



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2021 – 12:27 PM JST

PDB ID : 7EGV
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 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

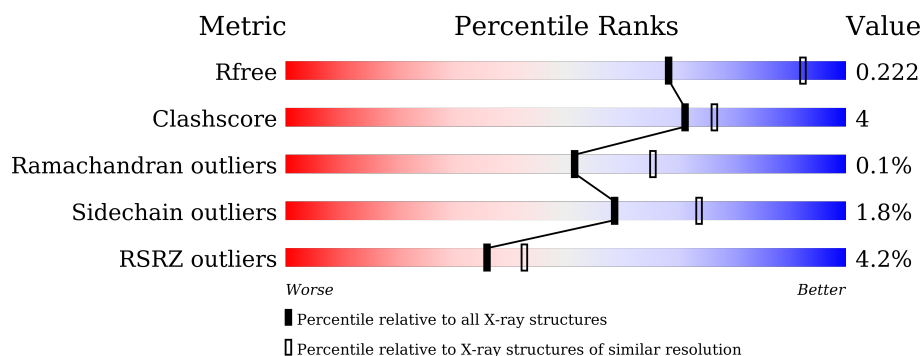
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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>4%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>
1	B	688	<div> <div>3%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>

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
9	J3L	B	701	-	-	-	X

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

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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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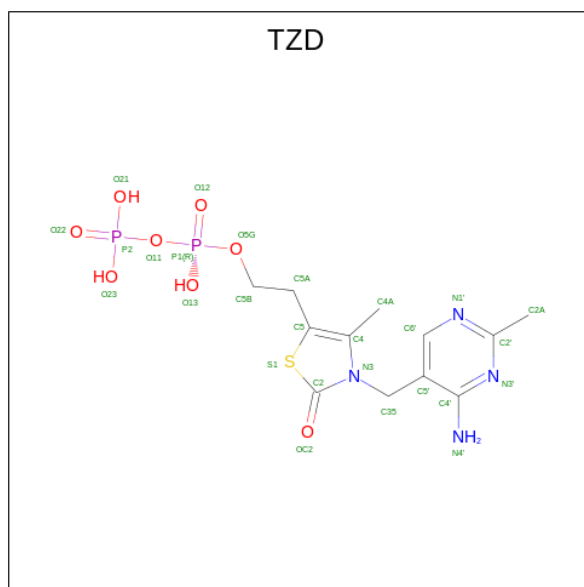
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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ARG	-	expression tag	UNP A0A2N1LPC4
B	16	GLY	-	expression tag	UNP A0A2N1LPC4
B	17	SER	-	expression tag	UNP A0A2N1LPC4
B	18	GLY	-	expression tag	UNP A0A2N1LPC4
B	19	MET	-	expression tag	UNP A0A2N1LPC4
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).

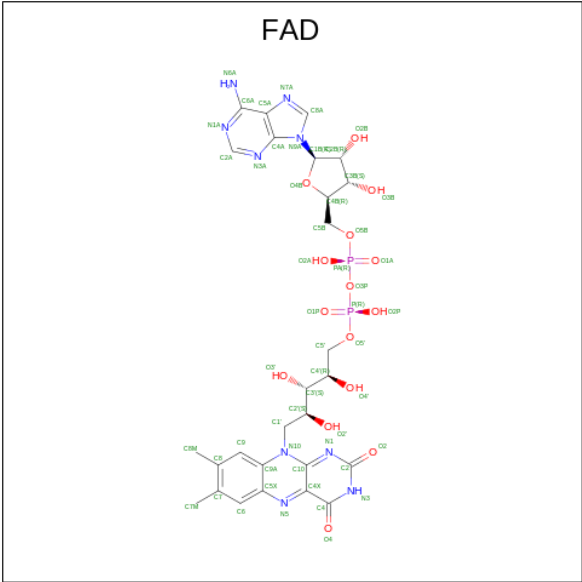
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is 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).



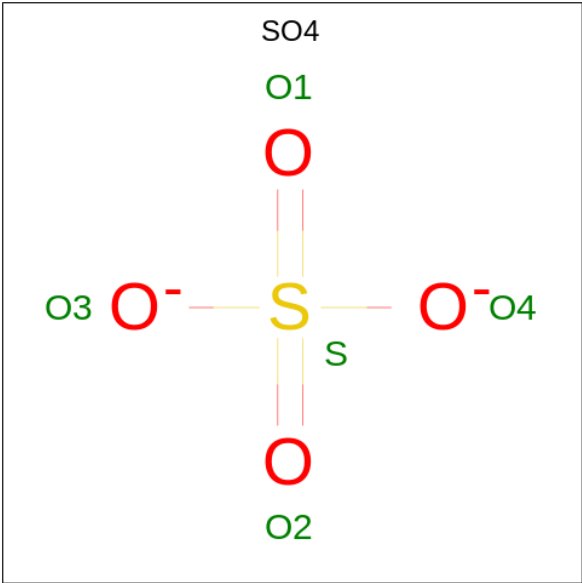
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		
3	B	1	Total	C	N	O	P	S	0	0
			27	12	4	8	2	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



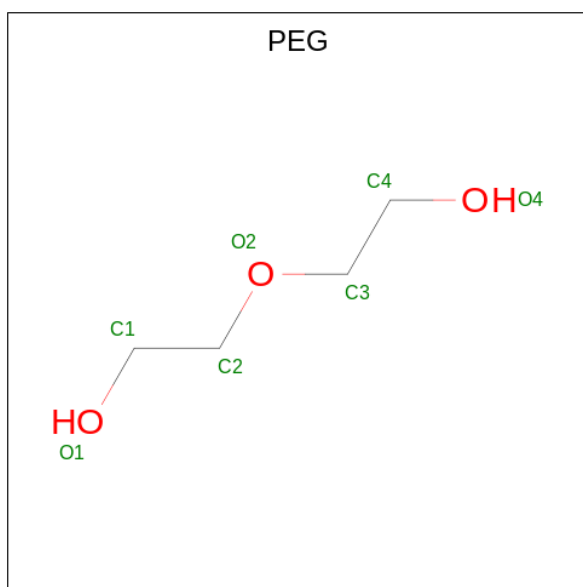
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



