



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:40 PM UTC

PDB ID : 5WKC / pdb_00005wkc
Title : Saccharomyces cerevisiae acetohydroxyacid synthase in complex with the herbicide penoxsulam
Authors : Guddat, W.L.; Lonhienne, G.T.
Deposited on : 2017-07-25
Resolution : 2.33 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

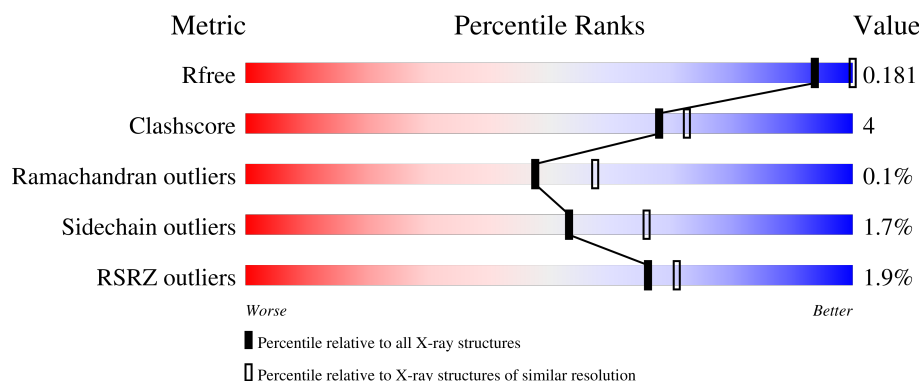
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	677	2% 80% 7% 13%
1	B	677	% 82% 6% 12%
1	E	677	3% 78% 9% 13%
2	D	677	% 81% 6% 12%

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
4	PXD	D	702	-	X	-	-
6	F50	A	704	-	-	X	-
6	F50	B	705	-	-	X	-
6	F50	E	705	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19824 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 catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	591	Total	C	N	O	S	0	3	0
			4526	2866	784	854	22			
1	B	598	Total	C	N	O	S	0	4	0
			4580	2898	792	868	22			
1	E	592	Total	C	N	O	S	0	2	0
			4528	2868	782	856	22			

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	initiating methionine	UNP P07342
A	12	HIS	-	expression tag	UNP P07342
A	13	HIS	-	expression tag	UNP P07342
A	14	HIS	-	expression tag	UNP P07342
A	15	HIS	-	expression tag	UNP P07342
A	16	HIS	-	expression tag	UNP P07342
A	17	HIS	-	expression tag	UNP P07342
A	18	SER	-	expression tag	UNP P07342
A	19	SER	-	expression tag	UNP P07342
A	20	GLY	-	expression tag	UNP P07342
A	21	LEU	-	expression tag	UNP P07342
A	22	VAL	-	expression tag	UNP P07342
A	23	PRO	-	expression tag	UNP P07342
A	24	ARG	-	expression tag	UNP P07342
A	25	GLY	-	expression tag	UNP P07342
A	26	SER	-	expression tag	UNP P07342
A	27	GLY	-	expression tag	UNP P07342
A	28	MET	-	expression tag	UNP P07342
A	29	LYS	-	expression tag	UNP P07342
A	30	GLU	-	expression tag	UNP P07342
A	31	THR	-	expression tag	UNP P07342
A	32	ALA	-	expression tag	UNP P07342
A	33	ALA	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342
A	36	PHE	-	expression tag	UNP P07342
A	37	GLU	-	expression tag	UNP P07342
A	38	ARG	-	expression tag	UNP P07342
A	39	GLN	-	expression tag	UNP P07342
A	40	HIS	-	expression tag	UNP P07342
A	41	MET	-	expression tag	UNP P07342
A	42	ASP	-	expression tag	UNP P07342
A	43	SER	-	expression tag	UNP P07342
A	44	PRO	-	expression tag	UNP P07342
A	45	ASP	-	expression tag	UNP P07342
A	46	LEU	-	expression tag	UNP P07342
A	47	GLY	-	expression tag	UNP P07342
A	48	THR	-	expression tag	UNP P07342
A	49	ASP	-	expression tag	UNP P07342
A	50	ASP	-	expression tag	UNP P07342
A	51	ASP	-	expression tag	UNP P07342
A	52	ASP	-	expression tag	UNP P07342
A	53	LYS	-	expression tag	UNP P07342
A	54	ALA	-	expression tag	UNP P07342
A	55	MET	-	expression tag	UNP P07342
A	56	GLY	-	expression tag	UNP P07342
A	57	SER	-	expression tag	UNP P07342
B	11	MET	-	initiating methionine	UNP P07342
B	12	HIS	-	expression tag	UNP P07342
B	13	HIS	-	expression tag	UNP P07342
B	14	HIS	-	expression tag	UNP P07342
B	15	HIS	-	expression tag	UNP P07342
B	16	HIS	-	expression tag	UNP P07342
B	17	HIS	-	expression tag	UNP P07342
B	18	SER	-	expression tag	UNP P07342
B	19	SER	-	expression tag	UNP P07342
B	20	GLY	-	expression tag	UNP P07342
B	21	LEU	-	expression tag	UNP P07342
B	22	VAL	-	expression tag	UNP P07342
B	23	PRO	-	expression tag	UNP P07342
B	24	ARG	-	expression tag	UNP P07342
B	25	GLY	-	expression tag	UNP P07342
B	26	SER	-	expression tag	UNP P07342
B	27	GLY	-	expression tag	UNP P07342
B	28	MET	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression tag	UNP P07342
B	37	GLU	-	expression tag	UNP P07342
B	38	ARG	-	expression tag	UNP P07342
B	39	GLN	-	expression tag	UNP P07342
B	40	HIS	-	expression tag	UNP P07342
B	41	MET	-	expression tag	UNP P07342
B	42	ASP	-	expression tag	UNP P07342
B	43	SER	-	expression tag	UNP P07342
B	44	PRO	-	expression tag	UNP P07342
B	45	ASP	-	expression tag	UNP P07342
B	46	LEU	-	expression tag	UNP P07342
B	47	GLY	-	expression tag	UNP P07342
B	48	THR	-	expression tag	UNP P07342
B	49	ASP	-	expression tag	UNP P07342
B	50	ASP	-	expression tag	UNP P07342
B	51	ASP	-	expression tag	UNP P07342
B	52	ASP	-	expression tag	UNP P07342
B	53	LYS	-	expression tag	UNP P07342
B	54	ALA	-	expression tag	UNP P07342
B	55	MET	-	expression tag	UNP P07342
B	56	GLY	-	expression tag	UNP P07342
B	57	SER	-	expression tag	UNP P07342
E	11	MET	-	initiating methionine	UNP P07342
E	12	HIS	-	expression tag	UNP P07342
E	13	HIS	-	expression tag	UNP P07342
E	14	HIS	-	expression tag	UNP P07342
E	15	HIS	-	expression tag	UNP P07342
E	16	HIS	-	expression tag	UNP P07342
E	17	HIS	-	expression tag	UNP P07342
E	18	SER	-	expression tag	UNP P07342
E	19	SER	-	expression tag	UNP P07342
E	20	GLY	-	expression tag	UNP P07342
E	21	LEU	-	expression tag	UNP P07342
E	22	VAL	-	expression tag	UNP P07342
E	23	PRO	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
E	24	ARG	-	expression tag	UNP P07342
E	25	GLY	-	expression tag	UNP P07342
E	26	SER	-	expression tag	UNP P07342
E	27	GLY	-	expression tag	UNP P07342
E	28	MET	-	expression tag	UNP P07342
E	29	LYS	-	expression tag	UNP P07342
E	30	GLU	-	expression tag	UNP P07342
E	31	THR	-	expression tag	UNP P07342
E	32	ALA	-	expression tag	UNP P07342
E	33	ALA	-	expression tag	UNP P07342
E	34	ALA	-	expression tag	UNP P07342
E	35	LYS	-	expression tag	UNP P07342
E	36	PHE	-	expression tag	UNP P07342
E	37	GLU	-	expression tag	UNP P07342
E	38	ARG	-	expression tag	UNP P07342
E	39	GLN	-	expression tag	UNP P07342
E	40	HIS	-	expression tag	UNP P07342
E	41	MET	-	expression tag	UNP P07342
E	42	ASP	-	expression tag	UNP P07342
E	43	SER	-	expression tag	UNP P07342
E	44	PRO	-	expression tag	UNP P07342
E	45	ASP	-	expression tag	UNP P07342
E	46	LEU	-	expression tag	UNP P07342
E	47	GLY	-	expression tag	UNP P07342
E	48	THR	-	expression tag	UNP P07342
E	49	ASP	-	expression tag	UNP P07342
E	50	ASP	-	expression tag	UNP P07342
E	51	ASP	-	expression tag	UNP P07342
E	52	ASP	-	expression tag	UNP P07342
E	53	LYS	-	expression tag	UNP P07342
E	54	ALA	-	expression tag	UNP P07342
E	55	MET	-	expression tag	UNP P07342
E	56	GLY	-	expression tag	UNP P07342
E	57	SER	-	expression tag	UNP P07342

- Molecule 2 is a protein called Acetolactate synthase catalytic subunit, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	596	Total	C	N	O	S	0	1	0
			4553	2880	789	862	22			

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	11	MET	-	initiating methionine	UNP P07342
D	12	HIS	-	expression tag	UNP P07342
D	13	HIS	-	expression tag	UNP P07342
D	14	HIS	-	expression tag	UNP P07342
D	15	HIS	-	expression tag	UNP P07342
D	16	HIS	-	expression tag	UNP P07342
D	17	HIS	-	expression tag	UNP P07342
D	18	SER	-	expression tag	UNP P07342
D	19	SER	-	expression tag	UNP P07342
D	20	GLY	-	expression tag	UNP P07342
D	21	LEU	-	expression tag	UNP P07342
D	22	VAL	-	expression tag	UNP P07342
D	23	PRO	-	expression tag	UNP P07342
D	24	ARG	-	expression tag	UNP P07342
D	25	GLY	-	expression tag	UNP P07342
D	26	SER	-	expression tag	UNP P07342
D	27	GLY	-	expression tag	UNP P07342
D	28	MET	-	expression tag	UNP P07342
D	29	LYS	-	expression tag	UNP P07342
D	30	GLU	-	expression tag	UNP P07342
D	31	THR	-	expression tag	UNP P07342
D	32	ALA	-	expression tag	UNP P07342
D	33	ALA	-	expression tag	UNP P07342
D	34	ALA	-	expression tag	UNP P07342
D	35	LYS	-	expression tag	UNP P07342
D	36	PHE	-	expression tag	UNP P07342
D	37	GLU	-	expression tag	UNP P07342
D	38	ARG	-	expression tag	UNP P07342
D	39	GLN	-	expression tag	UNP P07342
D	40	HIS	-	expression tag	UNP P07342
D	41	MET	-	expression tag	UNP P07342
D	42	ASP	-	expression tag	UNP P07342
D	43	SER	-	expression tag	UNP P07342
D	44	PRO	-	expression tag	UNP P07342
D	45	ASP	-	expression tag	UNP P07342
D	46	LEU	-	expression tag	UNP P07342
D	47	GLY	-	expression tag	UNP P07342
D	48	THR	-	expression tag	UNP P07342
D	49	ASP	-	expression tag	UNP P07342
D	50	ASP	-	expression tag	UNP P07342
D	51	ASP	-	expression tag	UNP P07342
D	52	ASP	-	expression tag	UNP P07342
D	53	LYS	-	expression tag	UNP P07342

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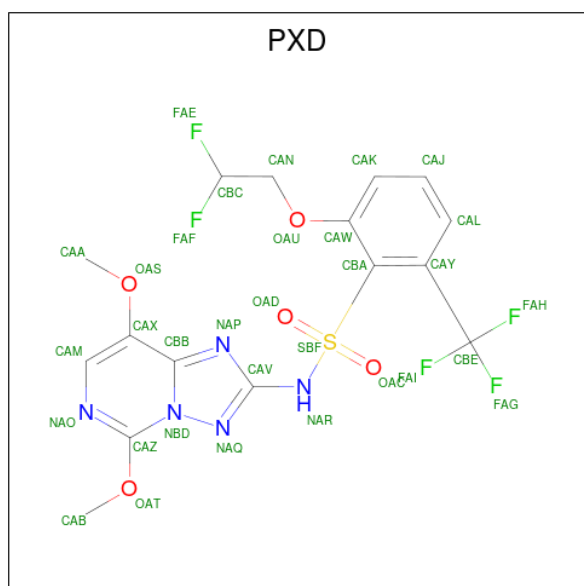
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Chain	Residue	Modelled	Actual	Comment	Reference
D	54	ALA	-	expression tag	UNP P07342
D	55	MET	-	expression tag	UNP P07342
D	56	GLY	-	expression tag	UNP P07342
D	57	SER	-	expression tag	UNP P07342

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is 2-(2,2-difluoroethoxy)-N-(5,8-dimethoxy[1,2,4]triazolo[1,5-c]pyrimidin-2-yl)-6-(trifluoromethyl)benzenesulfonamide (CCD ID: PXD) (formula: C₁₆H₁₄F₅N₅O₅S).



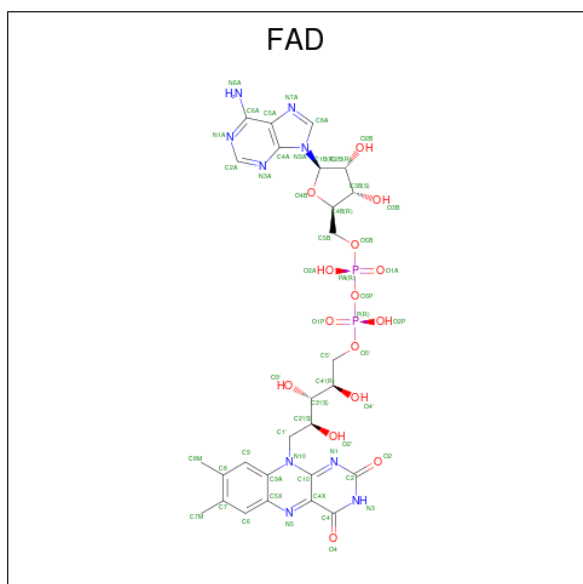
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F N O S 32 16 5 5 5 1	0	0
4	B	1	Total C F N O S 32 16 5 5 5 1	0	0
4	E	1	Total C F N O S 32 16 5 5 5 1	0	0

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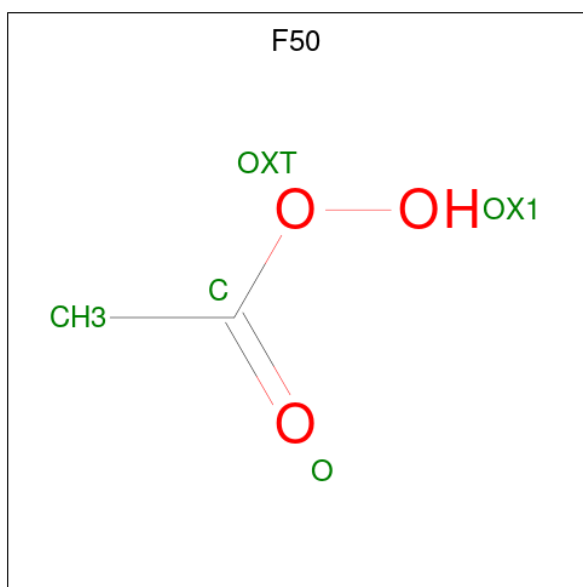
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	D	1	Total	C	F	N	O	S	0	0
			32	16	5	5	5	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



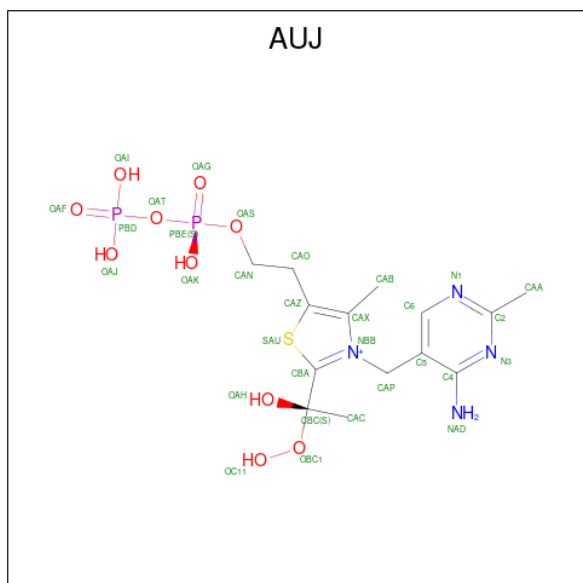
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	E	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is ETHANPEROXOIC ACID (CCD ID: F50) (formula: $\text{C}_2\text{H}_4\text{O}_3$).



