



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 04:40 PM UTC

PDB ID : 4FEG / pdb_00004feg
Title : High-resolution structure of pyruvate oxidase in complex with reaction intermediate 2-hydroxyethyl-thiamin diphosphate carbanion-enamine, crystal A
Authors : Meyer, D.; Neumann, P.; Koers, E.; Sjuts, H.; Luedtke, S.; Sheldrick, G.M.; Ficner, R.; Tittmann, K.
Deposited on : 2012-05-30
Resolution : 1.09 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](#) ①) 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

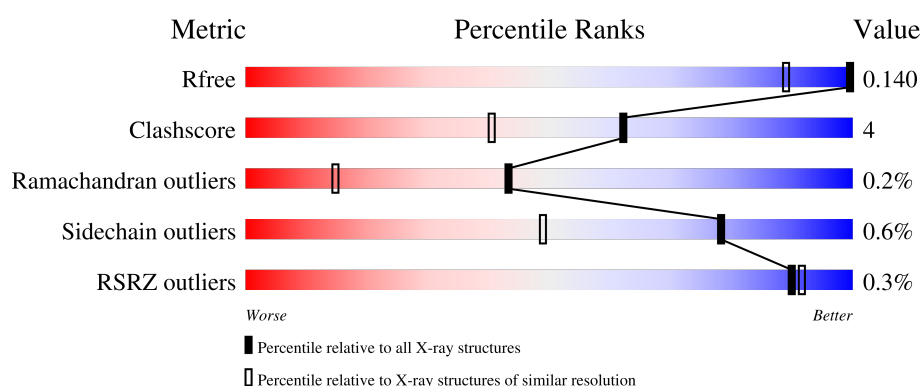
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.09 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	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	603	88% 7% . .
1	B	603	87% 9% . .

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
3	PO4	A	703	-	-	X	-
4	GOL	B	704[A]	-	X	X	-
4	GOL	B	704[B]	-	X	-	-

2 Entry composition [i](#)

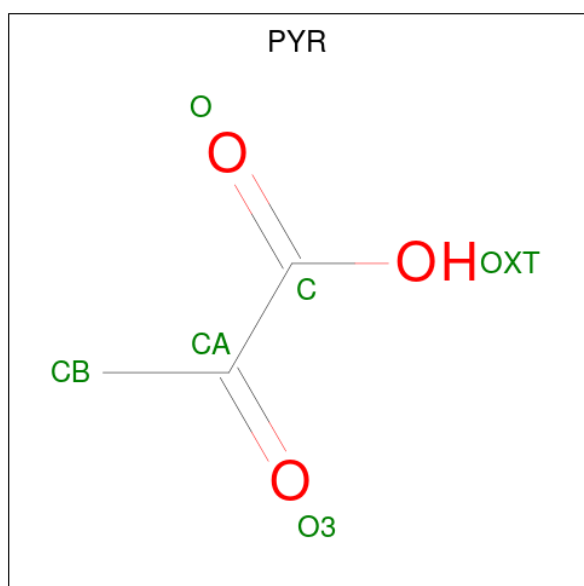
There are 8 unique types of molecules in this entry. The entry contains 12015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pyruvate oxidase.

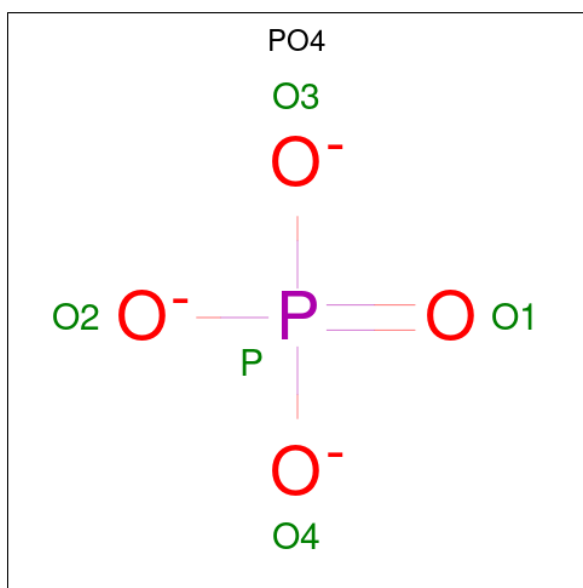
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	40	0
			4838	3067	840	913	18			
1	B	583	Total	C	N	O	S	2	48	0
			4899	3103	854	923	19			

- Molecule 2 is PYRUVIC ACID (CCD ID: PYR) (formula: C₃H₄O₃).



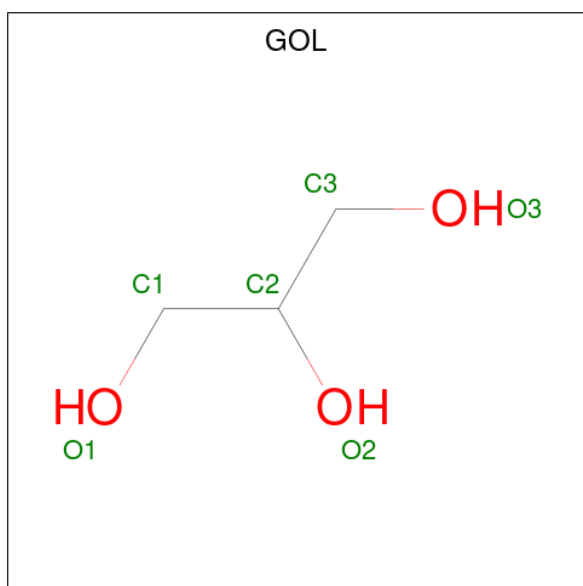
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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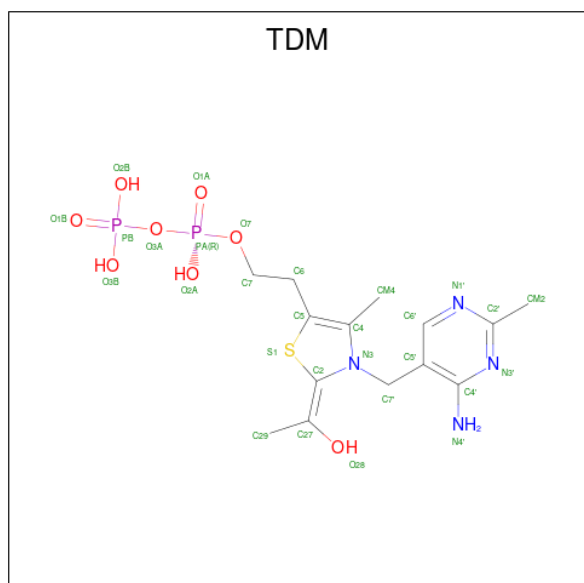
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

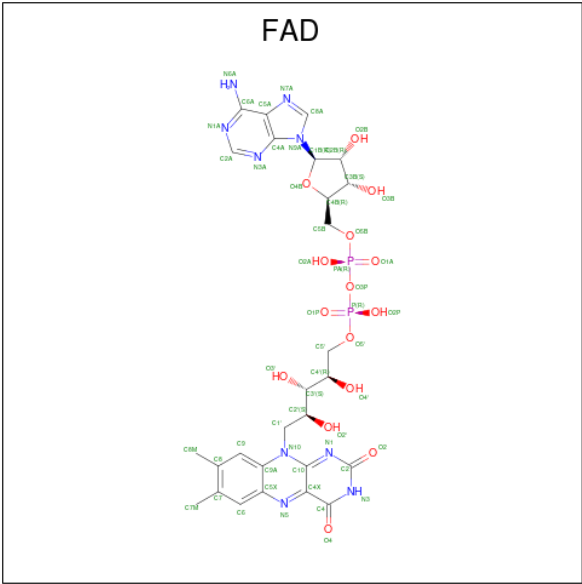
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2-[(2E)-3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-(1-HYDROXYETHYLIDENE)-4-METHYL-2,3-DIHYDRO-1,3-THIAZOL-5-YL]ETHYL TRIHYDROGEN DIPHOSPHATE (CCD ID: TDM) (formula: C₁₄H₂₂N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
6	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	974	Total	O	0	42
			1015	1015		
8	B	960	Total	O	0	48
			1009	1009		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