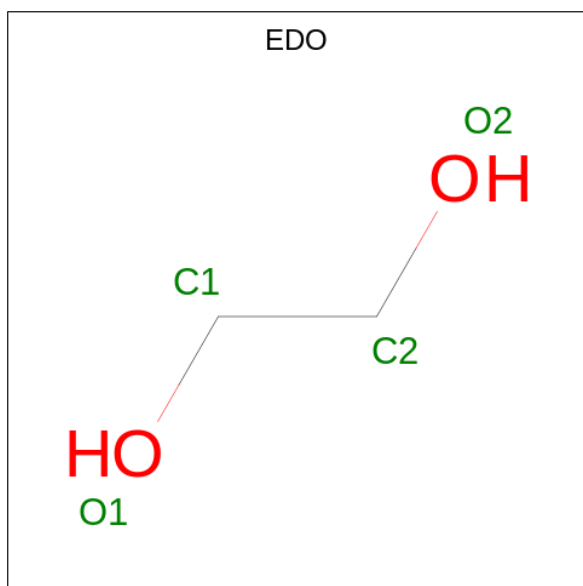
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: 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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



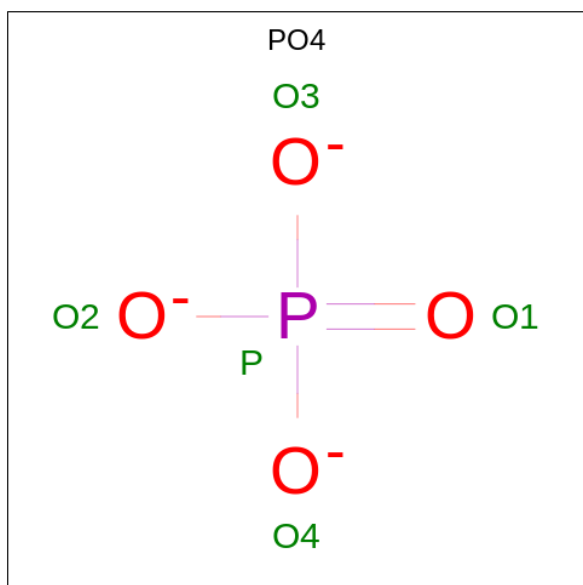
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		

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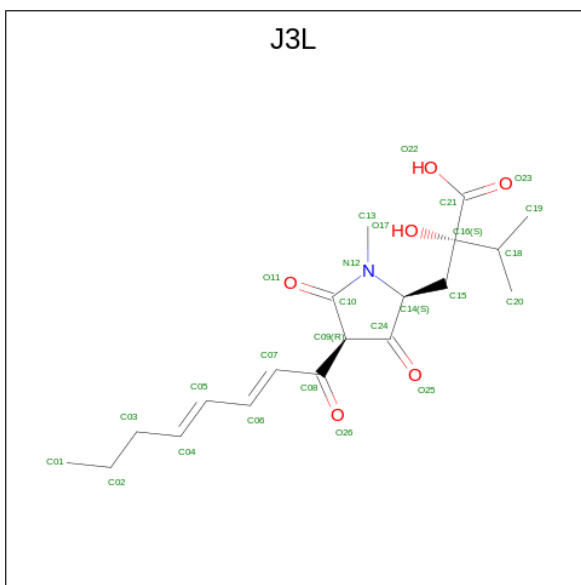
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is PHOSPHATE ION (three-letter code: 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(oxidanilidene)pyrrolidin-2-yl]methyl]-2-oxidanyl-butanoic acid (three-letter code: 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 45 45	0	0
10	B	33	Total O 33 33	0	0

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 0.175 , 0.222	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)	0.36 , 46.9	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: EDO, SO4, MG, J3L, PO4, PEG, FAD, TZD

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	0.42	0/4611	0.56	0/6234
1	B	0.42	0/4472	0.59	0/6052
All	All	0.42	0/9083	0.58	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	36	0
1	B	4383	0	4402	26	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	0	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

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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	64	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 (64) 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:A:167:ILE:HA	1:A:170:MET:HE3	1.80	0.63
1:B:132:PRO:HG3	1:B:138:ALA:HB2	1.78	0.63
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:577:ASN:ND2	1:A:643:GLU:OE1	2.35	0.56
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: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: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
1:B:498:VAL:HG21	1:B:524:GLY:C	2.35	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:142:ALA:HB3	1:A:180:MET:HE2	1.98	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: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: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:336:LEU:HA	1:B:336:LEU:HD23	1.84	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
1:A:157:VAL:O	1:A:184:CYS:HA	2.21	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
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:B:407:MET:HE3	1:B:409:LYS:HD3	2.02	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	584/688 (85%)	563 (96%)	20 (3%)	1 (0%)	47	60
1	B	569/688 (83%)	556 (98%)	13 (2%)	0	100	100
All	All	1153/1376 (84%)	1119 (97%)	33 (3%)	1 (0%)	51	65

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	603	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	474/556 (85%)	466 (98%)	8 (2%)	60	75
1	B	458/556 (82%)	449 (98%)	9 (2%)	55	70
All	All	932/1112 (84%)	915 (98%)	17 (2%)	59	74

All (17) 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	225	ARG
1	A	435	GLN

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Mol	Chain	Res	Type
1	A	517	MET
1	A	549	ASP
1	A	556	MET
1	B	133	ARG
1	B	286	SER
1	B	303	TYR
1	B	376	ASP
1	B	517	MET
1	B	556	MET
1	B	584	VAL
1	B	648	LYS
1	B	667	VAL

