



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:17 pm BST

PDB ID : 4FEG
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

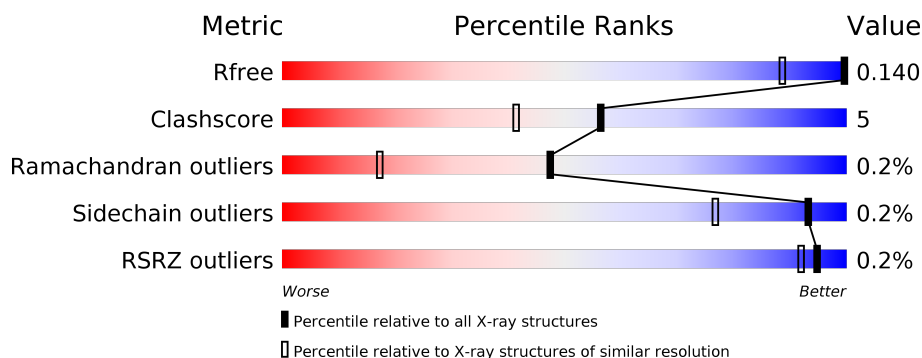
1 Overall quality at a glance ⓘ

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}	130704	1619 (1.14-1.06)
Clashscore	141614	1671 (1.14-1.06)
Ramachandran outliers	138981	1615 (1.14-1.06)
Sidechain outliers	138945	1613 (1.14-1.06)
RSRZ outliers	127900	1588 (1.14-1.06)

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 on 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	
1	B	603	

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
2	PYR	A	701	-	-	X	-
3	PO4	A	703	-	-	X	-
4	GOL	B	704[A]	-	X	X	-
4	GOL	B	704[B]	-	X	-	-

2 Entry composition [i](#)

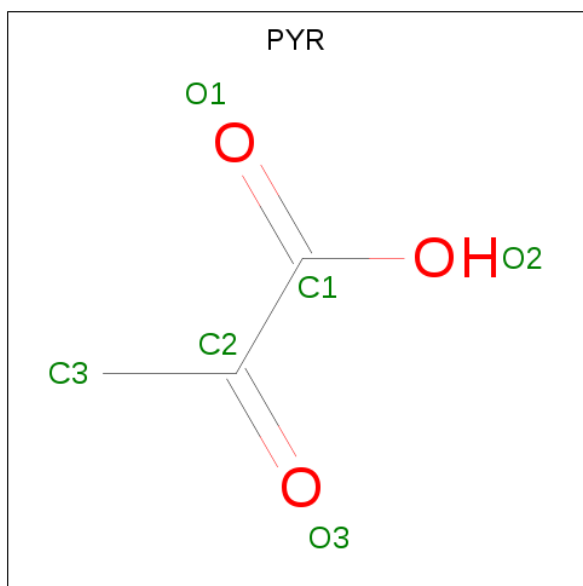
There are 8 unique types of molecules in this entry. The entry contains 12015 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (three-letter code: PYR) (formula: $C_3H_4O_3$).



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 (three-letter code: 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 (three-letter code: 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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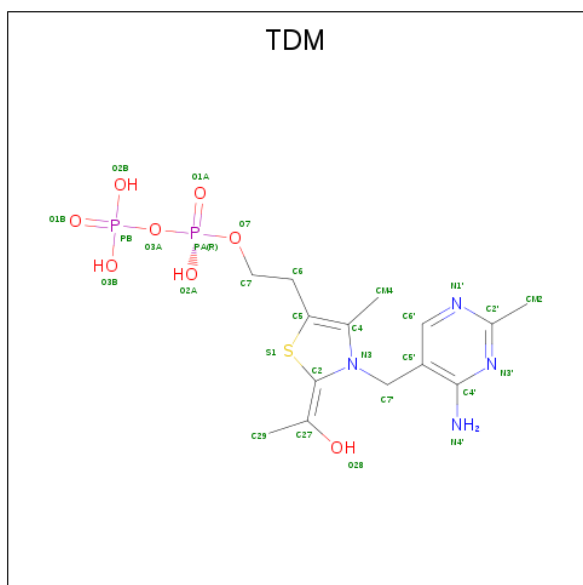
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

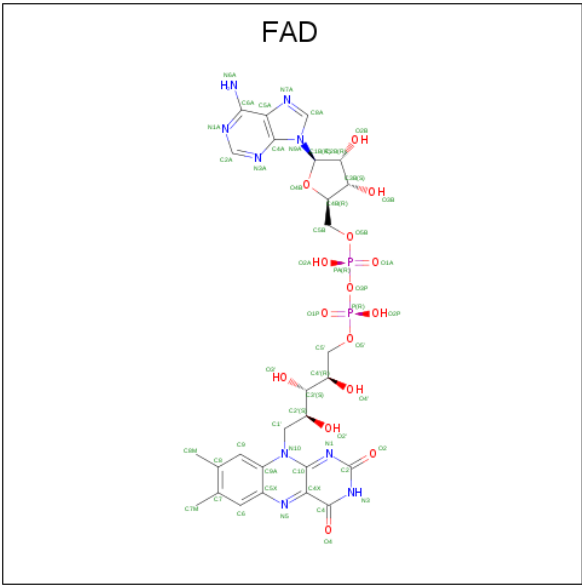
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- 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 (three-letter code: 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 (three-letter code: 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		

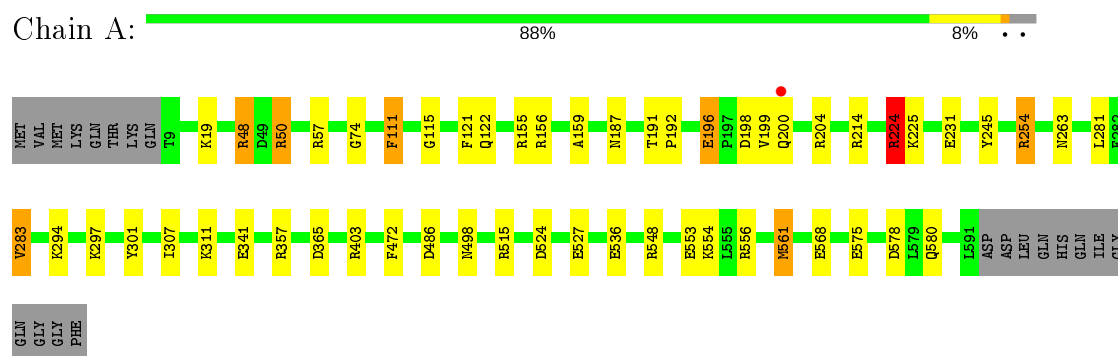
- Molecule 8 is water.

