



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:46 am BST

PDB ID : 5IMS
Title : Saccharomyces cerevisiae acetohydroxyacid synthase
Authors : Guddat, L.W.; Lonhienne, T.
Deposited on : 2016-03-06
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 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

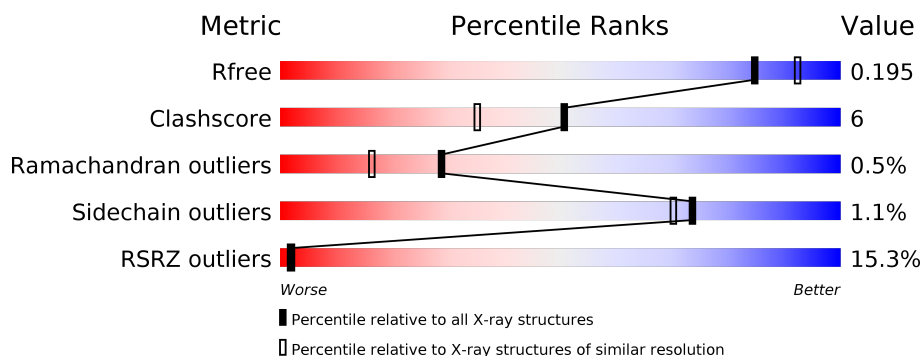
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

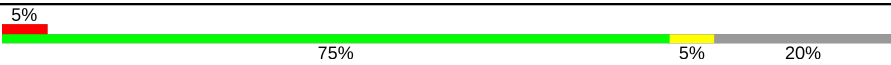

The reported resolution of this entry is 1.98 Å.

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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	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
7	ACT	A	708	-	-	X	-
7	ACT	B	712	-	-	X	-
7	ACT	B	713	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9452 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	541	Total	C	N	O	S	0	3	0
			4111	2604	709	779	19			
1	B	567	Total	C	N	O	S	0	1	0
			4325	2740	747	818	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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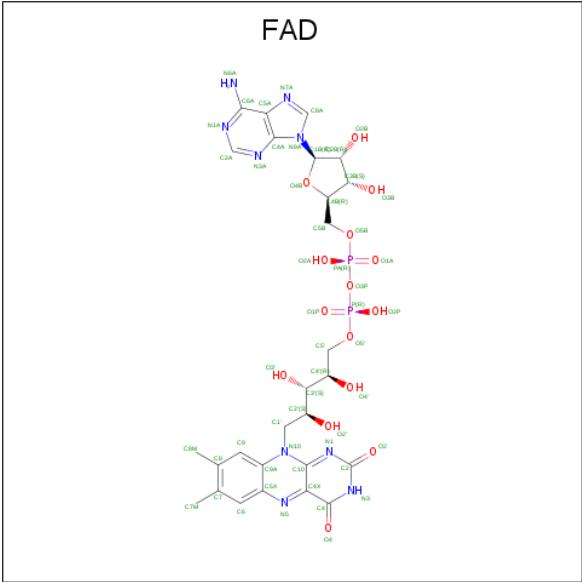
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Chain	Residue	Modelled	Actual	Comment	Reference
B	31	THR	-	expression tag	UNP P07342
B	32	ALA	-	expression tag	UNP P07342
B	33	ALA	-	expression tag	UNP P07342
B	34	ALA	-	expression tag	UNP P07342
B	35	LYS	-	expression tag	UNP P07342
B	36	PHE	-	expression 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 (three-letter code: K) (formula: K).

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

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

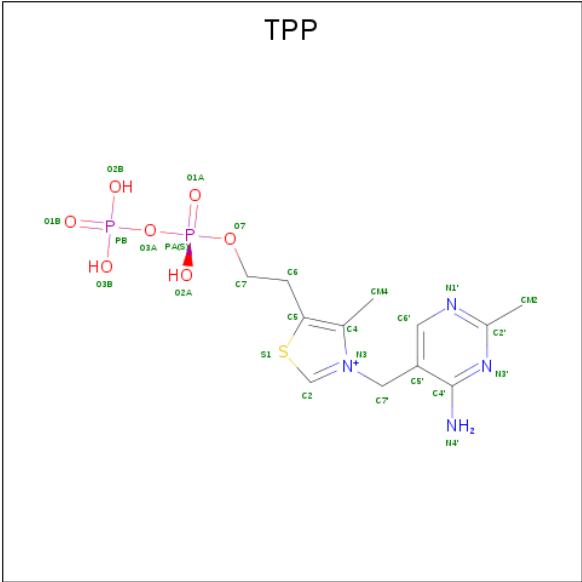


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

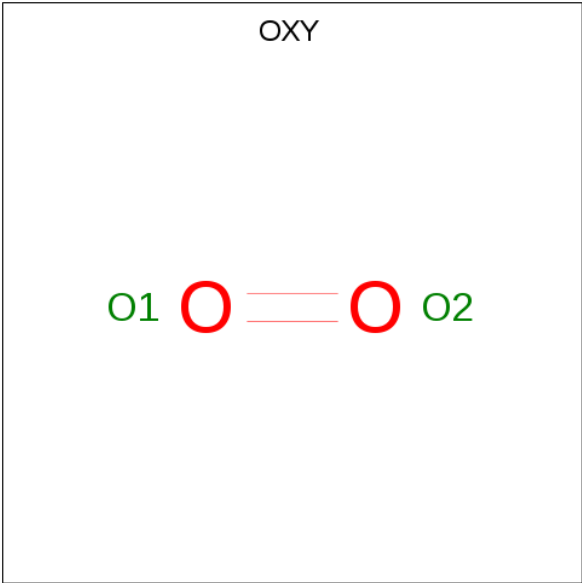
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

- Molecule 6 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



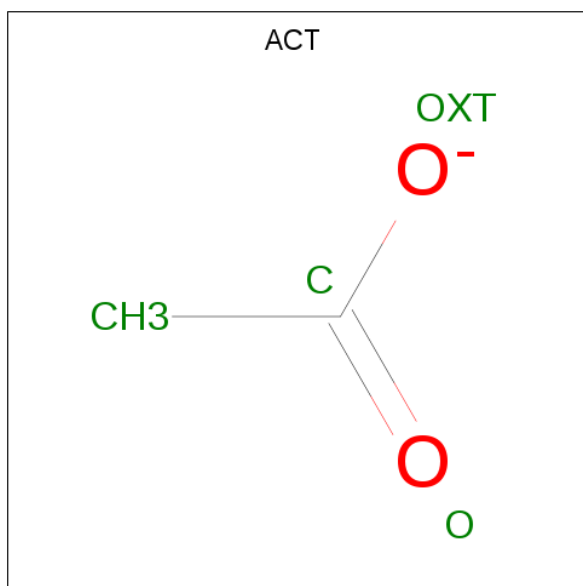
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			2	2		
6	A	1	Total	O	0	0
			2	2		