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

Mol	Chain	Res	Type
1	B	334	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 monosaccharides 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	$\# Z > 2$
5	SO4	A	704	-	4,4,4	0.12	0	6,6,6	0.18	0
8	PO4	A	709	-	4,4,4	0.92	0	6,6,6	0.68	0
3	TZD	A	702	2	23,28,28	3.14	5 (21%)	28,42,42	1.77	7 (25%)
9	J3L	B	701	-	21,26,26	3.01	5 (23%)	15,37,37	1.35	2 (13%)
7	EDO	A	708	-	3,3,3	0.13	0	2,2,2	0.30	0
4	FAD	B	704	-	51,58,58	1.11	2 (3%)	60,89,89	1.74	7 (11%)
7	EDO	A	707	-	3,3,3	0.09	0	2,2,2	0.03	0
7	EDO	B	705	-	3,3,3	0.18	0	2,2,2	0.24	0
7	EDO	A	706	-	3,3,3	0.08	0	2,2,2	0.28	0
3	TZD	B	703	2	23,28,28	3.18	5 (21%)	28,42,42	1.78	8 (28%)
7	EDO	B	706	-	3,3,3	0.06	0	2,2,2	0.19	0
4	FAD	A	703	-	51,58,58	1.09	2 (3%)	60,89,89	1.73	7 (11%)
6	PEG	A	705	-	6,6,6	0.15	0	5,5,5	0.09	0

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	TZD	A	702	2	-	1/16/17/17	0/2/2/2
9	J3L	B	701	-	-	13/20/48/48	0/1/1/1
7	EDO	A	708	-	-	0/1/1/1	-
4	FAD	B	704	-	-	2/30/50/50	0/6/6/6
7	EDO	A	707	-	-	0/1/1/1	-
7	EDO	B	705	-	-	0/1/1/1	-
7	EDO	A	706	-	-	0/1/1/1	-
3	TZD	B	703	2	-	2/16/17/17	0/2/2/2
7	EDO	B	706	-	-	0/1/1/1	-
4	FAD	A	703	-	-	2/30/50/50	0/6/6/6
6	PEG	A	705	-	-	1/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	701	J3L	C10-N12	12.30	1.51	1.34
3	A	702	TZD	C4-N3	11.21	1.64	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	703	TZD	C4-N3	11.17	1.64	1.39
3	A	702	TZD	C5-S1	-6.98	1.61	1.74
3	B	703	TZD	C5-S1	-6.34	1.62	1.74
4	B	704	FAD	C4X-C10	5.79	1.44	1.38
4	A	703	FAD	C4X-C10	5.73	1.44	1.38
3	B	703	TZD	C5A-C5	4.98	1.53	1.50
3	A	702	TZD	C4'-N4'	4.55	1.45	1.34
3	B	703	TZD	C4'-N4'	3.80	1.43	1.34
9	B	701	J3L	C14-C24	-3.06	1.48	1.53
9	B	701	J3L	C06-C05	2.84	1.52	1.44
4	A	703	FAD	C4-N3	2.69	1.37	1.33
4	B	704	FAD	C4-N3	2.66	1.37	1.33
3	A	702	TZD	C5A-C5	2.62	1.52	1.50
9	B	701	J3L	C15-C14	-2.45	1.50	1.54
3	A	702	TZD	C35-N3	-2.26	1.44	1.48
9	B	701	J3L	O26-C08	-2.06	1.19	1.22
3	B	703	TZD	C4'-N3'	-2.01	1.32	1.35

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	704	FAD	C4-N3-C2	8.13	122.01	115.14
4	A	703	FAD	C4-N3-C2	8.08	121.97	115.14
4	B	704	FAD	C4-C4X-C10	-5.81	116.10	119.95
4	A	703	FAD	C4-C4X-C10	-5.31	116.44	119.95
4	A	703	FAD	C10-C4X-N5	4.87	124.63	121.26
4	B	704	FAD	C10-C4X-N5	4.43	124.32	121.26
4	B	704	FAD	C4X-C4-N3	-4.32	117.52	123.43
4	A	703	FAD	C4X-C4-N3	-4.16	117.74	123.43
3	A	702	TZD	C5A-C5-C4	-4.12	124.13	127.43
3	B	703	TZD	C5'-C35-N3	-3.78	107.01	113.26
3	A	702	TZD	C2A-C2'-N1'	3.75	121.27	117.14
4	A	703	FAD	C4X-C10-N10	-3.60	116.60	120.30
3	B	703	TZD	C6'-N1'-C2'	3.52	121.95	115.96
4	B	704	FAD	C4X-C10-N10	-3.29	116.92	120.30
3	B	703	TZD	C5'-C6'-N1'	-3.11	118.63	123.82
3	B	703	TZD	P1-O11-P2	-3.04	122.38	132.83
3	B	703	TZD	N1'-C2'-N3'	-2.91	120.53	125.54
9	B	701	J3L	C13-N12-C10	2.85	125.96	122.09
3	B	703	TZD	C5A-C5-C4	-2.77	125.21	127.43
3	A	702	TZD	C5'-C35-N3	-2.74	108.74	113.26
3	A	702	TZD	C2'-N3'-C4'	2.72	122.32	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	TZD	C6'-N1'-C2'	2.69	120.54	115.96
3	B	703	TZD	C2A-C2'-N1'	2.69	120.09	117.14
3	A	702	TZD	N1'-C2'-N3'	-2.54	121.17	125.54
4	A	703	FAD	C1'-N10-C9A	2.39	120.17	118.29
3	A	702	TZD	C5'-C6'-N1'	-2.31	119.96	123.82
4	B	704	FAD	C5A-C6A-N6A	2.30	123.85	120.35
9	B	701	J3L	C06-C05-C04	-2.21	112.77	125.51
4	B	704	FAD	C1'-N10-C9A	2.12	119.96	118.29
4	A	703	FAD	C5A-C6A-N6A	2.10	123.55	120.35
3	B	703	TZD	O21-P2-O11	2.09	111.65	104.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