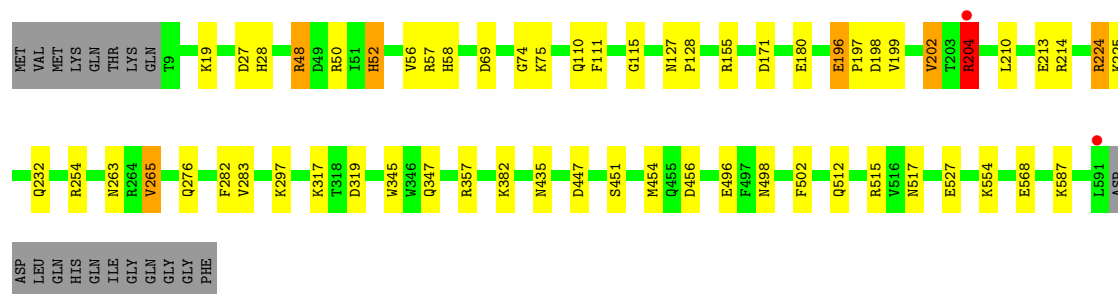
• Molecule 1: Pyruvate oxidase

Chain A: 



• Molecule 1: Pyruvate oxidase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.60Å 154.40Å 165.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.09 30.00 – 1.09	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.00-1.09) 91.8 (30.00-1.09)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.09Å)	Xtriage
Refinement program	SHELX, SHELXL-97	Depositor
R, R_{free}	0.119 , 0.142 0.122 , 0.140	Depositor DCC
R_{free} test set	30569 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	7.0	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 109.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12015	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: MG, GOL, PO4, TDM, FAD, PYR

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	0.88	3/4944 (0.1%)	1.19	31/6715 (0.5%)
1	B	0.87	2/5008 (0.0%)	1.19	38/6801 (0.6%)
All	All	0.87	5/9952 (0.1%)	1.19	69/13516 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	6
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	CD-NE	6.07	1.54	1.46
1	B	57	ARG	CD-NE	6.01	1.54	1.46
1	A	74	GLY	C-N	-5.90	1.25	1.33
1	A	283	VAL	CA-CB	5.66	1.61	1.54
1	B	58	HIS	CG-ND1	-5.07	1.32	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	357	ARG	NH1-CZ-NH2	11.63	134.41	119.30
1	B	347	GLN	OE1-CD-NE2	-9.53	113.07	122.60
1	B	155	ARG	NE-CZ-NH2	9.26	127.54	119.20
1	A	74	GLY	CA-C-N	9.07	134.47	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	GLY	C-N-CA	9.07	134.47	121.50
1	B	496	GLU	CG-CD-OE1	9.07	139.26	118.40
1	B	180	GLU	CB-CG-CD	9.05	127.99	112.60
1	A	155	ARG	NE-CZ-NH2	8.88	127.19	119.20
1	A	357	ARG	NE-CZ-NH1	-8.78	112.72	121.50
1	A	204	ARG	CD-NE-CZ	8.55	136.37	124.40
1	A	57	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	A	10	ASN	OD1-CG-ND2	-8.32	114.28	122.60
1	B	155	ARG	NE-CZ-NH1	-8.15	113.35	121.50
1	A	447	ASP	CA-CB-CG	8.14	120.74	112.60
1	B	357[A]	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	B	357[C]	ARG	NE-CZ-NH2	-7.90	112.09	119.20
1	B	155	ARG	CD-NE-CZ	7.87	135.42	124.40
1	A	155	ARG	CD-NE-CZ	7.40	134.76	124.40
1	A	155	ARG	NE-CZ-NH1	-7.35	114.15	121.50
1	B	74	GLY	CA-C-O	7.32	126.84	119.09
1	B	57	ARG	NE-CZ-NH1	7.22	128.72	121.50
1	A	357	ARG	NE-CZ-NH2	-7.07	112.84	119.20
1	B	345	TRP	CA-C-N	7.06	129.61	120.44
1	B	345	TRP	C-N-CA	7.06	129.61	120.44
1	A	232	GLN	OE1-CD-NE2	-7.05	115.55	122.60
1	B	447	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	52	HIS	CA-CB-CG	-6.88	106.92	113.80
1	B	265	VAL	N-CA-CB	6.87	122.57	111.23
1	A	196	GLU	OE1-CD-OE2	6.58	138.69	122.90
1	B	265	VAL	CB-CA-C	6.56	122.05	111.29
1	A	74	GLY	O-C-N	-6.54	114.08	122.39
1	B	357[A]	ARG	NH1-CZ-NH2	6.42	127.65	119.30
1	B	357[C]	ARG	NH1-CZ-NH2	6.42	127.65	119.30
1	A	254	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	521	GLN	OE1-CD-NE2	-6.29	116.31	122.60
1	B	496	GLU	OE1-CD-OE2	-6.29	107.81	122.90
1	B	276	GLN	OE1-CD-NE2	6.20	128.80	122.60
1	B	196	GLU	CB-CG-CD	5.95	122.72	112.60
1	A	69	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	282	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	515	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	B	204[A]	ARG	NH1-CZ-NH2	5.81	126.85	119.30
1	B	204[B]	ARG	NH1-CZ-NH2	5.81	126.85	119.30
1	A	298	ASN	CA-CB-CG	-5.69	106.91	112.60
1	A	298	ASN	CB-CG-ND2	5.62	124.83	116.40
1	A	561	MET	CA-C-O	5.61	124.97	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	GLN	OE1-CD-NE2	5.60	128.20	122.60
1	B	69	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	202[A]	VAL	CA-C-O	5.54	126.45	120.47
1	B	202[B]	VAL	CA-C-O	5.54	126.45	120.47
1	B	74	GLY	O-C-N	-5.53	115.50	122.41
1	B	52[A]	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	52[B]	HIS	CA-CB-CG	-5.50	108.30	113.80
1	B	171	ASP	CA-CB-CG	5.50	118.10	112.60
1	B	512	GLN	OE1-CD-NE2	5.48	128.08	122.60
1	A	396	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	156	ARG	NE-CZ-NH2	-5.46	114.28	119.20
1	A	57	ARG	NE-CZ-NH1	5.37	126.87	121.50
1	B	265	VAL	CG1-CB-CG2	5.37	122.61	110.80
1	A	298	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	A	283	VAL	CG1-CB-CG2	5.31	122.49	110.80
1	B	319	ASP	CA-CB-CG	-5.18	107.42	112.60
1	B	57	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	B	517	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	B	282	PHE	CA-CB-CG	5.10	118.90	113.80
1	A	196	GLU	CA-CB-CG	-5.09	103.93	114.10
1	B	180	GLU	CG-CD-OE1	5.07	130.05	118.40
1	A	346	TRP	CA-CB-CG	5.05	123.20	113.60
1	B	345	TRP	O-C-N	-5.04	116.88	122.07

