



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 20, 2025 – 09:25 pm GMT

PDB ID : 9GJ0
Title : Eugenol Oxidase (EUGO) from *Rhodococcus jostii* RHA1, mutant B1
Authors : Rozeboom, H.J.; Fraaije, M.W.
Deposited on : 2024-08-20
Resolution : 2.76 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

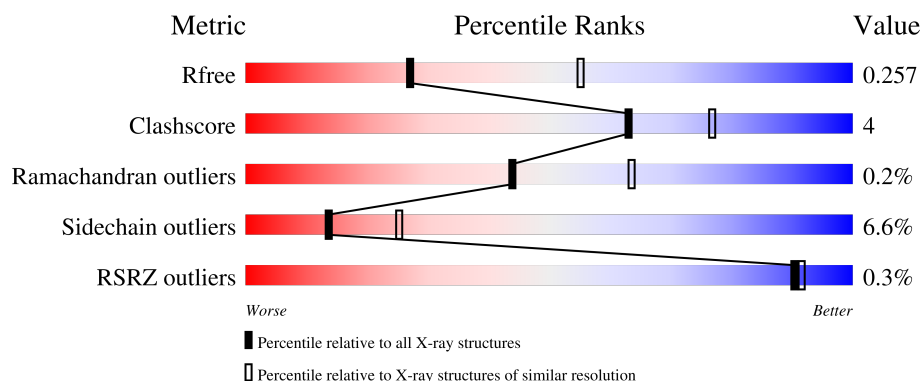
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.76 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	552	
1	B	552	
1	C	552	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12362 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 Probable vanillyl-alcohol oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	0	0
			4112	2622	697	769	24			
1	B	521	Total	C	N	O	S	0	0	0
			4099	2615	694	766	24			
1	C	515	Total	C	N	O	S	0	0	0
			4045	2577	686	758	24			