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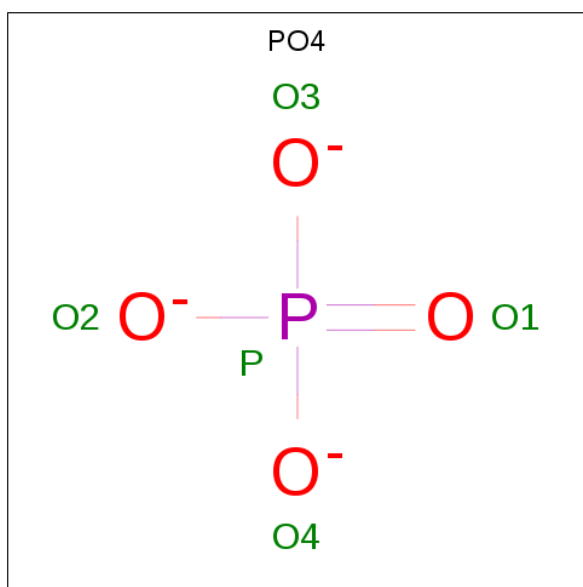
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0
6	B	1	Total O 2 2	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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	492	Total	O	0	0
			492	492		
9	B	327	Total	O	0	0
			327	327		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 5% 75% 5% 20%
- MET HIS HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY GLY MET LYS GLU THR ALA ALA LYS PHE GLU ARG ALN HIS MET ASP SER PRO LEU GLY THR ASP ASP ASP LYS ALA MET GLY SER ALA PRO SER PHE ASN VAL ASP PRO LEU GLU GLN PRO ALA
- R376 R385 R386 R387 R388 R393 R410 R413 R417 R421 R454 R455 R456 R457 R458 R459 R460 R461 R462 R463 R464 R465 R466 R467 R468 R469 R470 R494 R495 R517 R518 R519 R520 R521 R522 R529 R547 R571 R579 R580 R581 R582 R583 R584 R585 R586 R587 R588 R589 R590 R591 R592 R593 R594 R595 R596 R597 R598 R599 R600 R601 R602 R603 R604 R605 R606 R607 R608 R609 R610 R611 R612 R613 R614 R615 R616 R617 R618 R619 R620 R621 R622 R623 R624 R625 R626 R627 R628 R629 R630 R631 R632 R633 R634 R635 R636 R637 R638 R639 R640 R641 R642 R643 R644 R645 R646 R647 R648 R649 R650 R651 R652 R653 R654 R655 R656 R657 R658 R659 R660 R661 R662 R663 R664 R665 R666 R667 R668 R669 R670 R671 R672 R673 R674 R675 R676 R677 R678 R679 R680 R681 R682 R683 R684 R685 R686 R687 R688 R689 R690 R691 R692 R693 R694 R695 R696 R697 R698 R699 R700 R701 R702 R703 R704 R705 R706 R707 R708 R709 R710 R711 R712 R713 R714 R715 R716 R717 R718 R719 R720 R721 R722 R723 R724 R725 R726 R727 R728 R729 R730 R731 R732 R733 R734 R735 R736 R737 R738 R739 R740 R741 R742 R743 R744 R745 R746 R747 R748 R749 R750 R751 R752 R753 R754 R755 R756 R757 R758 R759 R760 R761 R762 R763 R764 R765 R766 R767 R768 R769 R770 R771 R772 R773 R774 R775 R776 R777 R778 R779 R780 R781 R782 R783 R784 R785 R786 R787 R788 R789 R790 R791 R792 R793 R794 R795 R796 R797 R798 R799 R800 R801 R802 R803 R804 R805 R806 R807 R808 R809 R810 R811 R812 R813 R814 R815 R816 R817 R818 R819 R820 R821 R822 R823 R824 R825 R826 R827 R828 R829 R830 R831 R832 R833 R834 R835 R836 R837 R838 R839 R840 R841 R842 R843 R844 R845 R846 R847 R848 R849 R850 R851 R852 R853 R854 R855 R856 R857 R858 R859 R860 R861 R862 R863 R864 R865 R866 R867 R868 R869 R870 R871 R872 R873 R874 R875 R876 R877 R878 R879 R880 R881 R882 R883 R884 R885 R886 R887 R888 R889 R890 R891 R892 R893 R894 R895 R896 R897 R898 R899 R900 R901 R902 R903 R904 R905 R906 R907 R908 R909 R910 R911 R912 R913 R914 R915 R916 R917 R918 R919 R920 R921 R922 R923 R924 R925 R926 R927 R928 R929 R930 R931 R932 R933 R934 R935 R936 R937 R938 R939 R940 R941 R942 R943 R944 R945 R946 R947 R948 R949 R950 R951 R952 R953 R954 R955 R956 R957 R958 R959 R960 R961 R962 R963 R964 R965 R966 R967 R968 R969 R970 R971 R972 R973 R974 R975 R976 R977 R978 R979 R980 R981 R982 R983 R984 R985 R986 R987 R988 R989 R990 R991 R992 R993 R994 R995 R996 R997 R998 R999 R1000

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LEU
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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	95.68Å 110.18Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 1.98 42.18 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.18-1.98) 99.0 (42.18-1.98)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.166 , 0.193 0.168 , 0.195	Depositor DCC
R_{free} test set	2000 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9452	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, OXY, PO4, TPP, ACT, K, 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	0.73	0/4195	0.69	1/5689 (0.0%)
1	B	0.68	0/4414	0.70	1/5989 (0.0%)
All	All	0.70	0/8609	0.70	2/11678 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	555	MET	CA-CB-CG	-9.17	97.72	113.30
1	A	129	ASP	CB-CG-OD1	5.83	123.54	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	4111	0	4143	23	0
1	B	4325	0	4349	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	53	0	31	0	0
3	B	53	0	31	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	26	0	16	1	0
5	B	26	0	16	1	0
6	A	6	0	0	1	0
6	B	12	0	0	1	0
7	A	4	0	3	2	0
7	B	8	0	6	2	0
8	B	5	0	0	0	0
9	A	492	0	0	5	1
9	B	327	0	0	11	1
All	All	9452	0	8595	99	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 6.