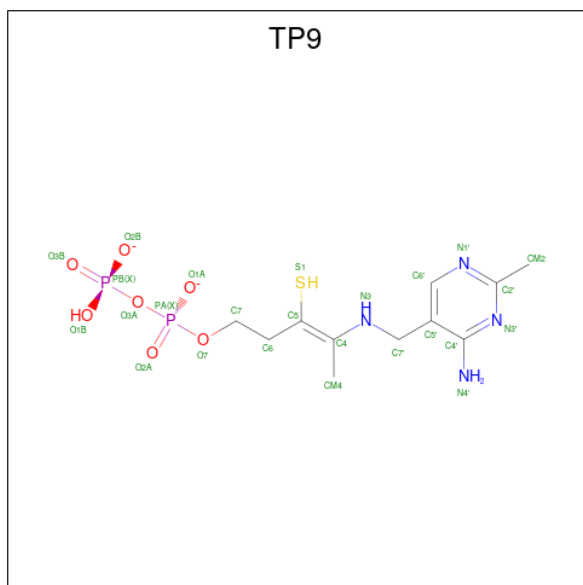
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	2	3		
6	B	1	Total	C	O	0	0
			5	2	3		
6	E	1	Total	C	O	0	0
			5	2	3		

- Molecule 7 is 2-[3-[(4-azanyl-2-methyl-pyrimidin-5-yl)methyl]-2-[(1 {S})-1-(dioxidanyl)-1-oxidanyl-ethyl]-4-methyl-1,3-thiazol-5-yl]ethyl phosphono hydrogen phosphate (CCD ID: AUJ) (formula: C₁₄H₂₃N₄O₁₀P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	S	0	0
			31	14	4	10	2	1		

- Molecule 8 is (3Z)-4-[[[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]AMINO}-3-MERCAPTOPENT-3-EN-1-YL TRIHYDROGEN DIPHOSPHATE (CCD ID: TP9) (formula: $C_{11}H_{18}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	B	1	Total 25	C 11	N 4	O 7	P 2	S 1	0	0
8	E	1	Total 25	C 11	N 4	O 7	P 2	S 1	0	0
8	D	1	Total 25	C 11	N 4	O 7	P 2	S 1	0	0

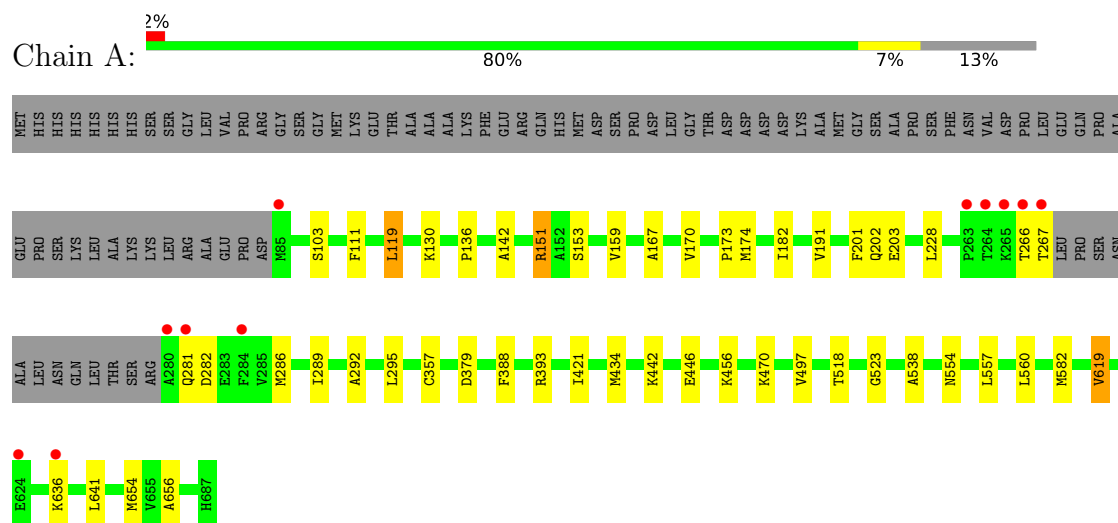
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	260	Total	O	0	0
			260	260		
9	B	357	Total	O	0	0
			357	357		
9	E	177	Total	O	0	0
			177	177		
9	D	378	Total	O	0	0
			378	378		

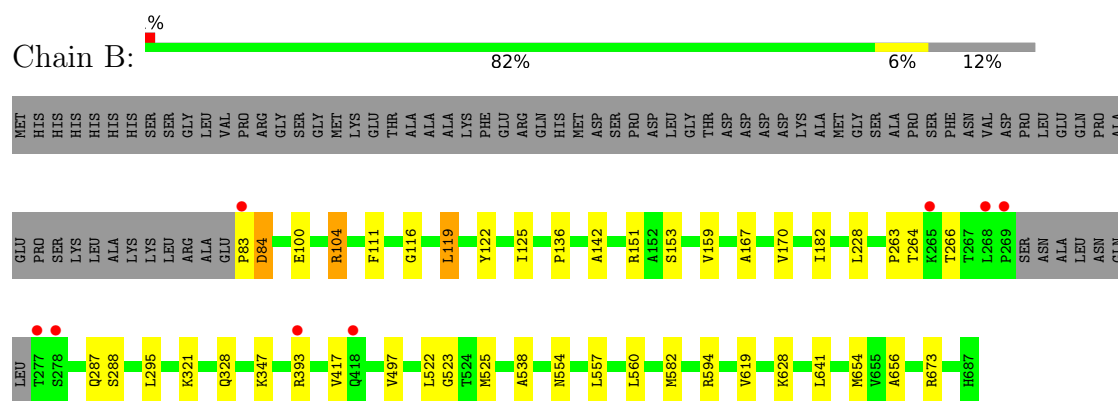
3 Residue-property plots [i](#)

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.

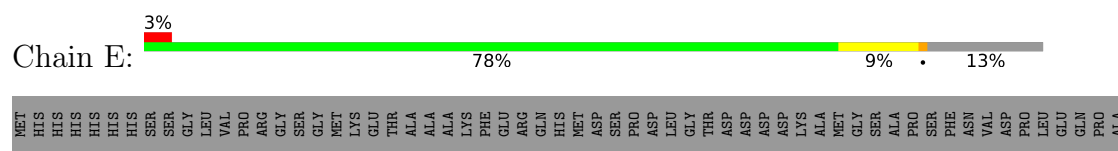
- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial

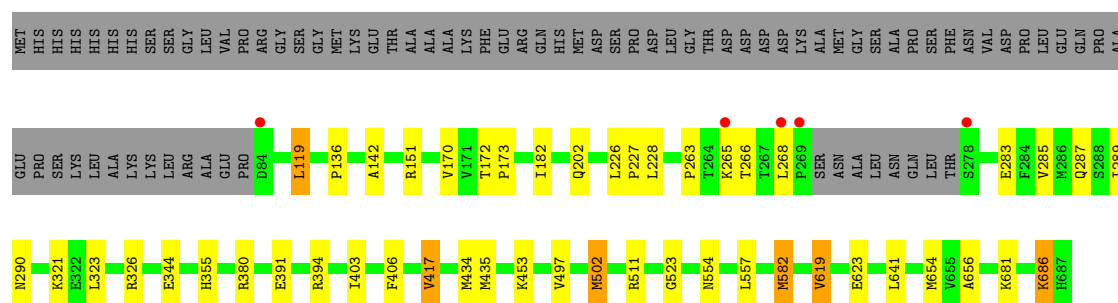


- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial



- Molecule 1: Acetolactate synthase catalytic subunit, mitochondrial





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	218.21Å 218.21Å 361.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 2.33 48.79 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.79-2.33) 99.9 (48.79-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.150 , 0.180 0.157 , 0.181	Depositor DCC
R_{free} test set	2000 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19824	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% 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: TP9, SME, F50, FAD, PXD, MG, AUJ

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	0.48	1/4630 (0.0%)	0.75	1/6276 (0.0%)
1	B	0.49	3/4688 (0.1%)	0.75	2/6356 (0.0%)
1	E	0.38	1/4629 (0.0%)	0.74	3/6275 (0.0%)
2	D	0.51	4/4641 (0.1%)	0.74	1/6291 (0.0%)
All	All	0.47	9/18588 (0.0%)	0.74	7/25198 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	119	LEU	C-O	-7.16	1.17	1.24
2	D	119	LEU	C-O	-6.89	1.18	1.24
1	E	119	LEU	C-O	-6.53	1.18	1.24
2	D	202	GLN	C-O	-5.76	1.16	1.23
1	B	288[A]	SER	C-O	-5.63	1.17	1.24
1	B	288[B]	SER	C-O	-5.63	1.17	1.24
1	A	119	LEU	C-O	-5.61	1.19	1.24
2	D	380	ARG	C-O	-5.44	1.17	1.24
2	D	290	ASN	C-O	-5.06	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288[A]	SER	N-CA-C	8.65	121.80	111.33
1	B	288[B]	SER	N-CA-C	8.65	121.80	111.33
2	D	380	ARG	N-CA-C	-5.50	106.53	113.18
1	A	281	GLN	N-CA-C	-5.26	107.23	113.97
1	E	112	GLY	N-CA-C	5.10	118.02	110.42
1	E	409	SER	CA-C-N	5.08	125.11	119.32
1	E	409	SER	C-N-CA	5.08	125.11	119.32

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	4526	0	4542	25	0
1	B	4580	0	4591	32	0
1	E	4528	0	4544	38	0
2	D	4553	0	4559	29	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	32	0	0	0	0
4	B	32	0	0	1	0
4	D	32	0	0	0	0
4	E	32	0	0	0	0
5	A	53	0	30	1	0
5	B	53	0	30	0	0
5	D	53	0	30	1	0
5	E	53	0	30	2	0
6	A	5	0	4	5	0
6	B	5	0	4	4	0
6	E	5	0	4	5	0
7	A	31	0	0	1	0
8	B	25	0	17	3	0
8	D	25	0	17	3	0
8	E	25	0	17	3	0
9	A	260	0	0	3	0
9	B	357	0	0	5	1
9	D	378	0	0	3	0
9	E	177	0	0	2	1
All	All	19824	0	18419	134	1

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 (134) 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)
6:A:704:F50:HH33	8:D:704:TP9:S1	1.83	1.17
6:A:704:F50:HH31	2:D:582[A]:MET:HG2	1.49	0.93
8:B:704:TP9:S1	6:E:705:F50:HH33	2.11	0.90
2:D:151:ARG:HD3	2:D:182:ILE:HD12	1.57	0.87
6:A:704:F50:CH3	8:D:704:TP9:S1	2.64	0.85
1:A:388:PHE:O	1:A:393:ARG:NH1	2.10	0.84
6:B:705:F50:HH33	8:E:704:TP9:S1	2.17	0.84
1:E:295:LEU:HD21	1:E:401:GLY:HA2	1.62	0.79
1:B:84:ASP:OD2	1:B:264:THR:OG1	1.99	0.79
2:D:326:ARG:HD3	2:D:435:MET:HE2	1.67	0.77
1:B:151:ARG:HD3	1:B:182:ILE:HD12	1.70	0.72
1:B:393:ARG:HH11	1:B:393:ARG:HG3	1.57	0.70
1:E:282:ASP:O	1:E:285:VAL:N	2.14	0.70
2:D:344:GLU:HG3	2:D:511:ARG:HE	1.57	0.70
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.77	0.67
1:E:87:THR:HG22	1:E:261:PRO:HG3	1.79	0.65
1:B:151:ARG:NH2	9:B:802:HOH:O	2.29	0.65
6:A:704:F50:CH3	2:D:582[A]:MET:HG2	2.24	0.64
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.80	0.64
1:A:103:SER:HB2	1:A:130:LYS:HD3	1.80	0.64
1:B:83:PRO:O	1:B:84:ASP:HB3	1.98	0.63
1:E:285:VAL:O	1:E:289:ILE:HG13	1.99	0.63
2:D:151:ARG:NH2	9:D:802:HOH:O	2.32	0.63
1:B:673:ARG:NH2	9:B:803:HOH:O	2.33	0.62
1:E:355:HIS:HB2	1:E:502:MET:HE2	1.81	0.62
1:A:151:ARG:NH2	1:A:518:THR:O	2.32	0.62
1:E:151:ARG:NH2	1:E:518:THR:O	2.33	0.62
2:D:355:HIS:HB2	2:D:502:SME:HE3	1.81	0.61
1:E:136:PRO:HG3	1:E:142:ALA:HB2	1.81	0.61
1:E:251:LYS:NZ	9:E:804:HOH:O	2.33	0.61
2:D:136:PRO:HG3	2:D:142:ALA:HB2	1.84	0.60
2:D:321:LYS:NZ	9:D:803:HOH:O	2.35	0.59
6:A:704:F50:C	8:D:704:TP9:HN3	2.16	0.59
4:B:702:PXD:CAM	6:E:705:F50:HH31	2.32	0.59
1:B:582[A]:MET:HG2	6:E:705:F50:CH3	2.32	0.58
2:D:283:GLU:OE1	9:D:801:HOH:O	2.17	0.58
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.86	0.57
1:B:263:PRO:HB2	1:B:266:THR:HG23	1.85	0.57
1:E:456:LYS:N	1:E:456:LYS:HD2	2.19	0.57
1:E:554:ASN:HA	1:E:557:LEU:HD23	1.86	0.57
2:D:554:ASN:HA	2:D:557:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103[B]:SER:HB2	1:E:130:LYS:HD3	1.88	0.56
2:D:435:MET:HE3	2:D:435:MET:HA	1.86	0.56
1:A:379:ASP:OD1	9:A:801:HOH:O	2.18	0.56
1:E:151:ARG:HD3	1:E:182:ILE:HD12	1.89	0.54
1:E:103[A]:SER:HB2	1:E:130:LYS:HD3	1.89	0.54
1:B:594:ARG:NH1	1:E:123:ASP:OD1	2.40	0.54
2:D:323:LEU:HA	2:D:435:MET:HE1	1.90	0.53
1:B:328:GLN:NE2	9:B:801:HOH:O	2.28	0.52
1:E:435:MET:HE3	1:E:435:MET:HA	1.90	0.52
1:B:228:LEU:HB2	1:B:266:THR:HB	1.91	0.52
1:E:323:LEU:HA	1:E:435:MET:HE1	1.90	0.52
2:D:263:PRO:HB2	2:D:266:THR:HG23	1.92	0.52
2:D:228:LEU:HB2	2:D:266:THR:HB	1.91	0.52
1:B:347:LYS:NZ	9:B:807:HOH:O	2.40	0.51
2:D:403:ILE:HD12	2:D:417:VAL:HG11	1.91	0.50
1:B:554:ASN:HA	1:B:557:LEU:HD23	1.94	0.50
1:A:470:LYS:NZ	9:A:807:HOH:O	2.43	0.49
1:B:393:ARG:HH22	1:B:417:VAL:HG23	1.78	0.48
6:B:705:F50:CH3	8:E:704:TP9:S1	2.95	0.48
1:E:594:ARG:NH2	9:E:806:HOH:O	2.46	0.48
1:A:170:VAL:HG23	1:A:174:MET:HE2	1.95	0.48
1:A:357:CYS:SG	9:A:1052:HOH:O	2.60	0.48
1:E:122:TYR:HA	1:E:125:ILE:HG12	1.96	0.48
8:B:704:TP9:HN3	6:E:705:F50:C	2.27	0.48
1:B:116:GLY:N	6:B:705:F50:OX1	2.36	0.47
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.96	0.47
2:D:686:LYS:HB2	2:D:686:LYS:HE3	1.65	0.47
2:D:497:VAL:HG21	2:D:523:GLY:C	2.39	0.47
1:B:497:VAL:HG21	1:B:523:GLY:C	2.40	0.47
1:E:282:ASP:OD1	1:E:283:GLU:N	2.48	0.47
1:A:554:ASN:HA	1:A:557:LEU:HD23	1.97	0.47
1:E:286:MET:SD	1:E:437:LYS:NZ	2.88	0.47
1:B:525:MET:SD	8:B:704:TP9:H61	2.54	0.46
2:D:170:VAL:C	2:D:173:PRO:HD2	2.41	0.46
1:B:122:TYR:HA	1:B:125:ILE:HG12	1.98	0.46
1:E:167:ALA:O	1:E:170:VAL:HG22	2.15	0.46
2:D:619:VAL:HG23	2:D:641:LEU:HD11	1.96	0.46
1:A:619:VAL:HG23	1:A:641:LEU:HD11	1.96	0.46
2:D:285:VAL:O	2:D:289:ILE:HG13	2.15	0.46
1:A:582[A]:MET:HG2	7:A:705:AUJ:CAC	2.45	0.46
1:E:170:VAL:C	1:E:173:PRO:HD2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:MET:HE2	1:B:656:ALA:HB2	1.99	0.45
6:B:705:F50:C	8:E:704:TP9:HN3	2.30	0.45
1:E:282:ASP:C	1:E:284:PHE:N	2.72	0.44
1:B:167:ALA:O	1:B:170:VAL:HG22	2.18	0.44
1:E:407:GLU:OE2	5:E:703:FAD:O2B	2.33	0.44
2:D:654:MET:HE2	2:D:656:ALA:HB2	1.98	0.44
1:A:228:LEU:HB2	1:A:266:THR:HB	1.99	0.44
2:D:406:PHE:HZ	2:D:434:MET:HE1	1.81	0.44
2:D:681:LYS:HB2	2:D:681:LYS:HE3	1.67	0.44
1:B:100:GLU:HB3	1:B:104:ARG:HH21	1.81	0.44
1:E:170:VAL:HG23	1:E:174:MET:HE2	2.00	0.43
1:E:358:ALA:HB3	1:E:458:TYR:HB3	2.01	0.43
5:E:703:FAD:H9	5:E:703:FAD:H1'1	1.76	0.43
1:A:282:ASP:OD1	1:A:282:ASP:N	2.51	0.43
1:B:111:PHE:O	1:B:159:VAL:HA	2.19	0.43
1:A:170:VAL:C	1:A:173:PRO:HD2	2.44	0.43
1:B:393:ARG:HH11	1:B:393:ARG:CG	2.29	0.42
1:B:522:LEU:O	1:E:202:GLN:HG2	2.19	0.42
1:B:619:VAL:HG22	1:B:628:LYS:HG3	2.00	0.42
1:E:304:LEU:HD23	1:E:371:ILE:HB	2.01	0.42
1:B:582[A]:MET:HG2	6:E:705:F50:HH31	2.01	0.42
1:A:191:VAL:HG11	1:A:203:GLU:HB2	2.02	0.42
1:E:226:LEU:HB3	1:E:227:PRO:HD3	2.02	0.42
1:A:295:LEU:HD12	1:A:421:ILE:HD12	2.00	0.42
1:E:494:THR:HG22	1:E:517:ILE:HB	2.02	0.42
1:A:151:ARG:HD3	1:A:182:ILE:HD12	2.00	0.42
1:A:153:SER:HB3	1:A:538:ALA:HB1	2.01	0.42
2:D:172:THR:HB	2:D:173:PRO:HD3	2.01	0.42
1:A:289:ILE:HG23	1:A:434:MET:HB2	2.02	0.41
1:A:497:VAL:HG21	1:A:523:GLY:C	2.45	0.41
1:E:282:ASP:O	1:E:284:PHE:N	2.54	0.41
2:D:268:LEU:HD23	2:D:268:LEU:HA	1.85	0.41
2:D:226:LEU:HB3	2:D:227:PRO:HD3	2.01	0.41
1:A:201:PHE:CE2	1:A:202:GLN:HG3	2.54	0.41
1:A:292:ALA:HB2	1:A:421:ILE:HG21	2.02	0.41
1:B:393:ARG:HG3	1:B:393:ARG:NH1	2.30	0.41
1:E:295:LEU:HD22	1:E:369:LEU:HD13	2.02	0.41
1:E:654:MET:HE2	1:E:656:ALA:HB2	2.02	0.41
5:D:703:FAD:H9	5:D:703:FAD:H1'1	1.76	0.41
5:A:703:FAD:H8A	5:A:703:FAD:H2B	1.91	0.41
1:E:263:PRO:HB2	1:E:266:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:442:LYS:HB2	1:E:443:GLU:H	1.59	0.41
2:D:151:ARG:HD3	2:D:182:ILE:CD1	2.40	0.41
1:A:111:PHE:O	1:A:159:VAL:HA	2.21	0.41
1:A:167:ALA:O	1:A:170:VAL:HG22	2.20	0.41
1:E:463:MET:HE3	1:E:463:MET:HA	2.02	0.41
1:B:321:LYS:NZ	9:B:810:HOH:O	2.53	0.41
1:B:295:LEU:HD23	1:B:295:LEU:HA	1.82	0.40
1:E:394:ARG:HH21	1:E:400:ARG:NH2	2.19	0.40
1:E:409:SER:HA	1:E:410:PRO:HD3	1.95	0.40
2:D:391:GLU:OE2	2:D:394:ARG:NH1	2.54	0.40
1:A:654:MET:HE2	1:A:656:ALA:HB2	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:1097:HOH:O	9:E:806:HOH:O[3_775]	2.19	0.01