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

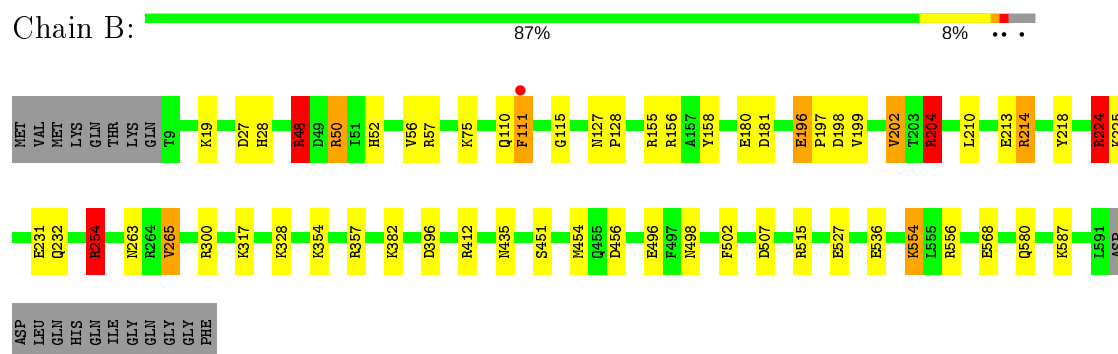
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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



• Molecule 1: Pyruvate oxidase



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 48.20 – 1.09	Depositor EDS
% Data completeness (in resolution range)	92.7 (30.00-1.09) 91.8 (48.20-1.09)	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	30568 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)	0.37 , 111.1	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, TDM, PO4, PYR, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	2/4944 (0.0%)	1.37	58/6715 (0.9%)
1	B	0.78	1/5008 (0.0%)	1.36	73/6801 (1.1%)
All	All	0.77	3/9952 (0.0%)	1.37	131/13516 (1.0%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	496	GLU	CD-OE1	-6.94	1.18	1.25
1	A	231	GLU	CD-OE1	-6.73	1.18	1.25
1	A	575	GLU	CD-OE2	5.01	1.31	1.25

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48[A]	ARG	NE-CZ-NH2	25.71	133.16	120.30
1	A	48[B]	ARG	NE-CZ-NH2	25.71	133.16	120.30
1	B	357[A]	ARG	NE-CZ-NH2	-19.00	110.80	120.30
1	B	357[C]	ARG	NE-CZ-NH2	-19.00	110.80	120.30
1	A	57	ARG	NE-CZ-NH2	-17.33	111.63	120.30
1	B	57	ARG	NE-CZ-NH1	16.85	128.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204[A]	ARG	NE-CZ-NH2	-16.49	112.05	120.30
1	B	204[B]	ARG	NE-CZ-NH2	-16.49	112.05	120.30
1	A	357	ARG	NE-CZ-NH1	-15.16	112.72	120.30
1	A	357	ARG	NE-CZ-NH2	-14.93	112.84	120.30
1	B	155	ARG	NE-CZ-NH2	14.48	127.54	120.30
1	B	155	ARG	NE-CZ-NH1	-13.91	113.35	120.30
1	A	155	ARG	NE-CZ-NH2	13.78	127.19	120.30
1	A	357	ARG	NH1-CZ-NH2	13.65	134.41	119.40
1	A	57	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	B	496	GLU	OE1-CD-OE2	-12.91	107.81	123.30
1	A	196	GLU	OE1-CD-OE2	12.83	138.69	123.30
1	A	155	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	A	156	ARG	NE-CZ-NH2	-12.03	114.28	120.30
1	B	57	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	B	224	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	B	224	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	B	496	GLU	CG-CD-OE1	10.48	139.26	118.30
1	A	254	ARG	NE-CZ-NH1	-10.32	115.14	120.30
1	B	111[A]	PHE	CD1-CE1-CZ	10.24	132.39	120.10
1	B	111[B]	PHE	CD1-CE1-CZ	10.24	132.39	120.10
1	B	50[A]	ARG	NE-CZ-NH2	10.21	125.41	120.30
1	B	50[B]	ARG	NE-CZ-NH2	10.21	125.41	120.30
1	B	204[A]	ARG	NH1-CZ-NH2	10.17	130.58	119.40
1	B	204[B]	ARG	NH1-CZ-NH2	10.17	130.58	119.40
1	B	111[A]	PHE	CB-CG-CD2	10.10	127.87	120.80
1	B	111[B]	PHE	CB-CG-CD2	10.10	127.87	120.80
1	A	48[A]	ARG	NE-CZ-NH1	-9.73	115.44	120.30
1	A	48[B]	ARG	NE-CZ-NH1	-9.73	115.44	120.30
1	A	156	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	515	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	A	204	ARG	CD-NE-CZ	9.12	136.37	123.60
1	B	204[A]	ARG	CD-NE-CZ	-9.02	110.97	123.60
1	B	204[B]	ARG	CD-NE-CZ	-9.02	110.97	123.60
1	A	403	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	A	214[A]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	214[B]	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	B	155	ARG	CD-NE-CZ	8.44	135.42	123.60
1	A	548	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	515	ARG	NE-CZ-NH2	8.32	124.46	120.30
1	B	180	GLU	OE1-CD-OE2	-8.30	113.33	123.30
1	B	254	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	515	ARG	NE-CZ-NH1	8.23	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	556	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	231	GLU	OE1-CD-OE2	-8.00	113.70	123.30
1	A	155	ARG	CD-NE-CZ	7.97	134.76	123.60
1	B	196	GLU	OE1-CD-OE2	-7.77	113.97	123.30
1	B	111[A]	PHE	CG-CD1-CE1	-7.54	112.51	120.80
1	B	111[B]	PHE	CG-CD1-CE1	-7.54	112.51	120.80
1	B	507	ASP	CB-CG-OD1	7.50	125.05	118.30
1	B	357[A]	ARG	NH1-CZ-NH2	7.50	127.65	119.40
1	B	357[C]	ARG	NH1-CZ-NH2	7.50	127.65	119.40
1	B	156	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	515	ARG	NE-CZ-NH1	-7.37	116.61	120.30
1	B	265	VAL	CG1-CB-CG2	7.32	122.61	110.90
1	B	554[A]	LYS	CD-CE-NZ	7.29	128.46	111.70
1	B	554[B]	LYS	CD-CE-NZ	7.29	128.46	111.70
1	A	48[A]	ARG	NH1-CZ-NH2	-7.27	111.40	119.40
1	A	48[B]	ARG	NH1-CZ-NH2	-7.27	111.40	119.40
1	A	283	VAL	CG1-CB-CG2	7.24	122.49	110.90
1	B	181	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	111[A]	PHE	CG-CD2-CE2	7.22	128.74	120.80
1	B	111[B]	PHE	CG-CD2-CE2	7.22	128.74	120.80
1	B	156	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	300	ARG	NE-CZ-NH1	-6.93	116.83	120.30
1	A	198	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	556	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	536	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	A	365	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	204[A]	ARG	CG-CD-NE	-6.47	98.20	111.80
1	B	204[B]	ARG	CG-CD-NE	-6.47	98.20	111.80
1	A	50[A]	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	A	50[B]	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	B	204[A]	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	B	204[B]	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	A	548	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	50[A]	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	B	50[B]	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	561	MET	CG-SD-CE	-6.14	90.37	100.20
1	A	111[A]	PHE	CG-CD1-CE1	-5.97	114.24	120.80
1	A	111[B]	PHE	CG-CD1-CE1	-5.97	114.24	120.80
1	B	180	GLU	CG-CD-OE1	5.88	130.05	118.30
1	A	204	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	B	48	ARG	NE-CZ-NH1	5.84	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	B	254	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	231	GLU	OE1-CD-OE2	-5.74	116.42	123.30
1	B	412	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	50[A]	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	50[B]	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	A	198	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	B	218	TYR	CB-CG-CD1	5.63	124.38	121.00
1	B	265	VAL	CB-CA-C	5.61	122.05	111.40
1	A	283	VAL	CA-CB-CG1	-5.59	102.52	110.90
1	A	245	TYR	CB-CG-CD1	5.56	124.33	121.00
1	B	111[A]	PHE	CB-CG-CD1	-5.51	116.95	120.80
1	B	111[B]	PHE	CB-CG-CD1	-5.51	116.95	120.80
1	A	365	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	224	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	301	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	403	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	202[A]	VAL	CA-C-N	5.40	129.09	117.20
1	B	202[B]	VAL	CA-C-N	5.40	129.09	117.20
1	A	74	GLY	O-C-N	-5.39	114.08	122.70
1	B	507	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	B	158	TYR	CB-CG-CD2	5.36	124.21	121.00
1	B	396	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	265	VAL	CA-CB-CG2	5.32	118.88	110.90
1	B	214[A]	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	214[B]	ARG	CD-NE-CZ	5.29	131.01	123.60
1	B	48	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	A	524	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	B	48	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	A	472	PHE	CB-CG-CD1	5.22	124.46	120.80
1	A	578	ASP	CB-CG-OD1	5.21	122.98	118.30
1	A	111[A]	PHE	CD1-CE1-CZ	5.16	126.29	120.10
1	A	111[B]	PHE	CD1-CE1-CZ	5.16	126.29	120.10
1	A	74	GLY	C-N-CA	5.11	134.47	121.70
1	B	180	GLU	CB-CG-CD	5.11	127.99	114.20
1	B	396	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	210	LEU	CB-CG-CD2	5.05	119.58	111.00
1	B	265	VAL	N-CA-CB	5.03	122.57	111.50
1	A	568[A]	GLU	N-CA-CB	-5.01	101.58	110.60
1	A	568[B]	GLU	N-CA-CB	-5.01	101.58	110.60
1	A	196	GLU	CG-CD-OE1	-5.00	108.29	118.30