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	224	ARG	Sidechain
1	A	254	ARG	Sidechain
1	A	48[A]	ARG	Sidechain
1	A	50[A]	ARG	Sidechain
1	B	204[A]	ARG	Sidechain
1	B	214[A]	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	254	ARG	Sidechain
1	B	48	ARG	Sidechain
1	B	50[A]	ARG	Sidechain

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	4838	0	4801	34	0
1	B	4899	0	4855	43	0
2	A	12	0	0	0	0
2	B	12	0	0	0	0
3	A	5	0	0	3	0
3	B	5	0	0	0	0
4	A	24	0	32	1	0
4	B	30	0	40	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	29	0	19	0	0
6	B	29	0	19	0	0
7	A	53	0	31	1	0
7	B	53	0	31	1	0
8	A	1015	0	0	21	0
8	B	1009	0	0	28	1
All	All	12015	0	9828	82	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 (82) 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)
3:A:703:PO4:O2	8:A:956[B]:HOH:O	1.71	1.08
1:B:27:ASP:H	4:B:704[A]:GOL:H11	1.22	1.05
3:A:703:PO4:P	8:A:956[B]:HOH:O	2.13	1.05
1:A:294:LYS:O	1:A:297[A]:LYS:HE3	1.72	0.89
1:B:75[B]:LYS:HB3	4:B:704[B]:GOL:H32	1.58	0.86
1:B:382[A]:LYS:HD2	8:B:7851:HOH:O	1.85	0.76
1:B:202[B]:VAL:HB	8:B:7614:HOH:O	1.86	0.75
1:B:568[B]:GLU:HG2	8:B:7816:HOH:O	1.86	0.75
1:B:232[A]:GLN:HG2	8:B:7870:HOH:O	1.87	0.73
1:A:199[B]:VAL:HG23	1:A:200[B]:GLN:OE1	1.88	0.72
3:A:703:PO4:O3	8:A:956[B]:HOH:O	2.06	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199[B]:VAL:HG22	8:A:1207:HOH:O	1.91	0.69
1:B:48:ARG:HD3	8:B:7715:HOH:O	1.94	0.68
1:B:75[B]:LYS:HG2	8:B:7802:HOH:O	1.94	0.67
1:B:27:ASP:HB3	4:B:704[A]:GOL:H12	1.76	0.66
8:A:1363:HOH:O	1:B:317:LYS:HE3	1.96	0.66
1:A:200[A]:GLN:HG3	8:A:1289:HOH:O	1.98	0.62
1:A:553:GLU:OE2	1:A:554[A]:LYS:HE2	2.02	0.59
1:B:75[B]:LYS:HD3	4:B:704[B]:GOL:O2	2.02	0.59
1:B:199[B]:VAL:HA	8:B:7614:HOH:O	2.03	0.59
1:B:27:ASP:N	4:B:704[A]:GOL:H11	2.06	0.58
1:B:225[B]:LYS:HE3	8:B:7281:HOH:O	2.05	0.57
1:A:297[A]:LYS:HE2	8:A:1589:HOH:O	2.05	0.56
1:A:498[B]:ASN:HB3	8:A:1202:HOH:O	2.06	0.56
1:A:294:LYS:CB	1:A:297[A]:LYS:HE3	2.35	0.56
1:A:297[A]:LYS:NZ	8:A:1665:HOH:O	2.27	0.56
1:B:382[A]:LYS:O	1:B:382[A]:LYS:HG3	2.04	0.56
1:A:111[A]:PHE:CE2	1:A:115:GLY:HA3	2.43	0.54
1:B:19[B]:LYS:HE3	8:B:7847:HOH:O	2.08	0.54
1:B:75[B]:LYS:HD3	8:B:7802:HOH:O	2.07	0.53
1:B:56[B]:VAL:HG13	1:B:456:ASP:OD1	2.09	0.53
1:B:111[A]:PHE:CE2	1:B:115:GLY:HA3	2.44	0.52
1:B:587:LYS:HG3	8:B:7842:HOH:O	2.09	0.52
1:B:454[B]:MET:HE3	1:B:502:PHE:CE1	2.45	0.52
1:B:198[B]:ASP:HA	8:B:7821:HOH:O	2.11	0.51
1:A:225[A]:LYS:NZ	8:A:1040:HOH:O	2.44	0.50
1:A:19[B]:LYS:HD2	8:A:1510:HOH:O	2.10	0.50
1:B:382[A]:LYS:HE3	8:B:7391:HOH:O	2.11	0.50
1:B:196:GLU:HG3	1:B:197[B]:PRO:O	2.13	0.49
1:B:225[B]:LYS:NZ	8:B:7800:HOH:O	2.45	0.49
1:A:294:LYS:HB3	1:A:297[A]:LYS:HE3	1.95	0.48
1:B:110:GLN:NE2	8:B:7157[B]:HOH:O	2.46	0.48
1:A:294:LYS:HB2	1:A:297[A]:LYS:CE	2.43	0.48
1:A:486:ASP:OD2	1:A:554[A]:LYS:HE3	2.14	0.48
1:A:580[B]:GLN:NE2	8:A:1158:HOH:O	2.45	0.48
1:B:382[C]:LYS:NZ	8:B:7684:HOH:O	2.47	0.47
1:A:111[A]:PHE:CD2	1:A:115:GLY:HA3	2.49	0.47
1:B:204[A]:ARG:NH2	8:B:7359:HOH:O	2.47	0.47
1:B:232[B]:GLN:HG3	8:B:7272:HOH:O	2.15	0.46
1:B:213[A]:GLU:HG2	8:B:7420:HOH:O	2.16	0.45
1:A:121:PHE:CE2	1:A:122[B]:GLN:HG3	2.50	0.45
1:A:307[A]:ILE:HD11	8:A:1627:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191[B]:THR:HG22	1:A:192:PRO:HD2	1.99	0.45
1:A:553:GLU:HG2	1:A:554[A]:LYS:HG3	1.99	0.45
1:B:435:ASN:OD1	4:B:704[A]:GOL:H32	2.17	0.45
1:A:192:PRO:HG3	8:A:1702:HOH:O	2.16	0.45
1:A:294:LYS:HB2	1:A:297[A]:LYS:HE2	1.99	0.44
1:B:27:ASP:HB3	4:B:704[A]:GOL:C1	2.46	0.44
1:A:311[B]:LYS:HE3	8:A:1050:HOH:O	2.16	0.44
1:A:196:GLU:HB3	8:A:1697:HOH:O	2.18	0.44
1:A:159:ALA:HA	8:A:1702:HOH:O	2.17	0.44
1:A:224:ARG:NE	8:A:1153:HOH:O	2.51	0.44
1:A:294:LYS:O	1:A:297[A]:LYS:CE	2.57	0.44
1:A:225[A]:LYS:NZ	8:A:1316:HOH:O	2.50	0.44
1:A:294:LYS:CB	1:A:297[A]:LYS:CE	2.96	0.44
1:B:28:HIS:HA	1:B:52[B]:HIS:O	2.17	0.44
1:A:307[B]:ILE:HG12	7:A:709:FAD:C4A	2.47	0.44
1:A:527[A]:GLU:HG2	8:A:1020:HOH:O	2.17	0.44
1:A:281:LEU:HG	1:A:283:VAL:CG2	2.49	0.43
1:B:498[B]:ASN:HB3	8:B:7384:HOH:O	2.18	0.43
1:B:451[B]:SER:O	1:B:454[B]:MET:HG2	2.19	0.43
1:B:224:ARG:NE	8:B:7613:HOH:O	2.51	0.42
1:B:297:LYS:NZ	8:B:7538:HOH:O	2.52	0.42
1:B:554[A]:LYS:NZ	8:B:7401:HOH:O	2.52	0.42
1:B:52[B]:HIS:HE1	8:B:7789:HOH:O	2.02	0.42
4:A:706:GOL:H12	8:A:1701:HOH:O	2.20	0.41
7:B:710:FAD:H8A	8:B:7744[A]:HOH:O	2.19	0.41
1:A:424[B]:VAL:C	1:A:427[B]:PRO:HD2	2.46	0.41
1:B:527[A]:GLU:HG2	8:B:7220:HOH:O	2.20	0.40
1:B:498[A]:ASN:HB2	8:B:7384:HOH:O	2.20	0.40
1:B:213[A]:GLU:HG2	8:B:7683:HOH:O	2.21	0.40
1:B:127:ASN:N	1:B:128[B]:PRO:HD2	2.36	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)
8:B:7280:HOH:O	8:B:7280:HOH:O[4_565]	2.16	0.04