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	590/677 (87%)	581 (98%)	9 (2%)	0	100	100
1	B	598/677 (88%)	589 (98%)	8 (1%)	1 (0%)	43	50
1	E	590/677 (87%)	577 (98%)	11 (2%)	2 (0%)	36	41
2	D	592/677 (87%)	585 (99%)	7 (1%)	0	100	100
All	All	2370/2708 (88%)	2332 (98%)	35 (2%)	3 (0%)	48	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	442	LYS
1	E	283	GLU
1	B	84	ASP

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	487/556 (88%)	477 (98%)	10 (2%)	47	60
1	B	494/556 (89%)	490 (99%)	4 (1%)	73	82
1	E	488/556 (88%)	478 (98%)	10 (2%)	48	61
2	D	488/555 (88%)	478 (98%)	10 (2%)	48	61
All	All	1957/2223 (88%)	1923 (98%)	34 (2%)	53	66

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	151	ARG
1	A	267	THR
1	A	286	MET
1	A	442	LYS
1	A	446	GLU
1	A	456	LYS
1	A	560	LEU
1	A	619	VAL
1	A	636	LYS
1	B	104	ARG
1	B	119	LEU
1	B	287	GLN
1	B	560	LEU
1	E	119	LEU
1	E	264	THR
1	E	269	PRO
1	E	286	MET
1	E	288	SER

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Mol	Chain	Res	Type
1	E	298	LEU
1	E	442	LYS
1	E	560	LEU
1	E	619	VAL
1	E	630	LYS
2	D	119	LEU
2	D	265	LYS
2	D	287	GLN
2	D	417	VAL
2	D	453	LYS
2	D	582[A]	MET
2	D	582[B]	MET
2	D	619	VAL
2	D	623	GLU
2	D	686	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	202	GLN
1	A	328	GLN
1	B	202	GLN
1	B	499	GLN
1	B	554	ASN
1	E	126	HIS
1	E	202	GLN
1	E	328	GLN
1	E	536	GLN
1	E	554	ASN
2	D	202	GLN
2	D	328	GLN
2	D	450	GLN
2	D	536	GLN
2	D	687	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SME	D	502	2	6,8,9	1.57	2 (33%)	3,9,11	6.53	3 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SME	D	502	2	-	1/6/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	502	SME	CB-CA	-2.36	1.50	1.53
2	D	502	SME	OE-S	-2.08	1.44	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	502	SME	CE-S-CG	9.57	121.39	97.45
2	D	502	SME	OE-S-CG	5.14	119.39	105.89
2	D	502	SME	OE-S-CE	3.14	118.71	106.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	502	SME	CB-CG-S-OE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	SME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	PXD	B	702	-	32,34,34	3.62	18 (56%)	37,51,51	2.46	14 (37%)
6	F50	A	704	-	4,4,4	1.67	1 (25%)	4,4,4	2.84	2 (50%)
8	TP9	B	704	3	22,25,25	3.04	11 (50%)	29,36,36	2.13	12 (41%)
4	PXD	E	702	-	32,34,34	3.50	18 (56%)	37,51,51	2.53	15 (40%)
5	FAD	D	703	-	58,58,58	1.58	11 (18%)	85,89,89	1.60	18 (21%)
5	FAD	A	703	-	58,58,58	1.62	12 (20%)	85,89,89	1.63	18 (21%)
6	F50	B	705	-	4,4,4	1.52	1 (25%)	4,4,4	3.23	2 (50%)
4	PXD	A	702	-	32,34,34	3.62	18 (56%)	37,51,51	2.76	16 (43%)
5	FAD	E	703	-	58,58,58	1.62	13 (22%)	85,89,89	1.62	19 (22%)
6	F50	E	705	-	4,4,4	1.44	1 (25%)	4,4,4	2.17	1 (25%)
8	TP9	D	704	3	22,25,25	3.03	12 (54%)	29,36,36	2.22	12 (41%)
4	PXD	D	702	-	32,34,34	3.89	20 (62%)	37,51,51	2.86	18 (48%)
7	AUJ	A	705	3	27,32,32	3.31	13 (48%)	36,49,49	1.46	8 (22%)
5	FAD	B	703	-	58,58,58	2.63	30 (51%)	85,89,89	1.79	21 (24%)
8	TP9	E	704	3	22,25,25	3.04	12 (54%)	29,36,36	2.15	10 (34%)

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	PXD	B	702	-	-	7/25/26/26	0/3/3/3
6	F50	A	704	-	-	0/0/2/2	-
8	TP9	B	704	3	-	6/17/22/22	0/1/1/1
4	PXD	E	702	-	-	8/25/26/26	0/3/3/3
5	FAD	D	703	-	-	4/34/50/50	0/6/6/6
5	FAD	A	703	-	-	5/34/50/50	0/6/6/6
6	F50	B	705	-	-	0/0/2/2	-
4	PXD	A	702	-	-	8/25/26/26	0/3/3/3
5	FAD	E	703	-	-	5/34/50/50	0/6/6/6
6	F50	E	705	-	-	0/0/2/2	-
8	TP9	D	704	3	-	6/17/22/22	0/1/1/1
4	PXD	D	702	-	-	10/25/26/26	0/3/3/3
7	AUJ	A	705	3	-	5/20/26/26	0/2/2/2
5	FAD	B	703	-	-	4/34/50/50	0/6/6/6
8	TP9	E	704	3	-	5/17/22/22	0/1/1/1

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	PXD	OAC-SBF	-12.42	1.29	1.43
4	A	702	PXD	OAC-SBF	-9.84	1.32	1.43
4	B	702	PXD	OAC-SBF	-9.27	1.32	1.43
4	E	702	PXD	OAC-SBF	-8.99	1.33	1.43
4	D	702	PXD	CBB-NBD	-8.80	1.25	1.38
8	E	704	TP9	PA-O3A	-8.76	1.50	1.59
5	B	703	FAD	PA-O3P	-8.69	1.50	1.59
4	E	702	PXD	CBB-NBD	-8.27	1.26	1.38
4	B	702	PXD	CBB-NBD	-8.16	1.26	1.38
4	A	702	PXD	CBB-NBD	-7.93	1.26	1.38
4	E	702	PXD	OAT-CAZ	7.62	1.41	1.33
8	B	704	TP9	PA-O3A	-7.58	1.51	1.59
7	A	705	AUJ	PBE-OAT	-7.35	1.51	1.59
7	A	705	AUJ	CAP-NBB	-7.30	1.40	1.47
4	A	702	PXD	OAT-CAZ	7.13	1.41	1.33
4	B	702	PXD	OAT-CAZ	7.02	1.41	1.33
8	D	704	TP9	PA-O3A	-6.93	1.52	1.59
7	A	705	AUJ	C4-N3	-6.49	1.26	1.35
8	D	704	TP9	C4-N3	6.39	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	702	PXD	OAT-CAZ	6.19	1.40	1.33
4	E	702	PXD	CAW-CBA	-6.13	1.35	1.41
4	B	702	PXD	CAW-CBA	-6.00	1.35	1.41
8	E	704	TP9	C4-N3	5.97	1.40	1.32
8	B	704	TP9	C4-N3	5.73	1.40	1.32
4	B	702	PXD	OAD-SBF	-5.66	1.37	1.43
5	B	703	FAD	C8A-N9A	-5.48	1.28	1.37
4	A	702	PXD	CAW-CBA	-5.16	1.36	1.41
5	E	703	FAD	C10-N1	5.14	1.43	1.33
4	A	702	PXD	OAD-SBF	-5.13	1.37	1.43
5	A	703	FAD	C10-N1	5.08	1.43	1.33
5	D	703	FAD	C10-N1	5.07	1.43	1.33
4	D	702	PXD	OAT-CAB	-4.92	1.34	1.45
4	D	702	PXD	OAD-SBF	-4.73	1.38	1.43
7	A	705	AUJ	PBD-OAF	-4.60	1.36	1.50
8	D	704	TP9	PA-O1A	-4.53	1.34	1.55
8	D	704	TP9	PB-O1B	-4.48	1.38	1.54
8	B	704	TP9	PB-O2B	-4.44	1.38	1.54
7	A	705	AUJ	PBD-OAI	-4.44	1.38	1.54
8	B	704	TP9	PA-O2A	-4.31	1.35	1.50
4	A	702	PXD	OAT-CAB	-4.28	1.35	1.45
4	E	702	PXD	OAT-CAB	-4.25	1.35	1.45
8	E	704	TP9	PB-O2B	-4.25	1.39	1.54
7	A	705	AUJ	C5-C4	4.23	1.49	1.42
5	B	703	FAD	O3'-C3'	-4.21	1.32	1.43
4	D	702	PXD	CAW-CBA	-4.21	1.37	1.41
7	A	705	AUJ	PBE-OAG	-4.19	1.36	1.50
4	B	702	PXD	OAT-CAB	-4.17	1.36	1.45
5	B	703	FAD	O4-C4	-4.16	1.15	1.23
5	B	703	FAD	O2-C2	-4.13	1.16	1.24
4	B	702	PXD	NBD-NAQ	-4.13	1.30	1.38
5	A	703	FAD	C4X-N5	4.13	1.39	1.30
5	B	703	FAD	P-O3P	-4.08	1.55	1.59
7	A	705	AUJ	C2-N1	-4.04	1.28	1.34
4	D	702	PXD	CAV-NAP	-4.01	1.28	1.36
5	E	703	FAD	C4X-N5	4.00	1.39	1.30
4	A	702	PXD	NBD-NAQ	-3.95	1.31	1.38
5	D	703	FAD	C4X-N5	3.90	1.39	1.30
4	B	702	PXD	CAV-NAP	-3.85	1.28	1.36
4	A	702	PXD	CBA-SBF	-3.84	1.72	1.78
7	A	705	AUJ	PBE-OAK	-3.83	1.37	1.55
5	B	703	FAD	C5A-N7A	-3.83	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	703	FAD	C5X-N5	-3.77	1.32	1.39
4	D	702	PXD	NBD-NAQ	-3.77	1.31	1.38
4	D	702	PXD	CAY-CBA	3.75	1.46	1.42
8	E	704	TP9	PA-O1A	-3.72	1.38	1.55
4	B	702	PXD	CBA-SBF	-3.70	1.73	1.78
5	B	703	FAD	PA-O2A	-3.65	1.38	1.55
8	B	704	TP9	PB-O3B	-3.64	1.39	1.50
4	E	702	PXD	NBD-NAQ	-3.63	1.31	1.38
8	D	704	TP9	PA-O2A	-3.62	1.38	1.50
4	A	702	PXD	CAY-CBA	3.58	1.46	1.42
4	A	702	PXD	CAV-NAP	-3.57	1.29	1.36
5	B	703	FAD	P-O2P	-3.56	1.38	1.55
4	D	702	PXD	FAH-CBE	-3.54	1.20	1.33
5	B	703	FAD	C10-N1	3.53	1.40	1.33
4	A	702	PXD	OAS-CAA	-3.50	1.37	1.45
4	A	702	PXD	SBF-NAR	-3.49	1.55	1.64
8	B	704	TP9	PA-O1A	-3.47	1.39	1.55
4	D	702	PXD	CAV-NAR	3.46	1.43	1.38
4	D	702	PXD	OAU-CAN	-3.45	1.33	1.44
4	E	702	PXD	CAV-NAP	-3.44	1.29	1.36
4	E	702	PXD	CBA-SBF	-3.39	1.73	1.78
4	B	702	PXD	OAS-CAA	-3.33	1.37	1.45
5	B	703	FAD	C1'-N10	-3.30	1.39	1.47
4	E	702	PXD	OAS-CAA	-3.30	1.37	1.45
4	D	702	PXD	SBF-NAR	-3.29	1.56	1.64
4	B	702	PXD	FAH-CBE	-3.23	1.21	1.33
4	D	702	PXD	CAN-CBC	-3.17	1.41	1.49
8	B	704	TP9	C4'-N3'	-3.15	1.30	1.35
4	B	702	PXD	OAU-CAN	-3.12	1.34	1.44
4	E	702	PXD	CAY-CBA	3.12	1.45	1.42
4	E	702	PXD	OAD-SBF	-3.09	1.40	1.43
4	A	702	PXD	FAH-CBE	-3.08	1.21	1.33
5	B	703	FAD	C2B-C1B	-3.08	1.43	1.53
4	E	702	PXD	CAV-NAR	3.07	1.43	1.38
6	A	704	F50	OXT-C	3.01	1.44	1.35
4	E	702	PXD	FAH-CBE	-2.98	1.22	1.33
4	D	702	PXD	OAS-CAA	-2.98	1.38	1.45
4	B	702	PXD	SBF-NAR	-2.97	1.57	1.64
8	D	704	TP9	PB-O2B	-2.96	1.43	1.54
5	B	703	FAD	C2B-C3B	-2.90	1.45	1.53
7	A	705	AUJ	C2-N3	2.86	1.39	1.34
4	A	702	PXD	FAG-CBE	-2.86	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	PXD	CAV-NAR	2.85	1.42	1.38
5	D	703	FAD	C2-N1	2.83	1.43	1.36
5	E	703	FAD	PA-O3P	-2.82	1.56	1.59
5	E	703	FAD	C2-N1	2.82	1.43	1.36
4	E	702	PXD	CAN-CBC	-2.80	1.42	1.49
8	D	704	TP9	PB-O3B	-2.77	1.41	1.50
4	E	702	PXD	SBF-NAR	-2.75	1.57	1.64
5	A	703	FAD	C2-N1	2.75	1.42	1.36
5	B	703	FAD	C1B-N9A	-2.75	1.38	1.46
5	A	703	FAD	PA-O3P	-2.75	1.56	1.59
5	A	703	FAD	C8A-N9A	-2.75	1.32	1.37
5	E	703	FAD	C8A-N9A	-2.75	1.32	1.37
4	E	702	PXD	OAU-CAN	-2.74	1.35	1.44
8	D	704	TP9	PA-O7	-2.73	1.48	1.59
5	B	703	FAD	C9-C8	-2.72	1.35	1.39
5	B	703	FAD	C4X-C10	-2.72	1.36	1.44
8	B	704	TP9	PB-O1B	-2.72	1.44	1.54
8	E	704	TP9	PB-O3B	-2.71	1.42	1.50
5	B	703	FAD	O2'-C2'	-2.70	1.37	1.43
5	B	703	FAD	C4A-N9A	-2.70	1.32	1.37
8	B	704	TP9	PA-O7	-2.70	1.48	1.59
8	D	704	TP9	C4'-N3'	-2.68	1.31	1.35
4	D	702	PXD	CBA-SBF	-2.67	1.74	1.78
5	E	703	FAD	O3'-C3'	-2.66	1.36	1.43
8	E	704	TP9	PB-O1B	-2.64	1.45	1.54
8	E	704	TP9	C5'-C4'	-2.63	1.38	1.42
6	B	705	F50	OXT-C	2.62	1.43	1.35
6	E	705	F50	OXT-C	2.61	1.43	1.35
7	A	705	AUJ	C6-C5	-2.61	1.32	1.37
5	A	703	FAD	C2'-C3'	2.60	1.58	1.53
4	A	702	PXD	CAV-NAR	2.60	1.42	1.38
8	E	704	TP9	C4'-N3'	-2.60	1.31	1.35
5	B	703	FAD	C5'-C4'	-2.58	1.48	1.51
5	D	703	FAD	C8A-N9A	-2.58	1.33	1.37
5	A	703	FAD	O3'-C3'	-2.57	1.36	1.43
5	B	703	FAD	C9A-N10	-2.55	1.36	1.41
5	D	703	FAD	O3'-C3'	-2.55	1.36	1.43
4	A	702	PXD	OAU-CAN	-2.51	1.36	1.44
8	E	704	TP9	PA-O7	-2.50	1.49	1.59
5	D	703	FAD	C2'-C3'	2.49	1.57	1.53
4	D	702	PXD	FAG-CBE	-2.47	1.24	1.33
5	D	703	FAD	PA-O3P	-2.47	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	PXD	CAN-CBC	-2.47	1.42	1.49
5	E	703	FAD	C2'-C3'	2.46	1.57	1.53
8	D	704	TP9	C5'-C4'	-2.46	1.38	1.42
4	B	702	PXD	FAG-CBE	-2.44	1.24	1.33
5	E	703	FAD	C1'-N10	-2.44	1.41	1.47
4	E	702	PXD	FAG-CBE	-2.41	1.24	1.33
5	D	703	FAD	C1'-N10	-2.40	1.42	1.47
5	B	703	FAD	PA-O1A	-2.40	1.42	1.50
8	E	704	TP9	PA-O2A	-2.40	1.42	1.50
5	B	703	FAD	C3B-C4B	-2.39	1.46	1.53
4	A	702	PXD	CAN-CBC	-2.39	1.43	1.49
4	B	702	PXD	CBB-NAP	2.39	1.38	1.33
4	D	702	PXD	CAM-NAO	-2.37	1.30	1.36
5	A	703	FAD	C1'-N10	-2.32	1.42	1.47
8	E	704	TP9	C7'-N3	-2.31	1.41	1.46
5	A	703	FAD	C1'-C2'	2.27	1.55	1.52
5	B	703	FAD	C9A-C5X	-2.26	1.37	1.41
5	B	703	FAD	C2A-N1A	-2.26	1.29	1.33
5	D	703	FAD	C1'-C2'	2.26	1.55	1.52
8	B	704	TP9	C7'-N3	-2.25	1.41	1.46
4	A	702	PXD	CBB-NAP	2.25	1.38	1.33
5	E	703	FAD	C2B-C3B	-2.25	1.47	1.53
7	A	705	AUJ	PBE-OAS	-2.23	1.50	1.59
5	A	703	FAD	C2B-C3B	-2.23	1.47	1.53
5	B	703	FAD	O4B-C4B	-2.21	1.40	1.45
5	B	703	FAD	C4-N3	-2.18	1.34	1.38
5	B	703	FAD	C2-N3	-2.16	1.34	1.39
5	D	703	FAD	C2B-C3B	-2.14	1.47	1.53
5	A	703	FAD	C4X-C4	2.13	1.52	1.44
4	D	702	PXD	CAJ-CAK	-2.10	1.35	1.38
5	B	703	FAD	P-O1P	-2.10	1.43	1.50
4	E	702	PXD	CBB-NAP	2.09	1.37	1.33
7	A	705	AUJ	PBD-OAJ	-2.09	1.47	1.54
5	E	703	FAD	C4X-C4	2.08	1.52	1.44
4	D	702	PXD	FAE-CBC	-2.07	1.25	1.35
8	B	704	TP9	O7-C7	-2.06	1.36	1.44
5	E	703	FAD	C1'-C2'	2.06	1.55	1.52
8	D	704	TP9	O7-C7	-2.05	1.36	1.44
5	E	703	FAD	C2B-C1B	-2.05	1.47	1.53
8	E	704	TP9	C4'-N4'	2.03	1.39	1.34
5	B	703	FAD	O4'-C4'	-2.03	1.39	1.43
8	D	704	TP9	C7'-N3	-2.03	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	FAD	C2B-C1B	-2.03	1.47	1.53
5	D	703	FAD	C2B-C1B	-2.02	1.47	1.53
4	B	702	PXD	CAY-CBA	2.02	1.44	1.42
5	E	703	FAD	C6A-N6A	2.01	1.39	1.34