All (99) 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:368:ASP:OD2	1:B:400:ARG:NH2	2.01	0.92
1:B:296:ILE:HD11	1:B:438:ILE:HD12	1.51	0.92
1:B:327:ALA:O	1:B:444:ARG:NH1	2.04	0.89
1:A:388:PHE:O	1:A:393:ARG:NH1	2.09	0.86
1:B:326:ARG:NH2	1:B:438:ILE:O	2.14	0.81
1:B:579:GLU:HB2	1:B:647:LYS:HE2	1.62	0.81
1:B:580:GLN:HB3	1:B:647:LYS:HB3	1.62	0.81
1:B:434:MET:HG2	1:B:438:ILE:HD11	1.64	0.79
1:A:385:ILE:HD11	1:A:417:VAL:HG12	1.64	0.78
6:B:708:OXY:O1	9:B:801:HOH:O	2.03	0.76
1:A:376:ARG:NH2	9:A:801:HOH:O	2.22	0.72
1:B:590:PHE:O	1:B:592:GLU:N	2.20	0.71
1:B:297:ASN:HD21	1:B:439:PHE:H	1.36	0.71
1:B:297:ASN:O	1:B:300:LYS:NZ	2.24	0.70
1:B:450:GLN:O	1:B:452:ASN:N	2.23	0.70
7:B:712:ACT:H2	7:B:713:ACT:H1	1.73	0.69
1:B:279:ARG:HH11	1:B:279:ARG:HG2	1.60	0.66
1:B:297:ASN:ND2	1:B:439:PHE:H	1.96	0.63
1:B:587:GLN:NE2	1:B:592:GLU:OE2	2.31	0.63
1:B:272:ALA:HA	1:B:275:GLN:HE21	1.64	0.62
1:B:272:ALA:HA	1:B:275:GLN:NE2	2.15	0.62
1:B:126:HIS:ND1	9:B:804:HOH:O	2.31	0.61
7:A:708:ACT:H3	9:B:875:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:582:MET:HG2	9:B:801:HOH:O	2.01	0.60
1:B:442:LYS:H	1:B:442:LYS:HD2	1.66	0.60
1:A:295:LEU:HD12	1:A:421:ILE:HD12	1.84	0.59
1:B:485:ASN:ND2	9:B:806:HOH:O	2.35	0.58
5:B:704:TPP:H2	9:B:875:HOH:O	2.03	0.58
1:B:297:ASN:HD21	1:B:439:PHE:N	2.01	0.58
1:B:151:ARG:NH2	9:B:802:HOH:O	2.09	0.57
1:B:579:GLU:CB	1:B:647:LYS:HE2	2.33	0.57
1:A:385:ILE:HD11	1:A:417:VAL:CG1	2.36	0.56
1:B:391:GLU:OE2	1:B:394:ARG:NH2	2.39	0.56
1:A:130:LYS:HD2	9:A:978:HOH:O	2.07	0.54
1:B:470:LYS:HE3	1:B:646:ASP:HA	1.91	0.53
1:B:324:SER:OG	1:B:347:LYS:HE2	2.08	0.53
1:A:263:PRO:HB3	1:A:265:LYS:HE2	1.92	0.52
1:B:450:GLN:NE2	1:B:454:TRP:HE1	2.08	0.52
1:A:335:LEU:HD22	9:A:1110:HOH:O	2.10	0.52
1:B:296:ILE:CD1	1:B:438:ILE:HD12	2.32	0.51
1:B:300:LYS:HA	1:B:444:ARG:NH2	2.26	0.51
1:B:443:GLU:CD	1:B:444:ARG:H	2.13	0.51
1:B:387:LYS:O	1:B:390:PRO:HD3	2.10	0.51
1:B:619:VAL:HG13	1:B:624:GLU:HG3	1.93	0.51
1:B:365:GLN:O	1:B:390:PRO:HD2	2.12	0.50
1:B:323:LEU:HA	1:B:435:MET:HE1	1.93	0.49
1:B:442:LYS:HD2	1:B:442:LYS:N	2.27	0.49
1:B:343:GLN:NE2	1:B:510:TRP:H	2.11	0.49
1:B:591:TYR:O	1:B:593:HIS:N	2.46	0.49
1:B:153:SER:HB3	1:B:538:ALA:HB1	1.95	0.48
1:B:413:ILE:HD13	1:B:422:ALA:HB1	1.96	0.48
1:B:344:GLU:HG3	1:B:511:ARG:NE	2.29	0.47
1:B:449:ALA:O	1:B:453:LYS:HE2	2.14	0.47
1:A:282:ASP:OD1	1:A:282:ASP:N	2.47	0.47
1:B:434:MET:CG	1:B:438:ILE:HD11	2.38	0.47
6:A:706:OXY:O1	7:A:708:ACT:O	2.31	0.47
1:A:324:SER:OG	1:A:347:LYS:HE2	2.14	0.47
1:A:597:HIS:HB2	9:A:1116:HOH:O	2.14	0.47
1:B:350:ASP:HB3	9:B:828:HOH:O	2.14	0.47
1:B:586:TRP:CZ3	1:B:595:TYR:CE1	3.03	0.47
1:A:268:LEU:HA	1:A:269:PRO:HD2	1.80	0.46
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.96	0.46
1:B:462:TYR:CE1	1:B:464:GLU:HG2	2.51	0.46
1:B:300:LYS:HA	1:B:444:ARG:HH21	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LYS:NZ	9:A:812:HOH:O	2.49	0.45
1:B:363:ALA:N	1:B:454:TRP:HZ3	2.15	0.45
1:B:413:ILE:HG22	1:B:414:ASN:ND2	2.32	0.45
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.99	0.45
1:A:136:PRO:HG3	1:A:142:ALA:HB2	2.00	0.44
7:B:712:ACT:CH3	7:B:713:ACT:H1	2.43	0.44
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.52	0.44
1:B:297:ASN:HA	1:B:297:ASN:HD22	1.60	0.44
1:B:299:ALA:O	1:B:300:LYS:HD2	2.18	0.44
1:A:137:LYS:O	1:B:555:MET:HG2	2.17	0.43
1:A:263:PRO:HB2	1:A:266:THR:HG23	2.00	0.43
1:A:335:LEU:HD21	1:A:518:THR:HG21	2.01	0.43
1:B:292:ALA:HB1	1:B:404:ILE:HD13	2.01	0.43
1:B:414:ASN:HA	1:B:417:VAL:O	2.19	0.43
1:B:579:GLU:H	1:B:647:LYS:HE2	1.84	0.42
1:A:410:PRO:HA	1:A:413:ILE:HD12	2.01	0.42
1:B:445:SER:O	1:B:449:ALA:HB3	2.18	0.42
1:B:279:ARG:CG	1:B:279:ARG:HH11	2.30	0.42
1:B:442:LYS:CD	1:B:442:LYS:H	2.32	0.41
1:B:443:GLU:OE2	1:B:448:PHE:HB3	2.18	0.41
1:B:470:LYS:NZ	9:B:805:HOH:O	2.34	0.41
1:A:465:GLU:N	1:A:465:GLU:OE2	2.52	0.41
5:A:704:TPP:H2	9:B:833:HOH:O	2.20	0.41
1:B:379:ASP:HB3	9:B:1065:HOH:O	2.18	0.41
1:B:136:PRO:HG3	1:B:142:ALA:HB2	2.02	0.41
1:B:296:ILE:CD1	1:B:438:ILE:HG23	2.51	0.41
1:B:579:GLU:H	1:B:647:LYS:CE	2.33	0.41
1:A:165:PRO:HD3	1:B:522:LEU:HG	2.03	0.41
1:B:304:LEU:HD23	1:B:371:ILE:HB	2.03	0.41
1:A:494:THR:HG22	1:A:517:ILE:HB	2.03	0.41
1:B:418:GLN:OE1	1:B:418:GLN:N	2.54	0.41
1:B:295:LEU:HD21	1:B:401:GLY:HA2	2.02	0.41
1:B:442:LYS:CD	1:B:442:LYS:N	2.84	0.41
1:A:385:ILE:HA	1:A:385:ILE:HD12	1.90	0.40
1:B:172:THR:HB	1:B:173:PRO:HD3	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1212:HOH:O	9:B:824:HOH:O[3_544]	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	538/677 (80%)	534 (99%)	3 (1%)	1 (0%)	47	38
1	B	566/677 (84%)	544 (96%)	18 (3%)	4 (1%)	22	11
All	All	1104/1354 (82%)	1078 (98%)	21 (2%)	5 (0%)	29	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	591	TYR
1	B	592	GLU
1	A	270	SER
1	B	367	ALA
1	B	366	ASN

