



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:47 AM UTC

PDB ID : 6BD9 / pdb_00006bd9
Title : Saccharomyces cerevisiae acetohydroxyacid synthase
Authors : Guddat, L.W.; Lonhienne, T.
Deposited on : 2017-10-22
Resolution : 1.98 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

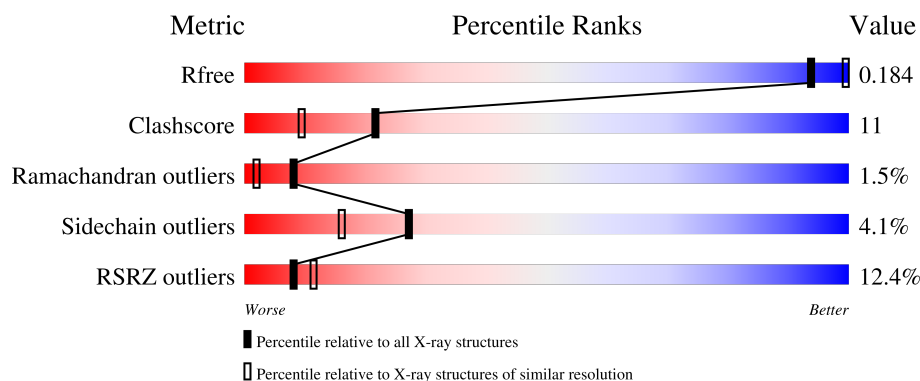
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	
1	B	677	

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
6	PYR	A	705	-	X	-	-
6	PYR	B	705	-	X	-	-
6	PYR	B	706	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9258 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	542	Total	C	N	O	S	0	3	0
			4122	2607	710	786	19			
1	B	564	Total	C	N	O	S	0	0	0
			4294	2718	741	815	20			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	expression tag	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
A	34	ALA	-	expression tag	UNP P07342
A	35	LYS	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-	expression tag	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
B	29	LYS	-	expression tag	UNP P07342
B	30	GLU	-	expression tag	UNP P07342

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

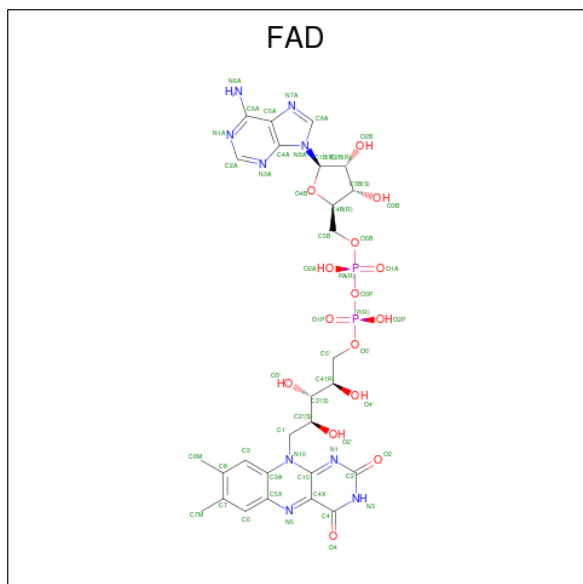
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

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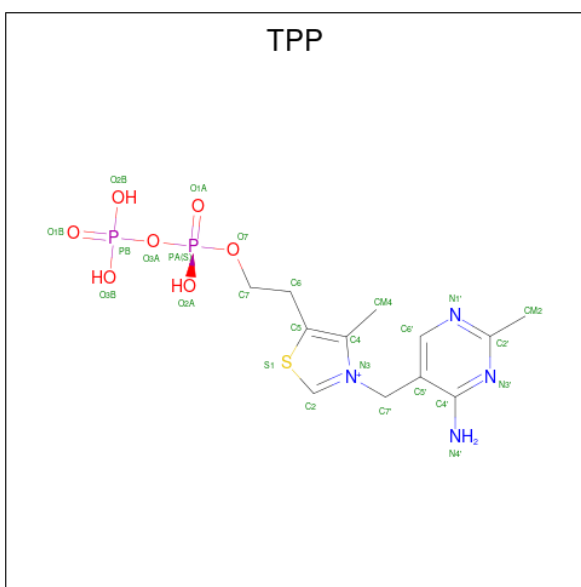
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0

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



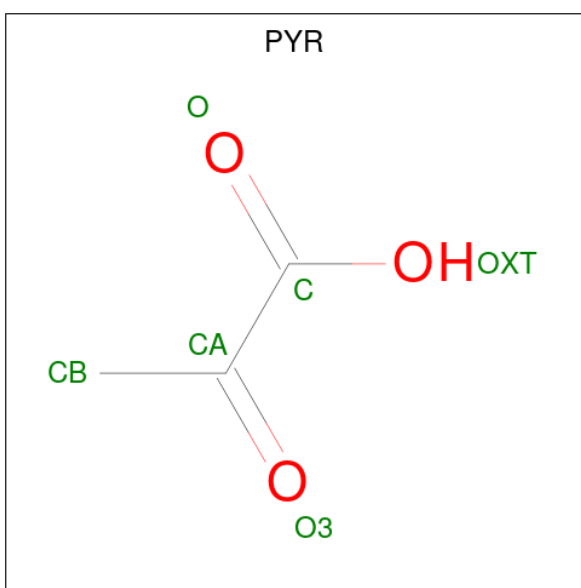
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $\text{C}_{12}\text{H}_{19}\text{N}_4\text{O}_7\text{P}_2\text{S}$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
5	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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



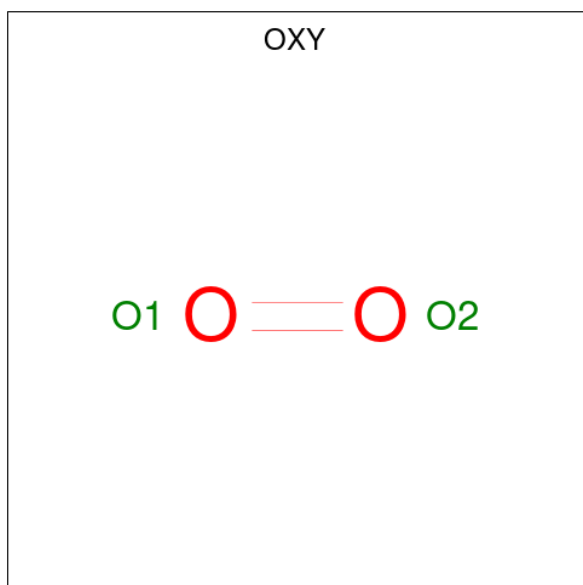
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0

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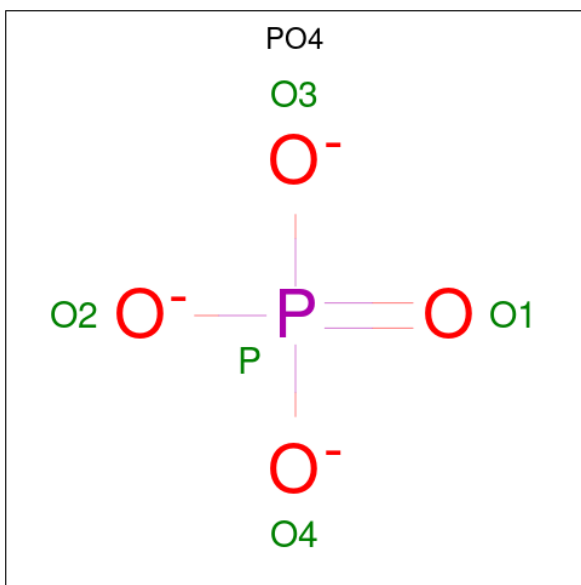
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

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



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	385	Total	O	0	0
			385	385		
9	B	250	Total	O	0	0
			250	250		

LEU	PRO	MET	VAL	ALA	GLY	GLY	SER	GLY	LEU	ASP	GLU	PHE	ILE	ASN	PHE	ASP	PRO	GLU	VAL	GLU	ARG	GLN	GLN	THR	GLU	LEU	ARG	HIS	LYS	ARG	THR	GLY	GLY	LYS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.02Å 110.97Å 180.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 1.98 29.93 – 1.98	Depositor EDS
% Data completeness (in resolution range)	95.2 (29.93-1.98) 95.2 (29.93-1.98)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.159 , 0.181 0.165 , 0.184	Depositor DCC
R_{free} test set	2000 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9258	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: MG, K, OXY, PO4, FAD, PYR, TPP