There are 111 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	HIS	SER	engineered mutation	UNP Q0SBK1
A	278	GLN	ARG	engineered mutation	UNP Q0SBK1
A	283	HIS	ASP	engineered mutation	UNP Q0SBK1
A	378	ASP	GLU	engineered mutation	UNP Q0SBK1
A	394	VAL	SER	engineered mutation	UNP Q0SBK1
A	423	MET	ALA	engineered mutation	UNP Q0SBK1
A	425	GLY	GLN	engineered mutation	UNP Q0SBK1
A	427	THR	ILE	engineered mutation	UNP Q0SBK1
A	434	TYR	HIS	engineered mutation	UNP Q0SBK1
A	445	ASP	ILE	engineered mutation	UNP Q0SBK1
A	518	PRO	SER	engineered mutation	UNP Q0SBK1
A	527	GLY	-	expression tag	UNP Q0SBK1
A	528	LYS	-	expression tag	UNP Q0SBK1
A	529	LEU	-	expression tag	UNP Q0SBK1
A	530	GLY	-	expression tag	UNP Q0SBK1
A	531	PRO	-	expression tag	UNP Q0SBK1
A	532	GLU	-	expression tag	UNP Q0SBK1
A	533	GLN	-	expression tag	UNP Q0SBK1
A	534	LYS	-	expression tag	UNP Q0SBK1
A	535	LEU	-	expression tag	UNP Q0SBK1
A	536	ILE	-	expression tag	UNP Q0SBK1
A	537	SER	-	expression tag	UNP Q0SBK1
A	538	GLU	-	expression tag	UNP Q0SBK1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	539	GLU	-	expression tag	UNP Q0SBK1
A	540	ASP	-	expression tag	UNP Q0SBK1
A	541	LEU	-	expression tag	UNP Q0SBK1
A	542	ASN	-	expression tag	UNP Q0SBK1
A	543	SER	-	expression tag	UNP Q0SBK1
A	544	ALA	-	expression tag	UNP Q0SBK1
A	545	VAL	-	expression tag	UNP Q0SBK1
A	546	ASP	-	expression tag	UNP Q0SBK1
A	547	HIS	-	expression tag	UNP Q0SBK1
A	548	HIS	-	expression tag	UNP Q0SBK1
A	549	HIS	-	expression tag	UNP Q0SBK1
A	550	HIS	-	expression tag	UNP Q0SBK1
A	551	HIS	-	expression tag	UNP Q0SBK1
A	552	HIS	-	expression tag	UNP Q0SBK1
B	81	HIS	SER	engineered mutation	UNP Q0SBK1
B	278	GLN	ARG	engineered mutation	UNP Q0SBK1
B	283	HIS	ASP	engineered mutation	UNP Q0SBK1
B	378	ASP	GLU	engineered mutation	UNP Q0SBK1
B	394	VAL	SER	engineered mutation	UNP Q0SBK1
B	423	MET	ALA	engineered mutation	UNP Q0SBK1
B	425	GLY	GLN	engineered mutation	UNP Q0SBK1
B	427	THR	ILE	engineered mutation	UNP Q0SBK1
B	434	TYR	HIS	engineered mutation	UNP Q0SBK1
B	445	ASP	ILE	engineered mutation	UNP Q0SBK1
B	518	PRO	SER	engineered mutation	UNP Q0SBK1
B	527	GLY	-	expression tag	UNP Q0SBK1
B	528	LYS	-	expression tag	UNP Q0SBK1
B	529	LEU	-	expression tag	UNP Q0SBK1
B	530	GLY	-	expression tag	UNP Q0SBK1
B	531	PRO	-	expression tag	UNP Q0SBK1
B	532	GLU	-	expression tag	UNP Q0SBK1
B	533	GLN	-	expression tag	UNP Q0SBK1
B	534	LYS	-	expression tag	UNP Q0SBK1
B	535	LEU	-	expression tag	UNP Q0SBK1
B	536	ILE	-	expression tag	UNP Q0SBK1
B	537	SER	-	expression tag	UNP Q0SBK1
B	538	GLU	-	expression tag	UNP Q0SBK1
B	539	GLU	-	expression tag	UNP Q0SBK1
B	540	ASP	-	expression tag	UNP Q0SBK1
B	541	LEU	-	expression tag	UNP Q0SBK1
B	542	ASN	-	expression tag	UNP Q0SBK1
B	543	SER	-	expression tag	UNP Q0SBK1