5.3.2 Protein sidechains [i](#)

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	442/556 (80%)	439 (99%)	3 (1%)	84	83
1	B	465/556 (84%)	458 (98%)	7 (2%)	65	59
All	All	907/1112 (82%)	897 (99%)	10 (1%)	73	70

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

Mol	Chain	Res	Type
1	A	119	LEU

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Mol	Chain	Res	Type
1	A	136	PRO
1	A	282	ASP
1	B	275	GLN
1	B	296	ILE
1	B	394	ARG
1	B	444	ARG
1	B	555	MET
1	B	614	LEU
1	B	649	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	275	GLN
1	B	297	ASN
1	B	587	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	ACT	A	708	-	1,3,3	1.15	0	0,3,3	0.00	-
8	PO4	B	711	-	4,4,4	0.87	0	6,6,6	0.97	0
6	OXY	A	705	-	1,1,1	0.14	0	-		
6	OXY	B	705	-	1,1,1	0.16	0	-		
3	FAD	B	702	-	51,58,58	2.16	12 (23%)	60,89,89	1.59	11 (18%)
5	TPP	A	704	4	22,27,27	1.81	6 (27%)	29,40,40	2.43	10 (34%)
6	OXY	B	706	-	1,1,1	0.16	0	-		
6	OXY	B	708	-	1,1,1	0.05	0	-		
6	OXY	B	707	-	1,1,1	0.18	0	-		
6	OXY	A	707	-	1,1,1	0.14	0	-		
3	FAD	A	702	-	51,58,58	2.09	10 (19%)	60,89,89	1.84	10 (16%)
7	ACT	B	713	-	1,3,3	0.09	0	0,3,3	0.00	-
6	OXY	B	709	-	1,1,1	0.00	0	-		
6	OXY	B	710	-	1,1,1	0.04	0	-		
5	TPP	B	704	4	22,27,27	2.13	5 (22%)	29,40,40	2.26	9 (31%)
6	OXY	A	706	-	1,1,1	0.15	0	-		
7	ACT	B	712	-	1,3,3	1.10	0	0,3,3	0.00	-

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
5	TPP	A	704	4	-	3/16/17/17	0/2/2/2
5	TPP	B	704	4	-	3/16/17/17	0/2/2/2
3	FAD	A	702	-	-	3/30/50/50	0/6/6/6
3	FAD	B	702	-	-	3/30/50/50	0/6/6/6

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	FAD	C10-N1	7.24	1.42	1.33
5	B	704	TPP	C6-C5	6.94	1.54	1.50
3	B	702	FAD	C10-N1	6.67	1.41	1.33
3	A	702	FAD	C4-C4X	6.12	1.51	1.41
3	B	702	FAD	C1'-N10	-5.81	1.42	1.48
3	A	702	FAD	C1'-N10	-5.58	1.42	1.48
3	B	702	FAD	C4-C4X	5.31	1.50	1.41
5	A	704	TPP	C6-C5	4.94	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	TPP	C4-N3	-4.76	1.35	1.39
3	B	702	FAD	C4X-N5	4.67	1.40	1.33
3	A	702	FAD	C4X-N5	4.51	1.39	1.33
3	B	702	FAD	C2B-C1B	-4.50	1.46	1.53
3	A	702	FAD	C2B-C1B	-3.76	1.48	1.53
3	B	702	FAD	C4-N3	3.63	1.39	1.33
3	B	702	FAD	O4B-C1B	3.20	1.45	1.41
3	A	702	FAD	C4-N3	3.15	1.38	1.33
5	A	704	TPP	C4'-N4'	3.06	1.41	1.34
5	A	704	TPP	C4-N3	-2.80	1.37	1.39
3	A	702	FAD	C2'-C3'	2.62	1.58	1.53
5	A	704	TPP	C6'-N1'	2.49	1.39	1.34
3	B	702	FAD	C2'-C3'	2.46	1.58	1.53
3	B	702	FAD	C7M-C7	2.46	1.55	1.51
5	A	704	TPP	C4'-N3'	2.45	1.38	1.35
5	B	704	TPP	C2'-N1'	2.42	1.38	1.34
3	B	702	FAD	O3'-C3'	-2.40	1.37	1.43
3	A	702	FAD	O4B-C1B	2.34	1.44	1.41
5	A	704	TPP	C7'-C5'	2.27	1.56	1.51
3	B	702	FAD	C8M-C8	2.24	1.55	1.51
5	B	704	TPP	C4'-N4'	2.19	1.39	1.34
3	A	702	FAD	C7M-C7	2.18	1.55	1.51
5	B	704	TPP	C7'-C5'	2.08	1.55	1.51
3	B	702	FAD	C2-N1	2.07	1.42	1.38
3	A	702	FAD	O3'-C3'	-2.00	1.38	1.43

