-O2-C3
9	B	701	J3L	C02-C03-C04-C05
4	A	703	FAD	C2B-C1B-N9A-C8A
4	B	704	FAD	PA-O3P-P-O2P

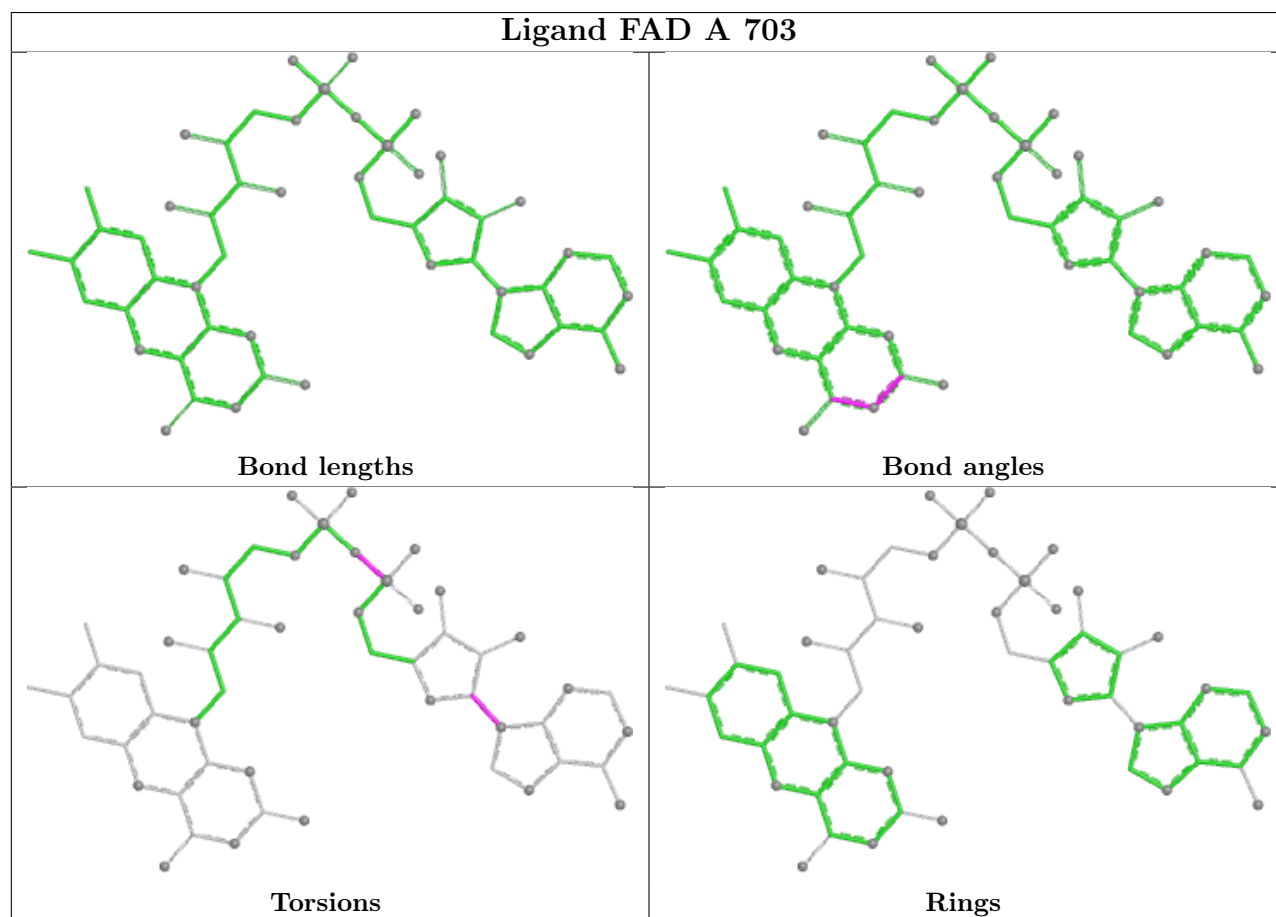
There are no ring outliers.