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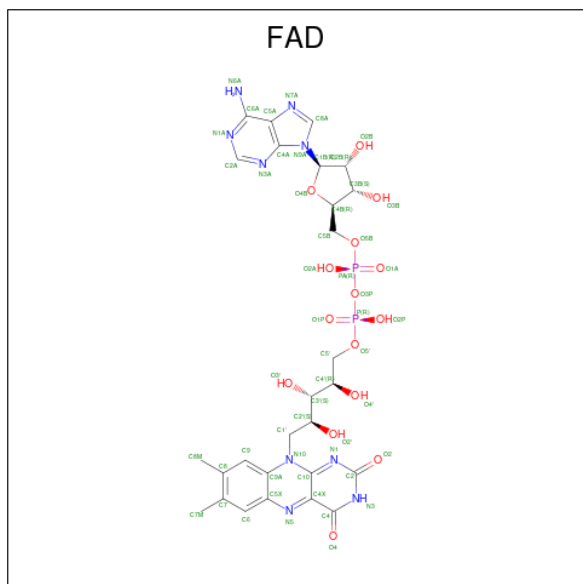
Chain	Residue	Modelled	Actual	Comment	Reference
B	544	ALA	-	expression tag	UNP Q0SBK1
B	545	VAL	-	expression tag	UNP Q0SBK1
B	546	ASP	-	expression tag	UNP Q0SBK1
B	547	HIS	-	expression tag	UNP Q0SBK1
B	548	HIS	-	expression tag	UNP Q0SBK1
B	549	HIS	-	expression tag	UNP Q0SBK1
B	550	HIS	-	expression tag	UNP Q0SBK1
B	551	HIS	-	expression tag	UNP Q0SBK1
B	552	HIS	-	expression tag	UNP Q0SBK1
C	81	HIS	SER	engineered mutation	UNP Q0SBK1
C	278	GLN	ARG	engineered mutation	UNP Q0SBK1
C	283	HIS	ASP	engineered mutation	UNP Q0SBK1
C	378	ASP	GLU	engineered mutation	UNP Q0SBK1
C	394	VAL	SER	engineered mutation	UNP Q0SBK1
C	423	MET	ALA	engineered mutation	UNP Q0SBK1
C	425	GLY	GLN	engineered mutation	UNP Q0SBK1
C	427	THR	ILE	engineered mutation	UNP Q0SBK1
C	434	TYR	HIS	engineered mutation	UNP Q0SBK1
C	445	ASP	ILE	engineered mutation	UNP Q0SBK1
C	518	PRO	SER	engineered mutation	UNP Q0SBK1
C	527	GLY	-	expression tag	UNP Q0SBK1
C	528	LYS	-	expression tag	UNP Q0SBK1
C	529	LEU	-	expression tag	UNP Q0SBK1
C	530	GLY	-	expression tag	UNP Q0SBK1
C	531	PRO	-	expression tag	UNP Q0SBK1
C	532	GLU	-	expression tag	UNP Q0SBK1
C	533	GLN	-	expression tag	UNP Q0SBK1
C	534	LYS	-	expression tag	UNP Q0SBK1
C	535	LEU	-	expression tag	UNP Q0SBK1
C	536	ILE	-	expression tag	UNP Q0SBK1
C	537	SER	-	expression tag	UNP Q0SBK1
C	538	GLU	-	expression tag	UNP Q0SBK1
C	539	GLU	-	expression tag	UNP Q0SBK1
C	540	ASP	-	expression tag	UNP Q0SBK1
C	541	LEU	-	expression tag	UNP Q0SBK1
C	542	ASN	-	expression tag	UNP Q0SBK1
C	543	SER	-	expression tag	UNP Q0SBK1
C	544	ALA	-	expression tag	UNP Q0SBK1
C	545	VAL	-	expression tag	UNP Q0SBK1
C	546	ASP	-	expression tag	UNP Q0SBK1
C	547	HIS	-	expression tag	UNP Q0SBK1
C	548	HIS	-	expression tag	UNP Q0SBK1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	549	HIS	-	expression tag	UNP Q0SBK1
C	550	HIS	-	expression tag	UNP Q0SBK1
C	551	HIS	-	expression tag	UNP Q0SBK1
C	552	HIS	-	expression tag	UNP Q0SBK1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).