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	1.07	4/4203 (0.1%)	1.04	7/5700 (0.1%)
1	B	1.03	3/4383 (0.1%)	1.10	12/5950 (0.2%)
All	All	1.05	7/8586 (0.1%)	1.07	19/11650 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	ALA	CA-CB	6.06	1.62	1.53
1	A	183	PRO	C-O	-5.63	1.17	1.23
1	B	183	PRO	C-O	-5.48	1.17	1.23
1	A	185	VAL	C-O	-5.38	1.18	1.24
1	B	151	ARG	C-O	-5.25	1.17	1.24
1	B	185	VAL	C-O	-5.23	1.18	1.24
1	A	228	LEU	C-O	-5.10	1.18	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	291	LYS	N-CA-C	-8.12	100.13	110.19
1	B	392	ALA	N-CA-C	-7.56	104.03	113.55
1	B	394	ARG	N-CA-C	-6.83	102.97	112.12
1	A	602	ASN	CA-C-N	-6.01	114.44	120.21
1	A	602	ASN	C-N-CA	-6.01	114.44	120.21
1	B	368	ASP	CA-C-N	6.00	131.38	122.86
1	B	368	ASP	C-N-CA	6.00	131.38	122.86
1	B	388	PHE	N-CA-C	5.93	118.33	109.25
1	B	301	LYS	CA-C-N	-5.86	114.27	120.66
1	B	301	LYS	C-N-CA	-5.86	114.27	120.66
1	A	375	ALA	CA-C-N	-5.60	113.87	122.60
1	A	375	ALA	C-N-CA	-5.60	113.87	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	ILE	N-CA-C	5.57	115.88	107.80
1	B	294	ASP	N-CA-C	-5.54	104.87	111.69
1	B	453	LYS	N-CA-C	-5.41	106.61	113.43
1	A	458	TYR	N-CA-C	5.20	118.11	109.79
1	A	529	LEU	CA-C-N	-5.10	113.67	119.28
1	A	529	LEU	C-N-CA	-5.10	113.67	119.28
1	B	118	ILE	N-CA-C	-5.05	107.83	112.83