3 monomers are involved in 4 short contacts:

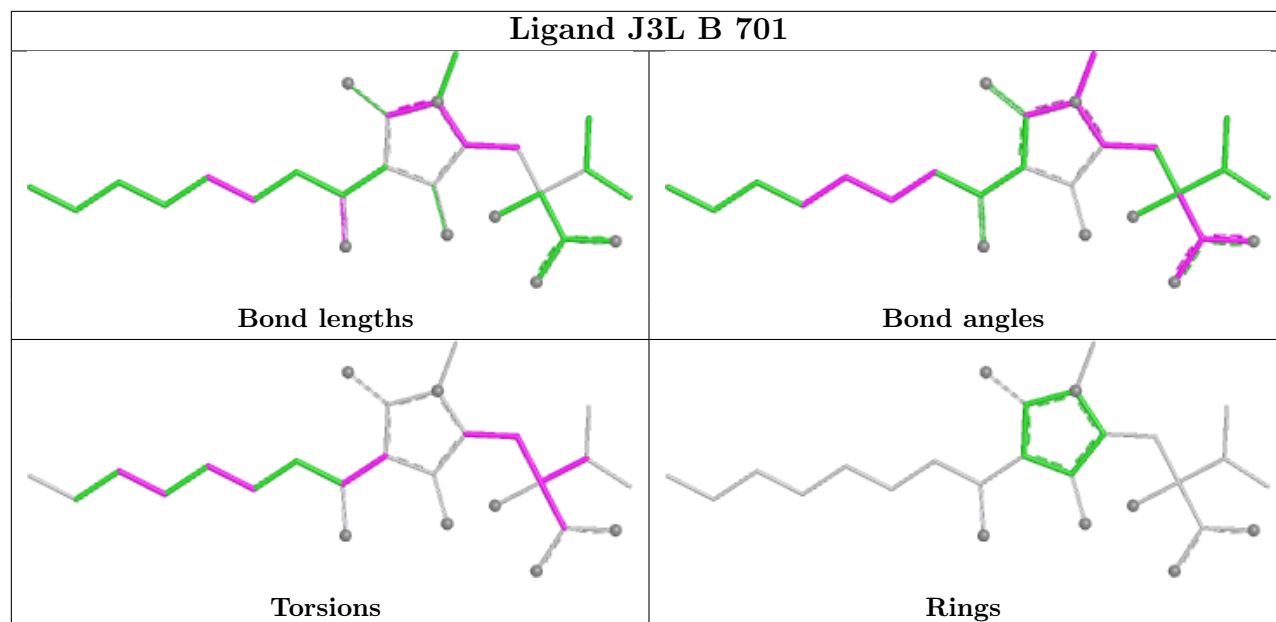
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	703	FAD	1	0
3	A	702	TZD	2	0
3	B	703	TZD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