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	FAD	C4-N3-C2	6.92	120.98	115.14
3	A	702	FAD	C1'-N10-C9A	6.60	123.49	118.29
5	A	704	TPP	C6-C5-C4	6.23	132.43	127.43
5	B	704	TPP	CM2-C2'-N1'	5.97	123.71	117.14
5	A	704	TPP	CM2-C2'-N1'	4.96	122.60	117.14
3	B	702	FAD	C4-N3-C2	4.84	119.23	115.14
5	B	704	TPP	N1'-C2'-N3'	-4.30	118.13	125.54
5	A	704	TPP	N1'-C2'-N3'	-4.28	118.17	125.54
3	A	702	FAD	N3A-C2A-N1A	-4.19	122.12	128.68
3	B	702	FAD	C4-C4X-C10	-4.19	117.18	119.95
5	B	704	TPP	C7'-N3-C2	-4.12	117.91	125.35
3	B	702	FAD	C9A-N10-C10	-3.92	116.77	121.91
3	B	702	FAD	N3A-C2A-N1A	-3.74	122.84	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	704	TPP	C7'-N3-C2	-3.70	118.67	125.35
5	B	704	TPP	C5-C4-N3	3.69	114.96	107.57
5	A	704	TPP	C6'-N1'-C2'	3.68	122.22	115.96
5	B	704	TPP	CM4-C4-C5	-3.49	119.98	127.60
3	B	702	FAD	C1'-N10-C9A	3.37	120.95	118.29
5	B	704	TPP	C6'-N1'-C2'	3.33	121.63	115.96
3	A	702	FAD	C4X-C4-N3	-3.29	118.93	123.43
3	A	702	FAD	C5X-C9A-N10	3.28	120.09	117.72
5	A	704	TPP	O2B-PB-O3A	3.27	115.59	104.64
3	B	702	FAD	C4-C4X-N5	3.26	122.33	118.60
5	A	704	TPP	C5-C4-N3	3.19	113.95	107.57
5	A	704	TPP	CM4-C4-C5	-3.18	120.64	127.60
5	A	704	TPP	PA-O3A-PB	-2.98	122.59	132.83
3	B	702	FAD	C4A-C5A-N7A	-2.85	106.43	109.40
3	A	702	FAD	C5'-C4'-C3'	-2.85	106.70	112.20
3	B	702	FAD	C1'-N10-C10	-2.81	115.89	118.41
5	B	704	TPP	C6-C5-C4	2.73	129.62	127.43
3	B	702	FAD	O4'-C4'-C3'	2.73	115.73	109.10
3	A	702	FAD	C4A-C5A-N7A	-2.70	106.58	109.40
3	A	702	FAD	C9A-N10-C10	-2.52	118.61	121.91
3	B	702	FAD	C5'-C4'-C3'	-2.38	107.60	112.20
3	A	702	FAD	C4X-N5-C5X	2.37	119.14	116.77
5	B	704	TPP	PA-O3A-PB	-2.34	124.80	132.83
5	A	704	TPP	CM4-C4-N3	2.26	125.41	122.53
5	B	704	TPP	O3B-PB-O2B	2.18	115.98	107.64
3	B	702	FAD	C1B-N9A-C4A	-2.15	122.87	126.64
3	A	702	FAD	C4-C4X-N5	2.04	120.93	118.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	702	FAD	P-O3P-PA-O5B
3	B	702	FAD	C2'-C1'-N10-C9A
5	A	704	TPP	C4-C5-C6-C7
5	A	704	TPP	PA-O3A-PB-O3B
3	A	702	FAD	P-O3P-PA-O5B
5	B	704	TPP	C4-C5-C6-C7
5	B	704	TPP	PA-O3A-PB-O2B
3	B	702	FAD	O4B-C4B-C5B-O5B
5	B	704	TPP	PA-O3A-PB-O3B
5	A	704	TPP	C7-O7-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	702	FAD	O4B-C4B-C5B-O5B
3	A	702	FAD	O3'-C3'-C4'-C5'

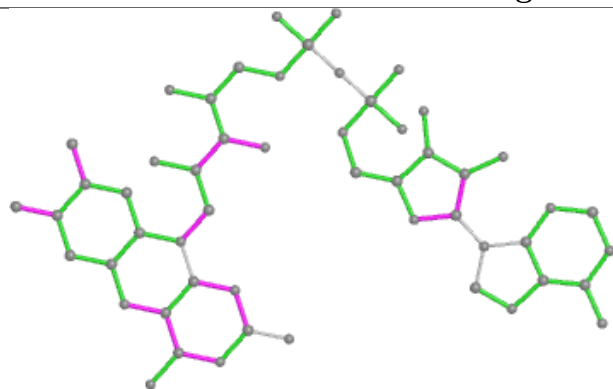
There are no ring outliers.

7 monomers are involved in 7 short contacts:

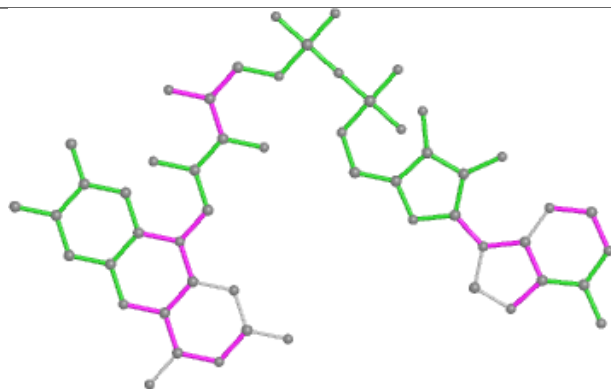
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	708	ACT	2	0
5	A	704	TPP	1	0
6	B	708	OXY	1	0
7	B	713	ACT	2	0
5	B	704	TPP	1	0
6	A	706	OXY	1	0
7	B	712	ACT	2	0

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.