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	702	PXD	OAD-SBF-OAC	-8.33	109.40	119.52
4	A	702	PXD	CBA-SBF-NAR	8.25	117.79	106.68
4	D	702	PXD	OAD-SBF-OAC	-7.98	109.83	119.52
4	D	702	PXD	NAQ-CAV-NAP	-7.52	106.65	116.67
4	E	702	PXD	NAQ-CAV-NAP	-6.71	107.72	116.67
4	D	702	PXD	CBA-SBF-NAR	6.35	115.23	106.68
4	B	702	PXD	NAQ-CAV-NAP	-6.21	108.39	116.67
4	A	702	PXD	NAQ-CAV-NAP	-6.18	108.43	116.67
4	B	702	PXD	CBA-SBF-NAR	6.15	114.96	106.68
5	B	703	FAD	C5A-C4A-N3A	-6.04	118.40	126.72
4	A	702	PXD	OAD-SBF-OAC	-5.85	112.42	119.52
4	B	702	PXD	OAD-SBF-OAC	-5.69	112.61	119.52
5	E	703	FAD	C5A-C4A-N3A	-5.36	119.34	126.72
5	A	703	FAD	C5A-C4A-N3A	-5.32	119.39	126.72
5	D	703	FAD	C5A-C4A-N3A	-5.21	119.55	126.72
6	B	705	F50	OXT-C-CH3	5.06	120.12	111.09
8	E	704	TP9	C5'-C7'-N3	5.02	123.26	113.15
4	E	702	PXD	CBA-SBF-NAR	5.00	113.42	106.68
5	B	703	FAD	N3A-C4A-N9A	4.80	135.33	127.17
8	D	704	TP9	C5'-C7'-N3	4.71	122.65	113.15
5	B	703	FAD	C4A-C5A-N7A	-4.57	105.36	110.58
8	D	704	TP9	C6'-C5'-C4'	4.52	121.11	115.55
8	D	704	TP9	O1A-PA-O2A	-4.47	91.63	112.44
4	D	702	PXD	OAU-CAW-CAK	-4.46	114.22	123.95
8	E	704	TP9	C7-C6-C5	4.44	126.67	112.73
8	B	704	TP9	C5'-C7'-N3	4.26	121.73	113.15
5	E	703	FAD	N3A-C4A-N9A	4.16	134.24	127.17
5	D	703	FAD	N3A-C2A-N1A	-4.14	122.32	128.58
5	A	703	FAD	N3A-C2A-N1A	-4.13	122.32	128.58
5	A	703	FAD	N3A-C4A-N9A	4.09	134.13	127.17
5	E	703	FAD	N3A-C2A-N1A	-4.04	122.46	128.58
5	D	703	FAD	N3A-C4A-N9A	4.04	134.04	127.17
6	A	704	F50	OX1-OXT-C	4.04	115.41	110.12
8	B	704	TP9	C6'-C5'-C4'	3.98	120.44	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	703	FAD	C5A-N7A-C8A	3.96	109.68	103.45
8	E	704	TP9	C6'-C5'-C4'	3.95	120.40	115.55
4	A	702	PXD	FAG-CBE-CAY	3.78	119.35	112.65
8	E	704	TP9	C7'-N3-C4	-3.71	120.03	125.47
5	E	703	FAD	C4A-C5A-N7A	-3.71	106.34	110.58
5	A	703	FAD	C2A-N3A-C4A	3.70	120.87	111.83
6	B	705	F50	OXT-C-O	-3.67	119.84	124.12
5	A	703	FAD	C4A-C5A-N7A	-3.67	106.39	110.58
4	A	702	PXD	OAU-CAW-CAK	-3.66	115.97	123.95
4	D	702	PXD	CBB-NBD-NAQ	-3.65	107.74	112.80
5	E	703	FAD	C2A-N3A-C4A	3.64	120.72	111.83
5	D	703	FAD	C2A-N3A-C4A	3.64	120.72	111.83
8	D	704	TP9	C5'-C6'-N1'	-3.61	117.96	123.83
8	B	704	TP9	C7-C6-C5	3.61	124.06	112.73
5	D	703	FAD	C4A-C5A-N7A	-3.59	106.48	110.58
8	B	704	TP9	C5'-C6'-N1'	-3.57	118.03	123.83
5	E	703	FAD	C5A-N7A-C8A	3.46	108.89	103.45
6	A	704	F50	OXT-C-CH3	3.42	117.19	111.09
6	E	705	F50	OXT-C-CH3	3.41	117.17	111.09
4	B	702	PXD	OAU-CAW-CAK	-3.40	116.54	123.95
5	D	703	FAD	C5A-N7A-C8A	3.40	108.79	103.45
5	A	703	FAD	C5A-N7A-C8A	3.39	108.78	103.45
4	B	702	PXD	OAT-CAZ-NBD	3.39	120.06	113.26
8	E	704	TP9	C5'-C6'-N1'	-3.36	118.36	123.83
4	B	702	PXD	CAA-OAS-CAX	3.35	123.48	116.96
4	D	702	PXD	CAK-CAW-CBA	3.34	125.14	119.14
4	A	702	PXD	OAT-CAZ-NBD	3.32	119.92	113.26
5	D	703	FAD	N9A-C8A-N7A	-3.28	109.28	113.94
5	B	703	FAD	C4-N3-C2	-3.26	119.86	125.64
5	B	703	FAD	C9A-N10-C10	-3.23	115.82	120.75
5	E	703	FAD	N9A-C8A-N7A	-3.22	109.36	113.94
5	A	703	FAD	C4-N3-C2	-3.22	119.92	125.64
4	A	702	PXD	NBD-CBB-NAP	-3.22	107.19	110.13
5	B	703	FAD	C4A-N9A-C8A	3.21	109.11	105.74
4	E	702	PXD	OAU-CAW-CAK	-3.21	116.94	123.95
4	D	702	PXD	CAB-OAT-CAZ	3.21	120.88	116.19
5	A	703	FAD	N9A-C8A-N7A	-3.19	109.41	113.94
4	D	702	PXD	FAG-CBE-CAY	3.18	118.29	112.65
5	E	703	FAD	C4-N3-C2	-3.18	119.99	125.64
4	D	702	PXD	CAA-OAS-CAX	3.18	123.15	116.96
5	D	703	FAD	C4-N3-C2	-3.15	120.04	125.64
8	B	704	TP9	CM4-C4-N3	3.15	121.44	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	703	FAD	C4A-N9A-C8A	3.14	109.04	105.74
4	D	702	PXD	CAJ-CAL-CAY	3.14	125.64	119.99
4	A	702	PXD	CAA-OAS-CAX	3.14	123.06	116.96
8	D	704	TP9	C7-C6-C5	3.14	122.58	112.73
5	B	703	FAD	C2A-N3A-C4A	3.13	119.47	111.83
4	D	702	PXD	OAT-CAZ-NBD	3.09	119.46	113.26
5	E	703	FAD	C4A-N9A-C8A	3.09	108.98	105.74
5	B	703	FAD	N9A-C8A-N7A	-3.07	109.58	113.94
5	A	703	FAD	C4A-N9A-C8A	3.04	108.93	105.74
4	A	702	PXD	CBE-CAY-CBA	3.04	126.14	124.15
4	B	702	PXD	CAK-CAW-CBA	3.04	124.59	119.14
8	D	704	TP9	O7-C7-C6	3.02	120.78	108.63
4	A	702	PXD	CAJ-CAL-CAY	3.02	125.42	119.99
5	B	703	FAD	C4X-C10-N10	3.01	120.79	116.48
4	E	702	PXD	CAY-CBA-SBF	2.94	127.30	120.12
4	E	702	PXD	OAT-CAZ-NBD	2.89	119.06	113.26
8	B	704	TP9	O1A-PA-O2A	-2.88	99.04	112.44
8	E	704	TP9	CM4-C4-N3	2.88	121.13	117.90
4	B	702	PXD	CBB-NBD-NAQ	-2.83	108.87	112.80
5	B	703	FAD	C4X-C10-N1	-2.82	117.67	124.59
8	B	704	TP9	O1B-PB-O3A	2.82	114.10	104.64
4	A	702	PXD	CAB-OAT-CAZ	2.81	120.29	116.19
8	D	704	TP9	C7'-C5'-C6'	-2.81	117.46	121.30
5	A	703	FAD	C4X-C4-N3	2.78	120.34	113.25
5	D	703	FAD	C4X-C4-N3	2.77	120.31	113.25
8	D	704	TP9	O1A-PA-O3A	2.76	114.74	107.27
5	B	703	FAD	C4X-C4-N3	2.76	120.27	113.25
5	E	703	FAD	C4X-C4-N3	2.75	120.25	113.25
5	A	703	FAD	C4X-C10-N10	2.74	120.41	116.48
7	A	705	AUJ	SAU-CBA-NBB	-2.74	109.55	112.24
7	A	705	AUJ	C5-C6-N1	-2.72	119.40	123.83
4	B	702	PXD	NBD-CBB-NAP	-2.71	107.65	110.13
5	B	703	FAD	O4B-C1B-N9A	2.70	113.27	108.09
5	B	703	FAD	C5X-C9A-N10	2.69	120.40	117.97
4	A	702	PXD	CAK-CAW-CBA	2.69	123.96	119.14
8	B	704	TP9	C7'-C5'-C6'	-2.68	117.63	121.30
4	E	702	PXD	CBB-NBD-NAQ	-2.68	109.09	112.80
4	E	702	PXD	CAK-CAW-CBA	2.68	123.95	119.14
4	E	702	PXD	NBD-CBB-NAP	-2.67	107.69	110.13
4	B	702	PXD	FAG-CBE-CAY	2.65	117.35	112.65
5	A	703	FAD	C4-C4X-N5	2.62	121.82	118.21
5	D	703	FAD	O4-C4-C4X	-2.61	119.64	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	702	PXD	OAU-CAW-CBA	2.60	120.62	116.68
7	A	705	AUJ	C6-C5-C4	2.60	118.75	115.55
4	D	702	PXD	NAR-CAV-NAQ	2.58	131.40	122.99
8	B	704	TP9	O2B-PB-O3A	2.57	113.25	104.64
5	E	703	FAD	C10-C4X-N5	-2.57	119.57	124.81
7	A	705	AUJ	OAK-PBE-OAG	-2.56	100.54	112.44
4	B	702	PXD	CAB-OAT-CAZ	2.55	119.92	116.19
5	A	703	FAD	C10-C4X-N5	-2.55	119.60	124.81
5	E	703	FAD	C4-C4X-N5	2.55	121.73	118.21
8	D	704	TP9	N4'-C4'-N3'	2.54	120.46	117.03
5	A	703	FAD	O4-C4-C4X	-2.52	119.89	126.53
4	D	702	PXD	CBE-CAY-CBA	2.52	125.80	124.15
5	E	703	FAD	O4-C4-C4X	-2.51	119.90	126.53
5	B	703	FAD	C10-N1-C2	2.51	122.28	116.85
8	E	704	TP9	O7-C7-C6	2.50	118.69	108.63
4	A	702	PXD	CBB-NBD-NAQ	-2.50	109.33	112.80
4	E	702	PXD	CAJ-CAL-CAY	2.50	124.48	119.99
4	B	702	PXD	CAY-CBA-SBF	2.48	126.17	120.12
5	D	703	FAD	C4X-C10-N10	2.48	120.03	116.48
5	B	703	FAD	N3A-C2A-N1A	-2.46	124.86	128.58
7	A	705	AUJ	C6-N1-C2	2.46	120.11	116.07
5	E	703	FAD	C4X-C10-N10	2.46	120.00	116.48
8	E	704	TP9	C7'-C5'-C4'	-2.37	120.26	122.56
7	A	705	AUJ	CAA-C2-N1	2.37	119.72	117.20
5	D	703	FAD	C10-C4X-N5	-2.36	120.00	124.81
4	D	702	PXD	CAY-CBA-SBF	2.35	125.86	120.12
8	B	704	TP9	O2B-PB-O3B	-2.34	101.72	110.83
4	E	702	PXD	CAL-CAJ-CAK	-2.34	117.24	120.24
5	A	703	FAD	C4X-C10-N1	-2.33	118.87	124.59
5	E	703	FAD	C4X-C10-N1	-2.31	118.92	124.59
5	D	703	FAD	C4X-C10-N1	-2.31	118.93	124.59
4	B	702	PXD	CAJ-CAL-CAY	2.31	124.14	119.99
4	A	702	PXD	OAD-SBF-NAR	-2.30	100.17	106.77
4	E	702	PXD	CAA-OAS-CAX	2.28	121.39	116.96
8	E	704	TP9	N4'-C4'-N3'	2.27	120.09	117.03
5	D	703	FAD	C4-C4X-N5	2.27	121.34	118.21
5	E	703	FAD	C9A-C5X-N5	-2.25	120.06	122.45
4	A	702	PXD	CAY-CBA-SBF	2.25	125.61	120.12
5	B	703	FAD	C10-C4X-N5	-2.24	120.24	124.81
5	B	703	FAD	N6A-C6A-N1A	2.23	123.34	118.38
4	E	702	PXD	OAD-SBF-CBA	2.23	111.98	108.74
4	A	702	PXD	OAU-CAW-CBA	2.22	120.04	116.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	702	PXD	NAR-CAV-NAQ	2.22	130.24	122.99
7	A	705	AUJ	CAO-CAZ-SAU	2.18	123.97	119.29
5	B	703	FAD	C9A-C5X-N5	-2.18	120.14	122.45
4	D	702	PXD	CAL-CAJ-CAK	-2.16	117.46	120.24
5	D	703	FAD	C6A-C5A-N7A	2.16	136.26	132.09
5	D	703	FAD	C9A-N10-C10	-2.16	117.46	120.75
5	D	703	FAD	C9A-C5X-N5	-2.16	120.17	122.45
5	A	703	FAD	C10-N1-C2	2.15	121.51	116.85
5	A	703	FAD	C6A-C5A-N7A	2.15	136.24	132.09
8	B	704	TP9	O7-C7-C6	2.15	117.27	108.63
5	B	703	FAD	C4-C4X-N5	2.14	121.16	118.21
8	B	704	TP9	C5'-C4'-N3'	-2.11	118.21	121.31
4	D	702	PXD	OAT-CAZ-NAO	-2.10	117.78	121.50
5	E	703	FAD	C6A-C5A-N7A	2.10	136.13	132.09
7	A	705	AUJ	C5-C4-N3	-2.09	118.24	121.31
8	E	704	TP9	O2B-PB-O3A	2.09	111.63	104.64
5	B	703	FAD	C6A-C5A-C4A	2.09	120.03	117.18
5	E	703	FAD	C9A-N10-C10	-2.08	117.57	120.75
5	A	703	FAD	C9A-C5X-N5	-2.08	120.25	122.45
8	D	704	TP9	O2B-PB-O3A	2.05	111.51	104.64
8	D	704	TP9	O1B-PB-O3B	-2.05	102.85	110.83
4	B	702	PXD	OAT-CAZ-NAO	-2.04	117.88	121.50
5	E	703	FAD	C10-N1-C2	2.03	121.25	116.85
4	E	702	PXD	CAB-OAT-CAZ	2.02	119.15	116.19
4	D	702	PXD	NBD-CBB-NAP	-2.02	108.28	110.13
8	D	704	TP9	C5'-C4'-N3'	-2.01	118.36	121.31