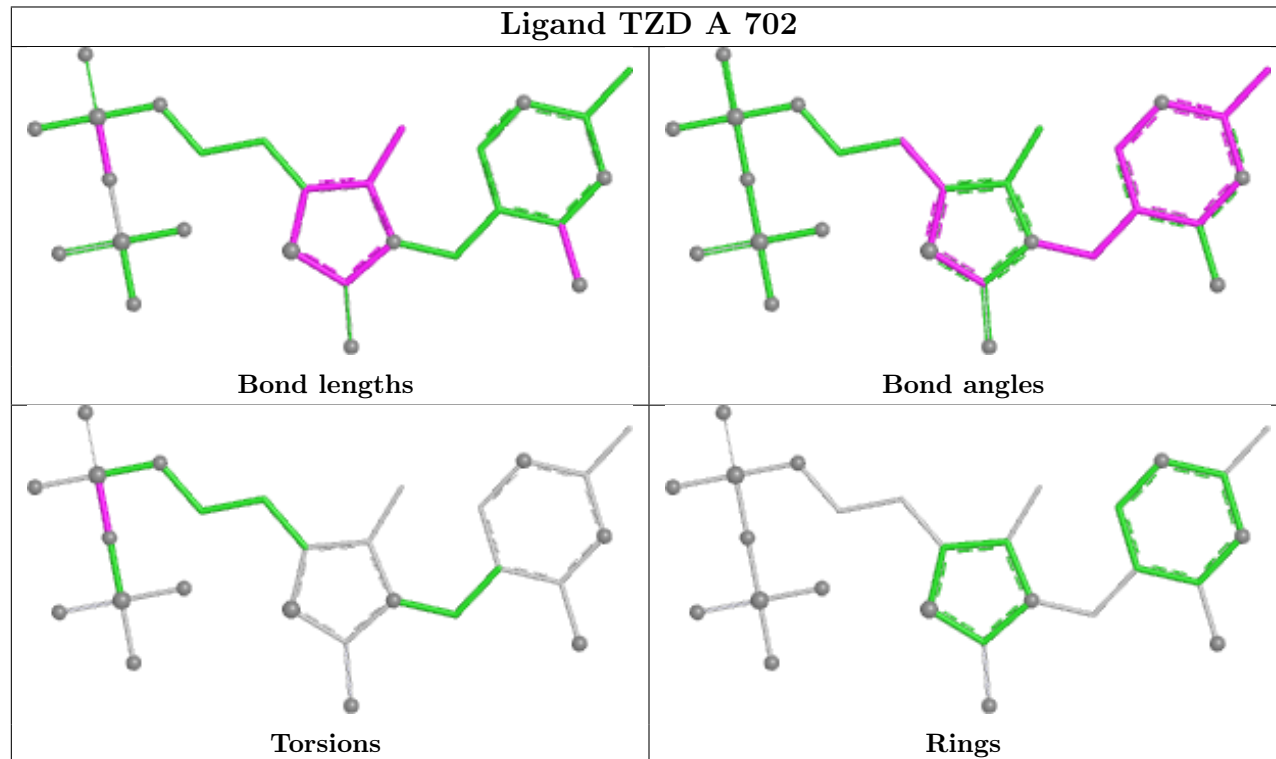
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