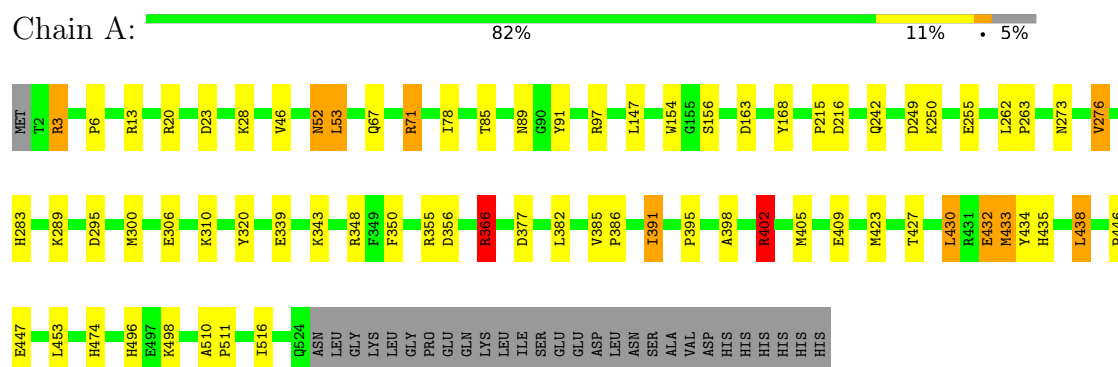


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

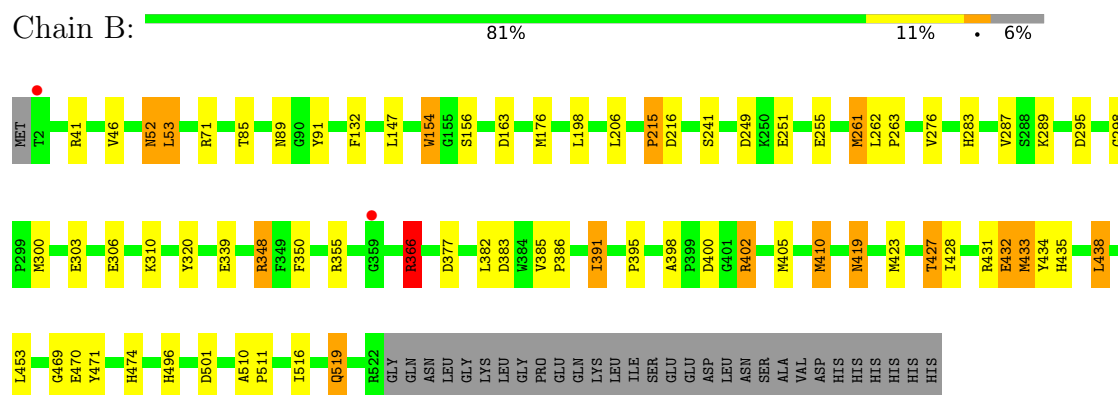
3 Residue-property plots

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

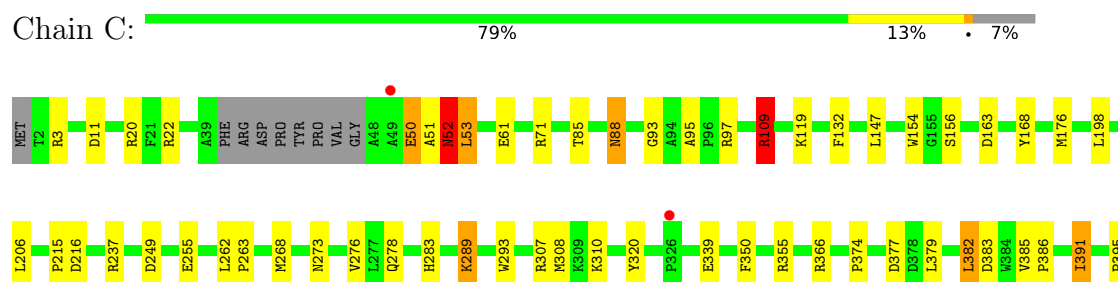
- Molecule 1: Probable vanillyl-alcohol oxidase

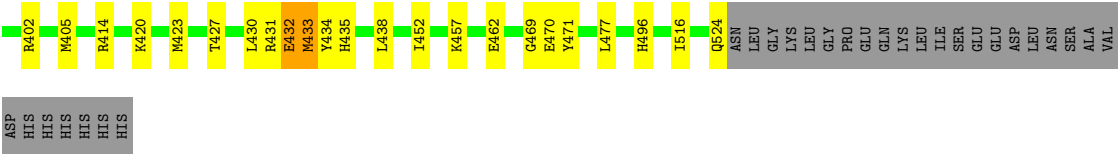


- Molecule 1: Probable vanillyl-alcohol oxidase



- Molecule 1: Probable vanillyl-alcohol oxidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.77 Å 109.77 Å 244.99 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	95.06 – 2.76 95.06 – 2.76	Depositor EDS
% Data completeness (in resolution range)	97.1 (95.06-2.76) 97.1 (95.06-2.76)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.77 Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.206 , 0.266 0.206 , 0.257	Depositor DCC
R_{free} test set	2245 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	87.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12362	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.38	0/4222	0.82	6/5731 (0.1%)
1	B	0.36	0/4209	0.78	7/5714 (0.1%)
1	C	0.37	0/4150	0.80	6/5630 (0.1%)
All	All	0.37	0/12581	0.80	19/17075 (0.1%)