There are no chirality outliers.

All (73) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	PXD	OAU-CAN-CBC-FAE
4	A	702	PXD	OAU-CAN-CBC-FAF
4	A	702	PXD	CAW-CBA-SBF-NAR
4	A	702	PXD	CAY-CBA-SBF-NAR
4	B	702	PXD	CAW-CBA-SBF-NAR
4	B	702	PXD	CAY-CBA-SBF-NAR
4	E	702	PXD	OAU-CAN-CBC-FAE
4	E	702	PXD	OAU-CAN-CBC-FAF
4	E	702	PXD	CAW-CBA-SBF-NAR
4	E	702	PXD	CAY-CBA-SBF-NAR
4	D	702	PXD	OAU-CAN-CBC-FAE

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Mol	Chain	Res	Type	Atoms
4	D	702	PXD	OAU-CAN-CBC-FAF
4	D	702	PXD	CAW-CBA-SBF-NAR
4	D	702	PXD	CAY-CBA-SBF-NAR
7	A	705	AUJ	CAN-OAS-PBE-OAG
7	A	705	AUJ	PBE-OAT-PBD-OAI
7	A	705	AUJ	SAU-CBA-CBC-CAC
7	A	705	AUJ	CAC-CBC-OBC1-OC11
8	B	704	TP9	C4-C5-C6-C7
8	B	704	TP9	C7-O7-PA-O2A
8	B	704	TP9	PA-O3A-PB-O2B
8	E	704	TP9	C4-C5-C6-C7
8	E	704	TP9	PA-O3A-PB-O1B
8	D	704	TP9	C4-C5-C6-C7
8	D	704	TP9	C7-O7-PA-O1A
8	D	704	TP9	PA-O3A-PB-O1B
5	A	703	FAD	O4'-C4'-C5'-O5'
4	A	702	PXD	CAW-CBA-SBF-OAD
4	B	702	PXD	CAW-CBA-SBF-OAD
4	B	702	PXD	CAY-CBA-SBF-OAD
5	A	703	FAD	C3'-C4'-C5'-O5'
5	B	703	FAD	C3'-C4'-C5'-O5'
5	E	703	FAD	C3'-C4'-C5'-O5'
4	B	702	PXD	CBA-CAW-OAU-CAN
4	D	702	PXD	CBA-CAW-OAU-CAN
8	B	704	TP9	CM4-C4-N3-C7'
8	D	704	TP9	CM4-C4-N3-C7'
4	A	702	PXD	CAY-CBA-SBF-OAD
8	B	704	TP9	C5-C4-N3-C7'
8	E	704	TP9	C5-C4-N3-C7'
8	D	704	TP9	C5-C4-N3-C7'
5	E	703	FAD	O4'-C4'-C5'-O5'
4	D	702	PXD	CAW-CBA-SBF-OAD
4	B	702	PXD	OAU-CAN-CBC-FAF
5	E	703	FAD	P-O3P-PA-O5B
5	D	703	FAD	P-O3P-PA-O5B
5	A	703	FAD	C2B-C1B-N9A-C8A
5	B	703	FAD	C2B-C1B-N9A-C8A
5	D	703	FAD	C2B-C1B-N9A-C8A
4	D	702	PXD	CAK-CAW-OAU-CAN
4	B	702	PXD	CAK-CAW-OAU-CAN
4	D	702	PXD	CAY-CBA-SBF-OAD
8	E	704	TP9	C7-O7-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	A	702	PXD	CBA-CAW-OAU-CAN
4	E	702	PXD	CBA-CAW-OAU-CAN
8	E	704	TP9	CM4-C4-N3-C7'
5	B	703	FAD	C2'-C3'-C4'-O4'
4	E	702	PXD	CAK-CAW-OAU-CAN
7	A	705	AUJ	PBE-OAT-PBD-OAF
4	A	702	PXD	CAK-CAW-OAU-CAN
5	E	703	FAD	C2B-C1B-N9A-C8A
4	E	702	PXD	CAV-NAR-SBF-OAD
4	E	702	PXD	CAW-CBA-SBF-OAD
5	B	703	FAD	O4B-C1B-N9A-C8A
5	D	703	FAD	PA-O3P-P-O2P
8	D	704	TP9	C5'-C7'-N3-C4
4	D	702	PXD	CBA-CAY-CBE-FAI
8	B	704	TP9	PA-O3A-PB-O3B
5	A	703	FAD	O4B-C4B-C5B-O5B
5	A	703	FAD	O4B-C1B-N9A-C8A
5	D	703	FAD	O4B-C1B-N9A-C8A
4	D	702	PXD	CBA-CAY-CBE-FAG
5	E	703	FAD	PA-O3P-P-O2P

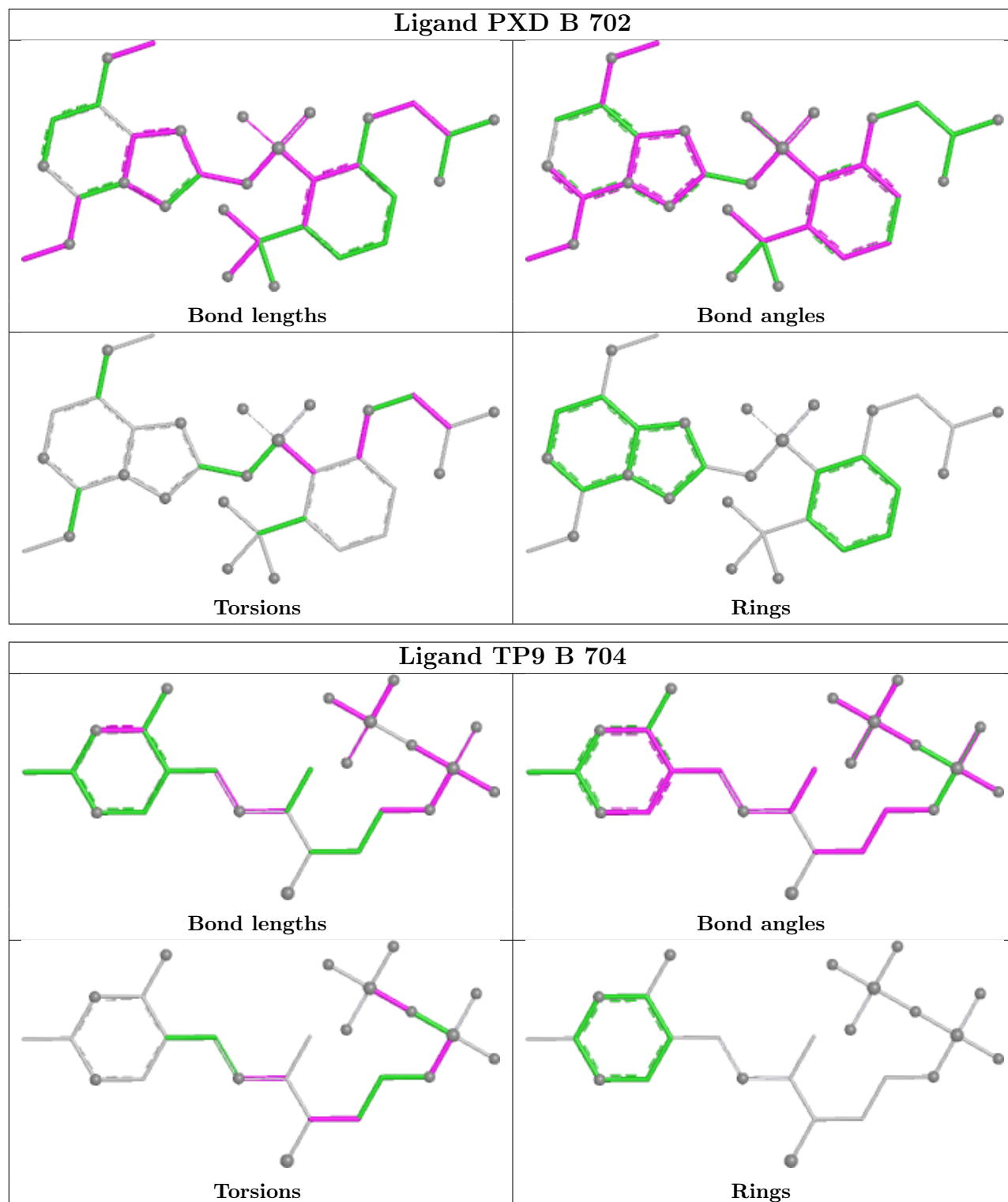
There are no ring outliers.

11 monomers are involved in 20 short contacts:

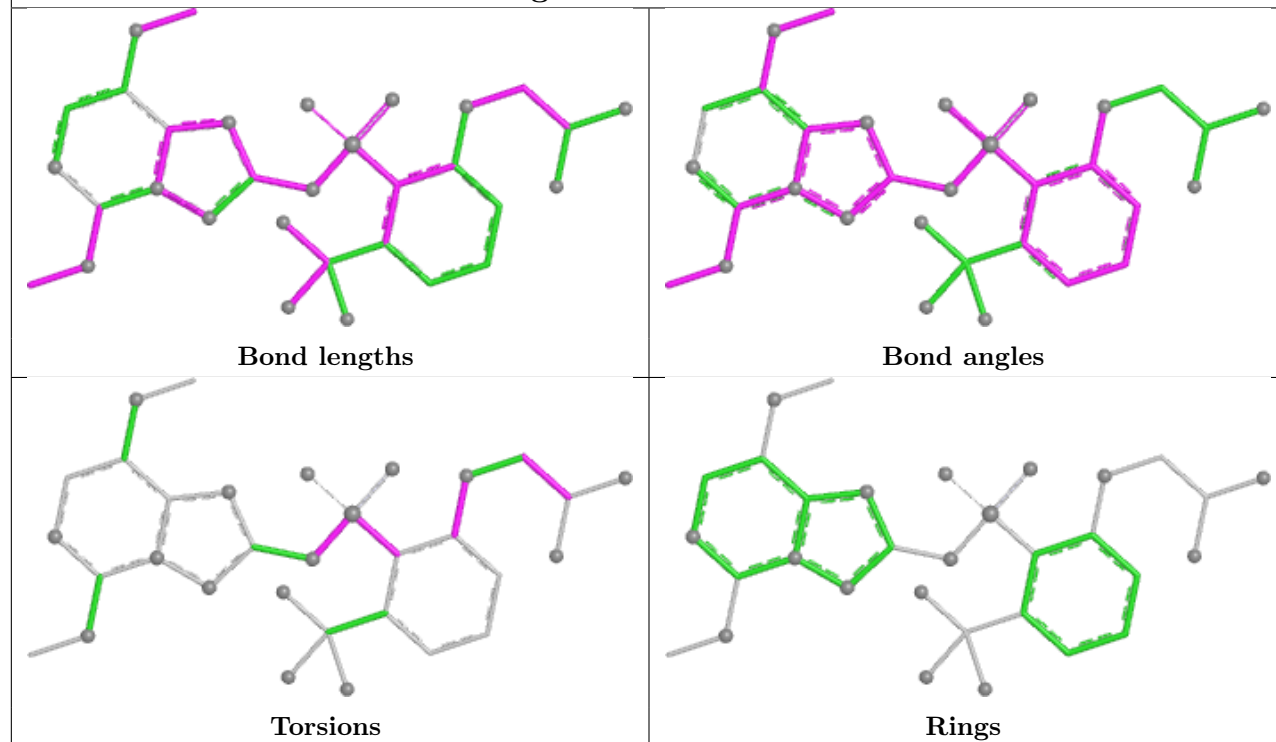
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	702	PXD	1	0
6	A	704	F50	5	0
8	B	704	TP9	3	0
5	D	703	FAD	1	0
5	A	703	FAD	1	0
6	B	705	F50	4	0
5	E	703	FAD	2	0
6	E	705	F50	5	0
8	D	704	TP9	3	0
7	A	705	AUJ	1	0
8	E	704	TP9	3	0

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.