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	620/603 (103%)	602 (97%)	17 (3%)	1 (0%)	43	15
1	B	629/603 (104%)	615 (98%)	13 (2%)	1 (0%)	43	15
All	All	1249/1206 (104%)	1217 (97%)	30 (2%)	2 (0%)	43	15

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	B	263	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	508/485 (105%)	502 (99%)	6 (1%)	63	26
1	B	515/485 (106%)	511 (99%)	4 (1%)	73	40
All	All	1023/970 (106%)	1013 (99%)	10 (1%)	78	33

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187[A]	ASN
1	A	187[B]	ASN
1	A	199[A]	VAL
1	A	199[B]	VAL

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Mol	Chain	Res	Type
1	A	225[A]	LYS
1	A	225[B]	LYS
1	B	210	LEU
1	B	265	VAL
1	B	283[A]	VAL
1	B	283[B]	VAL

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	127	ASN
1	A	167	GLN
1	A	175	GLN
1	A	190	GLN
1	A	276	GLN
1	A	347	GLN
1	A	417	ASN
1	A	489	GLN
1	A	572	GLN
1	B	127	ASN
1	B	167	GLN
1	B	276	GLN
1	B	347	GLN
1	B	417	ASN
1	B	490	ASN
1	B	572	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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$
6	TDM	A	708	5	28,30,30	1.62	8 (28%)	37,45,45	2.80	9 (24%)
4	GOL	A	704	-	5,5,5	0.62	0	5,5,5	1.25	0
2	PYR	B	701	-	5,5,5	2.17	2 (40%)	3,6,6	1.49	1 (33%)
2	PYR	A	701	-	5,5,5	4.45	3 (60%)	3,6,6	1.38	1 (33%)
4	GOL	A	710	-	5,5,5	0.44	0	5,5,5	1.05	0
4	GOL	B	706	-	5,5,5	0.76	0	5,5,5	0.97	0
2	PYR	B	702	-	5,5,5	2.83	2 (40%)	3,6,6	1.13	0
4	GOL	B	707	-	5,5,5	0.66	0	5,5,5	1.92	3 (60%)
4	GOL	B	705	-	5,5,5	1.35	1 (20%)	5,5,5	1.49	1 (20%)
2	PYR	A	702	-	5,5,5	2.81	2 (40%)	3,6,6	1.49	0
3	PO4	A	703	-	4,4,4	1.47	1 (25%)	6,6,6	0.93	0
4	GOL	B	704[B]	-	5,5,5	1.25	1 (20%)	5,5,5	2.95	3 (60%)
7	FAD	B	710	-	58,58,58	1.20	5 (8%)	85,89,89	1.13	6 (7%)
4	GOL	A	706	-	5,5,5	0.66	0	5,5,5	1.11	0
4	GOL	A	705	-	5,5,5	1.12	0	5,5,5	1.13	0
6	TDM	B	709	5	28,30,30	1.72	6 (21%)	37,45,45	3.31	11 (29%)
4	GOL	B	704[A]	-	5,5,5	0.85	0	5,5,5	2.06	2 (40%)
3	PO4	B	703	-	4,4,4	1.46	1 (25%)	6,6,6	0.77	0
7	FAD	A	709	-	58,58,58	1.14	4 (6%)	85,89,89	1.18	9 (10%)

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	PYR	A	701	-	-	0/4/4/4	-
7	FAD	B	710	-	-	4/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	706	-	-	0/4/4/4	-
4	GOL	A	705	-	-	0/4/4/4	-
4	GOL	B	707	-	-	0/4/4/4	-
4	GOL	B	705	-	-	0/4/4/4	-
4	GOL	A	710	-	-	2/4/4/4	-
2	PYR	B	702	-	-	3/4/4/4	-
6	TDM	A	708	5	-	2/17/21/21	0/2/2/2
6	TDM	B	709	5	-	2/17/21/21	0/2/2/2
4	GOL	B	704[A]	-	-	4/4/4/4	-
4	GOL	A	704	-	-	0/4/4/4	-
4	GOL	B	706	-	-	0/4/4/4	-
2	PYR	A	702	-	-	2/4/4/4	-
7	FAD	A	709	-	-	5/34/50/50	0/6/6/6
2	PYR	B	701	-	-	0/4/4/4	-
4	GOL	B	704[B]	-	-	2/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PYR	CB-CA	-8.94	1.32	1.50
2	B	702	PYR	CB-CA	-5.60	1.39	1.50
7	B	710	FAD	C4X-N5	4.86	1.41	1.30
2	A	702	PYR	CB-CA	-4.73	1.41	1.50
6	B	709	TDM	C7'-C5'	4.06	1.58	1.51
7	A	709	FAD	C4X-N5	3.92	1.39	1.30
2	B	701	PYR	CB-CA	-3.86	1.42	1.50
2	A	701	PYR	O-C	3.67	1.31	1.22
6	B	709	TDM	O28-C27	3.43	1.40	1.31
6	B	709	TDM	C2-N3	3.30	1.45	1.39
2	A	702	PYR	O-C	3.29	1.30	1.22
6	A	708	TDM	O28-C27	3.02	1.39	1.31
6	A	708	TDM	C6'-N1'	2.93	1.40	1.34
6	A	708	TDM	C6'-C5'	-2.88	1.32	1.37
6	A	708	TDM	C4'-N3'	2.87	1.38	1.35
6	B	709	TDM	C4'-N3'	2.86	1.38	1.35
7	A	709	FAD	C8A-N7A	2.77	1.37	1.31
7	B	710	FAD	O4-C4	2.74	1.28	1.23
6	A	708	TDM	C2-N3	2.67	1.44	1.39
2	B	702	PYR	O-C	2.60	1.29	1.22
7	B	710	FAD	C1'-C2'	2.52	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	PYR	OXT-C	-2.35	1.24	1.30
3	B	703	PO4	P-O1	-2.35	1.45	1.50
6	B	709	TDM	C4-N3	2.31	1.42	1.39
7	A	709	FAD	C3B-C4B	2.27	1.58	1.53
2	B	701	PYR	OXT-C	-2.20	1.24	1.30
7	B	710	FAD	P-O3P	2.20	1.61	1.59
4	B	704[B]	GOL	C3-C2	2.19	1.60	1.51
3	A	703	PO4	P-O4	-2.19	1.48	1.54
4	B	705	GOL	O3-C3	2.18	1.51	1.42
6	B	709	TDM	O7-C7	2.17	1.53	1.44
6	A	708	TDM	C7'-N3	2.14	1.51	1.47
7	A	709	FAD	O4-C4	2.14	1.27	1.23
6	A	708	TDM	C29-C27	2.09	1.53	1.48
7	B	710	FAD	C8A-N7A	2.02	1.35	1.31
6	A	708	TDM	C5'-C4'	2.01	1.46	1.42