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	5
1	C	0	4
All	All	0	13

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	C	268	MET	CG-SD-CE	6.71	110.93	100.20
1	A	300	MET	CG-SD-CE	-6.05	90.52	100.20
1	C	423	MET	CG-SD-CE	5.88	109.61	100.20
1	C	278	GLN	CB-CA-C	5.65	121.69	110.40
1	B	366	ARG	CD-NE-CZ	5.60	131.44	123.60
1	B	176	MET	CG-SD-CE	5.50	108.99	100.20
1	B	366	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	C	433	MET	CG-SD-CE	5.42	108.87	100.20
1	B	366	ARG	CG-CD-NE	5.33	123.00	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	366	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	B	215	PRO	N-CA-CB	-5.22	96.86	102.60
1	B	300	MET	CG-SD-CE	-5.20	91.89	100.20
1	A	366	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	176	MET	CG-SD-CE	5.11	108.37	100.20
1	A	3	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	3	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	366	ARG	CG-CD-NE	-5.03	101.25	111.80
1	A	71	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	ARG	Sidechain
1	A	366	ARG	Sidechain
1	A	402	ARG	Sidechain
1	A	97	ARG	Sidechain
1	B	348	ARG	Sidechain
1	B	366	ARG	Sidechain
1	B	402	ARG	Sidechain
1	B	41	ARG	Sidechain
1	B	71	ARG	Sidechain
1	C	109	ARG	Sidechain
1	C	20	ARG	Sidechain
1	C	22	ARG	Sidechain
1	C	71	ARG	Sidechain