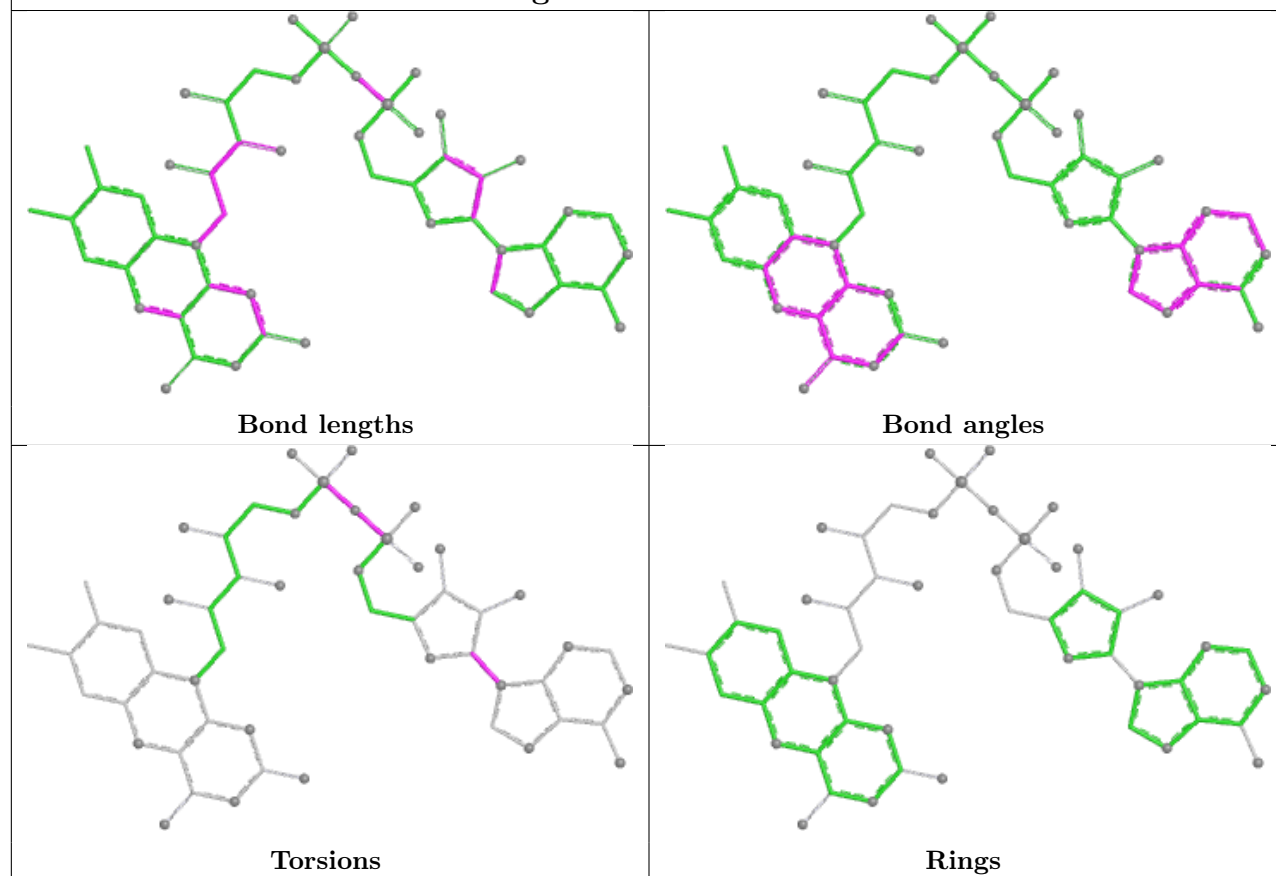
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



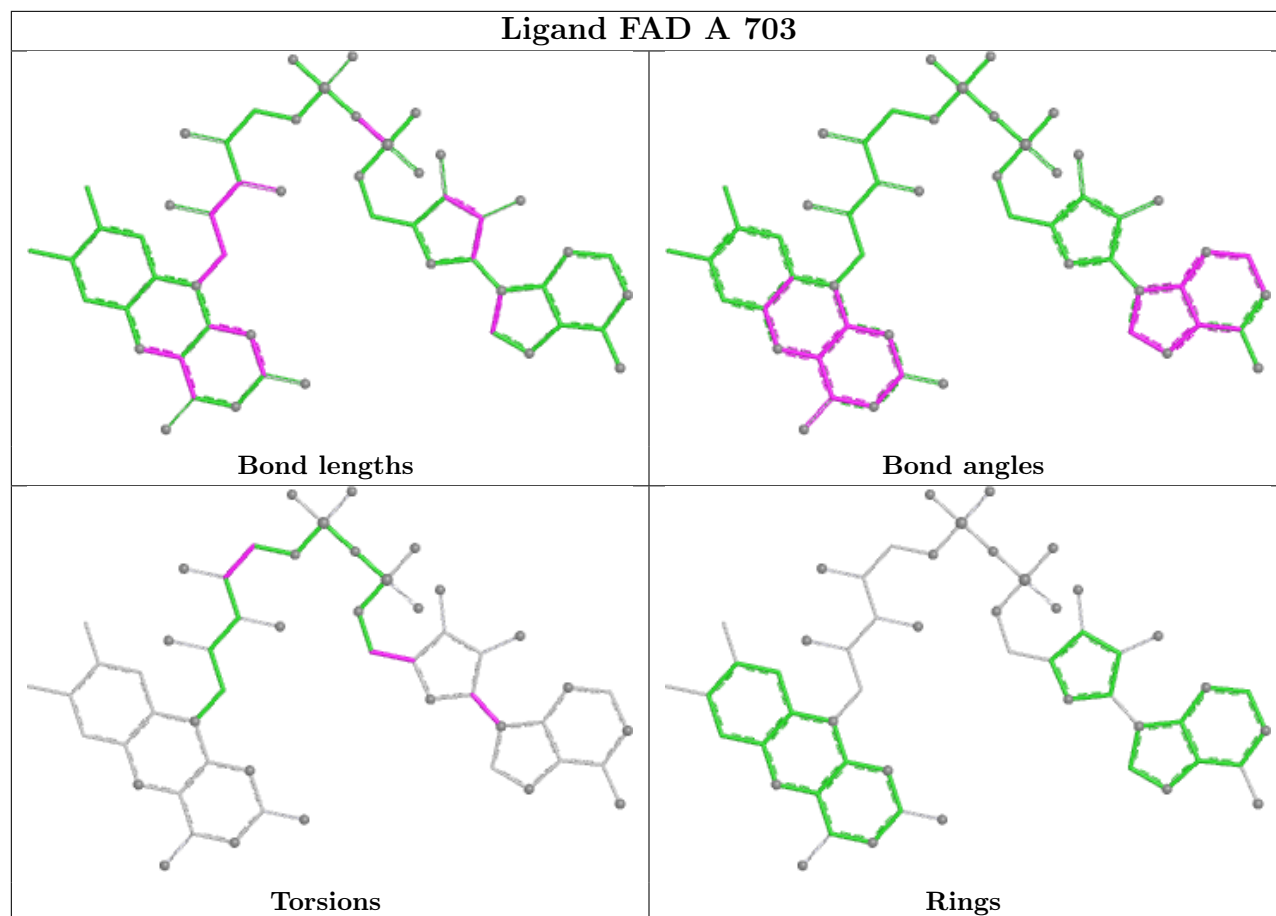
Ligand PXD E 702



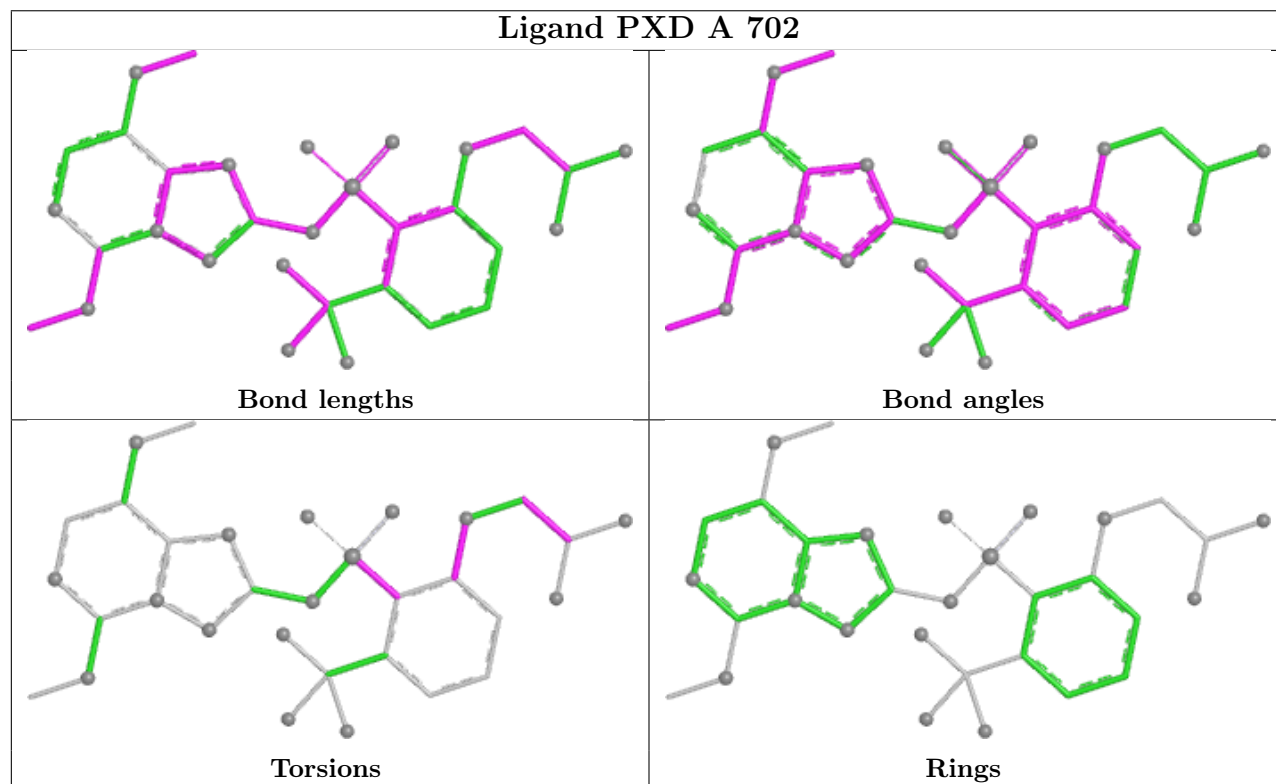
Ligand FAD D 703



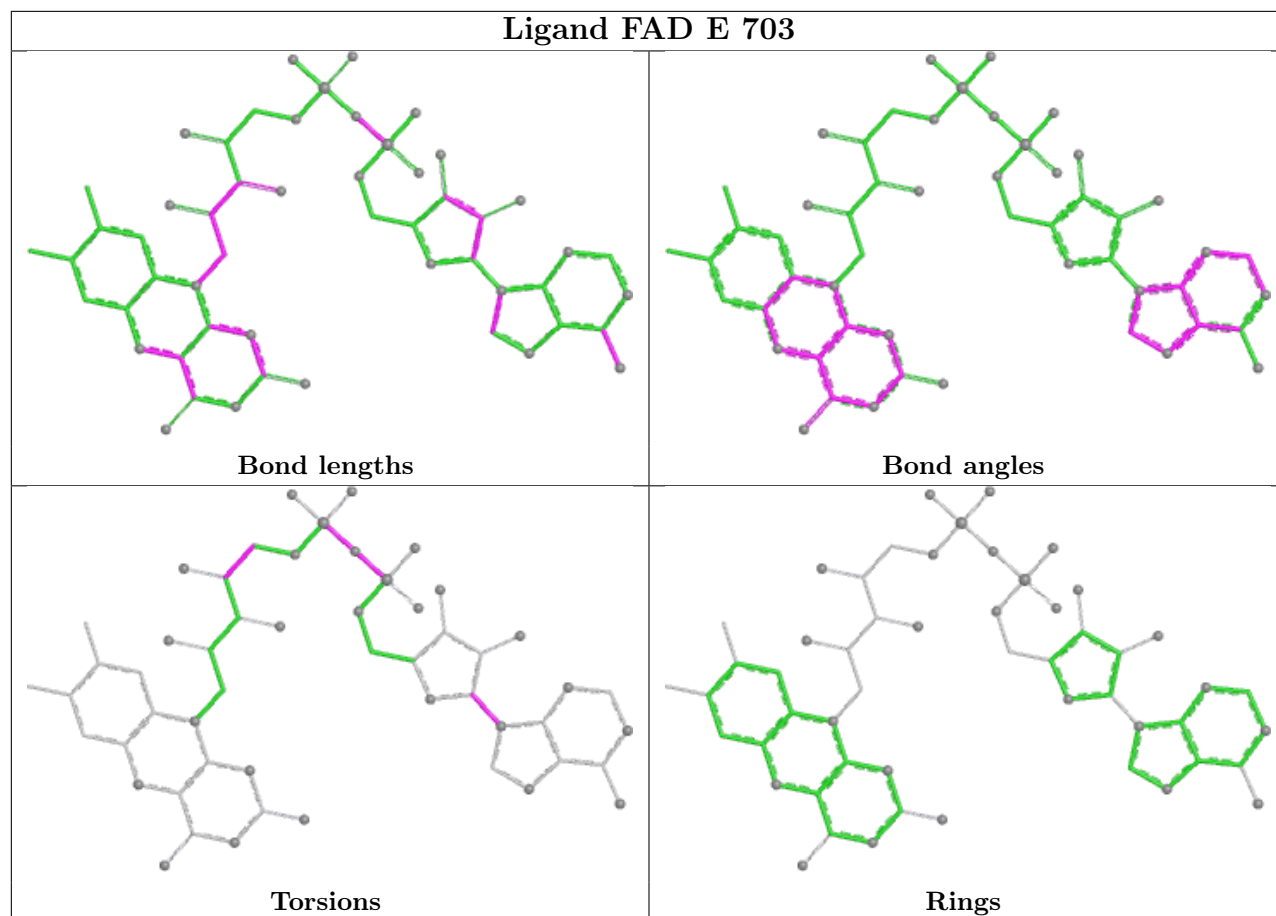
Ligand FAD A 703



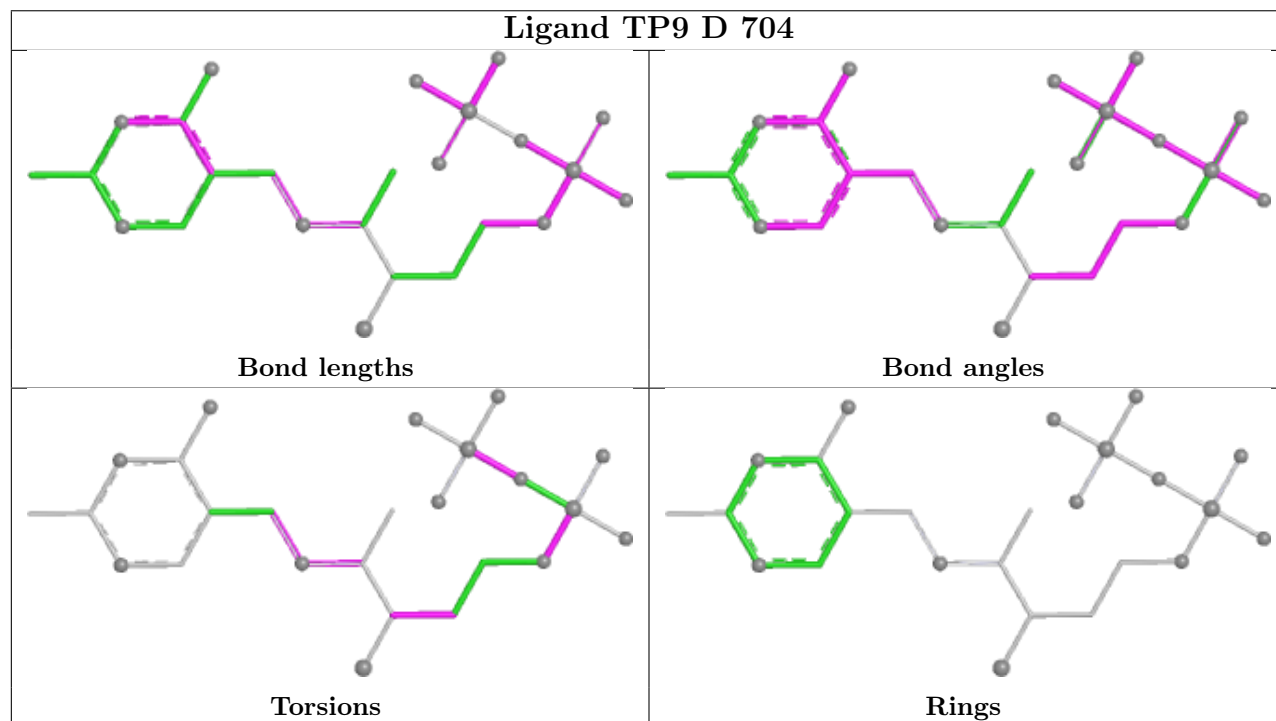
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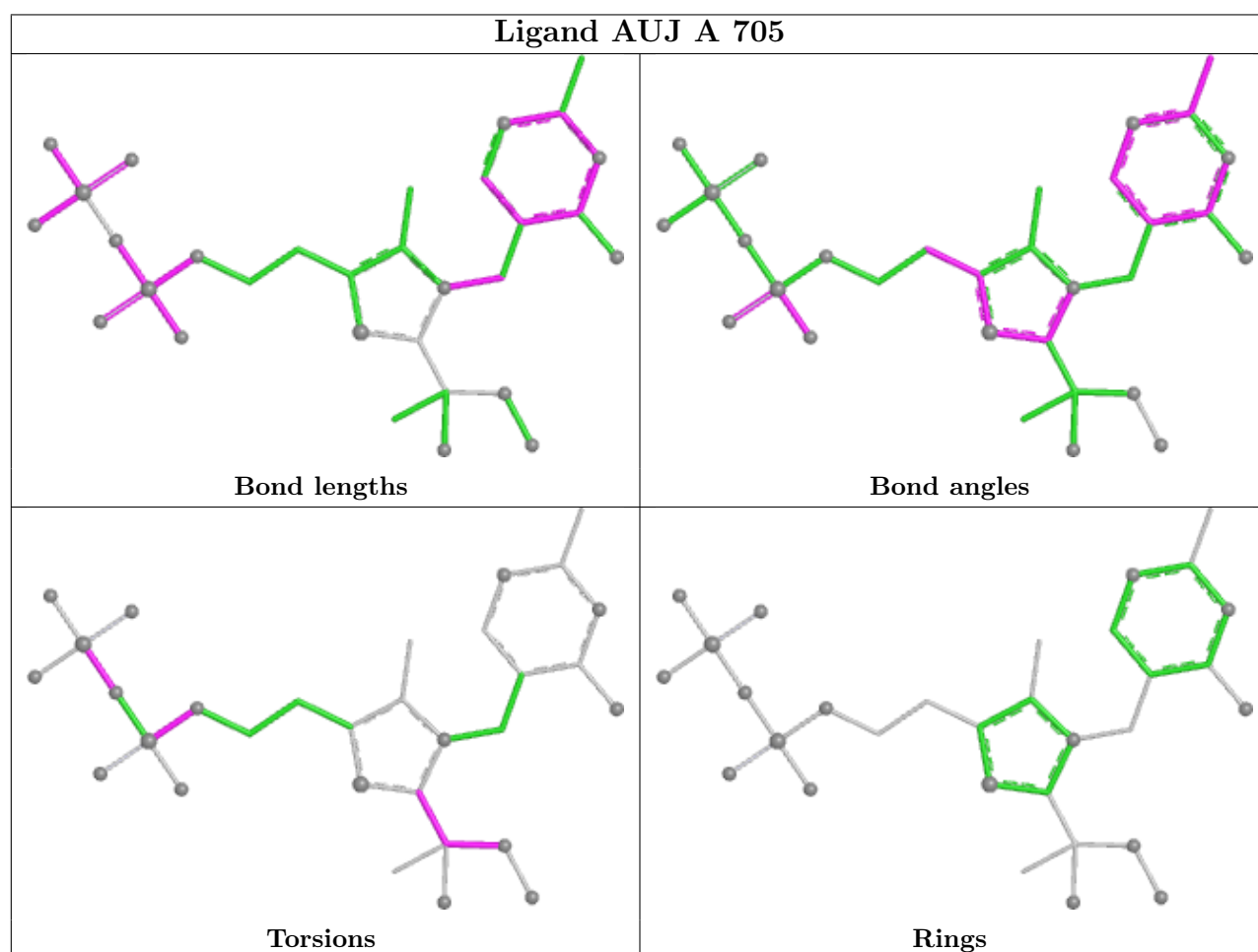
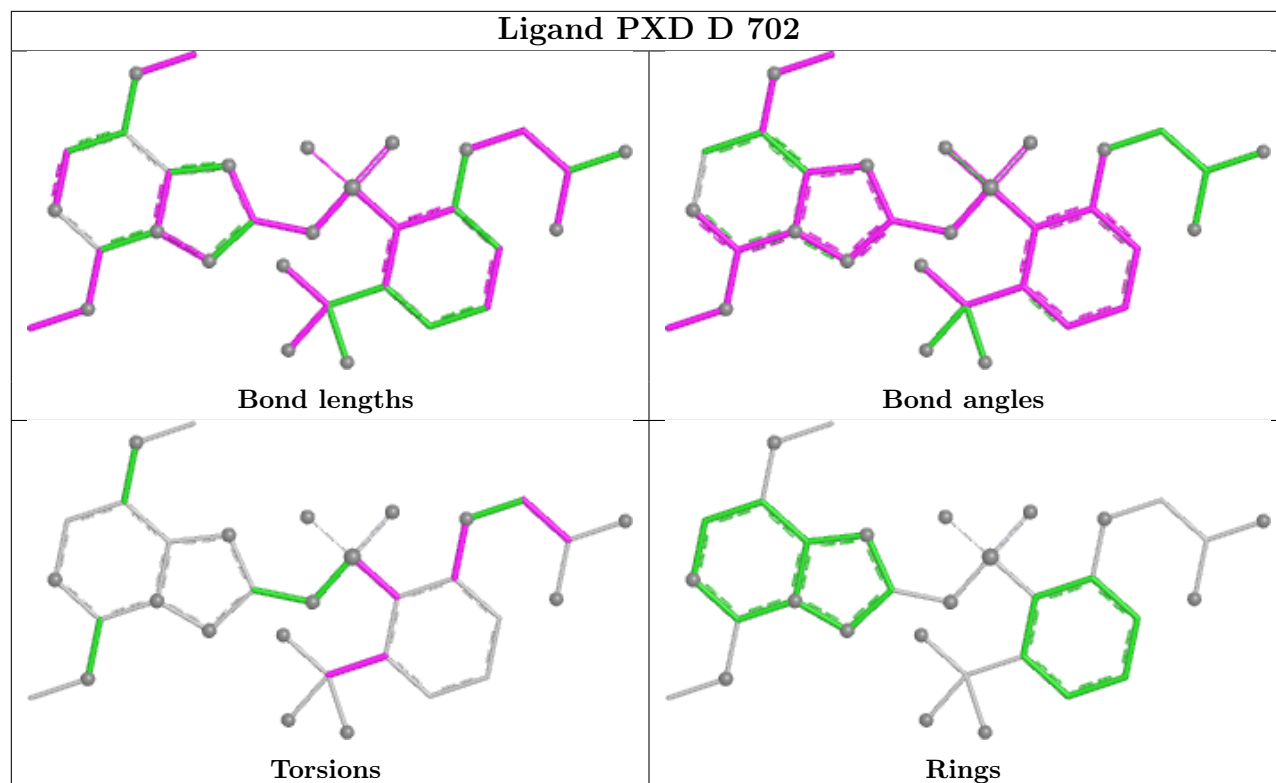