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	709	TDM	O28-C27-C2	-14.05	107.51	120.15
6	A	708	TDM	O28-C27-C2	-11.10	110.16	120.15
6	B	709	TDM	C29-C27-C2	-10.48	110.19	124.73
6	A	708	TDM	C29-C27-C2	-10.17	110.62	124.73
4	B	704[B]	GOL	O3-C3-C2	-4.18	91.54	110.38
4	B	704[B]	GOL	O1-C1-C2	3.90	127.94	110.38
6	B	709	TDM	C4-C5-S1	3.54	113.86	110.63
4	B	704[A]	GOL	O2-C2-C1	-3.39	95.13	109.18
7	B	710	FAD	C9A-C5X-N5	-3.29	118.96	122.45
7	A	709	FAD	C9A-C5X-N5	-3.09	119.18	122.45
4	B	704[B]	GOL	C3-C2-C1	-3.07	100.53	111.80
6	B	709	TDM	C5-S1-C2	3.05	92.56	90.80
6	B	709	TDM	O28-C27-C29	-2.96	108.73	114.60
6	A	708	TDM	C7'-N3-C2	-2.86	122.60	126.13
7	A	709	FAD	N3A-C2A-N1A	-2.85	124.26	128.58
6	B	709	TDM	C6'-N1'-C2'	2.71	120.52	116.07
4	B	707	GOL	C3-C2-C1	-2.69	101.94	111.80
6	A	708	TDM	O28-C27-C29	-2.64	109.36	114.60
6	B	709	TDM	C5'-C6'-N1'	-2.60	119.60	123.83
4	B	704[A]	GOL	O2-C2-C3	2.59	119.91	109.18
6	A	708	TDM	C6'-C5'-C4'	2.58	118.72	115.55
6	B	709	TDM	C7'-N3-C2	-2.58	122.95	126.13
6	B	709	TDM	C6'-C5'-C4'	2.50	118.62	115.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	PYR	O3-CA-CB	2.49	125.35	119.77
7	B	710	FAD	C10-C4X-N5	-2.42	119.87	124.81
7	A	709	FAD	N9A-C8A-N7A	-2.41	110.51	113.94
7	B	710	FAD	C4A-N9A-C8A	2.38	108.24	105.74
6	B	709	TDM	C7'-N3-C4	-2.35	122.01	124.98
4	B	705	GOL	O2-C2-C3	-2.30	99.66	109.18
7	A	709	FAD	C5A-C4A-N9A	2.24	108.25	105.81
4	B	707	GOL	O2-C2-C1	-2.23	99.94	109.18
7	A	709	FAD	C9A-C9-C8	2.22	123.69	119.22
6	B	709	TDM	C5'-C7'-N3	-2.18	110.50	113.14
6	A	708	TDM	C5-S1-C2	2.18	92.05	90.80
6	A	708	TDM	CM4-C4-N3	-2.17	119.08	122.27
7	B	710	FAD	O3P-PA-O1A	-2.13	104.29	110.70
7	A	709	FAD	C2A-N1A-C6A	2.12	122.22	118.73
7	B	710	FAD	C5'-C4'-C3'	-2.11	108.23	112.22
6	A	708	TDM	C6'-N1'-C2'	2.09	119.50	116.07
7	A	709	FAD	C5'-C4'-C3'	-2.07	108.30	112.22
7	A	709	FAD	C5X-N5-C4X	-2.07	114.74	118.09
7	B	710	FAD	O4B-C1B-C2B	-2.06	102.21	106.62
4	B	707	GOL	O1-C1-C2	-2.04	101.20	110.38
7	A	709	FAD	C4-C4X-N5	2.03	121.01	118.21
6	A	708	TDM	C5'-C6'-N1'	-2.02	120.55	123.83
2	A	701	PYR	OXT-C-O	2.02	128.70	123.90

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	PYR	OXT-C-CA-CB
2	B	702	PYR	O-C-CA-CB
2	B	702	PYR	OXT-C-CA-CB
4	A	710	GOL	C1-C2-C3-O3
4	B	704[A]	GOL	C1-C2-C3-O3
4	B	704[B]	GOL	C1-C2-C3-O3
6	A	708	TDM	PA-O3A-PB-O2B
6	B	709	TDM	PA-O3A-PB-O2B
6	B	709	TDM	PA-O3A-PB-O3B
7	B	710	FAD	C3'-C4'-C5'-O5'
7	B	710	FAD	O4'-C4'-C5'-O5'
4	B	704[A]	GOL	O1-C1-C2-C3
4	B	704[A]	GOL	O1-C1-C2-O2
4	B	704[A]	GOL	O2-C2-C3-O3

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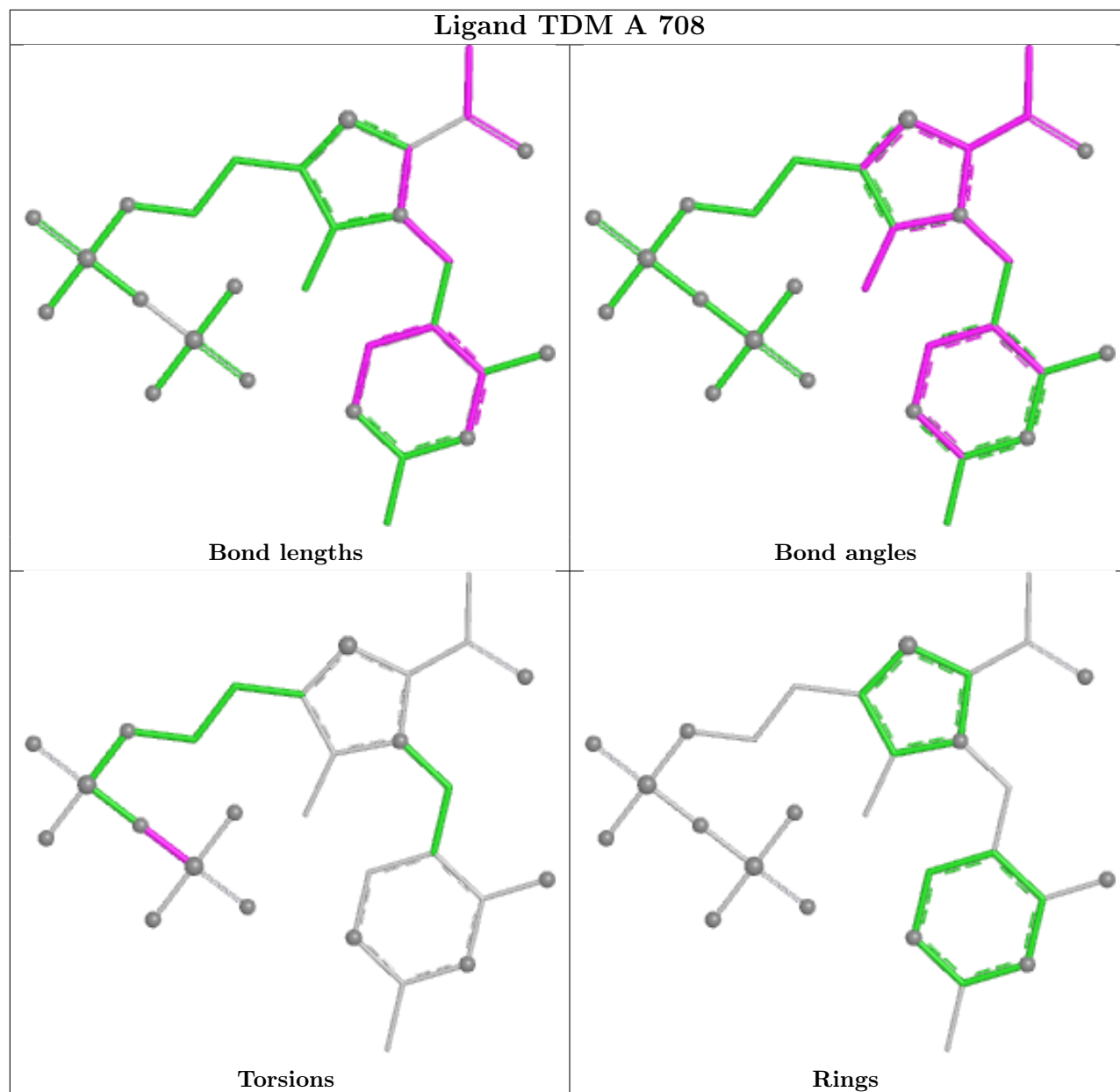
Mol	Chain	Res	Type	Atoms
4	B	704[B]	GOL	O2-C2-C3-O3
7	A	709	FAD	O4'-C4'-C5'-O5'
7	A	709	FAD	C3'-C4'-C5'-O5'
4	A	710	GOL	O2-C2-C3-O3
7	A	709	FAD	P-O3P-PA-O5B
7	B	710	FAD	P-O3P-PA-O5B
2	A	702	PYR	O-C-CA-CB
2	B	702	PYR	O-C-CA-O3
6	A	708	TDM	PA-O3A-PB-O1B
7	A	709	FAD	PA-O3P-P-O2P
7	B	710	FAD	PA-O3P-P-O2P
7	A	709	FAD	O4B-C4B-C5B-O5B