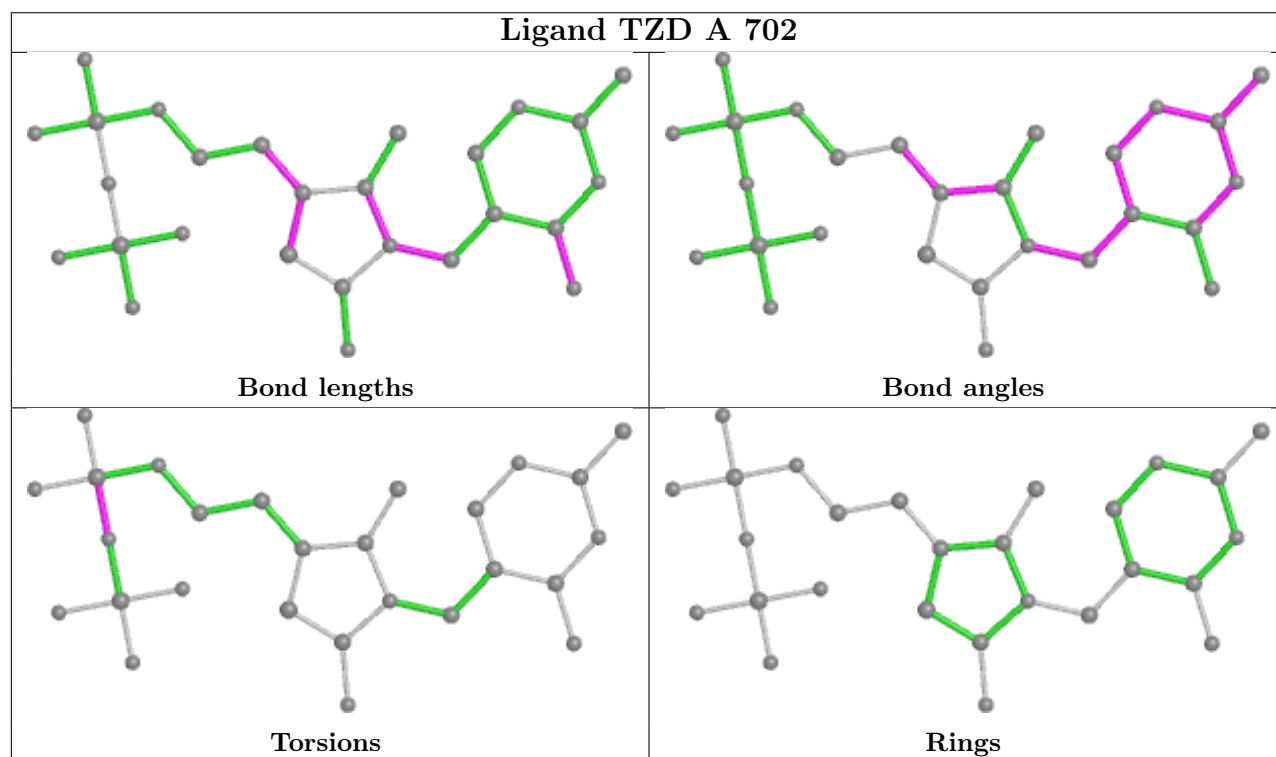
Mol	Chain	Res	Type	Atoms
3	A	702	TZD	P2-O11-P1-O5G
3	B	703	TZD	N3-C35-C5'-C4'
4	B	704	FAD	P-O3P-PA-O5B
9	B	701	J3L	C14-C15-C16-C18
9	B	701	J3L	C14-C15-C16-C21
9	B	701	J3L	C14-C15-C16-O17
9	B	701	J3L	C15-C16-C18-C19
9	B	701	J3L	C15-C16-C18-C20
9	B	701	J3L	C21-C16-C18-C19
9	B	701	J3L	C21-C16-C18-C20
9	B	701	J3L	O17-C16-C18-C19
9	B	701	J3L	O17-C16-C18-C20
9	B	701	J3L	C04-C05-C06-C07
3	B	703	TZD	P2-O11-P1-O5G
4	A	703	FAD	P-O3P-PA-O5B
9	B	701	J3L	O26-C08-C09-C24
6	A	705	PEG	C1-C2-O2-C3
9	B	701	J3L	C02-C03-C04-C05
4	A	703	FAD	O4B-C4B-C5B-O5B
9	B	701	J3L	N12-C14-C15-C16
4	B	704	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

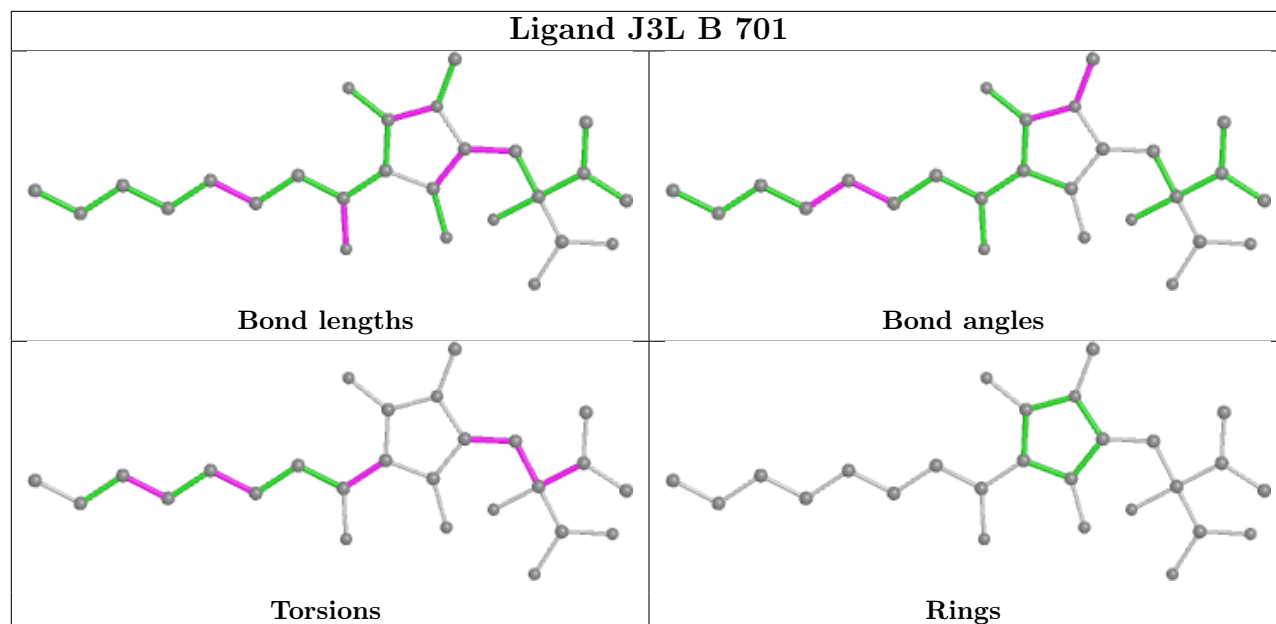
2 monomers are involved in 3 short contacts:

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

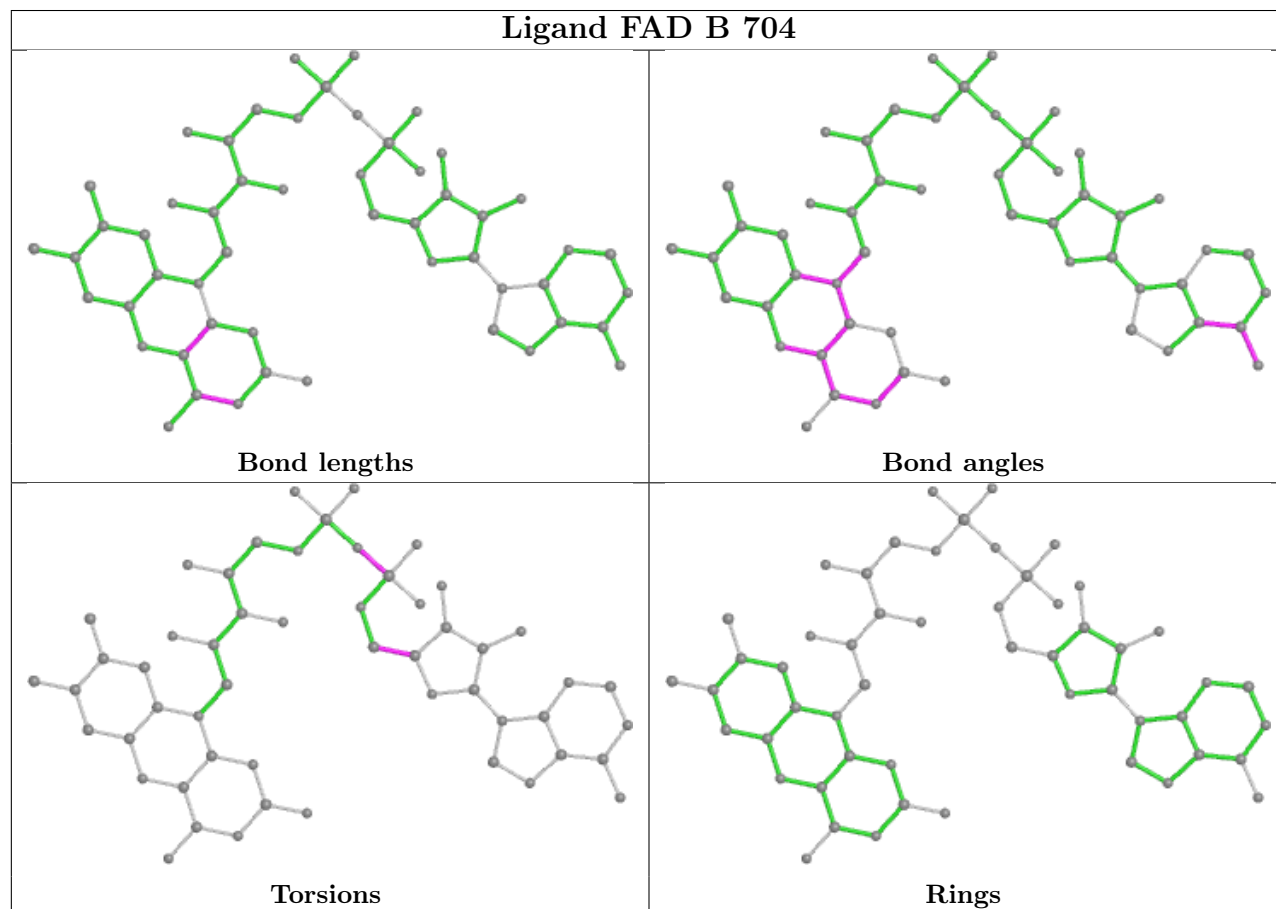
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