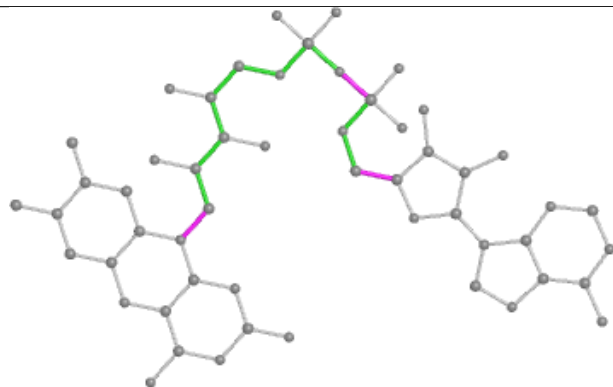
Ligand FAD B 702



Bond lengths



Bond angles

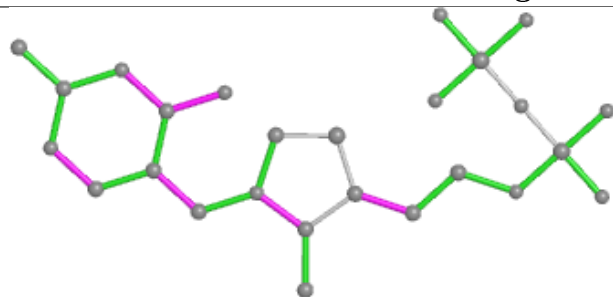


Torsions

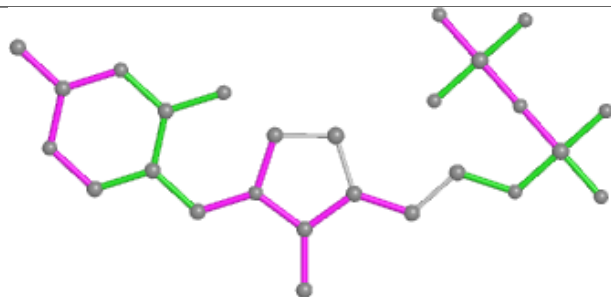


Rings

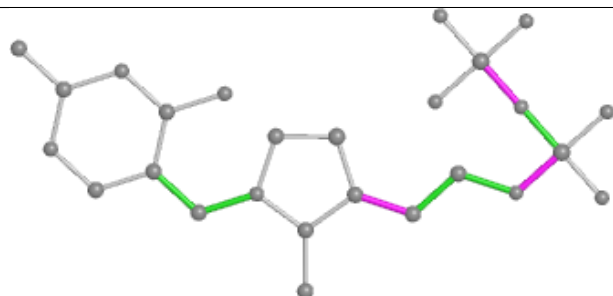
Ligand TPP A 704



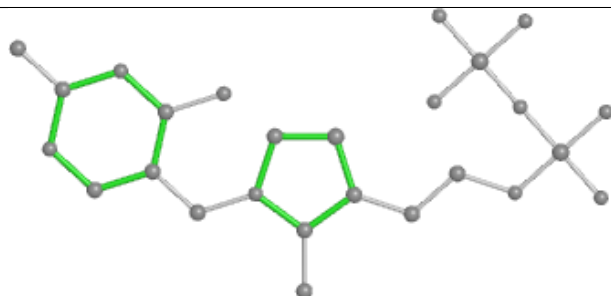
Bond lengths



Bond angles

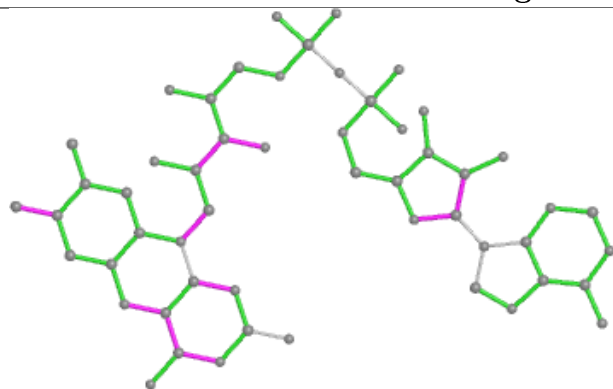


Torsions

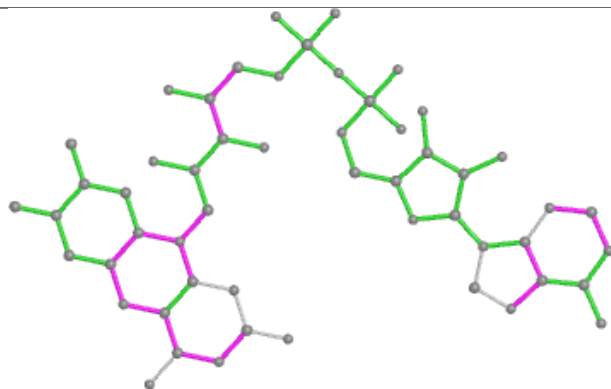


Rings

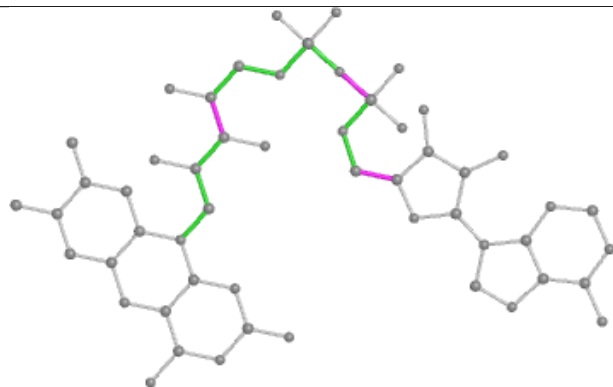
Ligand FAD A 702



Bond lengths



Bond angles

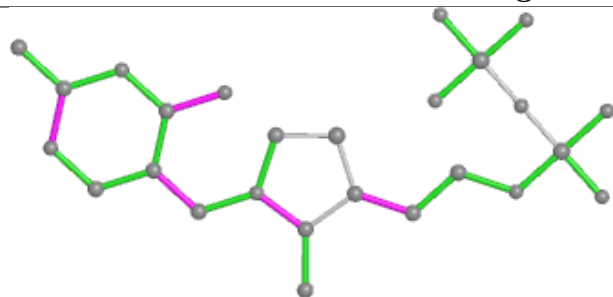


Torsions

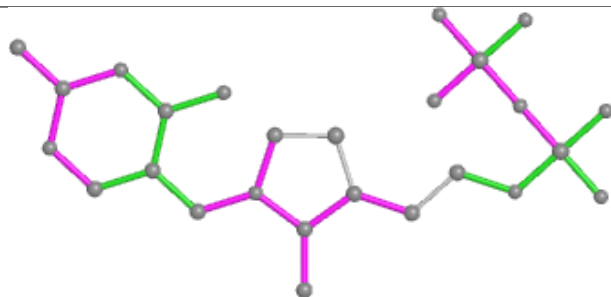


Rings

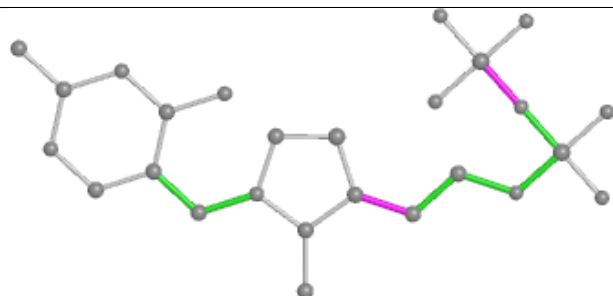
Ligand TPP B 704



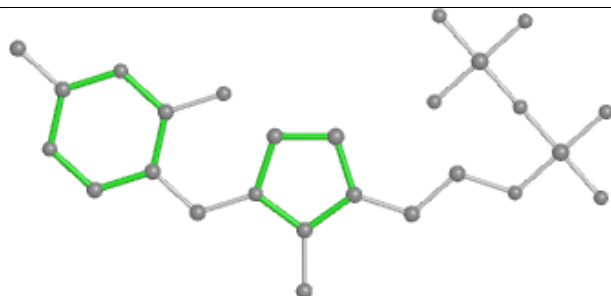
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	541/677 (79%)	0.28	37 (6%) 17 19	19, 29, 62, 112	0
1	B	567/677 (83%)	1.28	133 (23%) 0 0	19, 37, 117, 144	0
All	All	1108/1354 (81%)	0.79	170 (15%) 2 2	19, 32, 105, 144	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	591	TYR	10.6
1	B	448	PHE	9.2
1	B	451	ILE	8.9
1	B	387	LYS	8.2
1	B	396	ALA	8.1
1	B	454	TRP	8.1
1	B	273	LEU	7.9
1	B	458	TYR	7.9
1	B	390	PRO	7.8
1	B	362	LEU	7.7
1	B	649	VAL	7.6
1	B	296	ILE	7.3
1	B	449	ALA	7.2
1	B	392	ALA	7.0
1	B	385	ILE	6.9
1	B	463	MET	6.7
1	B	394	ARG	6.6
1	B	274	ASN	6.6
1	B	365	GLN	6.6
1	B	402	GLY	6.6
1	B	364	VAL	6.3
1	B	397	ALA	6.1
1	B	590	PHE	6.0
1	A	458	TYR	5.9