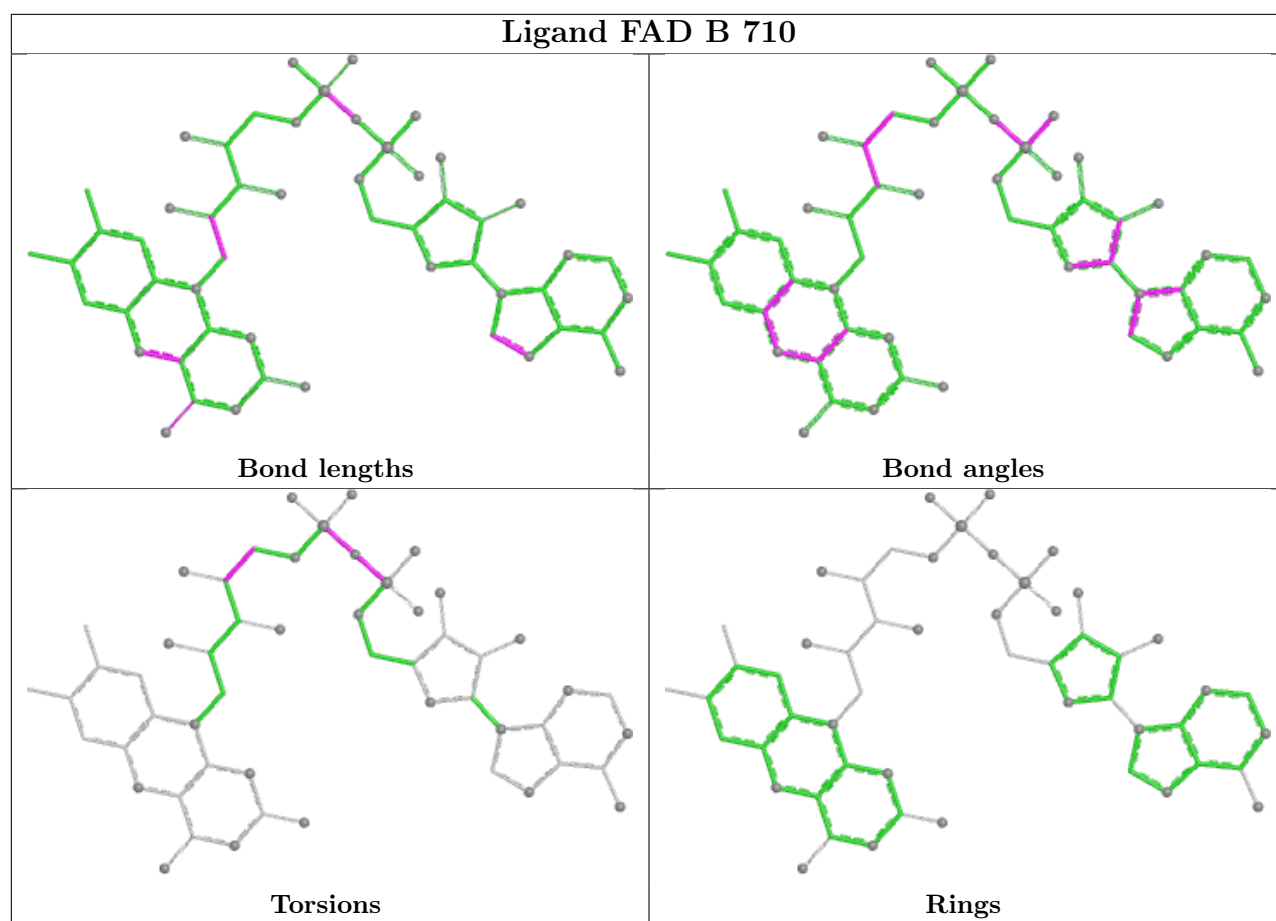
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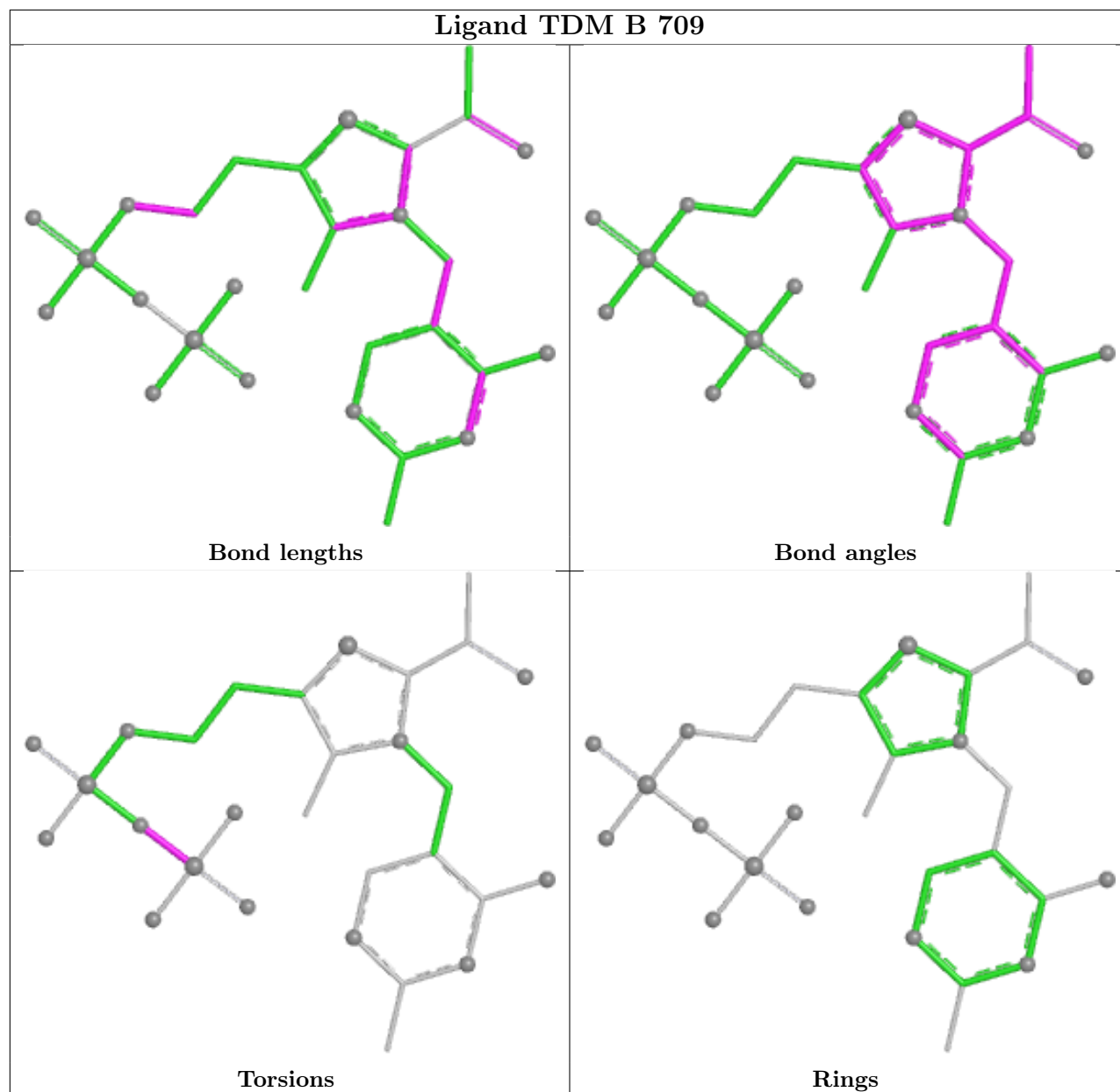
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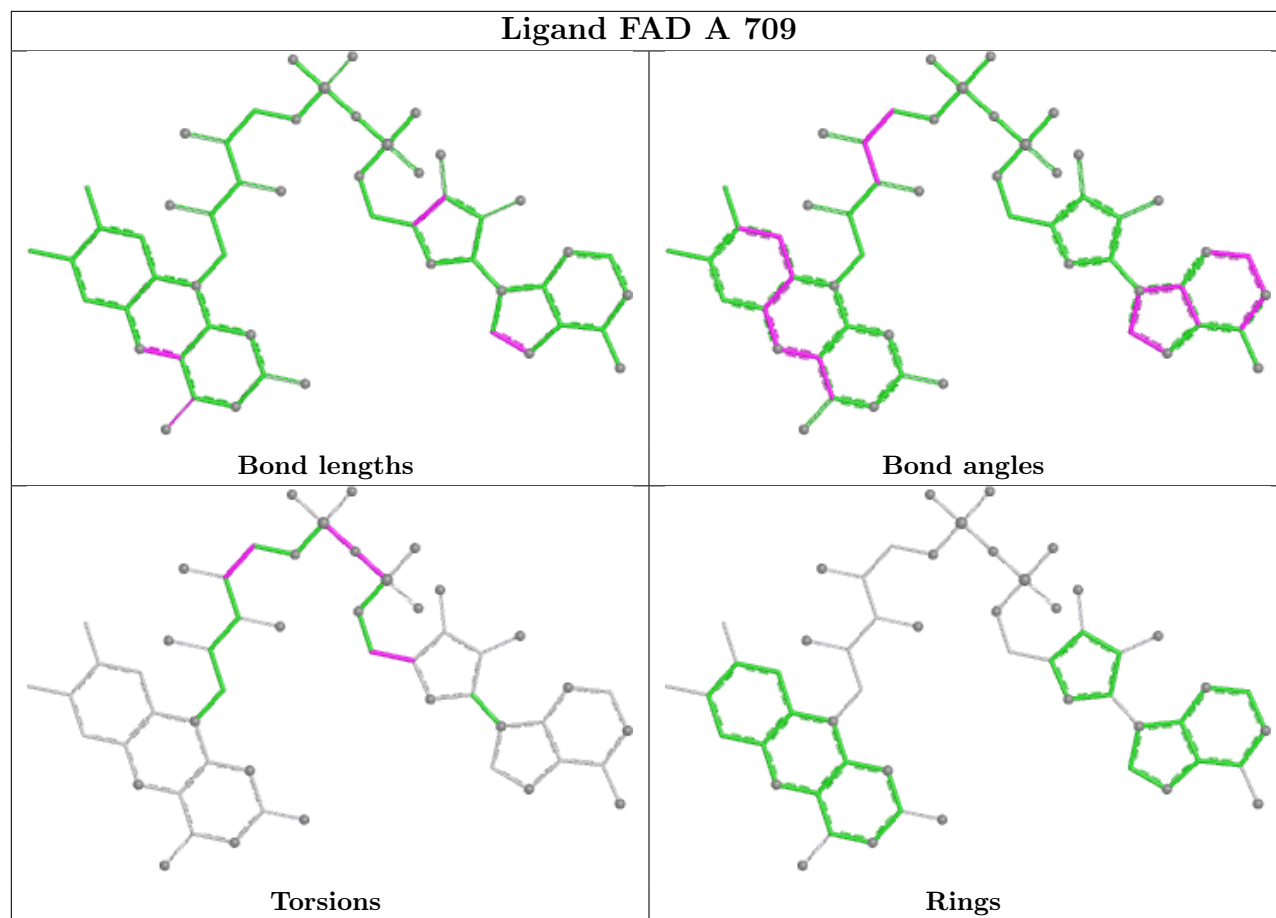
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	PO4	3	0
4	B	704[B]	GOL	2	0
7	B	710	FAD	1	0
4	A	706	GOL	1	0
4	B	704[A]	GOL	5	0
7	A	709	FAD	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	583/603 (96%)	-0.53	1 (0%) 91 92	3, 8, 18, 33	44 (7%)
1	B	583/603 (96%)	-0.59	2 (0%) 90 91	3, 7, 16, 30	52 (8%)
All	All	1166/1206 (96%)	-0.56	3 (0%) 90 91	3, 8, 17, 33	96 (8%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	THR	3.1
1	B	204[A]	ARG	2.0
1	B	591	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	704[A]	6/6	0.87	0.12	9,10,14,16	6
4	GOL	B	704[B]	6/6	0.87	0.12	9,9,15,21	6