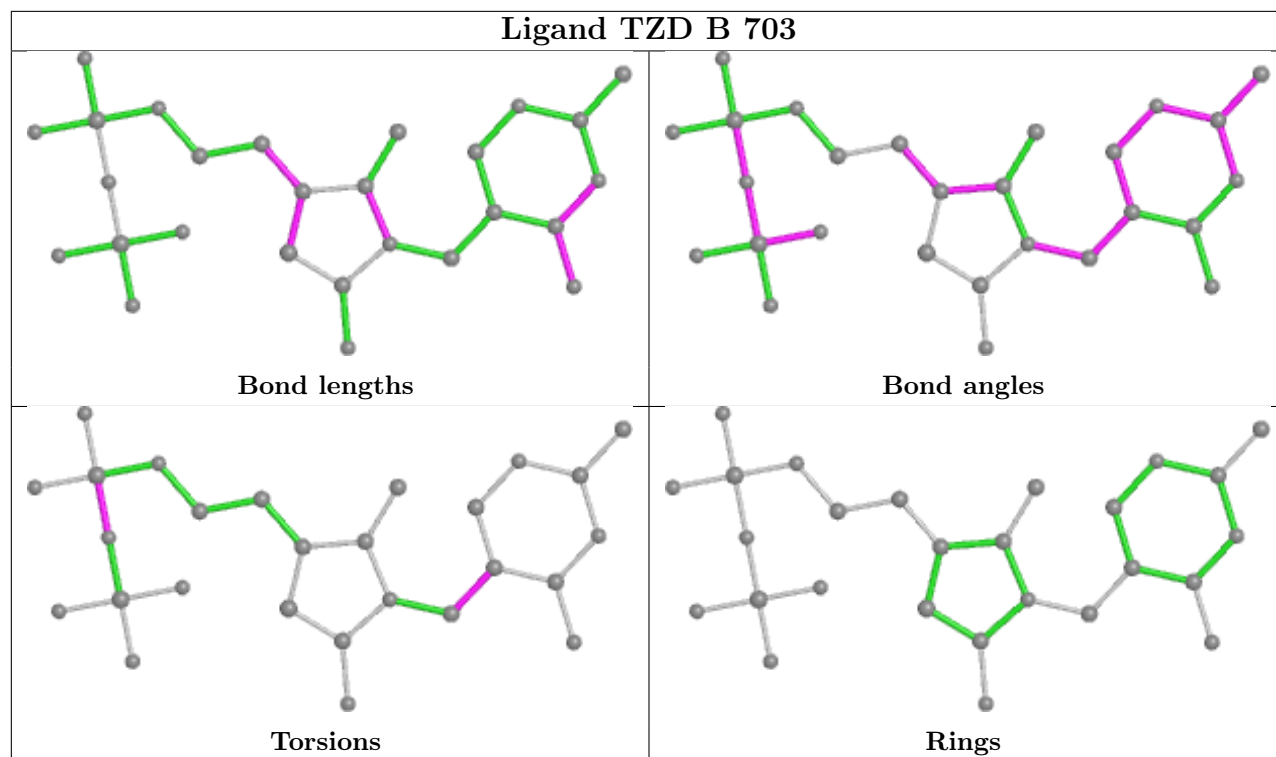
Ligand J3L B 701



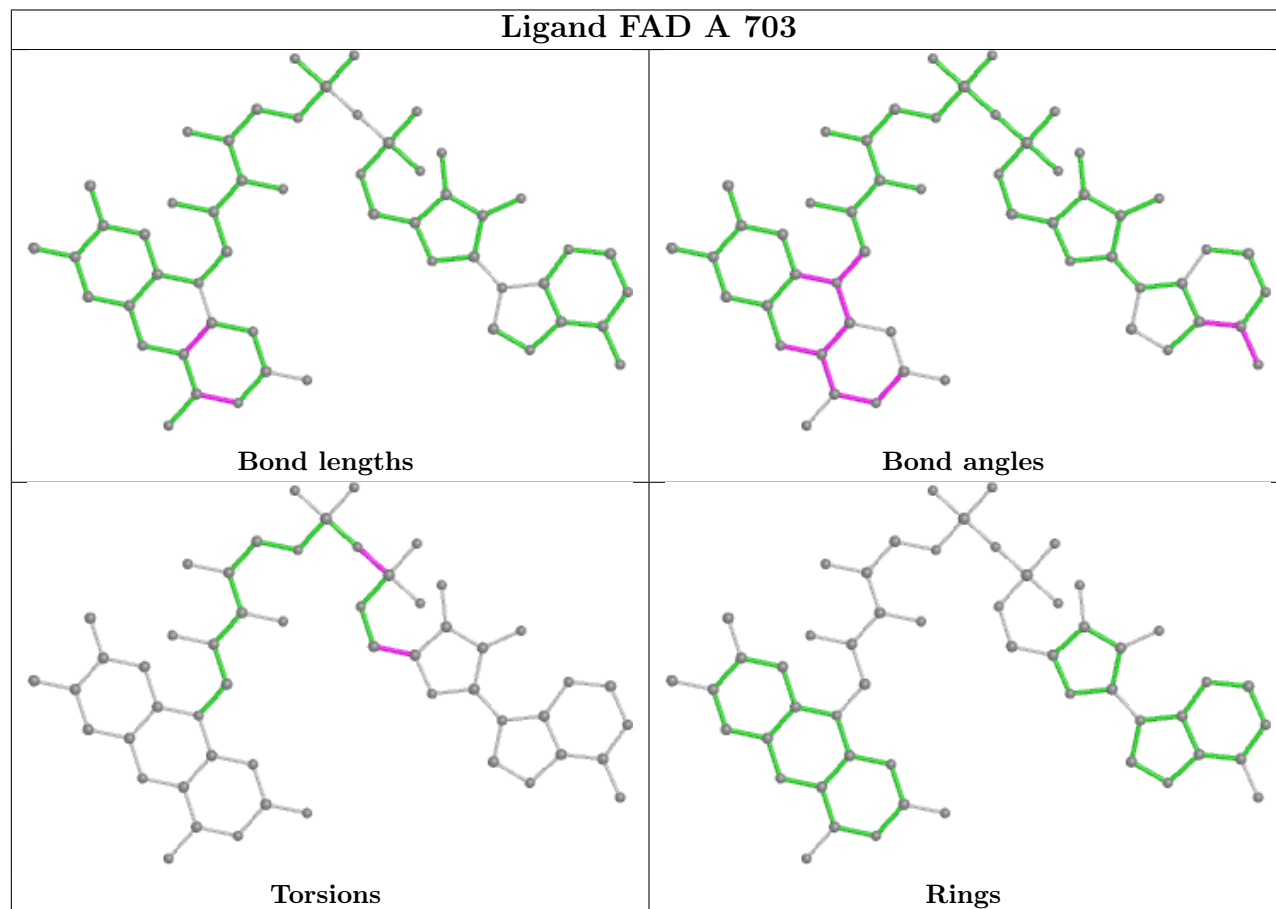
Ligand FAD B 704



Ligand TZD B 703



Ligand FAD 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	590/688 (85%)	0.09	26 (4%) 34 41	22, 35, 67, 93	0
1	B	576/688 (83%)	-0.01	23 (3%) 38 45	22, 32, 63, 88	0
All	All	1166/1376 (84%)	0.04	49 (4%) 36 42	22, 34, 65, 93	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	668	PHE	6.2
1	A	468	ARG	5.5
1	A	469	THR	5.1
1	B	591	PHE	5.1
1	B	669	ASP	5.0
1	A	278	LEU	4.5
1	A	274	ALA	4.3
1	B	592	TYR	4.2
1	A	688	HIS	4.2
1	B	665	PHE	4.1
1	A	257	ALA	4.1
1	B	589	ASN	4.0
1	B	657	PRO	3.9
1	B	667	VAL	3.8
1	B	268	PRO	3.7
1	B	666	LEU	3.7
1	A	281	GLN	3.7
1	B	596	TYR	3.6
1	A	256	ARG	3.5
1	A	687	VAL	3.5
1	B	658	ALA	3.1
1	A	85	PHE	3.1
1	A	276	LYS	3.0
1	A	277	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	85	PHE	2.8
1	B	659	GLY	2.8
1	B	660	SER	2.8
1	A	681	LYS	2.7
1	B	661	ALA	2.7
1	A	675	GLN	2.6
1	B	600	HIS	2.6
1	A	258	ILE	2.6
1	A	684	THR	2.5
1	A	671	GLU	2.5
1	B	590	LEU	2.5
1	A	669	ASP	2.5
1	B	258	ILE	2.4
1	B	656	VAL	2.3
1	B	664	GLU	2.3
1	B	80	ASP	2.3
1	A	83	GLU	2.2
1	B	257	ALA	2.1
1	A	685	LYS	2.1
1	A	470	GLY	2.1
1	A	682	GLU	2.1
1	A	280	THR	2.0
1	A	686	GLY	2.0
1	A	672	LYS	2.0
1	A	255	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