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	4122	0	4146	21	0
1	B	4294	0	4307	156	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	30	3	0
5	A	26	0	16	2	0
5	B	26	0	16	2	0
6	A	12	0	0	3	0
6	B	12	0	0	3	0
7	A	4	0	0	1	0
7	B	12	0	0	0	0
8	B	5	0	0	0	0
9	A	385	0	0	4	0
9	B	250	0	0	5	0
All	All	9258	0	8546	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (185) 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:B:383:GLY:HA3	1:B:384:ASN:CB	1.69	1.19
1:B:383:GLY:CA	1:B:384:ASN:HB2	1.74	1.17
1:B:386:SER:HA	1:B:393:ARG:NH1	1.68	1.06
1:B:385:ILE:HD12	1:B:386:SER:H	1.24	0.99
1:B:297:ASN:OD1	1:B:439:PHE:N	1.95	0.99
1:B:300:LYS:NZ	1:B:400:ARG:HH22	1.60	0.98
1:B:386:SER:HA	1:B:393:ARG:HH12	1.31	0.94
1:B:442:LYS:HG2	1:B:443:GLU:H	1.32	0.93
1:B:326:ARG:HH21	1:B:326:ARG:HG3	1.34	0.92
1:B:368:ASP:H	1:B:392:ALA:HB2	1.33	0.91
1:B:385:ILE:CD1	1:B:386:SER:H	1.87	0.88
1:B:300:LYS:NZ	1:B:400:ARG:NH2	2.22	0.88
1:B:125:ILE:HD11	1:B:160:LEU:HD22	1.56	0.87
1:B:300:LYS:HZ1	1:B:400:ARG:HH22	1.17	0.86
1:A:357:CYS:SG	9:A:1116:HOH:O	2.35	0.85
1:B:302:PRO:O	1:B:447:TRP:HZ3	1.62	0.83
1:B:445:SER:HA	1:B:448:PHE:HB2	1.62	0.80
1:B:298:LEU:HD12	1:B:298:LEU:O	1.83	0.78
1:B:442:LYS:HG2	1:B:443:GLU:N	1.95	0.78
1:B:442:LYS:HD3	1:B:442:LYS:H	1.48	0.77
6:A:705:PYR:CB	5:B:704:TPP:H2	2.14	0.77
1:B:388:PHE:C	1:B:390:PRO:HD3	2.10	0.76
1:B:300:LYS:HZ1	1:B:400:ARG:NH2	1.80	0.76
1:B:270:SER:OG	1:B:271:ASN:N	2.18	0.76
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.70	0.73
1:B:385:ILE:HD12	1:B:386:SER:N	2.02	0.73
1:B:367:ALA:HB3	1:B:392:ALA:HB2	1.71	0.72
1:B:291:LYS:O	1:B:293:ALA:N	2.21	0.72
1:B:299:ALA:O	1:B:300:LYS:HB2	1.89	0.71
1:B:298:LEU:HD12	1:B:298:LEU:C	2.15	0.71
1:B:302:PRO:O	1:B:447:TRP:CZ3	2.43	0.71
1:B:325:ASP:OD1	1:B:347:LYS:NZ	2.22	0.71
1:B:344:GLU:HG3	1:B:511:ARG:HH21	1.55	0.71
1:B:365:GLN:O	1:B:366:ASN:HB3	1.91	0.70
1:B:347:LYS:HG2	1:B:448:PHE:HZ	1.54	0.70
1:B:296:ILE:O	1:B:299:ALA:N	2.22	0.69
1:B:385:ILE:CG1	1:B:386:SER:H	2.02	0.69
1:B:347:LYS:HG2	1:B:448:PHE:CZ	2.28	0.68
1:B:352:LEU:HD13	1:B:381:VAL:HG13	1.74	0.68
1:B:326:ARG:HG3	1:B:326:ARG:NH2	2.00	0.67
1:B:584:THR:OG1	1:B:594:ARG:NE	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:ALA:O	1:B:444:ARG:NH2	2.21	0.66
1:B:366:ASN:HA	1:B:391:GLU:HB2	1.78	0.66
1:B:398:GLU:HB2	1:B:400:ARG:HE	1.60	0.65
1:B:301:LYS:HG3	1:B:368:ASP:HB2	1.77	0.64
1:B:383:GLY:HA3	1:B:384:ASN:HB2	0.81	0.64
1:B:395:ALA:HA	1:B:400:ARG:HG2	1.80	0.63
1:B:302:PRO:HG2	1:B:329:ILE:HG23	1.80	0.63
1:B:392:ALA:C	1:B:394:ARG:H	2.07	0.62
1:B:395:ALA:O	1:B:400:ARG:N	2.28	0.62
1:B:470:LYS:HE2	1:B:646:ASP:HA	1.82	0.62
1:A:499:GLN:OE1	1:A:648:LYS:HD3	1.99	0.61
1:B:435:MET:HA	1:B:435:MET:HE3	1.81	0.61
1:B:299:ALA:HB1	1:B:444:ARG:HH12	1.65	0.60
1:B:456:LYS:N	1:B:456:LYS:HD2	2.16	0.60
1:B:324:SER:O	1:B:328:GLN:HA	2.01	0.60
1:B:365:GLN:HA	1:B:389:ALA:HA	1.84	0.59
1:B:368:ASP:HA	1:B:391:GLU:O	2.03	0.59
1:B:365:GLN:HE21	1:B:387:LYS:HE2	1.66	0.59
1:B:297:ASN:OD1	1:B:439:PHE:HB2	2.03	0.58
1:B:300:LYS:HZ3	1:B:400:ARG:HH22	1.44	0.58
1:B:368:ASP:H	1:B:392:ALA:CB	2.13	0.58
1:B:300:LYS:HZ3	1:B:400:ARG:NH2	2.00	0.57
1:B:295:LEU:HD12	1:B:295:LEU:O	2.04	0.57
1:B:436:SER:C	1:B:438:ILE:H	2.12	0.57
1:B:451:ILE:C	1:B:453:LYS:H	2.13	0.56
1:B:291:LYS:O	1:B:292:ALA:HB3	2.06	0.56
1:B:367:ALA:O	1:B:368:ASP:HB2	2.06	0.56
1:B:367:ALA:O	1:B:368:ASP:CB	2.53	0.56
1:B:389:ALA:O	1:B:392:ALA:N	2.30	0.55
1:B:385:ILE:O	1:B:388:PHE:N	2.24	0.55
1:B:301:LYS:HB2	1:B:447:TRP:CZ2	2.42	0.55
1:B:397:ALA:C	1:B:399:GLY:H	2.13	0.55
1:B:123:ASP:O	1:B:127:ASN:ND2	2.41	0.54
1:B:297:ASN:OD1	1:B:439:PHE:CB	2.56	0.54
6:B:705:PYR:CB	6:B:706:PYR:O	2.55	0.54
1:A:410:PRO:HG3	1:A:424:GLU:OE2	2.09	0.53
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.91	0.53
1:B:391:GLU:HA	1:B:391:GLU:OE1	2.09	0.53
1:B:395:ALA:O	1:B:401:GLY:N	2.40	0.53
1:B:368:ASP:O	1:B:392:ALA:HA	2.09	0.53
1:A:270:SER:HA	1:A:271:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:VAL:HG23	1:B:447:TRP:HH2	1.74	0.52
6:A:705:PYR:CB	5:B:704:TPP:HN42	2.23	0.52
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.92	0.52
1:B:151:ARG:CD	9:B:1030:HOH:O	2.57	0.52
1:B:385:ILE:HD12	1:B:386:SER:CB	2.40	0.52
1:B:299:ALA:HB1	1:B:444:ARG:NH1	2.25	0.51
1:B:393:ARG:O	1:B:393:ARG:HG2	2.09	0.51
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.40	0.51
1:A:295:LEU:HD22	1:A:421:ILE:HD12	1.93	0.51
1:B:364:VAL:O	1:B:365:GLN:C	2.54	0.51
1:B:291:LYS:C	1:B:293:ALA:N	2.66	0.51
1:B:315:ASP:OD1	1:B:318:ARG:NH1	2.44	0.51
1:B:326:ARG:NE	1:B:438:ILE:O	2.39	0.51