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	4112	0	3975	28	1
1	B	4099	0	3964	38	0
1	C	4045	0	3913	34	1
2	A	53	0	30	3	0
2	B	53	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12362	0	11912	95	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (95) 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:89:ASN:O	2:A:600:FAD:H9	1.87	0.74
1:A:85:THR:OG1	2:A:600:FAD:O1P	2.08	0.71
1:B:89:ASN:O	2:B:600:FAD:H9	1.92	0.70
1:A:262:LEU:HB3	1:A:263:PRO:HD3	1.78	0.66
1:C:52:ASN:HB3	1:C:95:ALA:HB1	1.77	0.65
1:C:52:ASN:O	1:C:53:LEU:HD23	1.97	0.64
1:C:262:LEU:HB3	1:C:263:PRO:HD3	1.79	0.64
1:C:457:LYS:HG3	1:C:477:LEU:HD22	1.82	0.60
1:A:52:ASN:O	1:A:53:LEU:HD23	2.01	0.60
1:B:262:LEU:HB3	1:B:263:PRO:HD3	1.82	0.60
1:B:431:ARG:O	1:C:206:LEU:HB3	2.01	0.60
1:A:276:VAL:HG11	1:A:366:ARG:HH21	1.67	0.60
1:C:496:HIS:HB3	1:C:516:ILE:HD13	1.82	0.60
1:B:52:ASN:O	1:B:53:LEU:HD23	2.02	0.60
1:B:261:MET:SD	1:B:428:ILE:HD13	2.42	0.59
1:C:391:ILE:HG21	1:C:452:ILE:HG23	1.85	0.58
1:B:91:TYR:HA	1:B:474:HIS:HA	1.86	0.58
1:B:391:ILE:HD12	1:B:474:HIS:CD2	2.40	0.57
1:A:91:TYR:HA	1:A:474:HIS:HA	1.86	0.56
1:A:385:VAL:HB	1:A:386:PRO:HD2	1.88	0.56
1:C:385:VAL:HB	1:C:386:PRO:HD2	1.87	0.56
1:A:391:ILE:HD12	1:A:474:HIS:CD2	2.41	0.56
1:C:88:ASN:HB3	1:C:93:GLY:HA2	1.89	0.55
1:A:402:ARG:HH11	1:A:402:ARG:HG3	1.72	0.55
1:B:255:GLU:HB2	1:B:405:MET:CE	2.37	0.55
1:A:446:PRO:HB2	1:B:132:PHE:HB3	1.88	0.54
1:C:414:ARG:HG3	1:C:462:GLU:OE1	2.06	0.54
1:B:427:THR:C	1:B:428:ILE:HD12	2.29	0.53
1:C:524:GLN:N	1:C:524:GLN:OE1	2.41	0.52
1:C:379:LEU:O	1:C:382:LEU:HB2	2.10	0.52
1:B:385:VAL:HB	1:B:386:PRO:HD2	1.90	0.52
1:B:496:HIS:HB3	1:B:516:ILE:HD13	1.92	0.51
1:B:46:VAL:HG12	1:B:453:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:GLU:HB2	1:C:405:MET:CE	2.39	0.51
1:B:501:ASP:OD1	1:B:519:GLN:HG3	2.11	0.51
1:A:306:GLU:O	1:A:310:LYS:HG2	2.12	0.50
1:A:496:HIS:HB3	1:A:516:ILE:HD13	1.94	0.49
1:B:395:PRO:HG2	1:B:435:HIS:HB3	1.94	0.49
1:B:306:GLU:O	1:B:310:LYS:HG2	2.13	0.49
1:B:85:THR:OG1	2:B:600:FAD:O1P	2.31	0.48
1:A:255:GLU:HB2	1:A:405:MET:CE	2.43	0.48
1:A:350:PHE:CD2	1:A:355:ARG:HD2	2.50	0.47
1:C:50:GLU:OE1	1:C:51:ALA:HB3	2.14	0.47
1:A:6:PRO:HG2	1:A:78:ILE:HD12	1.96	0.47
2:A:600:FAD:H8A	2:A:600:FAD:O5B	2.14	0.47
1:A:395:PRO:HG2	1:A:435:HIS:HB3	1.96	0.47
1:C:283:HIS:CD2	1:C:320:TYR:HH	2.31	0.47
1:B:350:PHE:CD2	1:B:355:ARG:HD2	2.50	0.47
1:C:395:PRO:HG2	1:C:435:HIS:HB3	1.97	0.46
1:A:423:MET:HB2	1:A:438:LEU:O	2.16	0.46
1:B:423:MET:HB2	1:B:438:LEU:O	2.15	0.46
1:A:168:TYR:O	1:A:273:ASN:HB2	2.16	0.46
1:C:432:GLU:OE1	1:C:434:TYR:OH	2.30	0.46
1:A:283:HIS:CD2	1:A:320:TYR:HH	2.30	0.46
1:A:46:VAL:HG12	1:A:453:LEU:HD13	1.97	0.46