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	4800	43	0
1	B	4899	0	4855	50	0
2	A	12	0	6	4	0
2	B	12	0	6	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	31	0
8	B	1009	0	0	35	1
All	All	12015	0	9839	100	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 5.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199[B]:VAL:CG2	8:A:1543:HOH:O	1.84	1.24
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:225[B]:LYS:CD	8:A:1734:HOH:O	2.12	0.95
1:B:328[B]:LYS:HD3	8:B:7858:HOH:O	1.70	0.91
1:A:294:LYS:O	1:A:297[A]:LYS:HE3	1.72	0.89
1:B:328[B]:LYS:CE	8:B:7858:HOH:O	2.24	0.86
1:A:199[B]:VAL:HG22	8:A:1543:HOH:O	1.61	0.86
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:A:225[B]:LYS:HD3	8:A:1734:HOH:O	1.80	0.75
1:B:328[B]:LYS:HE2	8:B:7858:HOH:O	1.81	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:B:328[B]:LYS:CD	8:B:7858:HOH:O	2.29	0.72
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
1:A:199[B]:VAL:HG22	8:A:1207:HOH:O	1.91	0.69
1:B:580[B]:GLN:OE1	8:B:7753:HOH:O	2.10	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
2:A:701:PYR:H33	8:A:1687:HOH:O	1.97	0.65
1:A:200[A]:GLN:HG3	8:A:1289:HOH:O	1.98	0.62
2:A:701:PYR:H31	8:A:1633:HOH:O	2.00	0.60
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:A:225[B]:LYS:CE	8:A:1734:HOH:O	2.47	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:B:232[B]:GLN:OE1	8:B:7921:HOH:O	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:225[B]:LYS:NZ	8:A:1734:HOH:O	2.37	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:454[B]:MET:HE3	1:B:502:PHE:CE1	2.47	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:354[B]:LYS:HE3	8:B:7948:HOH:O	2.12	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:254:ARG:CZ	8:B:7959:HOH:O	2.56	0.47
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
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:341[B]:GLU:HG2	8:A:1376:HOH:O	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:196:GLU:CD	8:A:1697:HOH:O	2.58	0.42
1:B:224:ARG:NE	8:B:7613:HOH:O	2.51	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
1:A:225[B]:LYS:HD2	8:A:1734:HOH:O	1.96	0.42
1:A:561:MET:HE3	2:A:701:PYR:H32	2.02	0.41
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: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:A:561:MET:CE	2:A:701:PYR:H32	2.52	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	620/603 (103%)	602 (97%)	17 (3%)	1 (0%)	47	17
1	B	629/603 (104%)	615 (98%)	13 (2%)	1 (0%)	47	17
All	All	1249/1206 (104%)	1217 (97%)	30 (2%)	2 (0%)	47	17

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%)	506 (100%)	2 (0%)	91	74
1	B	515/485 (106%)	514 (100%)	1 (0%)	93	77
All	All	1023/970 (106%)	1020 (100%)	3 (0%)	93	76