1:B:366:ASN:C	1:B:391:GLU:HB3	2.35	0.51
5:A:704:TPP:H2	9:A:895:HOH:O	2.10	0.50
1:B:395:ALA:CA	1:B:400:ARG:HG2	2.41	0.50
1:B:151:ARG:HD2	9:B:1030:HOH:O	2.12	0.49
1:B:125:ILE:HD11	1:B:160:LEU:CD2	2.37	0.49
1:B:293:ALA:O	1:B:297:ASN:ND2	2.46	0.49
1:B:385:ILE:CG1	1:B:386:SER:N	2.72	0.49
1:A:623:GLU:H	1:A:623:GLU:CD	2.20	0.48
1:B:435:MET:O	1:B:438:ILE:N	2.46	0.48
1:B:296:ILE:C	1:B:298:LEU:N	2.68	0.48
1:B:388:PHE:C	1:B:390:PRO:CD	2.85	0.48
1:B:398:GLU:HB2	1:B:400:ARG:NE	2.28	0.48
1:B:285:VAL:O	1:B:289:ILE:HG13	2.14	0.48
1:B:300:LYS:HB3	1:B:368:ASP:OD1	2.14	0.48
1:B:350:ASP:HB3	9:B:863:HOH:O	2.14	0.48
1:B:397:ALA:C	1:B:399:GLY:N	2.72	0.48
1:B:435:MET:HA	1:B:435:MET:CE	2.44	0.48
1:B:436:SER:C	1:B:438:ILE:N	2.72	0.48
1:B:414:ASN:OD1	1:B:419:THR:HG22	2.14	0.47
1:B:586:TRP:CZ3	1:B:595:TYR:CE1	3.02	0.47
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.96	0.47
1:A:324:SER:OG	1:A:347:LYS:HE2	2.14	0.47
1:A:494:THR:HG22	1:A:517:ILE:HB	1.97	0.47
1:B:367:ALA:HB1	1:B:370:ILE:HG23	1.96	0.47
1:B:394:ARG:HE	1:B:400:ARG:HH11	1.62	0.47
1:B:434:MET:O	1:B:438:ILE:HG12	2.15	0.47
1:B:394:ARG:C	1:B:396:ALA:N	2.71	0.47
1:B:367:ALA:CB	1:B:392:ALA:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:704:TPP:H7'2	6:B:705:PYR:O3	2.15	0.46
1:B:364:VAL:HG12	1:B:365:GLN:N	2.30	0.46
1:B:392:ALA:C	1:B:394:ARG:N	2.73	0.46
1:A:119:LEU:HD12	1:A:119:LEU:HA	1.79	0.46
1:B:366:ASN:CG	1:B:366:ASN:O	2.58	0.45
1:B:436:SER:O	1:B:438:ILE:N	2.49	0.45
1:B:451:ILE:HA	1:B:454:TRP:CD1	2.51	0.45
1:B:456:LYS:N	1:B:456:LYS:CD	2.79	0.45
1:B:298:LEU:C	1:B:298:LEU:CD1	2.85	0.45
1:B:297:ASN:HD21	1:B:438:ILE:HA	1.81	0.45
1:B:364:VAL:HG12	1:B:365:GLN:H	1.81	0.45
1:B:151:ARG:HG3	9:B:968:HOH:O	2.17	0.45
1:B:301:LYS:C	1:B:447:TRP:CZ3	2.94	0.45
4:B:702:FAD:HM73	4:B:702:FAD:HM81	1.79	0.45
1:B:395:ALA:HB1	1:B:401:GLY:N	2.33	0.44
1:B:435:MET:O	1:B:438:ILE:HB	2.18	0.44
1:B:394:ARG:HE	1:B:400:ARG:NH1	2.15	0.44
1:B:136:PRO:HG3	1:B:142:ALA:HB2	2.00	0.44
1:A:597:HIS:CG	1:A:598:THR:H	2.36	0.44
1:B:324:SER:O	1:B:328:GLN:CA	2.65	0.44
1:A:579:GLU:O	1:A:579:GLU:HG3	2.18	0.43
1:A:295:LEU:CD2	1:A:421:ILE:HD12	2.48	0.43
6:A:705:PYR:CA	7:A:708:OXY:O2	2.66	0.43
1:B:273:LEU:HD12	1:B:275:GLN:HB2	1.99	0.43
1:B:640:LEU:C	1:B:640:LEU:HD23	2.43	0.43
1:B:390:PRO:HA	1:B:393:ARG:HB3	2.00	0.43
1:B:580:GLN:HG3	9:B:966:HOH:O	2.18	0.43
1:B:297:ASN:OD1	1:B:439:PHE:CA	2.65	0.43
1:B:395:ALA:CB	1:B:401:GLY:HA3	2.49	0.43
1:B:437:LYS:H	1:B:437:LYS:HG2	1.45	0.43
1:A:270:SER:HB2	1:A:271:ASN:O	2.19	0.43
9:A:895:HOH:O	6:B:705:PYR:CA	2.67	0.42
1:B:292:ALA:HA	1:B:295:LEU:HB3	2.02	0.42
1:B:380:ARG:HD3	4:B:702:FAD:N5	2.34	0.42
1:A:539:LYS:NZ	9:A:807:HOH:O	2.51	0.42
1:B:298:LEU:O	1:B:299:ALA:HB3	2.18	0.42
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.01	0.42
1:B:365:GLN:NE2	1:B:387:LYS:HE2	2.32	0.42
1:B:390:PRO:C	1:B:392:ALA:N	2.78	0.42
4:B:702:FAD:H8A	4:B:702:FAD:H2B	1.88	0.42
1:B:321:LYS:HE2	1:B:325:ASP:OD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:GLU:CB	1:B:400:ARG:HE	2.27	0.42
1:B:580:GLN:NE2	1:B:646:ASP:O	2.52	0.42
1:B:413:ILE:HG22	1:B:414:ASN:ND2	2.35	0.42
1:B:153:SER:HB3	1:B:538:ALA:HB1	2.02	0.41
1:A:647:LYS:H	1:A:647:LYS:HG2	1.52	0.41
1:B:338:LEU:HD22	1:B:510:TRP:CD1	2.56	0.41
1:B:301:LYS:H	1:B:301:LYS:HG2	1.61	0.41
1:A:226:LEU:HB3	1:A:227:PRO:HD3	2.02	0.41
1:B:172:THR:HB	1:B:173:PRO:HD3	2.03	0.41
1:B:390:PRO:C	1:B:392:ALA:H	2.27	0.41
1:B:465:GLU:OE1	1:B:475:THR:OG1	2.37	0.41
1:B:366:ASN:HA	1:B:391:GLU:CB	2.49	0.41
1:B:368:ASP:CA	1:B:392:ALA:HA	2.51	0.41
1:B:576:ASN:OD1	1:B:578:GLU:HB3	2.21	0.41
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.56	0.40
1:B:584:THR:HG1	1:B:594:ARG:HE	1.61	0.40
1:A:376:ARG:HD3	4:A:703:FAD:O2A	2.22	0.40
1:B:298:LEU:HD21	1:B:400:ARG:O	2.21	0.40
1:B:303:VAL:HB	1:B:370:ILE:HG22	2.03	0.40
1:B:329:ILE:HG22	1:B:330:PRO:HD2	2.03	0.40
1:B:394:ARG:HH11	1:B:400:ARG:NH1	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	539/677 (80%)	531 (98%)	8 (2%)	0	100	100
1	B	562/677 (83%)	515 (92%)	30 (5%)	17 (3%)	3	0
All	All	1101/1354 (81%)	1046 (95%)	38 (4%)	17 (2%)	8	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	272	ALA
1	B	300	LYS
1	B	364	VAL
1	B	367	ALA
1	B	368	ASP
1	B	385	ILE
1	B	591	TYR
1	B	270	SER
1	B	384	ASN
1	B	389	ALA
1	B	452	ASN
1	B	365	GLN
1	B	435	MET
1	B	437	LYS
1	B	273	LEU
1	B	328	GLN
1	B	366	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	445/556 (80%)	438 (98%)	7 (2%)	55	50
1	B	462/556 (83%)	432 (94%)	30 (6%)	15	6
All	All	907/1112 (82%)	870 (96%)	37 (4%)	27	16