Ligand FAD E 703

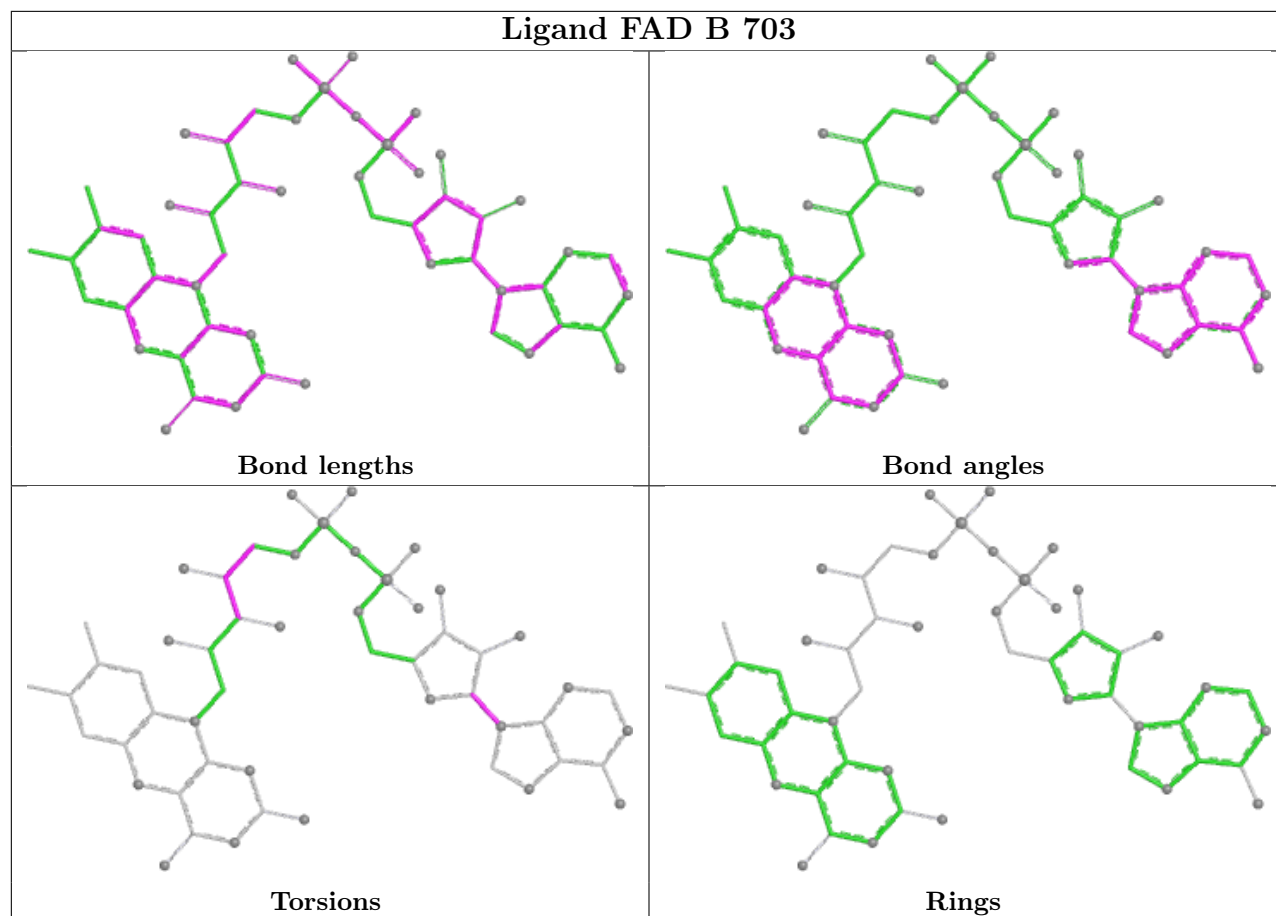


Ligand TP9 D 704

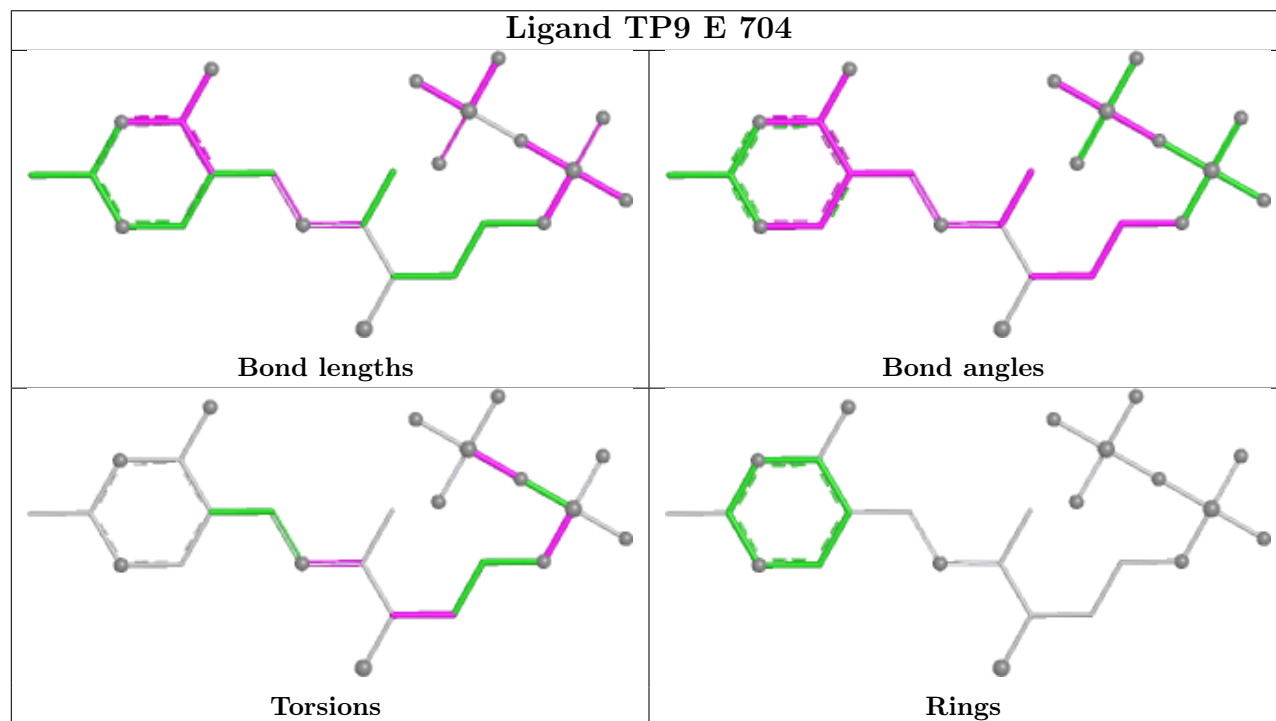




Ligand FAD B 703



Ligand TP9 E 704



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	591/677 (87%)	-0.39	11 (1%) 66 71	19, 34, 59, 97	3 (0%)
1	B	598/677 (88%)	-0.59	8 (1%) 75 79	16, 28, 47, 97	4 (0%)
1	E	592/677 (87%)	-0.01	20 (3%) 48 54	23, 44, 83, 128	2 (0%)
2	D	595/677 (87%)	-0.65	5 (0%) 82 85	16, 26, 47, 77	1 (0%)
All	All	2376/2708 (87%)	-0.41	44 (1%) 66 71	16, 32, 66, 128	10 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	7.6
1	A	280	ALA	6.9
1	B	277	THR	5.4
1	E	284	PHE	4.8
1	E	282	ASP	4.5
1	E	269	PRO	4.4
2	D	278	SER	4.4
1	E	84	ASP	4.2
1	E	268	LEU	4.1
1	B	268	LEU	4.0
2	D	268	LEU	4.0
1	E	442	LYS	3.9
1	E	266	THR	3.9
1	E	265	LYS	3.7
1	E	283	GLU	3.4
2	D	265	LYS	3.4
1	A	284	PHE	3.2
1	A	267	THR	3.2
1	E	439	PHE	3.2
1	E	263	PRO	3.2
1	E	264	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	269	PRO	3.0
1	E	456	LYS	2.8
1	E	295	LEU	2.8
1	E	453	LYS	2.8
1	A	265	LYS	2.8
1	A	85	MET	2.7
1	A	266	THR	2.7
1	E	300	LYS	2.7
2	D	269	PRO	2.7
1	E	417	VAL	2.6
1	E	393	ARG	2.6
1	B	393	ARG	2.5
1	A	264	THR	2.5
1	A	636	LYS	2.4
1	B	278	SER	2.3
1	A	624	GLU	2.3
1	A	263	PRO	2.2
2	D	84	ASP	2.1
1	E	267	THR	2.1
1	E	443	GLU	2.1
1	B	265	LYS	2.0
1	A	281	GLN	2.0
1	B	418	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	SME	D	502	9/10	0.98	0.08	22,23,38,63	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

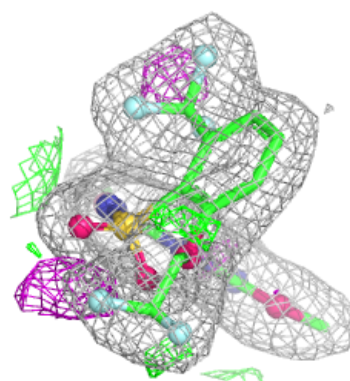
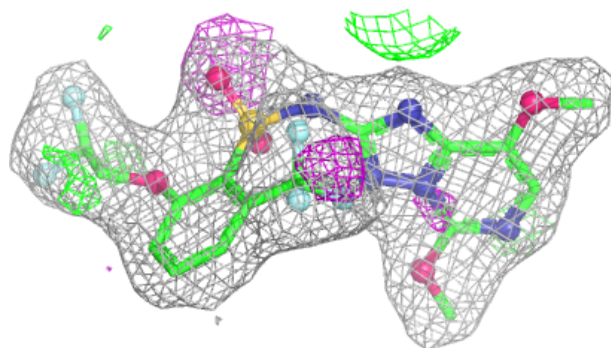
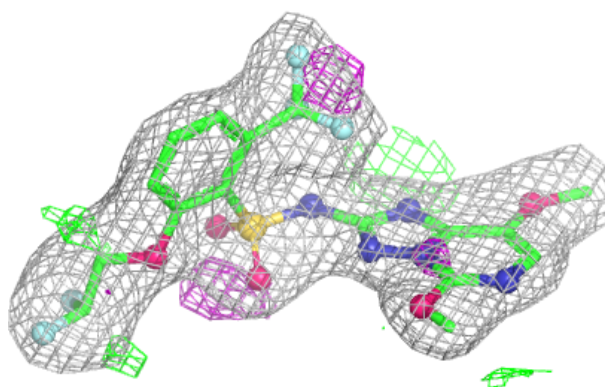
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	F50	B	705	5/5	0.87	0.19	27,30,35,35	5
6	F50	A	704	5/5	0.91	0.19	22,39,43,43	5
6	F50	E	705	5/5	0.94	0.15	38,39,42,43	5
4	PXD	E	702	32/32	0.96	0.08	33,38,60,66	0
4	PXD	A	702	32/32	0.97	0.07	23,30,52,58	0
8	TP9	E	704	25/25	0.97	0.06	22,26,34,40	0
5	FAD	A	703	53/53	0.98	0.05	21,29,34,36	0
5	FAD	B	703	53/53	0.98	0.05	16,24,27,30	0
5	FAD	E	703	53/53	0.98	0.06	32,39,50,50	0
3	MG	B	701	1/1	0.98	0.03	23,23,23,23	0
4	PXD	B	702	32/32	0.98	0.06	21,31,48,54	0
3	MG	D	701	1/1	0.98	0.02	20,20,20,20	0
7	AUJ	A	705	31/31	0.98	0.07	15,24,37,38	3
8	TP9	B	704	25/25	0.98	0.06	17,24,29,40	0
4	PXD	D	702	32/32	0.98	0.06	15,27,45,55	0
8	TP9	D	704	25/25	0.98	0.06	14,20,26,39	0
3	MG	E	701	1/1	0.99	0.02	26,26,26,26	0
5	FAD	D	703	53/53	0.99	0.04	13,20,24,33	0
3	MG	A	701	1/1	0.99	0.02	23,23,23,23	0