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187[A]	ASN
1	A	187[B]	ASN
1	B	265	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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
3	PO4	B	703	-	4,4,4	1.45	1 (25%)	6,6,6	0.75	0
4	GOL	A	706	-	5,5,5	0.65	0	5,5,5	1.06	0
2	PYR	A	702	-	2,5,5	2.18	1 (50%)	2,6,6	1.29	0
4	GOL	B	707	-	5,5,5	0.63	0	5,5,5	1.79	2 (40%)
4	GOL	A	705	-	5,5,5	1.07	0	5,5,5	1.04	0
4	GOL	B	705	-	5,5,5	1.32	1 (20%)	5,5,5	1.40	1 (20%)
4	GOL	B	704[A]	-	5,5,5	0.84	0	5,5,5	1.95	2 (40%)
2	PYR	B	702	-	2,5,5	2.48	1 (50%)	2,6,6	1.06	0
4	GOL	B	704[B]	-	5,5,5	1.19	1 (20%)	5,5,5	2.77	3 (60%)
7	FAD	A	709	-	51,58,58	1.37	6 (11%)	60,89,89	2.21	13 (21%)
4	GOL	B	706	-	5,5,5	0.76	0	5,5,5	0.89	0
3	PO4	A	703	-	4,4,4	1.43	1 (25%)	6,6,6	0.90	0
4	GOL	A	704	-	5,5,5	0.61	0	5,5,5	1.16	0
7	FAD	B	710	-	51,58,58	1.44	5 (9%)	60,89,89	1.84	9 (15%)
6	TDM	B	709	5	25,30,30	2.50	6 (24%)	32,45,45	3.51	9 (28%)
2	PYR	B	701	-	2,5,5	1.75	1 (50%)	2,6,6	1.64	1 (50%)
2	PYR	A	701	-	2,5,5	4.03	1 (50%)	2,6,6	1.13	0
6	TDM	A	708	5	25,30,30	1.91	6 (24%)	32,45,45	3.04	8 (25%)
4	GOL	A	710	-	5,5,5	0.43	0	5,5,5	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	706	-	-	0/4/4/4	-
2	PYR	A	702	-	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	707	-	-	1/4/4/4	-
4	GOL	A	705	-	-	0/4/4/4	-
4	GOL	B	705	-	-	0/4/4/4	-
4	GOL	B	704[A]	-	-	4/4/4/4	-
2	PYR	B	702	-	-	0/0/4/4	-
4	GOL	B	704[B]	-	-	2/4/4/4	-
7	FAD	A	709	-	-	4/30/50/50	0/6/6/6
4	GOL	B	706	-	-	0/4/4/4	-
4	GOL	A	704	-	-	0/4/4/4	-
7	FAD	B	710	-	-	4/30/50/50	0/6/6/6
6	TDM	B	709	5	-	2/16/21/21	0/2/2/2
2	PYR	B	701	-	-	0/0/4/4	-
2	PYR	A	701	-	-	0/0/4/4	-
6	TDM	A	708	5	-	2/16/21/21	0/2/2/2
4	GOL	A	710	-	-	2/4/4/4	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	709	TDM	C6-C5	9.18	1.55	1.50
2	A	701	PYR	C3-C2	-5.69	1.32	1.49
7	B	710	FAD	C4X-N5	5.54	1.41	1.33
6	A	708	TDM	C6-C5	5.10	1.53	1.50
6	B	709	TDM	C2-N3	4.15	1.45	1.38
7	A	709	FAD	C4X-N5	4.12	1.39	1.33
7	A	709	FAD	C9A-N10	3.57	1.43	1.38
6	B	709	TDM	C7'-C5'	3.55	1.58	1.51
2	B	702	PYR	C3-C2	-3.50	1.39	1.49
6	A	708	TDM	C2-N3	3.47	1.44	1.38
6	B	709	TDM	O28-C27	3.41	1.40	1.31
7	B	710	FAD	C5X-N5	3.29	1.40	1.35
7	A	709	FAD	C2A-N3A	3.14	1.37	1.32
6	A	708	TDM	O28-C27	3.01	1.39	1.31
7	B	710	FAD	C4-N3	2.99	1.38	1.33
2	A	702	PYR	C3-C2	-2.93	1.41	1.49
7	B	710	FAD	C9A-N10	2.85	1.42	1.38
6	A	708	TDM	C6'-N1'	2.83	1.40	1.34
6	A	708	TDM	C6'-C5'	-2.70	1.32	1.37
6	A	708	TDM	C4'-N3'	2.67	1.38	1.35
6	B	709	TDM	C4'-N3'	2.66	1.38	1.35
3	B	703	PO4	P-O1	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	PYR	C3-C2	-2.36	1.42	1.49
7	A	709	FAD	C3B-C4B	2.25	1.58	1.53
7	A	709	FAD	C2B-C1B	-2.19	1.50	1.53
7	B	710	FAD	O4B-C1B	2.18	1.44	1.41
4	B	705	GOL	O3-C3	2.17	1.51	1.42
3	A	703	PO4	P-O4	-2.11	1.48	1.54
6	B	709	TDM	O7-C7	2.09	1.53	1.44
4	B	704[B]	GOL	C3-C2	2.05	1.60	1.51
7	A	709	FAD	C5X-N5	2.01	1.38	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	709	TDM	O28-C27-C2	-12.74	107.51	120.05
7	A	709	FAD	C4-N3-C2	11.51	124.86	115.14
6	A	708	TDM	O28-C27-C2	-10.04	110.16	120.05
6	B	709	TDM	C29-C27-C2	-9.80	110.19	124.92
6	A	708	TDM	C29-C27-C2	-9.52	110.62	124.92
6	B	709	TDM	C2-N3-C4	8.66	113.46	108.64
7	B	710	FAD	C4-N3-C2	8.60	122.40	115.14
6	A	708	TDM	C2-N3-C4	7.01	112.54	108.64
7	A	709	FAD	C4X-C4-N3	-5.11	116.45	123.43
7	B	710	FAD	C4X-C4-N3	-5.08	116.48	123.43
7	A	709	FAD	C1'-N10-C9A	4.58	121.90	118.29
7	B	710	FAD	C1'-N10-C9A	4.40	121.75	118.29
7	A	709	FAD	C4-C4X-C10	-4.19	117.18	119.95
4	B	704[B]	GOL	O3-C3-C2	-3.89	91.54	110.20
4	B	704[B]	GOL	O1-C1-C2	3.70	127.94	110.20
7	B	710	FAD	O4B-C1B-C2B	-3.23	102.21	106.93
4	B	704[A]	GOL	O2-C2-C1	-3.18	95.13	109.12
6	A	708	TDM	C5-C4-N3	3.12	114.17	107.66
7	A	709	FAD	C9A-N10-C10	-3.01	117.97	121.91
6	B	709	TDM	O28-C27-C29	-2.89	108.73	114.59
4	B	704[B]	GOL	C3-C2-C1	-2.87	100.53	111.70
6	A	708	TDM	CM4-C4-N3	-2.86	119.08	122.69
7	A	709	FAD	N3A-C2A-N1A	-2.83	124.26	128.68
6	B	709	TDM	C6'-N1'-C2'	2.68	120.52	115.96
7	B	710	FAD	C9A-N10-C10	-2.67	118.41	121.91
7	A	709	FAD	C4X-C10-N10	-2.63	117.60	120.30
6	A	708	TDM	O28-C27-C29	-2.57	109.36	114.59
6	B	709	TDM	C5'-C6'-N1'	-2.53	119.60	123.82
4	B	707	GOL	C3-C2-C1	-2.51	101.94	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	709	TDM	CM4-C4-N3	-2.47	119.58	122.69
4	B	704[A]	GOL	O2-C2-C3	2.45	119.91	109.12
2	B	701	PYR	O3-C2-C3	2.30	125.35	120.17
7	B	710	FAD	C1B-N9A-C4A	-2.27	122.66	126.64
6	A	708	TDM	C6'-C5'-C4'	2.21	118.72	115.72
7	B	710	FAD	C9A-C5X-N5	-2.18	118.96	122.36
4	B	705	GOL	O2-C2-C3	-2.15	99.66	109.12
6	B	709	TDM	C6'-C5'-C4'	2.13	118.62	115.72
7	A	709	FAD	C4-C4X-N5	2.11	121.01	118.60
4	B	707	GOL	O2-C2-C1	-2.08	99.94	109.12
6	A	708	TDM	C6'-N1'-C2'	2.08	119.50	115.96
7	B	710	FAD	C5'-C4'-C3'	-2.05	108.23	112.20
7	A	709	FAD	C5A-C6A-N6A	2.05	123.47	120.35
6	B	709	TDM	C5-C4-N3	2.05	111.94	107.66
7	A	709	FAD	C9A-C5X-N5	-2.04	119.18	122.36
7	A	709	FAD	C4X-N5-C5X	-2.03	114.74	116.77
7	A	709	FAD	C2A-N1A-C6A	2.02	122.22	118.75
7	A	709	FAD	C5'-C4'-C3'	-2.02	108.30	112.20
7	B	710	FAD	C10-C4X-N5	-2.01	119.87	121.26