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	LEU
1	A	265	LYS
1	A	281	GLN
1	A	283	GLU
1	A	357	CYS
1	A	623	GLU

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Mol	Chain	Res	Type
1	A	636	LYS
1	B	127	ASN
1	B	265	LYS
1	B	273	LEU
1	B	274	ASN
1	B	287	GLN
1	B	298	LEU
1	B	300	LYS
1	B	301	LYS
1	B	302	PRO
1	B	326	ARG
1	B	329	ILE
1	B	347	LYS
1	B	352	LEU
1	B	362	LEU
1	B	366	ASN
1	B	370	ILE
1	B	371	ILE
1	B	385	ILE
1	B	386	SER
1	B	390	PRO
1	B	435	MET
1	B	437	LYS
1	B	440	PRO
1	B	443	GLU
1	B	453	LYS
1	B	457	GLU
1	B	463	MET
1	B	465	GLU
1	B	600	GLN
1	B	614	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	GLN
1	A	599	HIS
1	B	126	HIS
1	B	355	HIS
1	B	512	ASN
1	B	580	GLN
1	B	593	HIS

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, 4 are monoatomic - leaving 17 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	$\# Z > 2$
7	OXY	A	708	-	1,1,1	0.16	0	-		
7	OXY	B	712	-	1,1,1	0.28	0	-		
8	PO4	B	713	-	4,4,4	1.28	0	6,6,6	0.91	0
6	PYR	B	706	-	5,5,5	1.71	2 (40%)	3,6,6	1.47	1 (33%)
6	PYR	A	705	-	5,5,5	2.75	2 (40%)	3,6,6	1.37	1 (33%)
6	PYR	A	706	-	5,5,5	1.65	1 (20%)	3,6,6	1.22	0
6	PYR	B	705	-	5,5,5	2.47	3 (60%)	3,6,6	1.47	0
7	OXY	A	707	-	1,1,1	0.12	0	-		
7	OXY	B	707	-	1,1,1	0.09	0	-		
7	OXY	B	708	-	1,1,1	0.15	0	-		
5	TPP	B	704	3	26,27,27	1.48	4 (15%)	38,40,40	2.10	12 (31%)
4	FAD	A	703	-	58,58,58	1.56	10 (17%)	85,89,89	1.90	23 (27%)
4	FAD	B	702	-	58,58,58	2.10	21 (36%)	85,89,89	1.61	14 (16%)
5	TPP	A	704	3	26,27,27	1.63	6 (23%)	38,40,40	1.93	8 (21%)
7	OXY	B	710	-	1,1,1	0.11	0	-		
7	OXY	B	709	-	1,1,1	0.14	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	OXY	B	711	-	1,1,1	0.21	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
6	PYR	B	706	-	-	4/4/4/4	-
6	PYR	A	705	-	-	4/4/4/4	-
6	PYR	A	706	-	-	0/4/4/4	-
6	PYR	B	705	-	-	4/4/4/4	-
5	TPP	B	704	3	-	2/17/17/17	0/2/2/2
4	FAD	A	703	-	-	2/34/50/50	0/6/6/6
4	FAD	B	702	-	-	4/34/50/50	0/6/6/6
5	TPP	A	704	3	-	1/17/17/17	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	FAD	PA-O3P	-5.70	1.53	1.59
4	B	702	FAD	C8A-N9A	-4.61	1.29	1.37
4	A	703	FAD	C4X-N5	4.56	1.40	1.30
4	B	702	FAD	P-O3P	-4.21	1.55	1.59
6	A	705	PYR	OXT-C	-4.16	1.19	1.30
6	A	705	PYR	CA-C	-4.15	1.40	1.54
5	A	704	TPP	C5-C4	4.07	1.43	1.35
4	B	702	FAD	C10-N1	3.87	1.41	1.33
4	A	703	FAD	C10-N1	3.60	1.40	1.33
6	B	705	PYR	CA-C	-3.59	1.42	1.54
4	A	703	FAD	PA-O3P	-3.44	1.55	1.59
5	B	704	TPP	C5-C4	3.43	1.42	1.35
5	A	704	TPP	C2-S1	3.40	1.79	1.69
4	B	702	FAD	O4-C4	-3.37	1.17	1.23
4	B	702	FAD	O3'-C3'	-3.33	1.34	1.43
4	B	702	FAD	C1'-N10	-3.18	1.40	1.47
4	B	702	FAD	C4X-C10	-3.16	1.34	1.44
5	B	704	TPP	C2'-N1'	3.16	1.39	1.34
5	A	704	TPP	C4'-N4'	3.07	1.42	1.34
6	B	705	PYR	OXT-C	-2.97	1.22	1.30
6	A	706	PYR	CA-C	-2.96	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	704	TPP	C6'-N1'	2.94	1.40	1.34
4	B	702	FAD	C2B-C3B	-2.89	1.45	1.53
5	B	704	TPP	C2-S1	2.83	1.77	1.69
4	B	702	FAD	C2B-C1B	-2.80	1.44	1.53
4	A	703	FAD	C2'-C3'	2.78	1.58	1.53
4	A	703	FAD	P-O3P	2.76	1.62	1.59
6	B	706	PYR	CA-C	-2.76	1.45	1.54
4	B	702	FAD	O2-C2	-2.71	1.19	1.24
4	B	702	FAD	C4X-N5	2.70	1.36	1.30
5	B	704	TPP	C7'-C5'	2.68	1.56	1.51
4	A	703	FAD	C8A-N7A	2.60	1.36	1.31
4	B	702	FAD	C5X-N5	-2.59	1.34	1.39
6	B	705	PYR	O3-CA	-2.59	1.17	1.23
4	B	702	FAD	C2A-N1A	-2.57	1.29	1.33
4	B	702	FAD	PA-O2A	-2.48	1.43	1.55
5	A	704	TPP	C7'-C5'	2.46	1.55	1.51
4	B	702	FAD	O4B-C4B	-2.41	1.39	1.45
4	B	702	FAD	C1B-N9A	-2.40	1.39	1.46
4	B	702	FAD	C5A-N7A	-2.37	1.34	1.39
4	A	703	FAD	C1'-N10	-2.31	1.42	1.47
4	B	702	FAD	P-O2P	-2.29	1.44	1.55
4	A	703	FAD	C7M-C7	2.26	1.55	1.51
4	A	703	FAD	C2-N1	2.18	1.41	1.36
6	B	706	PYR	OXT-C	-2.17	1.24	1.30
5	A	704	TPP	PB-O2B	-2.08	1.47	1.54
4	A	703	FAD	C4X-C4	2.04	1.52	1.44
4	B	702	FAD	C2'-C3'	2.04	1.57	1.53
4	B	702	FAD	C3B-C4B	-2.01	1.47	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	TPP	CM2-C2'-N1'	7.13	124.80	117.20
5	A	704	TPP	CM2-C2'-N1'	6.81	124.45	117.20
4	A	703	FAD	C5A-C4A-N3A	-6.23	118.14	126.72
4	B	702	FAD	C5A-C4A-N3A	-5.76	118.79	126.72
5	B	704	TPP	N1'-C2'-N3'	-4.65	117.80	125.53
5	A	704	TPP	N1'-C2'-N3'	-4.53	118.00	125.53
4	B	702	FAD	C4A-C5A-N7A	-4.48	105.46	110.58
4	A	703	FAD	C4X-C10-N10	4.30	122.63	116.48
4	B	702	FAD	N3A-C4A-N9A	4.16	134.24	127.17
5	B	704	TPP	C6'-N1'-C2'	4.10	122.81	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	703	FAD	C4-C4X-N5	4.08	123.84	118.21
4	A	703	FAD	N3A-C4A-N9A	3.84	133.69	127.17
5	A	704	TPP	C6'-N1'-C2'	3.81	122.33	116.07
4	A	703	FAD	C2A-N3A-C4A	3.79	121.09	111.83
4	B	702	FAD	O4-C4-C4X	-3.78	116.54	126.53
4	B	702	FAD	C4-N3-C2	-3.72	119.03	125.64
4	A	703	FAD	C5'-C4'-C3'	-3.62	105.40	112.22
4	A	703	FAD	O2A-PA-O3P	3.47	116.65	107.27
4	B	702	FAD	C4X-C4-N3	3.39	121.89	113.25
4	B	702	FAD	C5A-N7A-C8A	3.36	108.74	103.45
4	A	703	FAD	C4A-C5A-N7A	-3.34	106.76	110.58
4	A	703	FAD	O2-C2-N1	-3.31	116.31	121.80
5	A	704	TPP	CM4-C4-C5	-3.25	119.42	127.75
4	A	703	FAD	C4-N3-C2	-3.21	119.94	125.64
5	B	704	TPP	CM4-C4-C5	-3.09	119.83	127.75
4	B	702	FAD	C2A-N3A-C4A	3.04	119.25	111.83
4	A	703	FAD	N9A-C8A-N7A	-3.01	109.67	113.94
4	A	703	FAD	N3A-C2A-N1A	-3.00	124.04	128.58
4	A	703	FAD	C10-C4X-N5	-3.00	118.68	124.81
4	A	703	FAD	O2-C2-N3	2.97	124.28	118.58
4	A	703	FAD	C10-N1-C2	2.94	123.21	116.85
4	A	703	FAD	C5A-N7A-C8A	2.91	108.03	103.45
5	A	704	TPP	C7'-N3-C2	-2.84	117.56	123.48
4	A	703	FAD	C4X-C4-N3	2.75	120.25	113.25
5	A	704	TPP	CM4-C4-N3	2.69	126.78	120.57
5	B	704	TPP	N4'-C4'-N3'	-2.62	113.50	117.03
5	B	704	TPP	O3B-PB-O2B	2.57	117.43	107.80
4	A	703	FAD	O4-C4-C4X	-2.56	119.78	126.53
4	B	702	FAD	N3A-C2A-N1A	-2.55	124.73	128.58
4	B	702	FAD	C9A-C5X-N5	-2.42	119.89	122.45
5	B	704	TPP	C7'-N3-C2	-2.39	118.50	123.48
4	B	702	FAD	C4X-C10-N1	-2.39	118.74	124.59
6	B	706	PYR	OXT-C-CA	2.36	120.14	113.59
5	A	704	TPP	C5'-C6'-N1'	-2.35	120.01	123.83
4	B	702	FAD	C4A-N9A-C8A	2.33	108.19	105.74
4	B	702	FAD	N9A-C8A-N7A	-2.32	110.64	113.94
6	A	705	PYR	O3-CA-CB	2.30	124.93	119.77
4	A	703	FAD	O4B-C4B-C5B	-2.29	101.99	109.33
5	B	704	TPP	C7'-N3-C4	2.29	128.42	122.36
4	B	702	FAD	C10-N1-C2	2.24	121.70	116.85
4	A	703	FAD	C1'-N10-C9A	2.22	124.94	120.63
5	B	704	TPP	C5'-C4'-N3'	2.15	124.46	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	704	TPP	O3A-PA-O1A	2.13	117.11	110.70
5	B	704	TPP	C5'-C6'-N1'	-2.07	120.46	123.83
4	A	703	FAD	O2P-P-O3P	-2.06	101.71	107.27
5	B	704	TPP	C7-C6-C5	-2.03	106.36	112.73
4	A	703	FAD	C5A-C4A-N9A	2.03	108.02	105.81
4	A	703	FAD	C4X-C10-N1	-2.01	119.67	124.59
5	A	704	TPP	C2'-N3'-C4'	2.00	121.18	118.10

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	702	FAD	P-O3P-PA-O5B
5	B	704	TPP	PA-O3A-PB-O2B
6	A	705	PYR	O-C-CA-O3
6	A	705	PYR	O-C-CA-CB
6	A	705	PYR	OXT-C-CA-O3
6	A	705	PYR	OXT-C-CA-CB
6	B	705	PYR	O-C-CA-O3
6	B	705	PYR	OXT-C-CA-O3
6	B	706	PYR	O-C-CA-O3
6	B	706	PYR	O-C-CA-CB
4	A	703	FAD	P-O3P-PA-O5B
4	A	703	FAD	C2B-C1B-N9A-C8A
6	B	705	PYR	O-C-CA-CB
5	B	704	TPP	PA-O3A-PB-O1B
4	B	702	FAD	C5'-O5'-P-O1P
6	B	705	PYR	OXT-C-CA-CB
6	B	706	PYR	OXT-C-CA-O3
6	B	706	PYR	OXT-C-CA-CB
4	B	702	FAD	C2B-C1B-N9A-C8A
5	A	704	TPP	C5-C6-C7-O7
4	B	702	FAD	PA-O3P-P-O2P

There are no ring outliers.

8 monomers are involved in 11 short contacts:

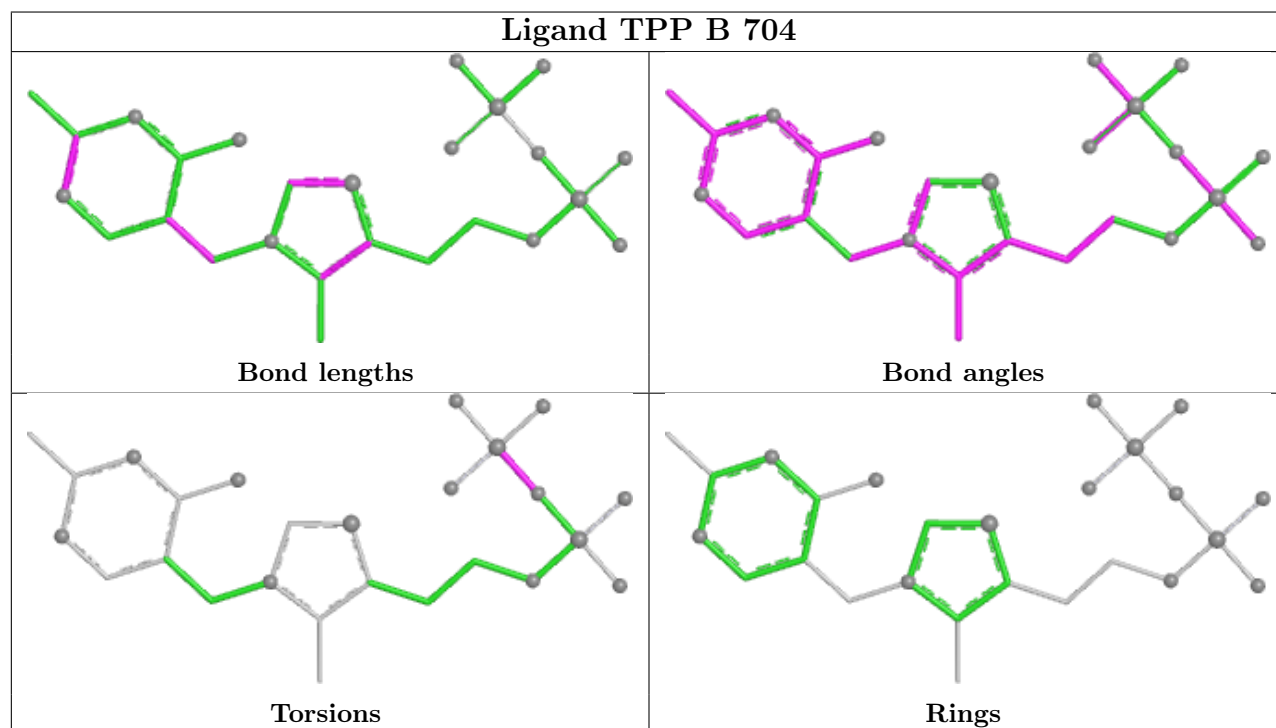
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	708	OXY	1	0
6	B	706	PYR	1	0
6	A	705	PYR	3	0