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Mol	Chain	Res	Type	RSRZ
1	B	401	GLY	5.8
1	B	388	PHE	5.8
1	A	280	ALA	5.6
1	B	447	TRP	5.2
1	A	281	GLN	5.2
1	B	293	ALA	5.2
1	B	369	LEU	5.2
1	B	326	ARG	5.1
1	B	595	TYR	5.1
1	B	467	PRO	5.1
1	A	268	LEU	5.0
1	A	467	PRO	5.0
1	B	461	ALA	5.0
1	A	271	ASN	4.9
1	B	462	TYR	4.9
1	B	438	ILE	4.9
1	A	463	MET	4.9
1	B	416	VAL	4.8
1	B	285	VAL	4.8
1	B	439	PHE	4.8
1	B	386	SER	4.7
1	B	417	VAL	4.7
1	B	441	VAL	4.7
1	B	292	ALA	4.6
1	B	436	SER	4.6
1	B	393	ARG	4.5
1	B	298	LEU	4.5
1	B	279	ARG	4.5
1	B	400	ARG	4.5
1	B	127	ASN	4.5
1	B	419	THR	4.5
1	B	395	ALA	4.5
1	B	466	THR	4.5
1	B	299	ALA	4.4
1	B	383	GLY	4.4
1	A	270	SER	4.4
1	B	435	MET	4.2
1	B	647	LYS	4.2
1	A	597	HIS	4.2
1	B	272	ALA	4.2
1	B	384	ASN	4.2
1	A	83	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	367	ALA	4.1
1	A	466	THR	4.1
1	B	468	GLY	4.1
1	A	599	HIS	4.0
1	B	324	SER	4.0
1	B	358	ALA	4.0
1	B	276	LEU	3.9
1	B	368	ASP	3.9
1	B	646	ASP	3.8
1	B	456	LYS	3.8
1	B	442	LYS	3.8
1	B	294	ASP	3.8
1	B	403	ILE	3.8
1	B	366	ASN	3.8
1	B	459	PRO	3.8
1	B	329	ILE	3.7
1	B	370	ILE	3.7
1	B	287	GLN	3.7
1	B	303	VAL	3.7
1	B	453	LYS	3.7
1	A	269	PRO	3.6
1	B	648	LYS	3.6
1	B	592	GLU	3.6
1	B	284	PHE	3.6
1	B	443	GLU	3.6
1	A	279	ARG	3.6
1	B	593	HIS	3.5
1	B	277	THR	3.5
1	B	460	TYR	3.5
1	B	418	GLN	3.4
1	B	302	PRO	3.4
1	B	275	GLN	3.4
1	B	398	GLU	3.4
1	B	361	ASN	3.3
1	B	271	ASN	3.3
1	B	420	GLN	3.2
1	A	265	LYS	3.2
1	B	586	TRP	3.2
1	B	389	ALA	3.2
1	B	589	LEU	3.0
1	B	301	LYS	3.0
1	B	286	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	468	GLY	2.9
1	B	280	ALA	2.9
1	B	399	GLY	2.8
1	A	469	SER	2.8
1	B	469	SER	2.8
1	B	83	PRO	2.8
1	B	289	ILE	2.8
1	B	527	TYR	2.8
1	B	283	GLU	2.8
1	B	431	LEU	2.7
1	B	444	ARG	2.7
1	A	283	GLU	2.7
1	A	456	LYS	2.7
1	B	335	LEU	2.7
1	B	129	ASP	2.6
1	B	531	ALA	2.6
1	B	126	HIS	2.6
1	A	457	GLU	2.6
1	A	517	ILE	2.6
1	B	270	SER	2.5
1	A	454	TRP	2.5
1	B	517	ILE	2.5
1	B	391	GLU	2.5
1	B	457	GLU	2.5
1	A	461	ALA	2.5
1	A	282	ASP	2.5
1	B	380	ARG	2.5
1	B	434	MET	2.5
1	B	325	ASP	2.4
1	A	647	LYS	2.4
1	B	446	GLU	2.4
1	A	529	LEU	2.3
1	B	182	ILE	2.3
1	B	290	ASN	2.3
1	A	459	PRO	2.3
1	B	291	LYS	2.3
1	B	516	PHE	2.3
1	B	288	SER	2.3
1	B	300	LYS	2.3
1	B	363	ALA	2.3
1	A	522	LEU	2.3
1	B	357	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	284	PHE	2.2
1	B	304	LEU	2.2
1	B	131	PHE	2.2
1	B	583	VAL	2.2
1	A	495	THR	2.1
1	A	518	THR	2.1
1	B	465	GLU	2.1
1	B	278	SER	2.1
1	B	440	PRO	2.1
1	B	323	LEU	2.1
1	A	547	ILE	2.1
1	B	421	ILE	2.1
1	B	529	LEU	2.1
1	A	520	GLY	2.1
1	A	387	LYS	2.1
1	A	84	ASP	2.1
1	A	144	HIS	2.0
1	A	636	LYS	2.0
1	B	404	ILE	2.0
1	B	432	GLY	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 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(\AA^2)	Q<0.9
6	OXY	A	705	2/2	0.74	0.22	55,55,55,60	0
6	OXY	B	706	2/2	0.80	0.38	84,84,84,85	0
6	OXY	B	709	2/2	0.83	0.36	64,64,64,69	0

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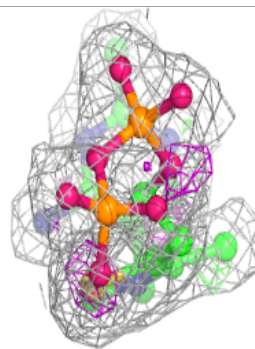
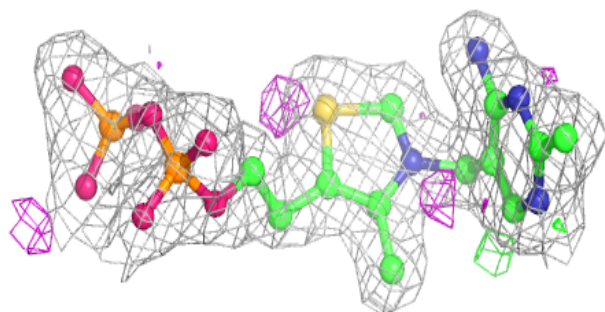
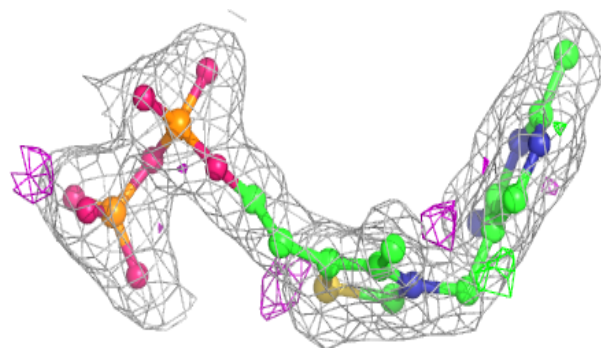
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	OXY	A	706	2/2	0.83	0.26	69,69,69,71	0
7	ACT	B	712	4/4	0.84	0.18	56,57,63,65	0
6	OXY	B	705	2/2	0.89	0.14	68,68,68,69	0
6	OXY	B	708	2/2	0.90	0.25	59,59,59,61	0
7	ACT	A	708	4/4	0.90	0.15	41,57,57,61	0
7	ACT	B	713	4/4	0.90	0.14	57,58,71,73	0
8	PO4	B	711	5/5	0.95	0.12	57,66,70,71	0
4	MG	B	703	1/1	0.95	0.05	25,25,25,25	0
4	MG	A	703	1/1	0.95	0.05	35,35,35,35	0
6	OXY	B	710	2/2	0.96	0.39	40,40,40,48	0
6	OXY	B	707	2/2	0.96	0.16	61,61,61,62	0
5	TPP	A	704	26/26	0.96	0.10	21,30,37,56	0
5	TPP	B	704	26/26	0.97	0.10	19,22,26,28	0
6	OXY	A	707	2/2	0.97	0.17	48,48,48,53	0
3	FAD	B	702	53/53	0.97	0.13	33,41,66,74	0
2	K	A	701	1/1	0.98	0.07	34,34,34,34	0
2	K	B	701	1/1	0.98	0.09	41,41,41,41	0
3	FAD	A	702	53/53	0.98	0.12	25,31,64,70	0