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	704[B]	GOL	C1-C2-C3-O3
4	B	704[A]	GOL	C1-C2-C3-O3
7	B	710	FAD	C3'-C4'-C5'-O5'
7	B	710	FAD	O4'-C4'-C5'-O5'
6	B	709	TDM	PA-O3A-PB-O2B
6	B	709	TDM	PA-O3A-PB-O3B
6	A	708	TDM	PA-O3A-PB-O2B
4	A	710	GOL	C1-C2-C3-O3
4	B	704[A]	GOL	O1-C1-C2-C3
7	A	709	FAD	O4'-C4'-C5'-O5'
4	B	704[B]	GOL	O2-C2-C3-O3
4	B	704[A]	GOL	O1-C1-C2-O2
4	B	704[A]	GOL	O2-C2-C3-O3
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
4	B	707	GOL	C1-C2-C3-O3

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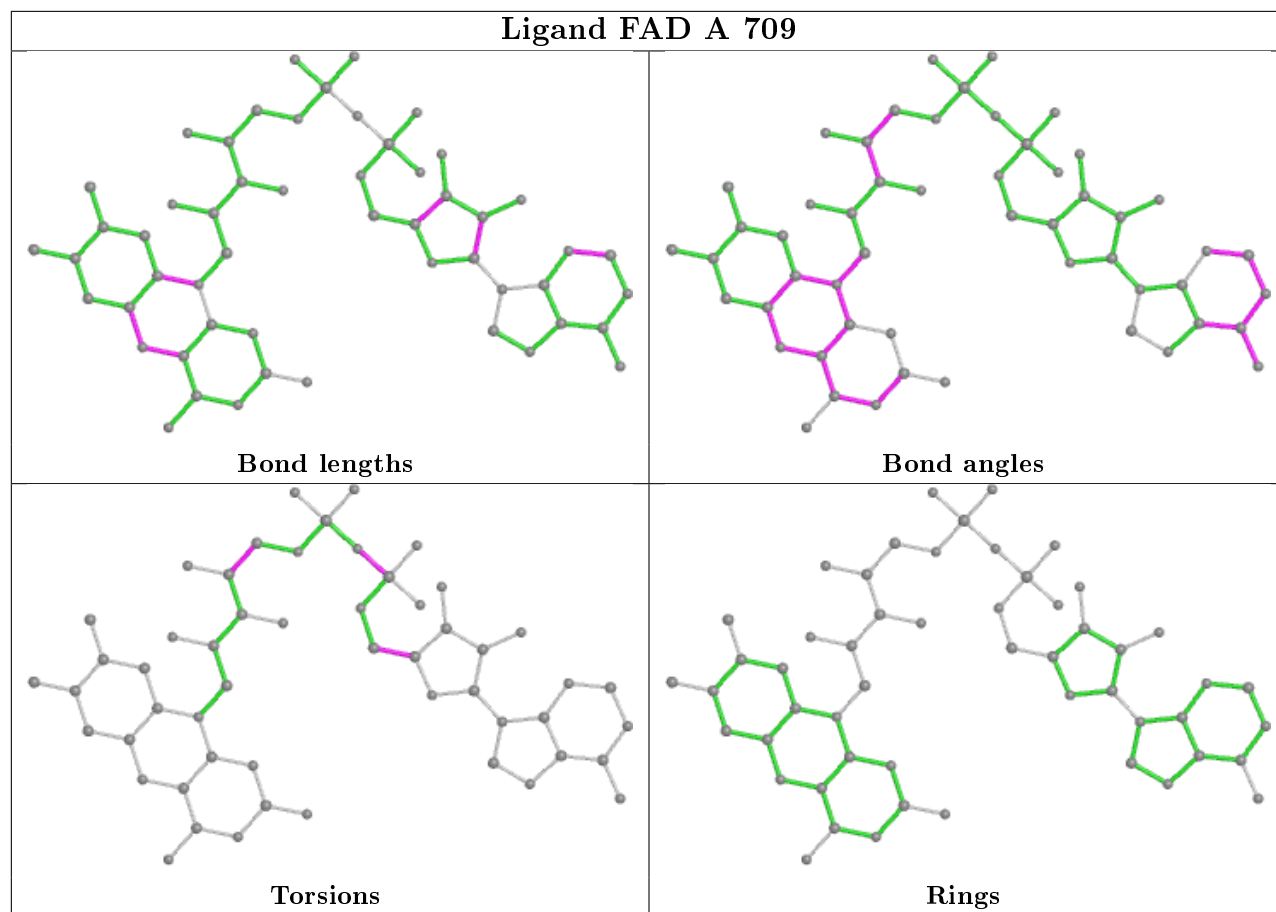
Mol	Chain	Res	Type	Atoms
7	A	709	FAD	O4B-C4B-C5B-O5B
7	B	710	FAD	O4B-C4B-C5B-O5B
6	A	708	TDM	PA-O3A-PB-O1B