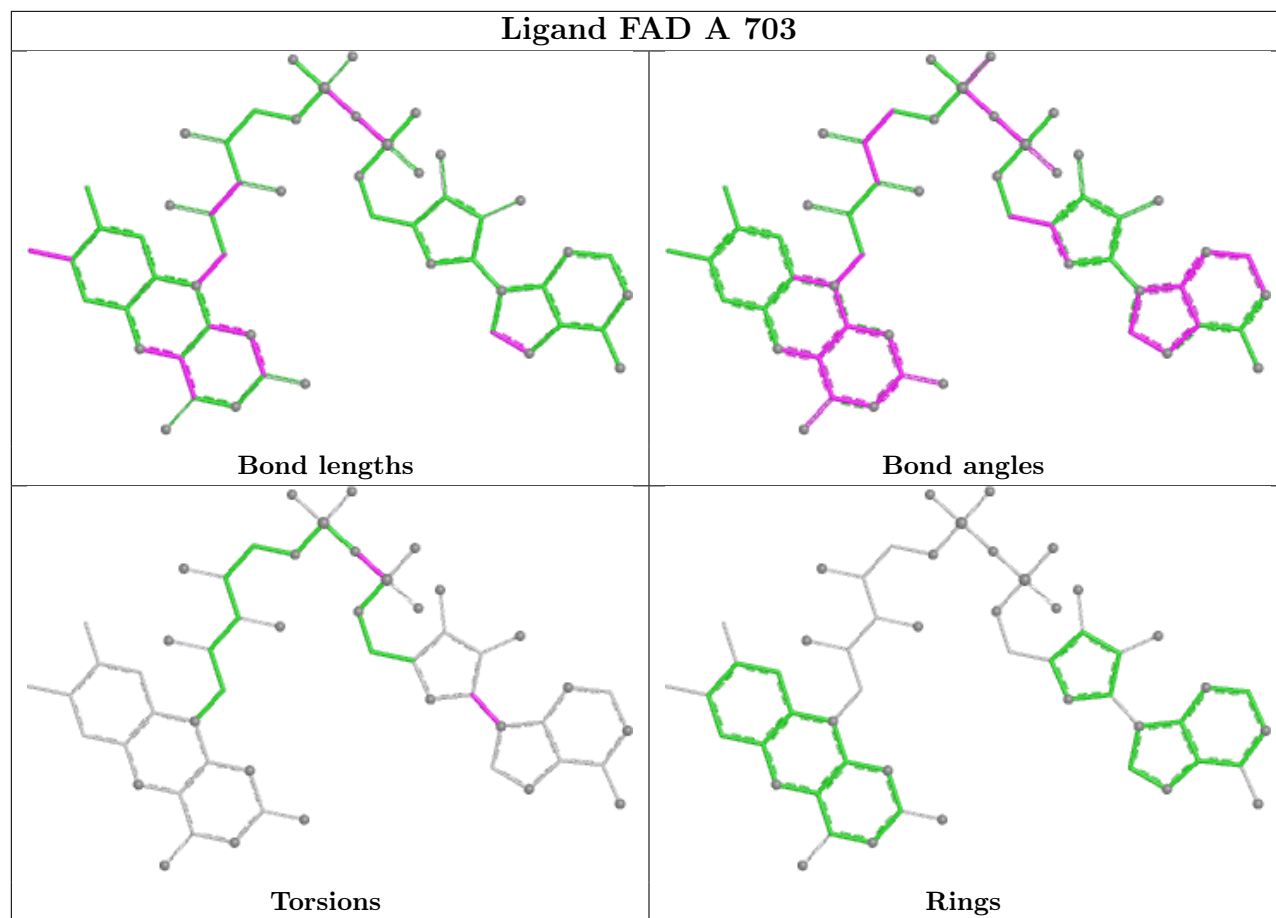
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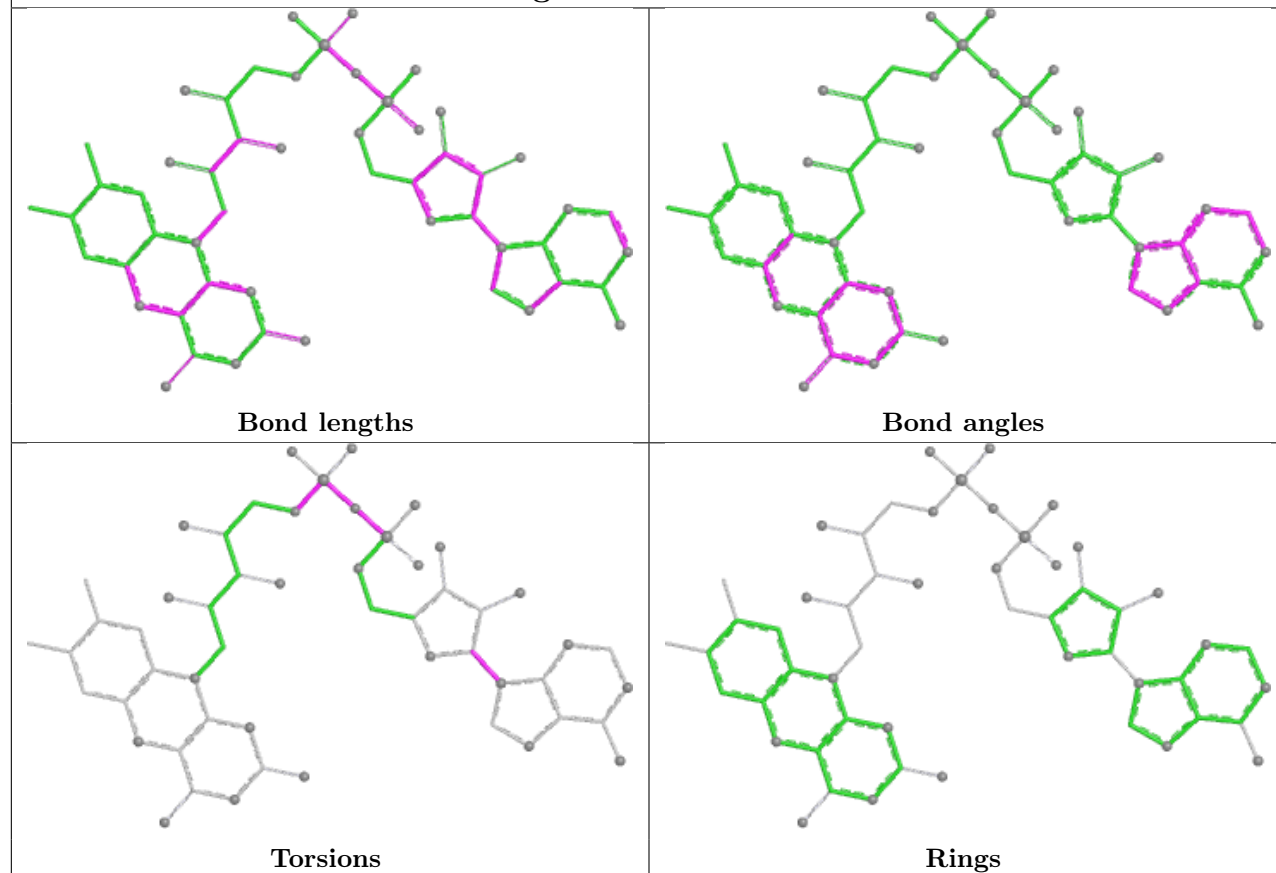
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	705	PYR	3	0
5	B	704	TPP	2	0
4	A	703	FAD	1	0
4	B	702	FAD	3	0
5	A	704	TPP	2	0

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.