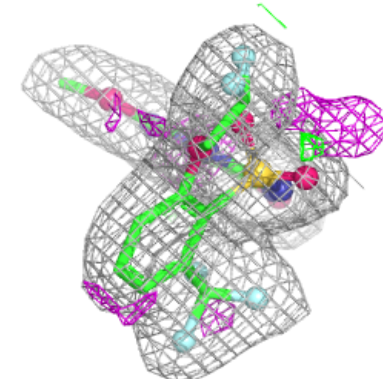
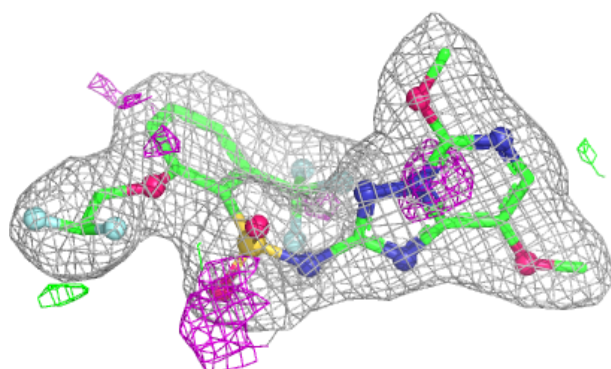
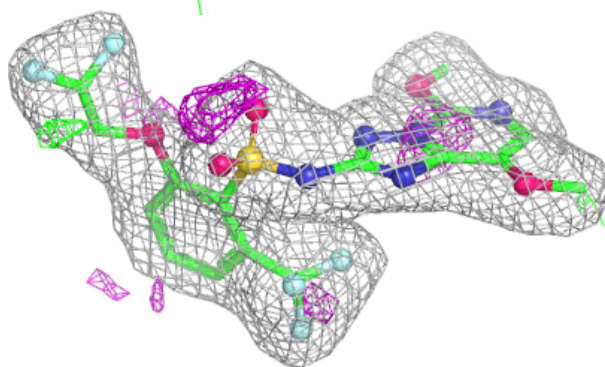
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PXD E 702:

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

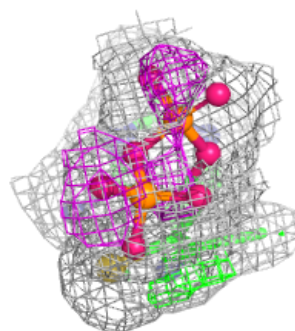
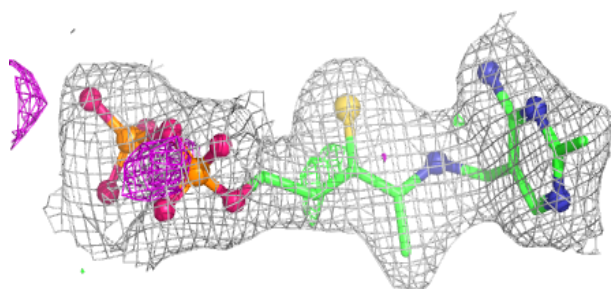
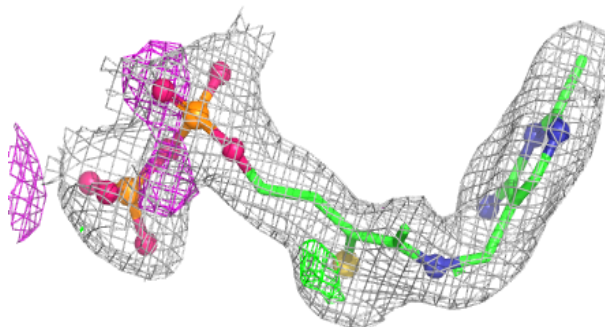
**Electron density around PXD A 702:**

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and green (positive)

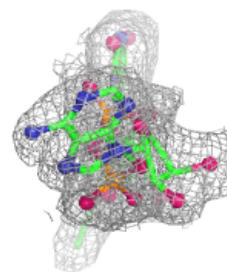
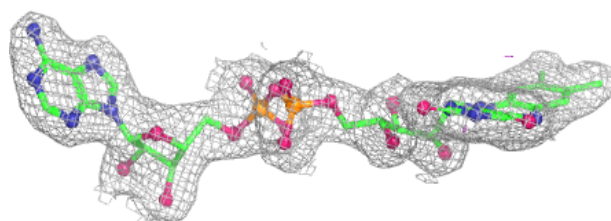
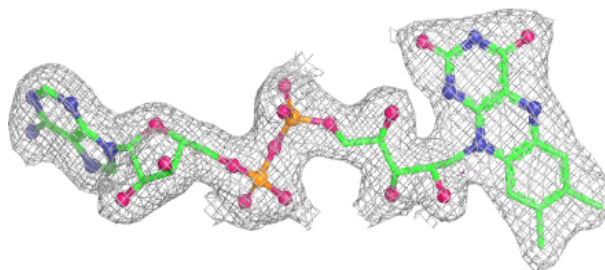


Electron density around TP9 E 704:

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and green (positive)

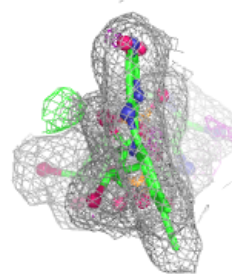
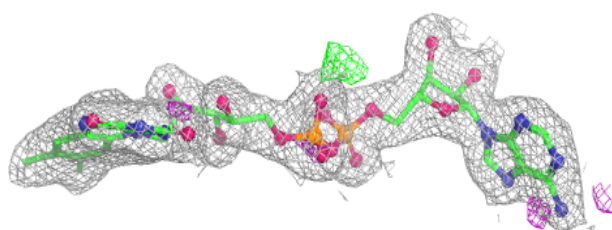
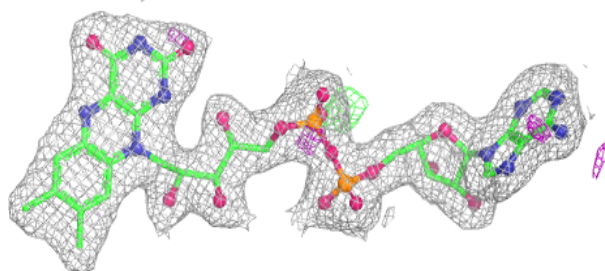
**Electron density around FAD A 703:**

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and green (positive)

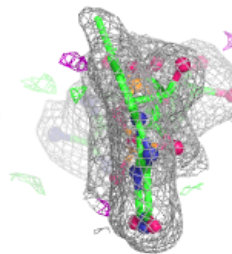
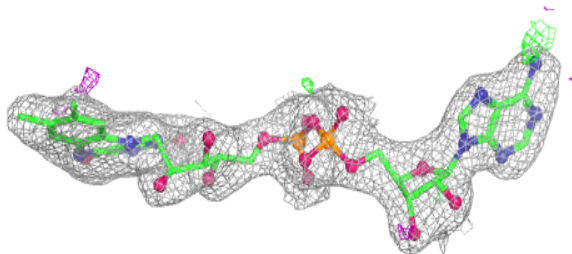
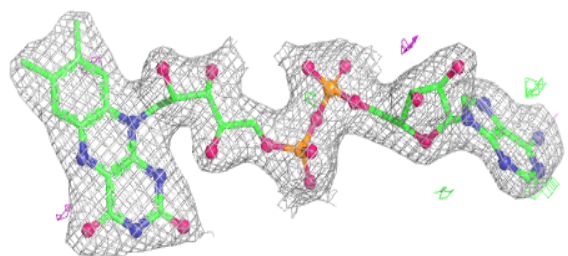


Electron density around FAD B 703:

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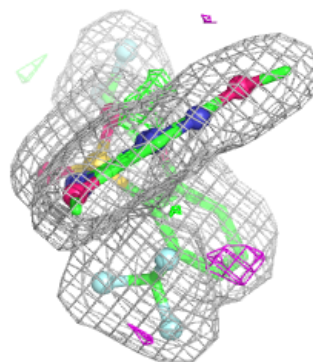
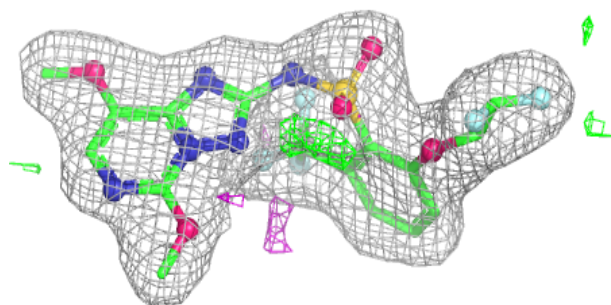
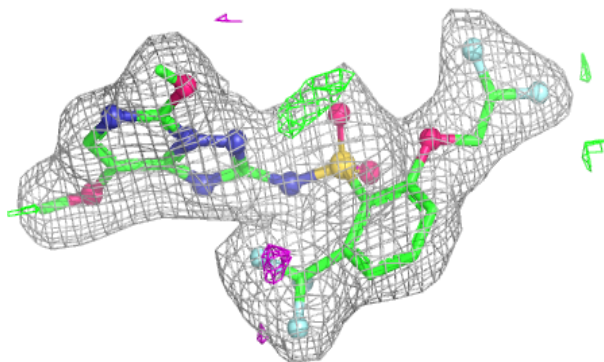
**Electron density around FAD E 703:**

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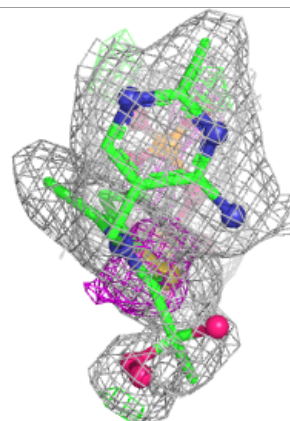
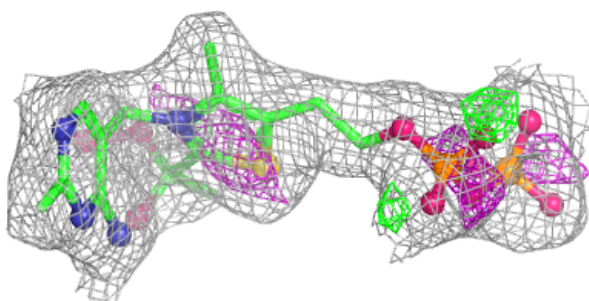
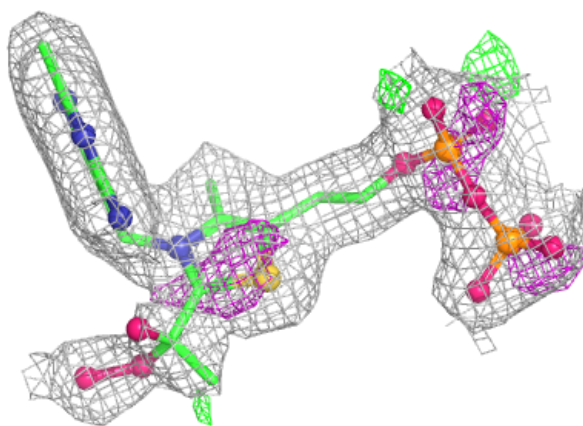


Electron density around PXD B 702:

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and green (positive)

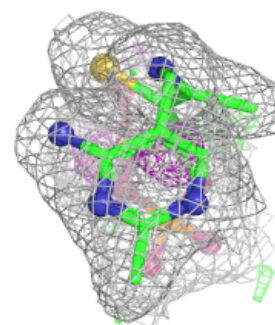
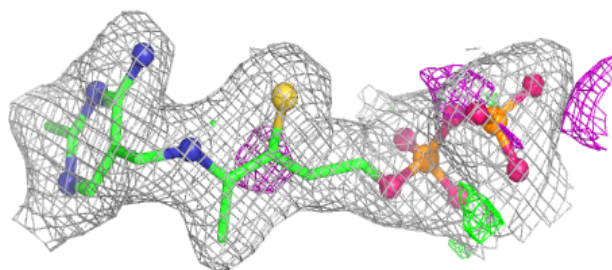
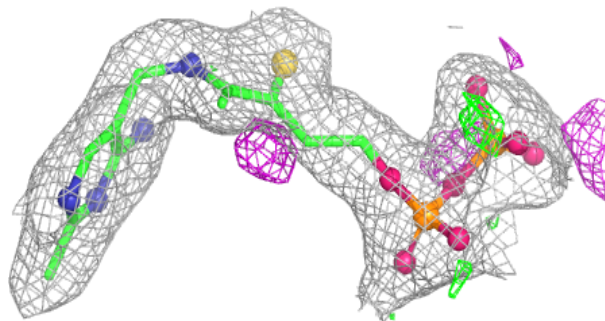
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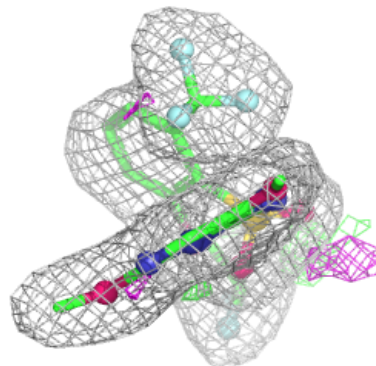
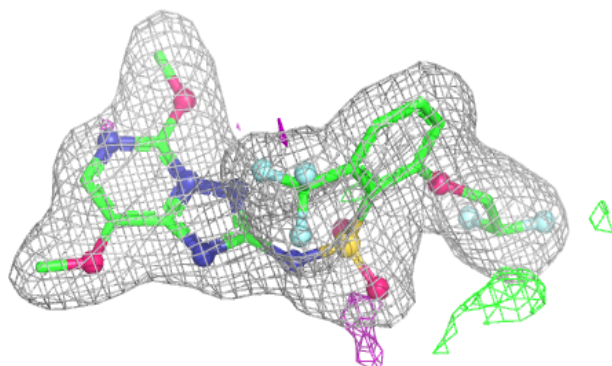
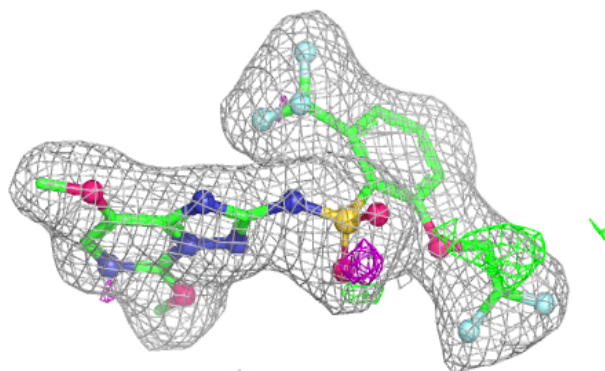


Electron density around TP9 B 704:

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and green (positive)

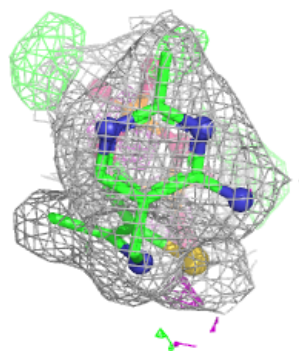
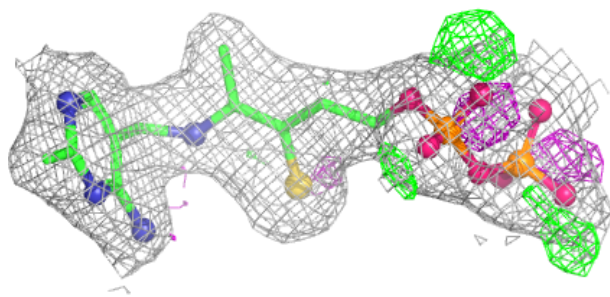
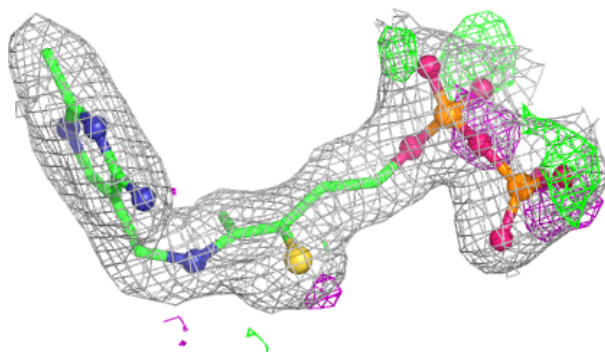
**Electron density around PXD D 702:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

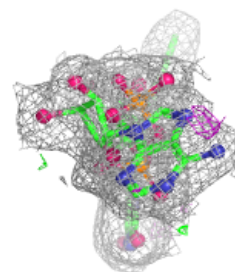
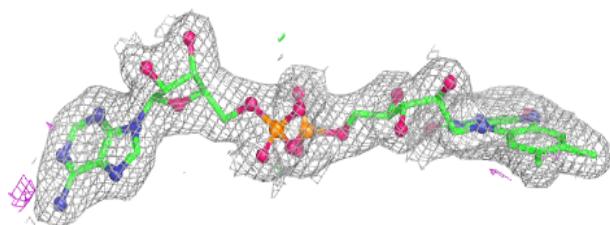
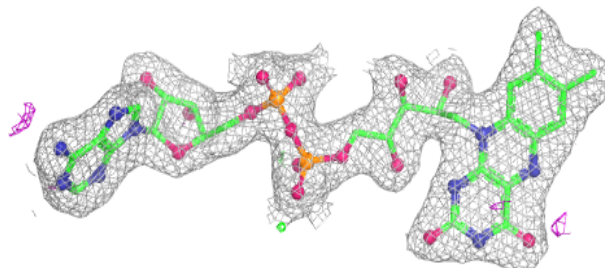


Electron density around TP9 D 704:

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

**Electron density around FAD D 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.