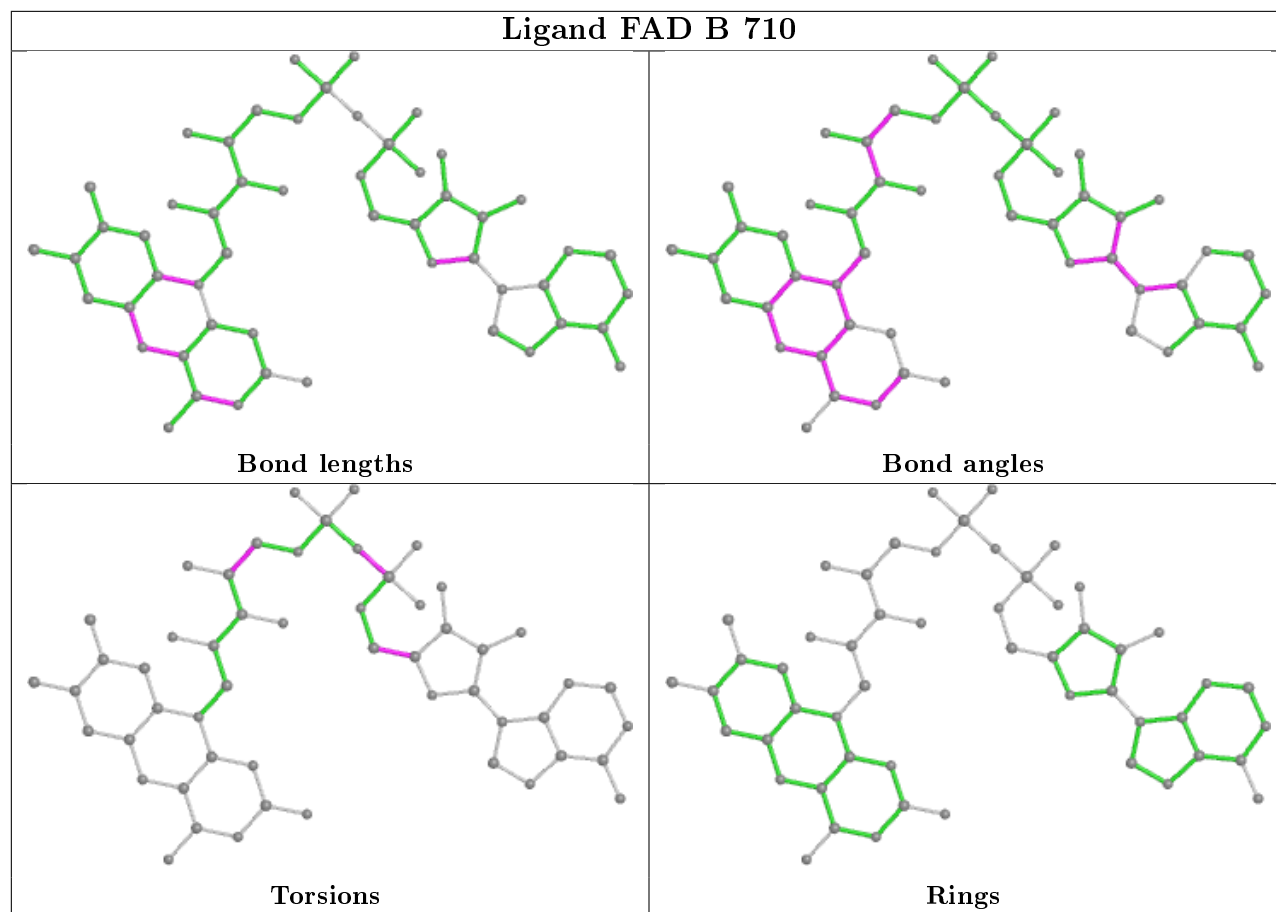
There are no ring outliers.

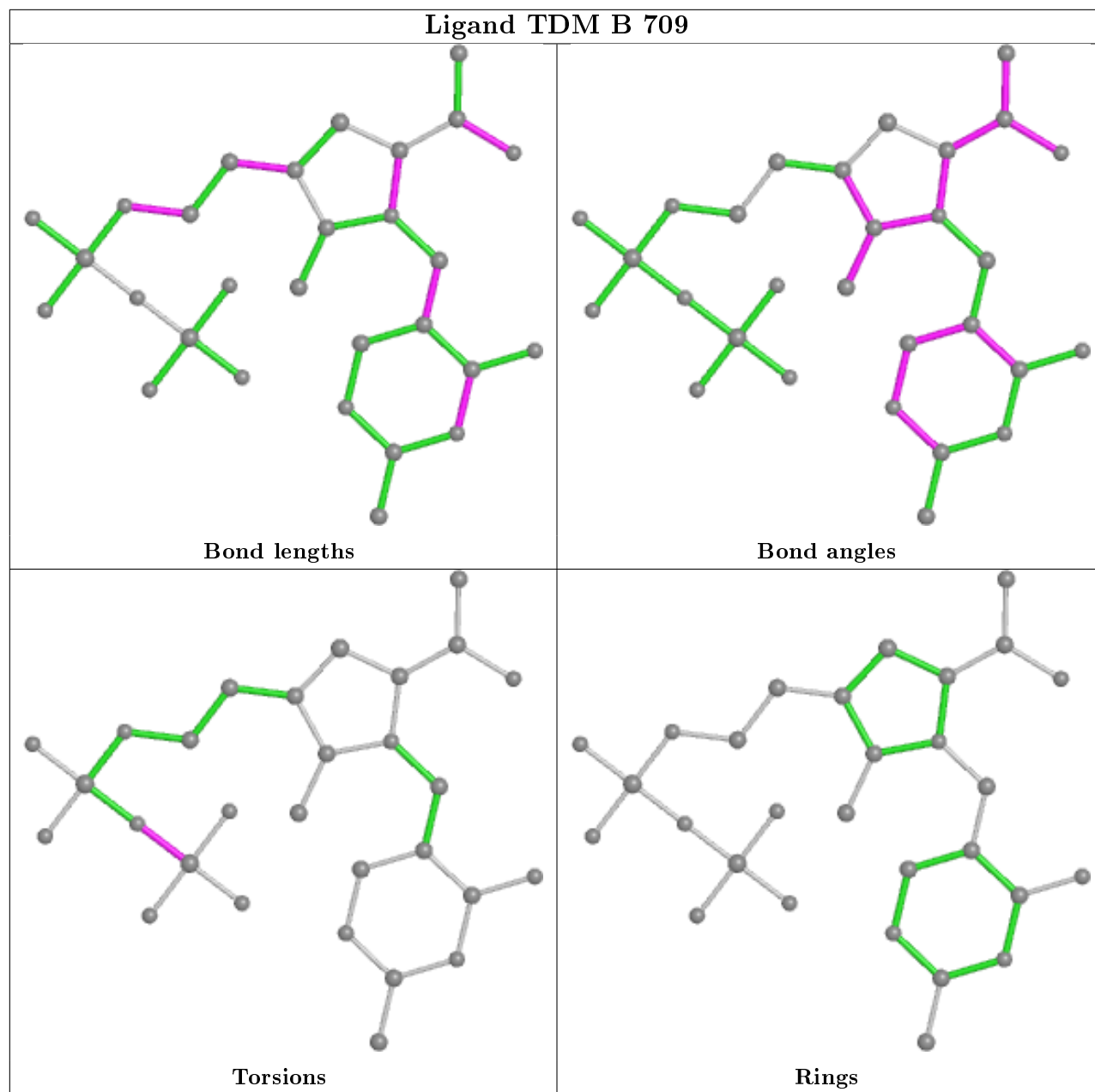
7 monomers are involved in 17 short contacts:

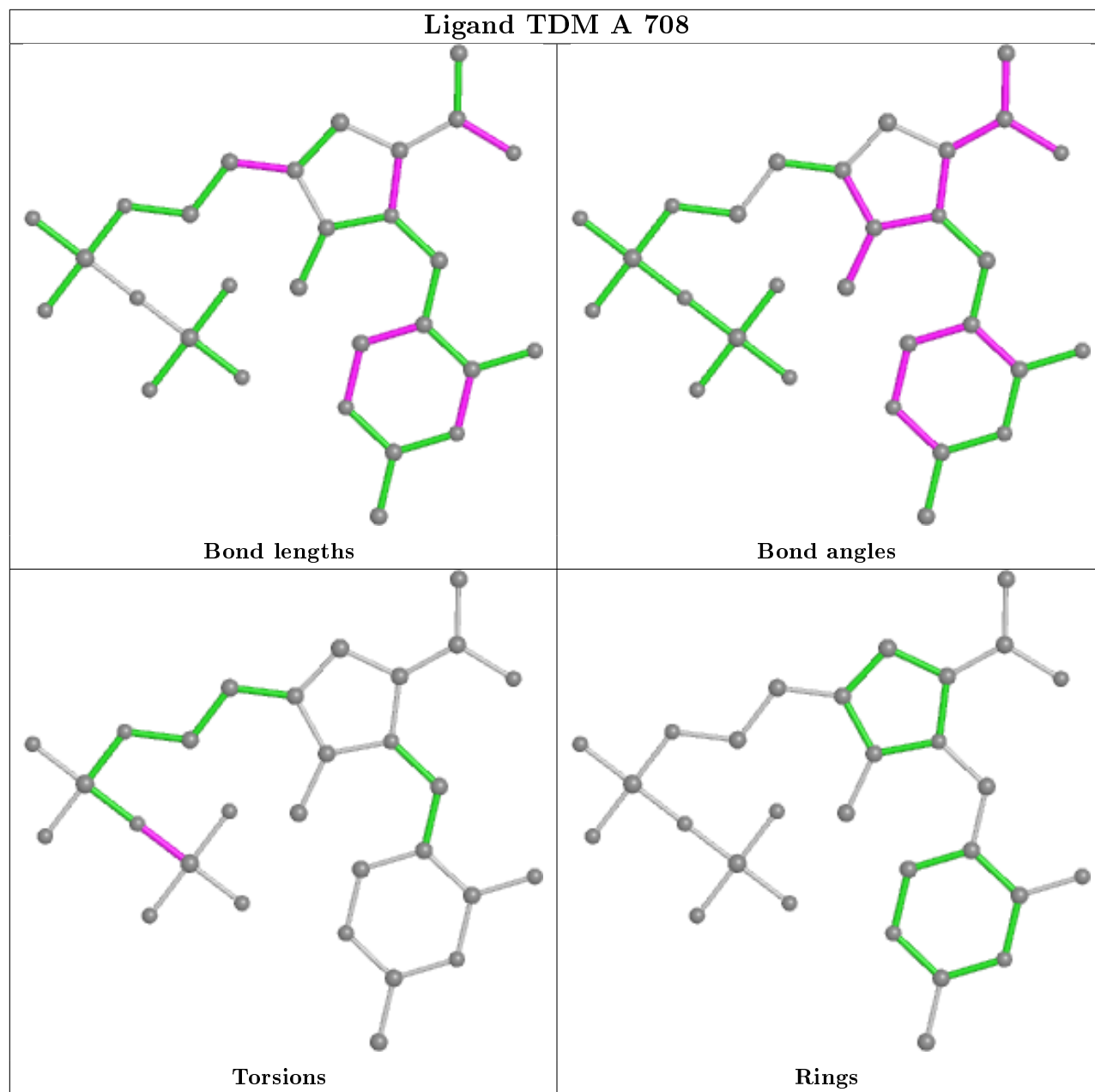
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	GOL	1	0
4	B	704[A]	GOL	5	0
4	B	704[B]	GOL	2	0
7	A	709	FAD	1	0
3	A	703	PO4	3	0
7	B	710	FAD	1	0
2	A	701	PYR	4	0

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%) 95 92	5, 8, 19, 36	4 (0%)
1	B	583/603 (96%)	-0.60	1 (0%) 95 92	5, 8, 17, 32	4 (0%)
All	All	1166/1206 (96%)	-0.56	2 (0%) 95 92	5, 8, 19, 36	8 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200[A]	GLN	2.4
1	B	111[A]	PHE	2.1

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 carbohydrates 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	707	6/6	0.84	0.15	29,32,34,42	0
4	GOL	B	704[B]	6/6	0.90	0.19	9,9,15,21	6
4	GOL	B	704[A]	6/6	0.90	0.19	9,10,14,16	6

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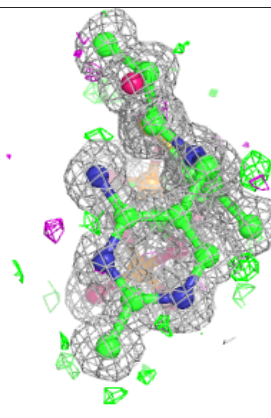
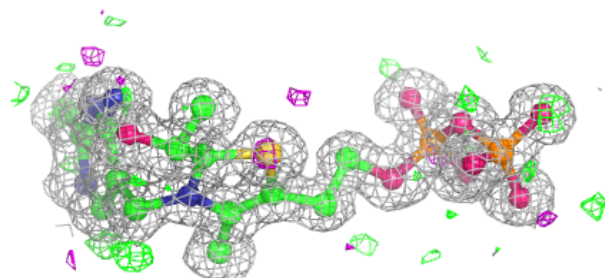
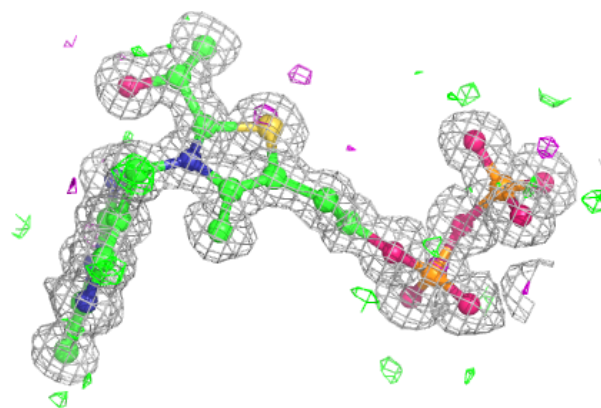
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	A	710	6/6	0.90	0.14	29,34,37,37	0
4	GOL	B	706	6/6	0.93	0.16	17,26,33,44	0
4	GOL	A	704	6/6	0.96	0.07	10,18,23,25	0
4	GOL	A	705	6/6	0.96	0.10	17,21,30,39	0
2	PYR	A	701	6/6	0.96	0.07	12,15,16,27	0
2	PYR	A	702	6/6	0.96	0.08	13,14,17,18	0
2	PYR	B	702	6/6	0.97	0.07	13,14,16,16	0
4	GOL	B	705	6/6	0.97	0.09	16,17,20,21	0
4	GOL	A	706	6/6	0.98	0.08	13,27,31,33	0
2	PYR	B	701	6/6	0.98	0.09	12,13,14,17	0
3	PO4	B	703	5/5	0.99	0.05	8,9,13,21	5
3	PO4	A	703	5/5	0.99	0.07	9,9,15,21	5
6	TDM	B	709	29/29	1.00	0.04	5,6,7,9	0
5	MG	B	708	1/1	1.00	0.01	5,5,5,5	0
5	MG	A	707	1/1	1.00	0.02	6,6,6,6	0
7	FAD	A	709	53/53	1.00	0.04	5,5,7,8	0
6	TDM	A	708	29/29	1.00	0.04	6,6,7,10	0
7	FAD	B	710	53/53	1.00	0.03	4,5,6,6	0