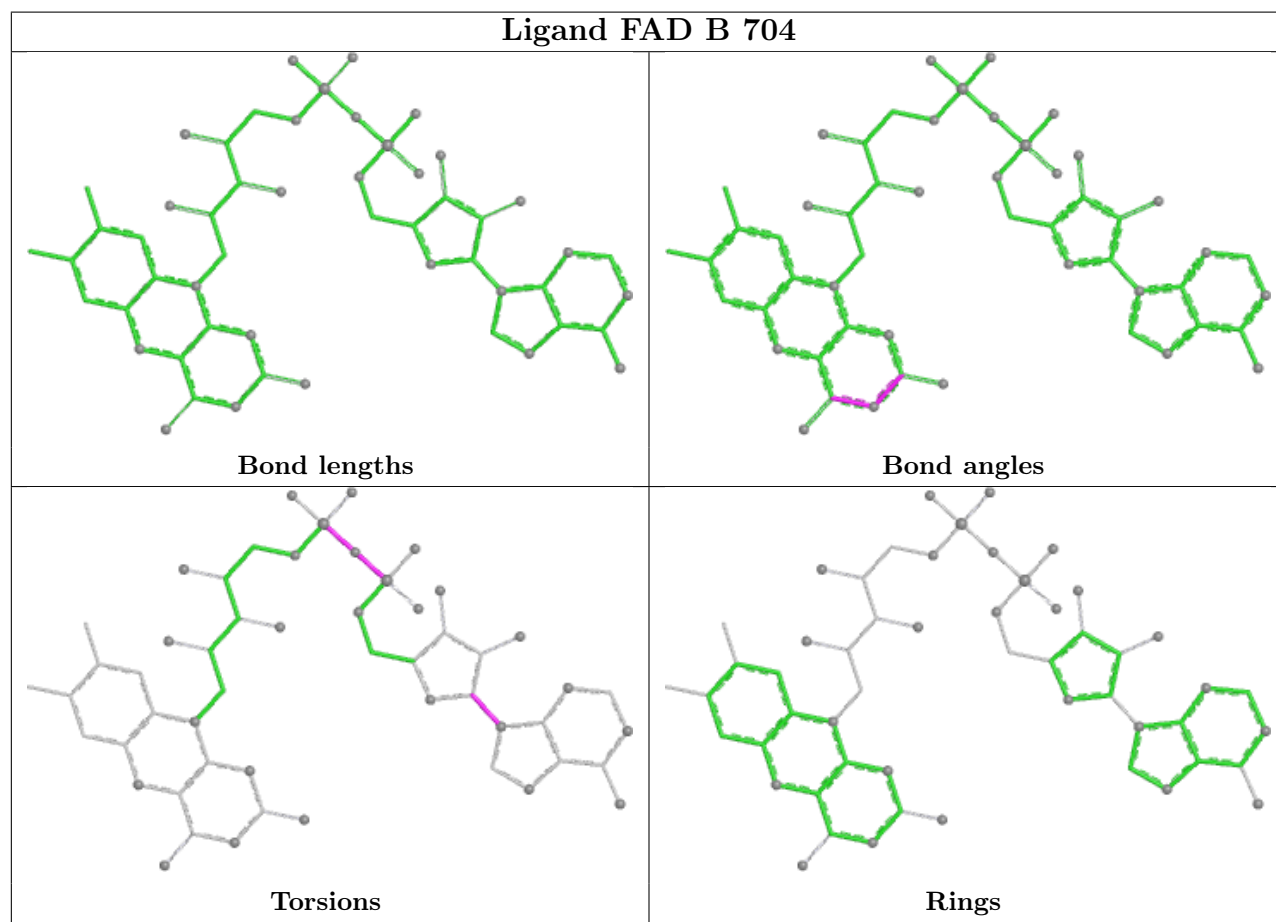
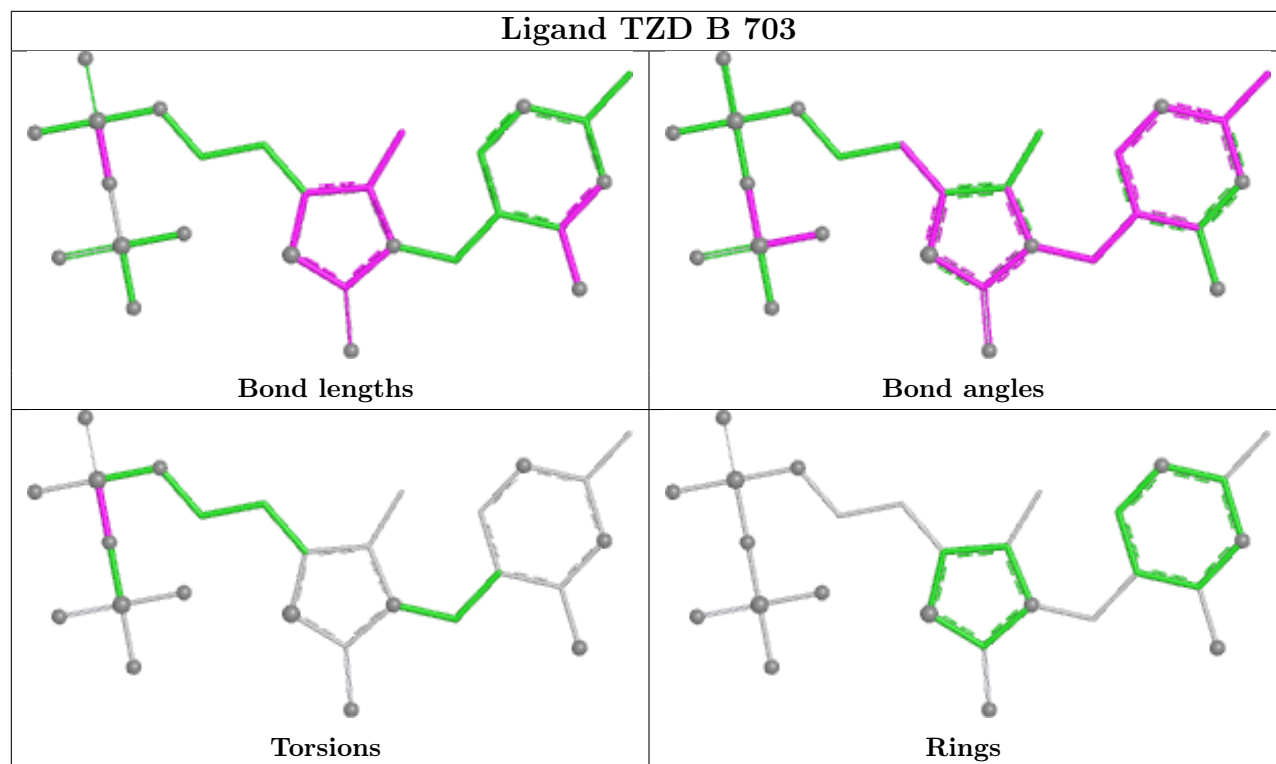