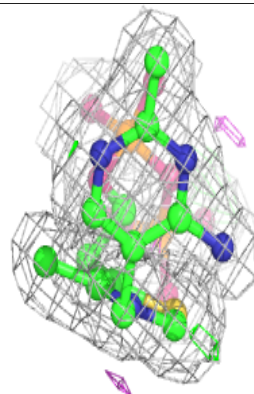
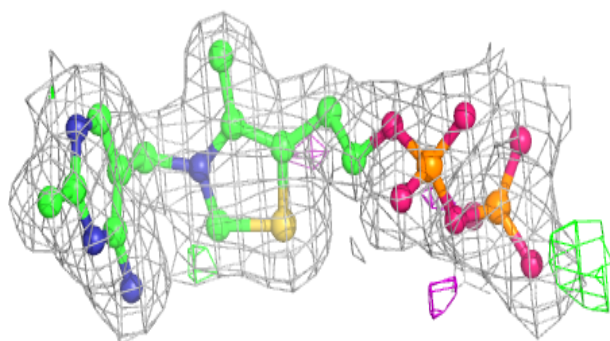
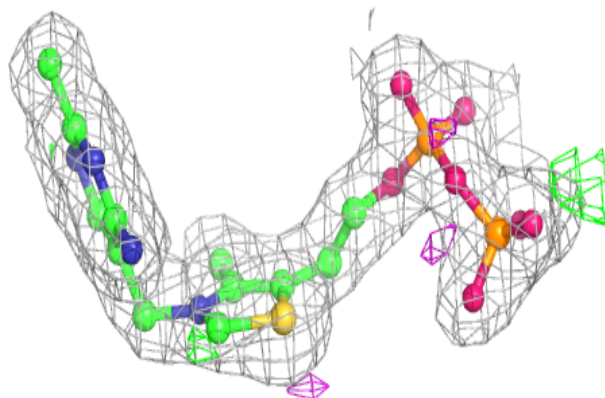
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

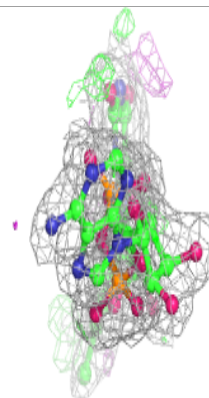
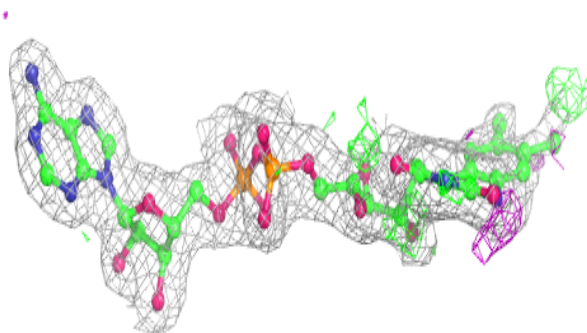
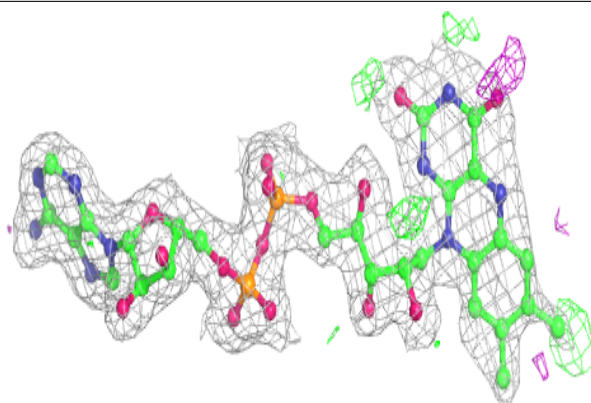
**Electron density around TPP B 704:**

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

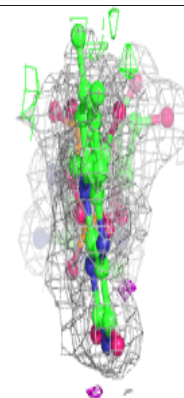
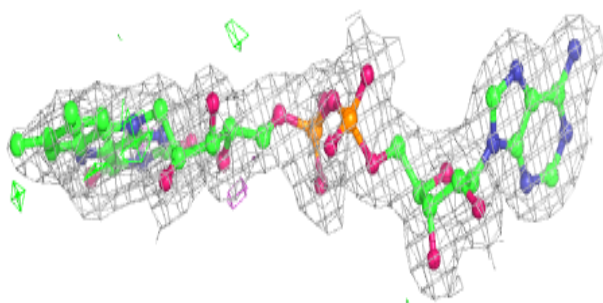
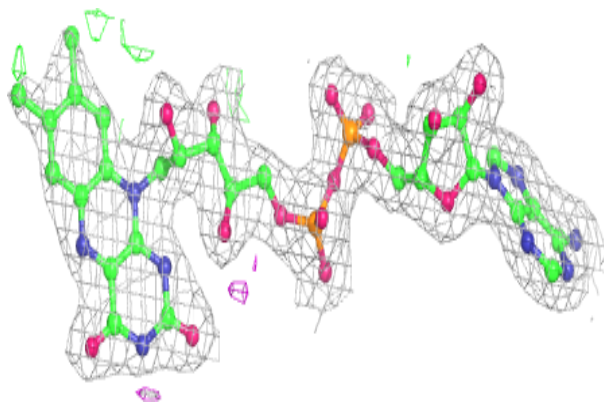


Electron density around FAD B 702:

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

**Electron density around FAD A 702:**

$2mF_o-DF_c$ (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.