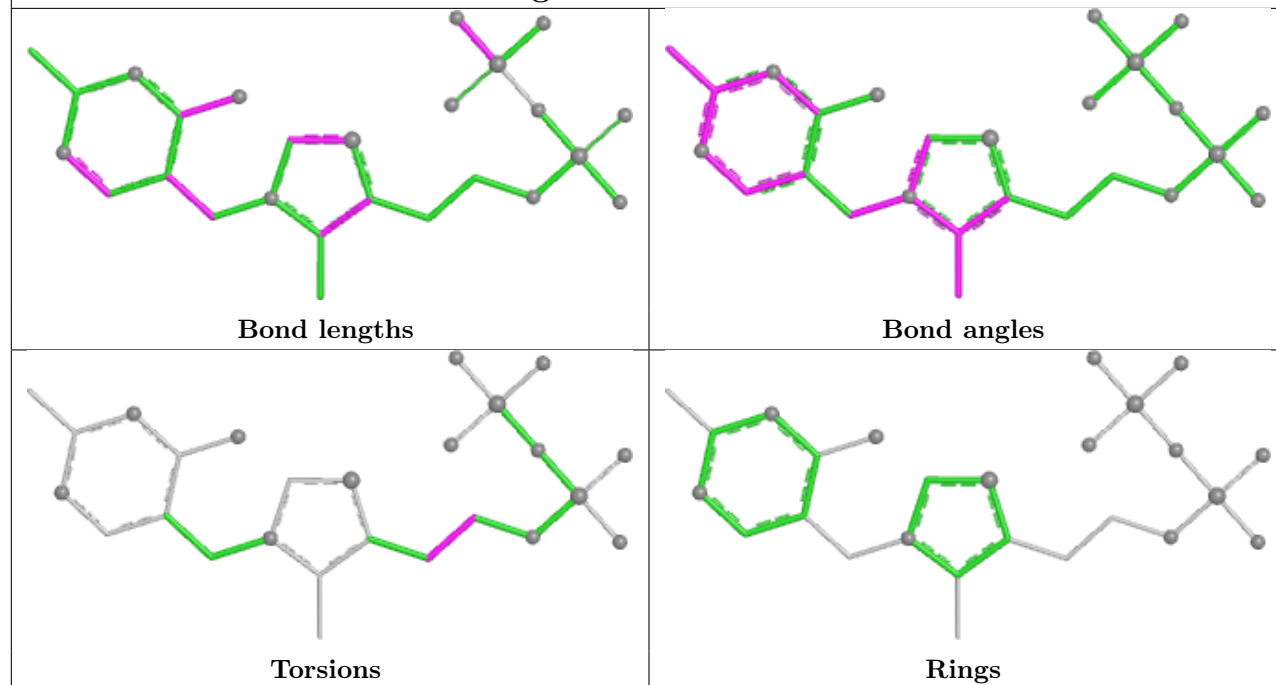




Ligand FAD B 702



Ligand TPP A 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	542/677 (80%)	-0.30	22 (4%) 41 51	11, 29, 66, 115	3 (0%)
1	B	564/677 (83%)	0.57	115 (20%) 3 3	18, 40, 122, 152	0
All	All	1106/1354 (81%)	0.14	137 (12%) 8 11	11, 32, 108, 152	3 (0%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	273	LEU	8.6
1	B	447	TRP	6.5
1	B	448	PHE	6.1
1	B	127	ASN	6.0
1	B	385	ILE	5.8
1	B	292	ALA	5.7
1	B	272	ALA	5.6
1	A	280	ALA	5.6
1	B	367	ALA	5.5
1	A	83	PRO	5.4
1	B	454	TRP	5.3
1	B	591	TYR	4.9
1	B	83	PRO	4.7
1	B	441	VAL	4.7
1	B	416	VAL	4.7
1	B	362	LEU	4.7
1	A	597	HIS	4.7
1	B	590	PHE	4.6
1	B	462	TYR	4.6
1	B	299	ALA	4.6
1	A	599	HIS	4.5
1	B	461	ALA	4.4
1	B	451	ILE	4.3
1	B	401	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	298	LEU	4.3
1	B	594	ARG	4.3
1	B	293	ALA	4.3
1	B	284	PHE	4.1
1	B	463	MET	4.0
1	B	369	LEU	4.0
1	B	458	TYR	3.8
1	B	396	ALA	3.8
1	B	276	LEU	3.7
1	B	445	SER	3.7
1	B	366	ASN	3.7
1	B	296	ILE	3.7
1	B	439	PHE	3.7
1	B	595	TYR	3.6
1	B	368	ASP	3.6
1	B	460	TYR	3.5
1	A	268	LEU	3.5
1	B	421	ILE	3.5
1	B	300	LYS	3.5
1	B	270	SER	3.4
1	A	271	ASN	3.4
1	B	295	LEU	3.4
1	A	270	SER	3.3
1	A	648	LYS	3.3
1	B	301	LYS	3.3
1	B	417	VAL	3.3
1	B	365	GLN	3.3
1	B	379	ASP	3.2
1	B	600	GLN	3.2
1	B	384	ASN	3.2
1	B	581	GLY	3.2
1	B	449	ALA	3.2
1	B	589	LEU	3.2
1	B	586	TRP	3.1
1	B	382	THR	3.1
1	B	370	ILE	3.1
1	B	593	HIS	3.1
1	B	302	PRO	3.1
1	B	347	LYS	3.1
1	A	596	SER	3.1
1	B	389	ALA	3.1
1	B	411	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	442	LYS	3.0
1	B	400	ARG	2.9
1	A	284	PHE	2.9
1	A	463	MET	2.9
1	B	388	PHE	2.9
1	B	303	VAL	2.9
1	B	646	ASP	2.8
1	B	418	GLN	2.8
1	B	452	ASN	2.8
1	A	265	LYS	2.8
1	B	275	GLN	2.7
1	B	467	PRO	2.7
1	B	468	GLY	2.7
1	B	436	SER	2.6
1	B	390	PRO	2.6
1	B	453	LYS	2.6
1	B	466	THR	2.6
1	B	329	ILE	2.6
1	B	457	GLU	2.6
1	B	197	GLY	2.6
1	A	269	PRO	2.5
1	B	291	LYS	2.5
1	A	282	ASP	2.5
1	B	380	ARG	2.5
1	B	444	ARG	2.5
1	B	327	ALA	2.5
1	B	285	VAL	2.5
1	B	125	ILE	2.4
1	B	392	ALA	2.4
1	B	279	ARG	2.4
1	B	386	SER	2.4
1	B	387	LYS	2.4
1	B	415	LYS	2.4
1	B	413	ILE	2.4
1	A	461	ALA	2.4
1	B	271	ASN	2.4
1	B	402	GLY	2.4
1	B	199	ASP	2.3
1	B	464	GLU	2.3
1	B	397	ALA	2.3
1	B	438	ILE	2.3
1	B	394	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	277	THR	2.3
1	B	440	PRO	2.3
1	A	579	GLU	2.3
1	B	420	GLN	2.3
1	A	462	TYR	2.2
1	B	410	PRO	2.2
1	A	281	GLN	2.2
1	B	580	GLN	2.2
1	B	357	CYS	2.2
1	B	584	THR	2.2
1	B	592	GLU	2.2
1	B	274	ASN	2.2
1	B	596	SER	2.2
1	B	459	PRO	2.2
1	B	446	GLU	2.1
1	B	399	GLY	2.1
1	A	647	LYS	2.1
1	B	297	ASN	2.1
1	A	266	THR	2.1
1	B	363	ALA	2.1
1	B	636	LYS	2.1
1	B	364	VAL	2.1
1	A	598	THR	2.0
1	B	126	HIS	2.0
1	B	328	GLN	2.0
1	B	283	GLU	2.0
1	A	354	MET	2.0
1	B	383	GLY	2.0
1	B	326	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