Ligand J3L B 701



Ligand TZD A 702





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	590/688 (85%)	-0.33	8 (1%) 73 74	22, 35, 67, 93	0
1	B	576/688 (83%)	-0.41	15 (2%) 57 58	22, 32, 63, 88	0
All	All	1166/1376 (84%)	-0.37	23 (1%) 65 65	22, 34, 65, 93	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ALA	4.2
1	B	591	PHE	3.8
1	A	258	ILE	3.4
1	A	275	ALA	3.3
1	B	596	TYR	3.2
1	B	666	LEU	3.1
1	B	657	PRO	3.1
1	B	658	ALA	3.1
1	A	122	TYR	2.9
1	B	665	PHE	2.9
1	B	592	TYR	2.7
1	B	601	GLN	2.5
1	A	276	LYS	2.5
1	A	469	THR	2.5
1	B	600	HIS	2.4
1	B	667	VAL	2.4
1	A	123	ASN	2.3
1	B	669	ASP	2.3
1	B	655	MET	2.2
1	A	688	HIS	2.1
1	B	668	PHE	2.1
1	B	656	VAL	2.0
1	B	268	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

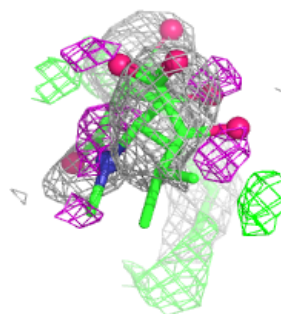
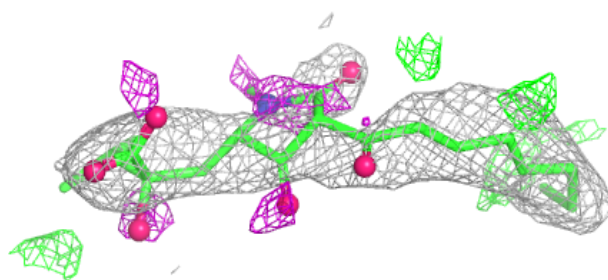
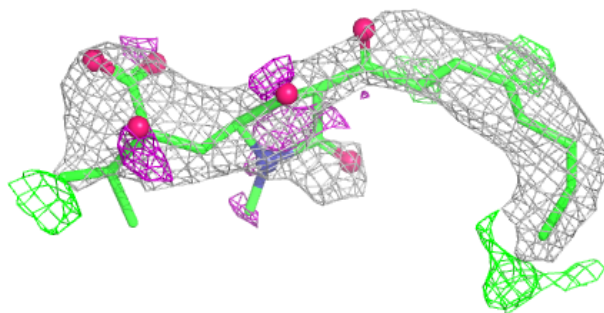
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	708	4/4	0.60	0.21	47,49,50,62	0
9	J3L	B	701	26/26	0.70	0.27	40,57,61,64	26
7	EDO	A	706	4/4	0.73	0.17	68,71,74,75	0
7	EDO	B	705	4/4	0.79	0.13	39,39,40,48	0
6	PEG	A	705	7/7	0.81	0.17	53,55,60,70	0
7	EDO	B	706	4/4	0.83	0.14	52,53,53,54	0
7	EDO	A	707	4/4	0.86	0.13	40,43,46,46	0
8	PO4	A	709	5/5	0.91	0.14	54,55,62,73	0
5	SO4	A	704	5/5	0.97	0.07	40,42,49,58	0
3	TZD	B	703	27/27	0.98	0.05	24,31,35,40	0
4	FAD	A	703	53/53	0.98	0.06	24,30,34,35	0
4	FAD	B	704	53/53	0.98	0.06	22,29,33,35	0
3	TZD	A	702	27/27	0.98	0.06	24,28,31,35	0
2	MG	B	702	1/1	0.99	0.10	24,24,24,24	0
2	MG	A	701	1/1	0.99	0.05	25,25,25,25	0