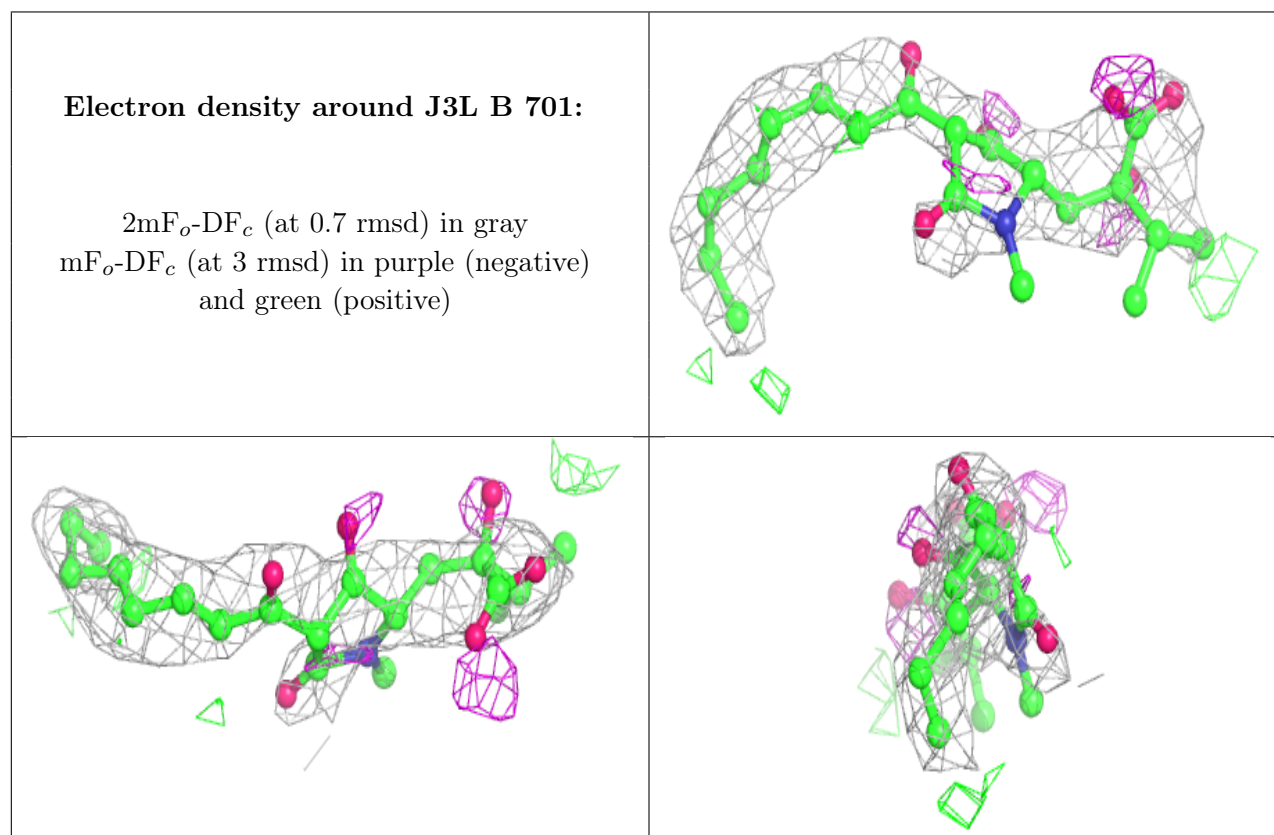
There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

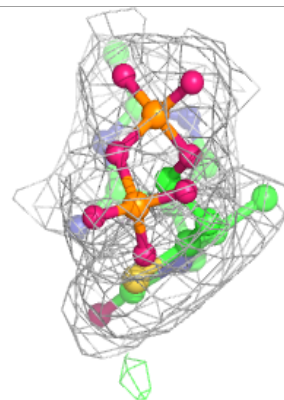
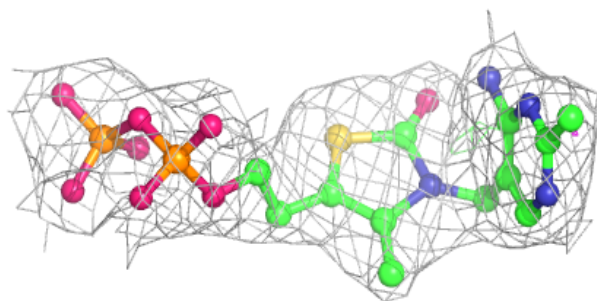
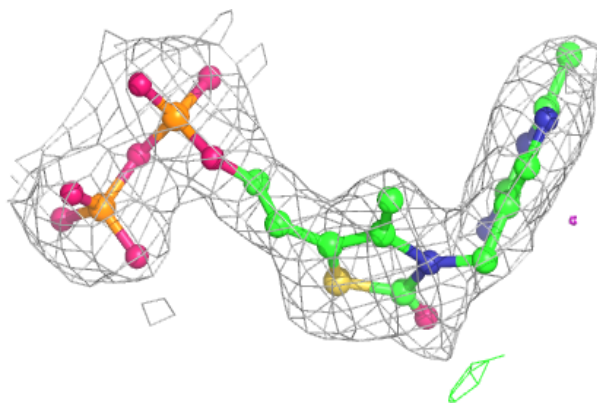
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	J3L	B	701	26/26	0.60	0.48	40,57,61,64	26
7	EDO	A	708	4/4	0.75	0.28	47,49,50,62	0
7	EDO	A	706	4/4	0.76	0.28	68,71,74,75	0
6	PEG	A	705	7/7	0.85	0.30	53,55,60,70	0
7	EDO	A	707	4/4	0.90	0.14	40,43,46,46	0
7	EDO	B	705	4/4	0.91	0.13	39,39,40,48	0
7	EDO	B	706	4/4	0.92	0.20	52,53,53,54	0
8	PO4	A	709	5/5	0.94	0.22	54,55,62,73	0
3	TZD	A	702	27/27	0.98	0.17	24,28,31,35	0
4	FAD	A	703	53/53	0.98	0.15	24,30,34,35	0
4	FAD	B	704	53/53	0.98	0.14	22,29,33,35	0
5	SO4	A	704	5/5	0.98	0.08	40,42,49,58	0
2	MG	A	701	1/1	0.98	0.14	25,25,25,25	0
2	MG	B	702	1/1	0.98	0.19	24,24,24,24	0
3	TZD	B	703	27/27	0.99	0.17	24,31,35,40	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.