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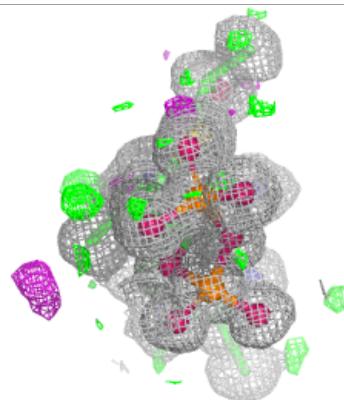
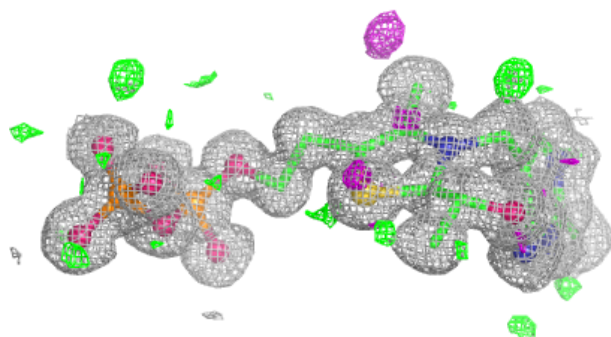
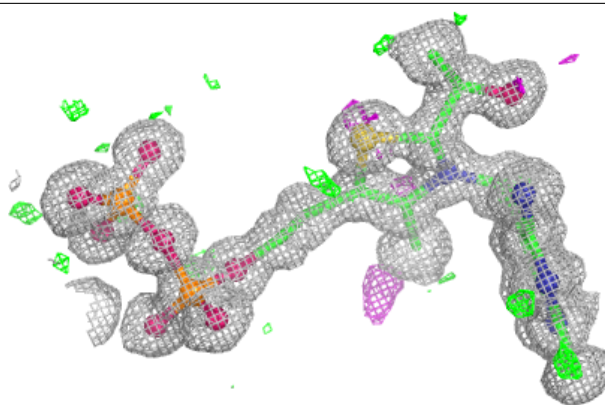
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	B	707	6/6	0.89	0.12	29,32,34,42	0
4	GOL	A	710	6/6	0.92	0.11	29,34,37,37	0
4	GOL	B	706	6/6	0.94	0.09	17,26,33,44	0
4	GOL	A	705	6/6	0.96	0.08	17,21,30,39	0
4	GOL	A	704	6/6	0.96	0.08	10,18,23,25	0
4	GOL	B	705	6/6	0.97	0.06	16,17,20,21	0
2	PYR	A	702	6/6	0.97	0.07	13,14,17,18	0
2	PYR	A	701	6/6	0.97	0.07	12,15,16,27	0
2	PYR	B	701	6/6	0.98	0.05	12,13,14,17	0
2	PYR	B	702	6/6	0.98	0.06	13,14,16,16	0
4	GOL	A	706	6/6	0.98	0.07	13,27,31,33	0
3	PO4	B	703	5/5	0.99	0.04	8,9,13,21	5
3	PO4	A	703	5/5	0.99	0.05	9,9,15,21	5
5	MG	A	707	1/1	1.00	0.01	6,6,6,6	0
5	MG	B	708	1/1	1.00	0.01	5,5,5,5	0
6	TDM	A	708	29/29	1.00	0.02	6,6,7,10	0
6	TDM	B	709	29/29	1.00	0.02	5,6,7,9	0
7	FAD	A	709	53/53	1.00	0.02	5,5,7,8	0
7	FAD	B	710	53/53	1.00	0.02	4,5,6,6	0