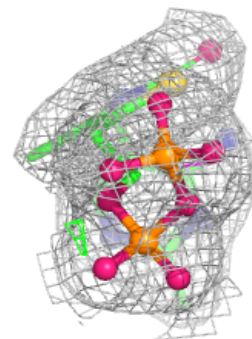
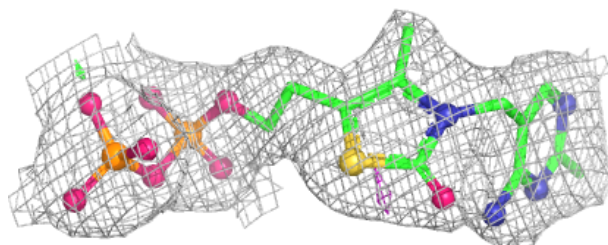
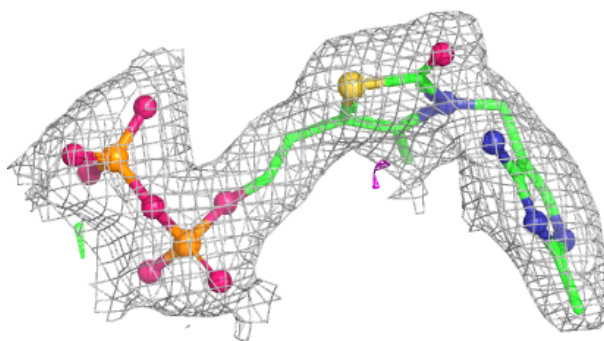
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around J3L B 701:

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

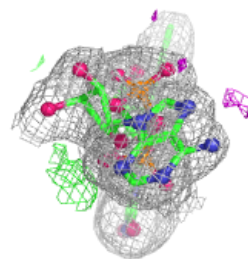
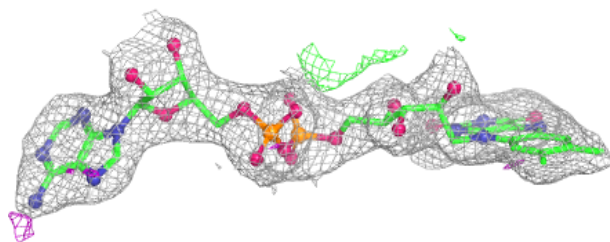
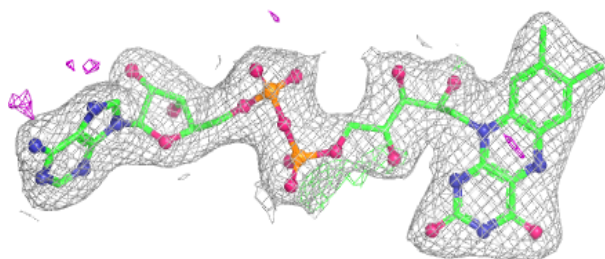
**Electron density around TZD B 703:**

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

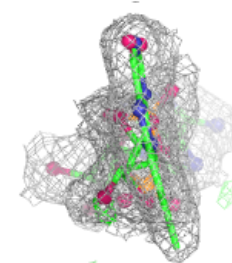
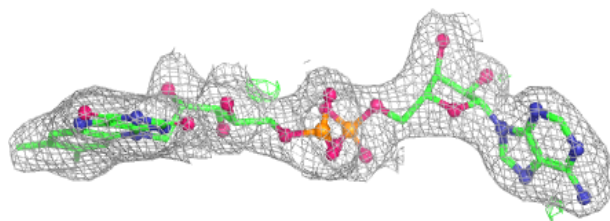
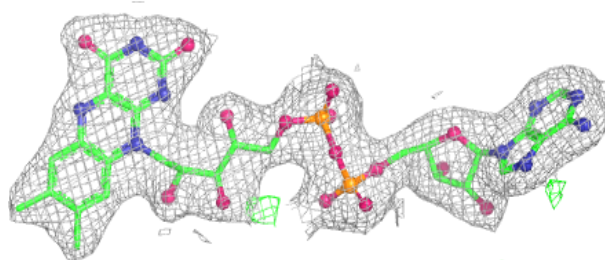