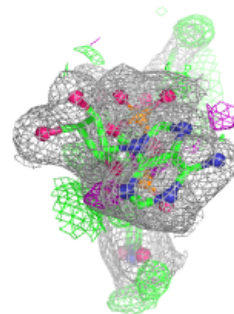
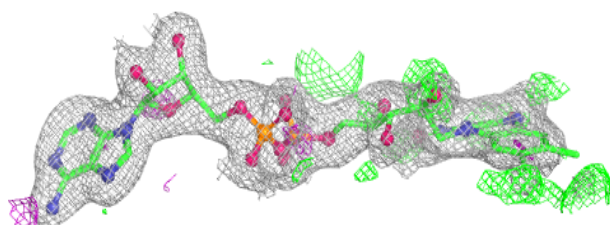
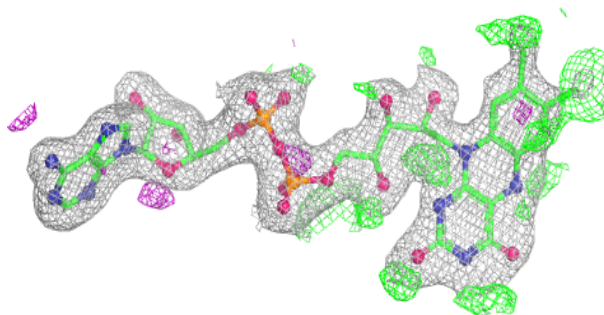
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PYR	A	705	6/6	0.75	0.18	41,58,60,72	0
6	PYR	A	706	6/6	0.82	0.29	110,110,111,111	0
6	PYR	B	706	6/6	0.82	0.27	87,89,91,91	0
7	OXY	B	712	2/2	0.82	0.18	54,54,54,56	0
7	OXY	B	711	2/2	0.83	0.28	60,60,60,62	0
7	OXY	B	709	2/2	0.84	0.20	57,57,57,60	0
8	PO4	B	713	5/5	0.84	0.15	74,75,77,79	0
7	OXY	B	708	2/2	0.90	0.19	56,56,56,59	0
7	OXY	B	710	2/2	0.91	0.35	67,67,67,67	0
6	PYR	B	705	6/6	0.92	0.14	53,54,65,68	0
7	OXY	A	707	2/2	0.92	0.37	74,74,74,76	0
7	OXY	A	708	2/2	0.92	0.26	61,61,61,63	0
7	OXY	B	707	2/2	0.93	0.23	68,68,68,70	0
4	FAD	B	702	53/53	0.95	0.10	33,42,69,74	0
2	K	B	701	1/1	0.97	0.08	39,39,39,39	0
3	MG	A	702	1/1	0.98	0.03	29,29,29,29	0
4	FAD	A	703	53/53	0.98	0.06	22,31,73,75	0
3	MG	B	703	1/1	0.99	0.02	27,27,27,27	0
5	TPP	A	704	26/26	0.99	0.05	20,26,29,31	0
5	TPP	B	704	26/26	0.99	0.04	18,23,26,28	0
2	K	A	701	1/1	0.99	0.07	31,31,31,31	0

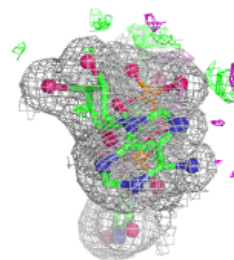
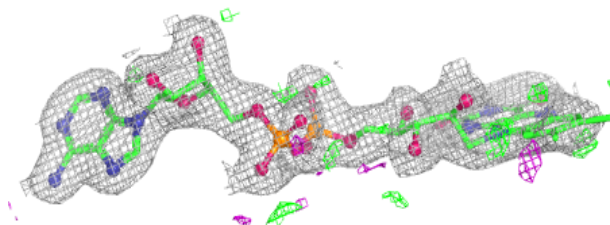
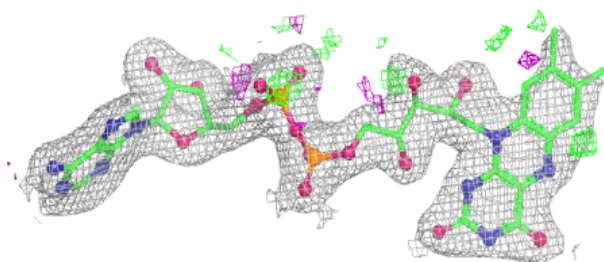
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 702:

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

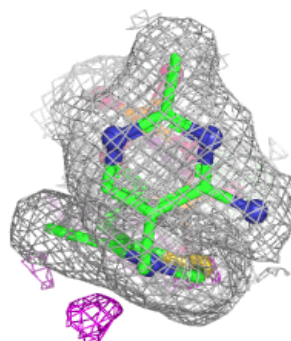
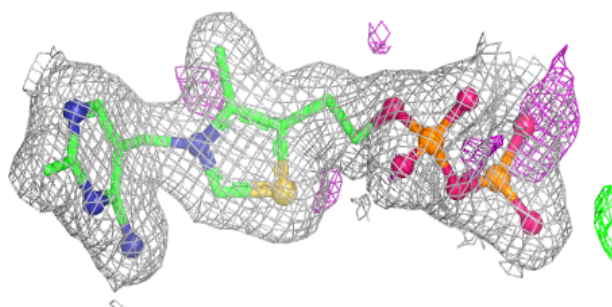
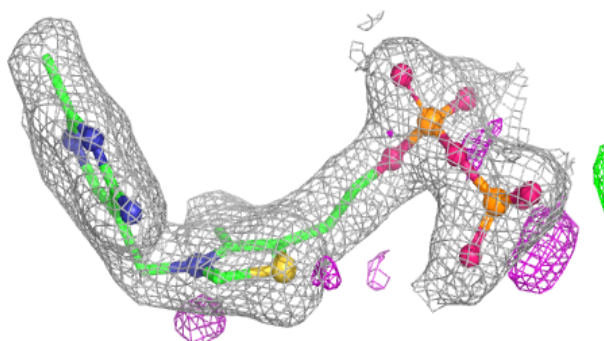
**Electron density around FAD A 703:**

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

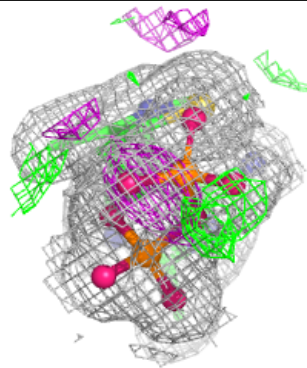
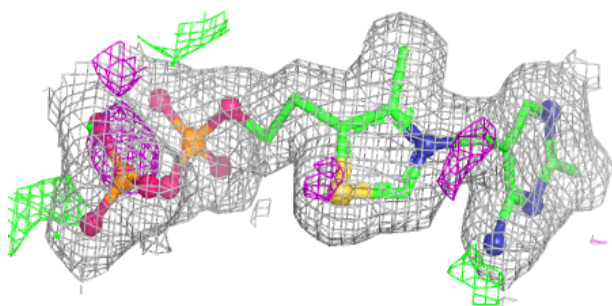
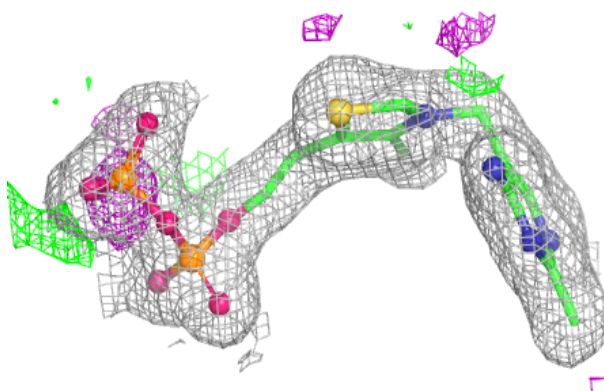


Electron density around TPP A 704:

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

**Electron density around TPP B 704:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.