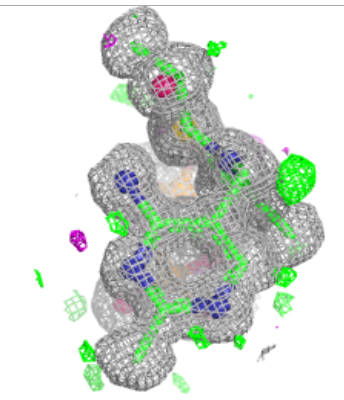
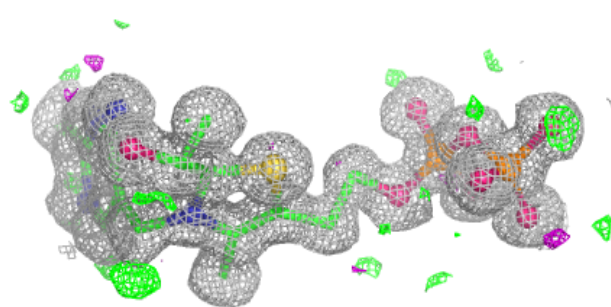
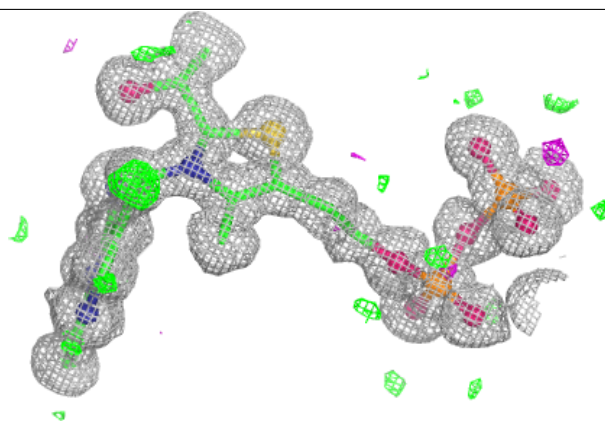
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TDM A 708:

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

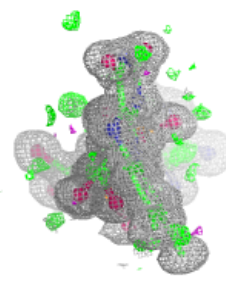
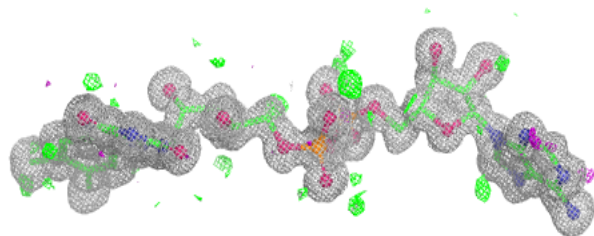
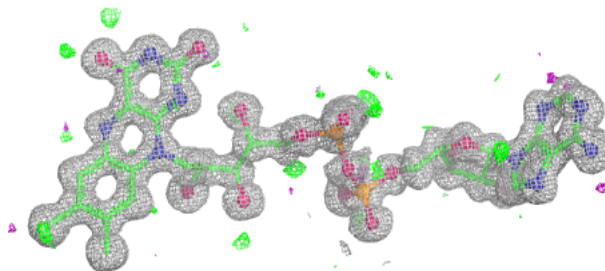
**Electron density around TDM B 709:**

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

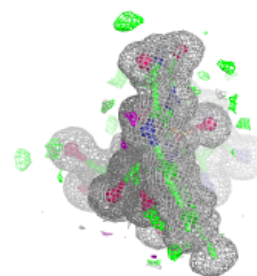
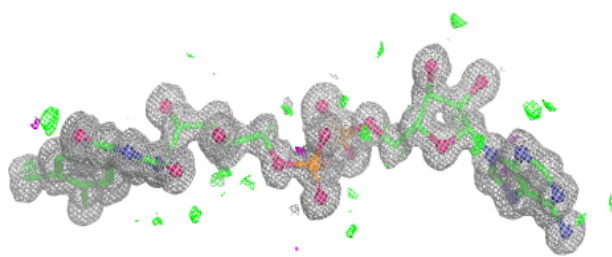
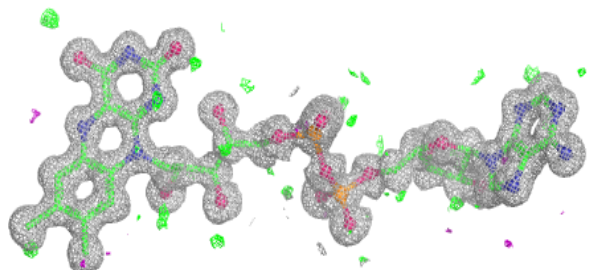


Electron density around FAD A 709:

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

**Electron density around FAD B 710:**

$2mF_o-DF_c$ (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.