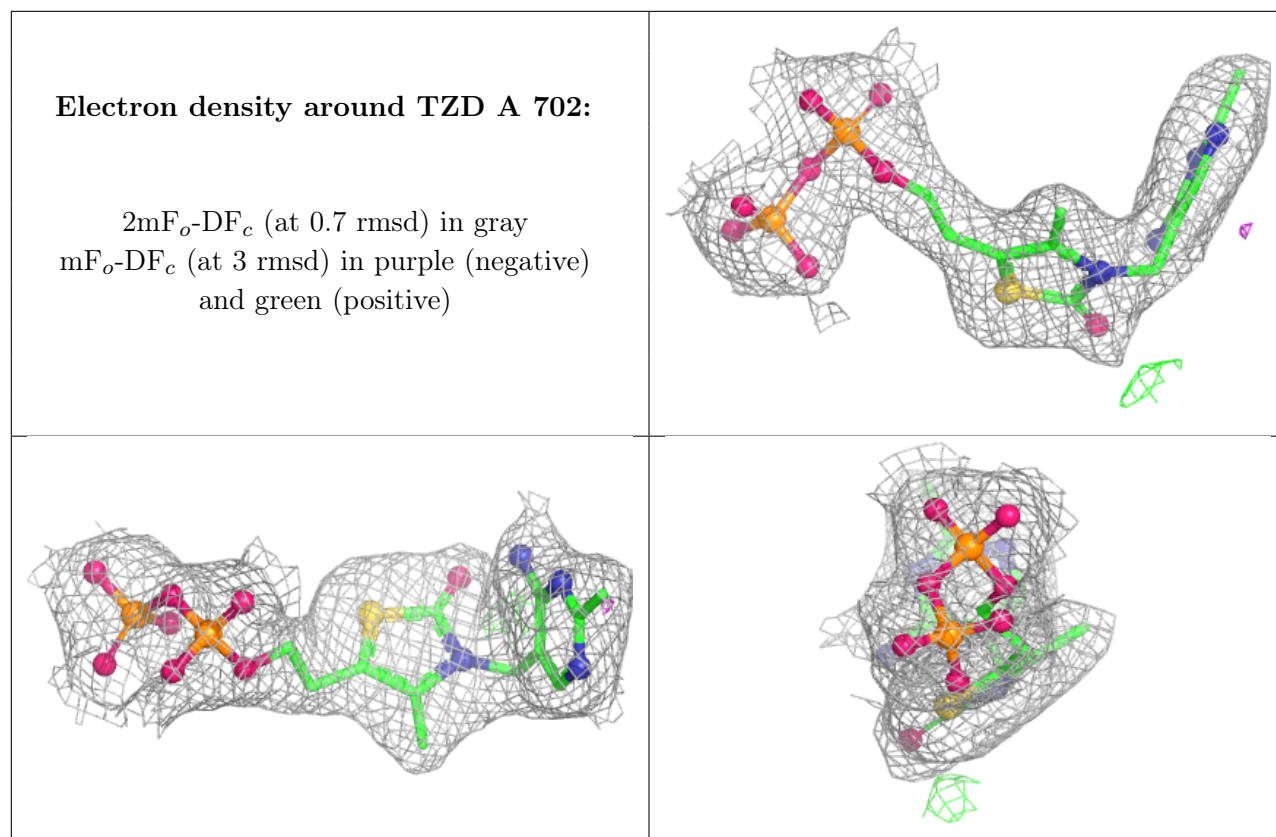
Electron density around FAD A 703:

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

**Electron density around FAD B 704:**

$2mF_o-DF_c$ (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.