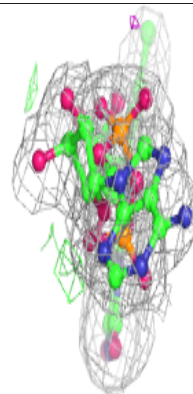
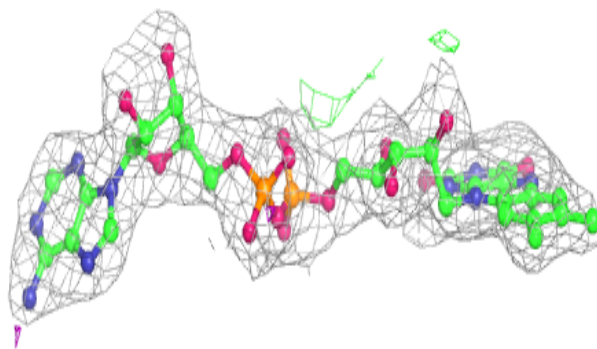
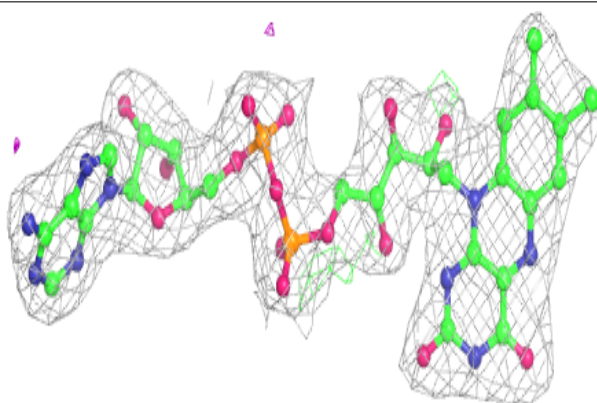


Electron density around TZD A 702:

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

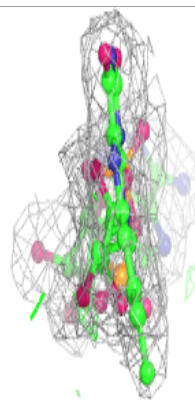
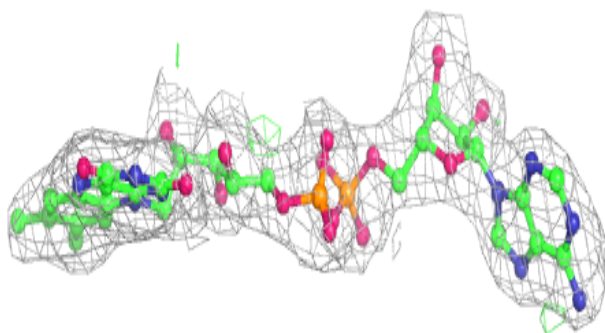
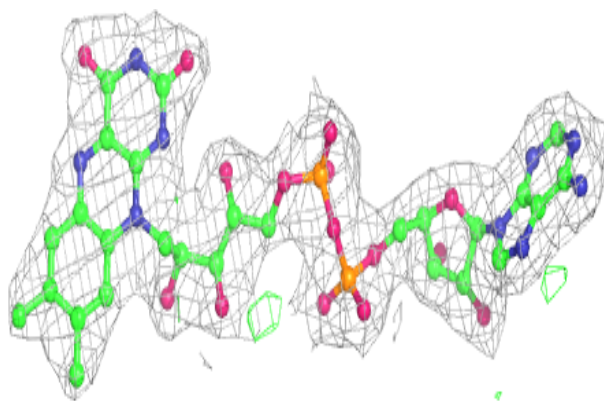
**Electron density around FAD A 703:**

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

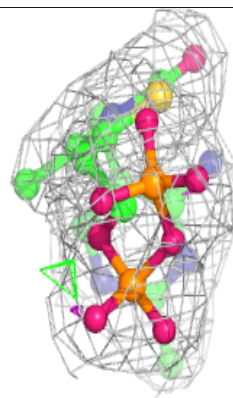
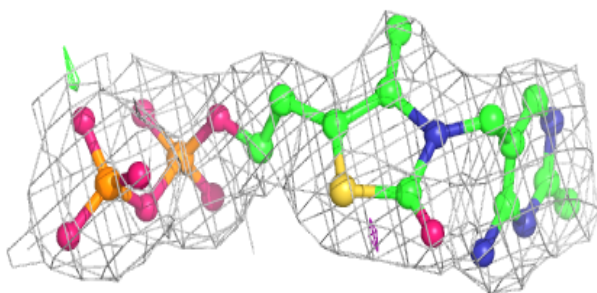
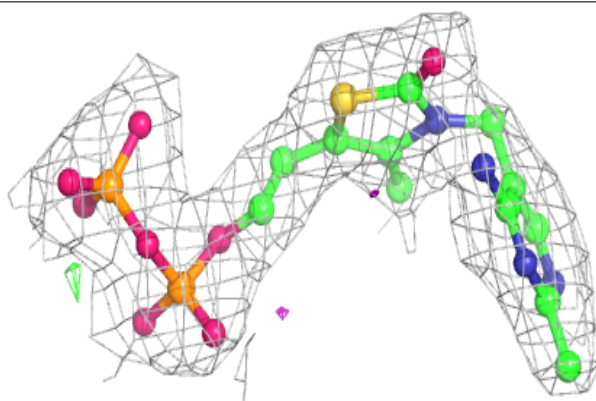


Electron density around FAD B 704:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.