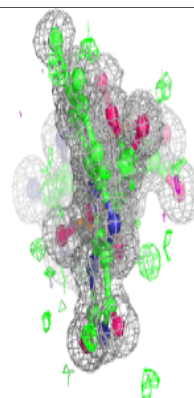
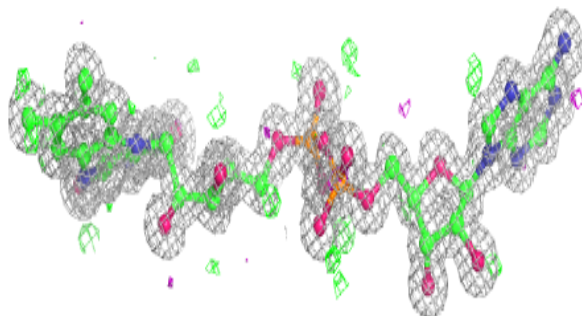
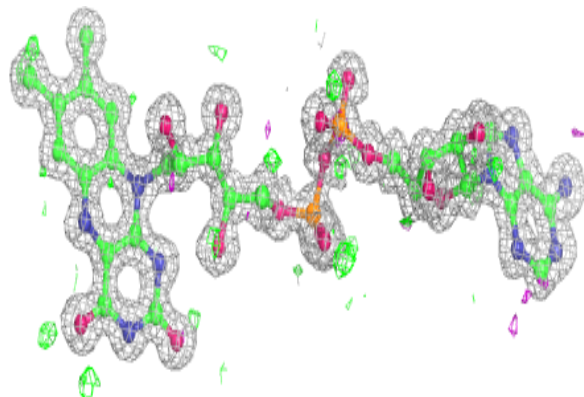
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TDM 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)

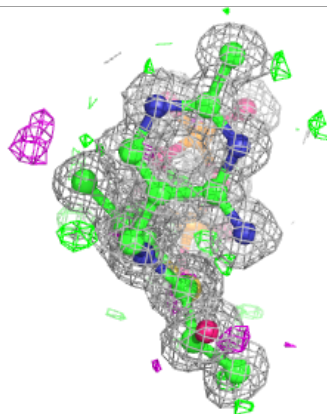
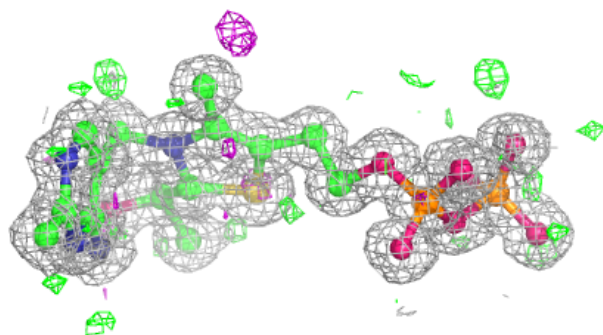
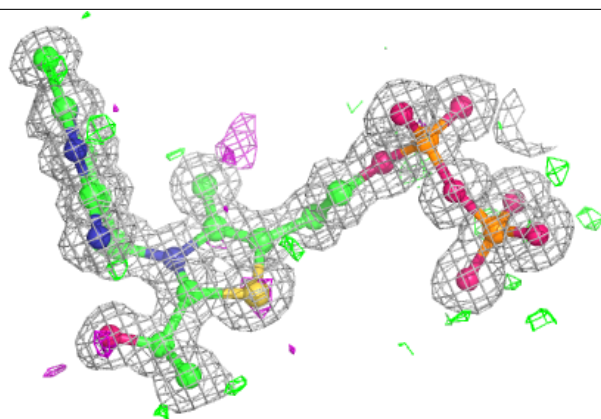
**Electron density around FAD A 709:**

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

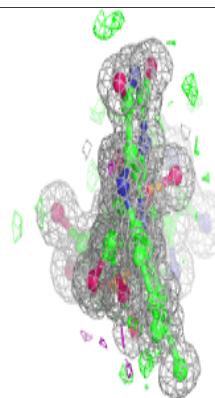
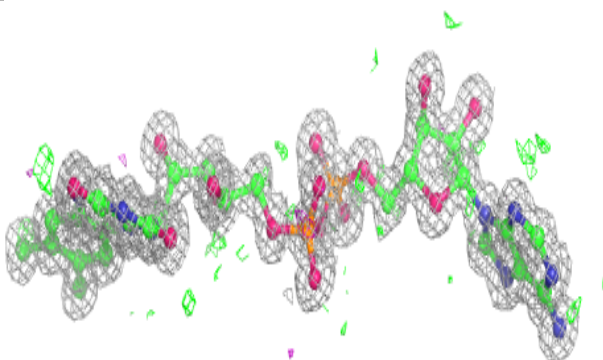
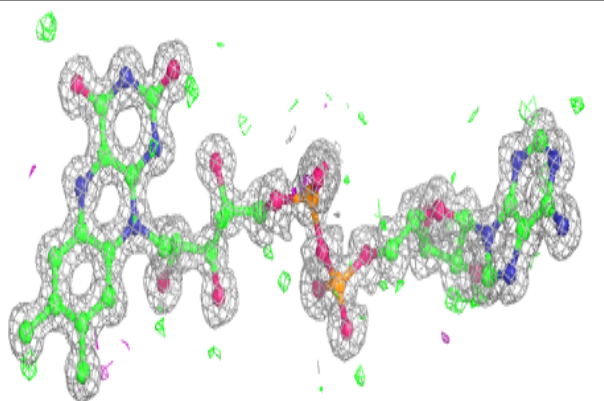


Electron density around TDM A 708:

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

**Electron density around 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

There are no such residues in this entry.