1:A:147:LEU:C	1:A:147:LEU:HD12	2.37	0.46
1:C:496:HIS:HB3	1:C:516:ILE:CD1	2.46	0.46
1:B:85:THR:HG23	1:B:156:SER:HB2	1.98	0.45
1:C:132:PHE:CE1	1:C:374:PRO:HB2	2.51	0.45
1:C:350:PHE:CD2	1:C:355:ARG:HD2	2.51	0.45
2:B:600:FAD:O5B	2:B:600:FAD:H8A	2.16	0.45
1:C:432:GLU:OE1	1:C:434:TYR:CZ	2.70	0.45
1:B:206:LEU:HB3	1:C:431:ARG:O	2.17	0.44
1:B:432:GLU:OE1	1:B:434:TYR:CZ	2.70	0.44
1:B:147:LEU:C	1:B:147:LEU:HD12	2.38	0.44
1:B:198:LEU:HD13	1:C:469:GLY:HA3	2.00	0.43
1:B:298:GLY:HA2	1:B:419:ASN:OD1	2.18	0.43
1:C:289:LYS:HG2	1:C:383:ASP:O	2.18	0.43
1:B:283:HIS:CD2	1:B:320:TYR:HH	2.35	0.43
1:B:432:GLU:OE1	1:B:434:TYR:OH	2.29	0.43
1:B:255:GLU:HB2	1:B:405:MET:HE3	2.00	0.43
1:A:398:ALA:O	1:A:433:MET:HE2	2.19	0.42
1:C:147:LEU:HD12	1:C:147:LEU:C	2.39	0.42
1:A:432:GLU:OE1	1:A:434:TYR:CZ	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ALA:N	1:A:511:PRO:HD3	2.33	0.42
1:B:398:ALA:O	1:B:433:MET:HE2	2.20	0.42
1:C:61:GLU:OE1	1:C:109:ARG:NH1	2.53	0.42
1:C:168:TYR:O	1:C:273:ASN:HB2	2.19	0.42
1:C:85:THR:HG23	1:C:156:SER:HB2	2.00	0.42
1:B:469:GLY:HA3	1:C:198:LEU:HD13	2.02	0.41
1:A:85:THR:HG23	1:A:156:SER:HB2	2.03	0.41
1:A:67:GLN:O	1:A:71:ARG:HG3	2.21	0.41
1:A:447:GLU:OE2	1:B:154:TRP:O	2.39	0.41
1:B:470:GLU:N	1:B:470:GLU:CD	2.74	0.41
1:C:293:TRP:O	1:C:307:ARG:NH2	2.54	0.41
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.90	0.40
1:B:289:LYS:HG2	1:B:383:ASP:O	2.21	0.40
1:B:400:ASP:OD1	1:C:119:LYS:NZ	2.54	0.40
1:B:410:MET:HE2	1:B:410:MET:HB2	2.00	0.40
1:C:293:TRP:CE3	1:C:308:MET:HG2	2.56	0.40
1:B:510:ALA:N	1:B:511:PRO:HD3	2.36	0.40
1:C:470:GLU:N	1:C:470:GLU:CD	2.75	0.40
1:B:366:ARG:HH21	1:B:366:ARG:HB3	1.87	0.40
1:B:496:HIS:HB3	1:B:516:ILE:CD1	2.51	0.40
1:C:391:ILE:HG21	1:C:452:ILE:CG2	2.50	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)
1:A:23:ASP:OD2	1:C:97:ARG:NH2[2_444]	2.18	0.02

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	521/552 (94%)	497 (95%)	23 (4%)	1 (0%)	44	63
1	B	519/552 (94%)	496 (96%)	22 (4%)	1 (0%)	44	63
1	C	511/552 (93%)	487 (95%)	23 (4%)	1 (0%)	44	63
All	All	1551/1656 (94%)	1480 (95%)	68 (4%)	3 (0%)	44	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	52	ASN
1	A	52	ASN
1	B	52	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	431/457 (94%)	402 (93%)	29 (7%)	13	25
1	B	430/457 (94%)	402 (94%)	28 (6%)	14	26
1	C	424/457 (93%)	396 (93%)	28 (7%)	14	25
All	All	1285/1371 (94%)	1200 (93%)	85 (7%)	14	25

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	20	ARG
1	A	28	LYS
1	A	53	LEU
1	A	154	TRP
1	A	163	ASP
1	A	215	PRO
1	A	216	ASP
1	A	242	GLN
1	A	249	ASP

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Mol	Chain	Res	Type
1	A	250	LYS
1	A	276	VAL
1	A	289	LYS
1	A	295	ASP
1	A	339	GLU
1	A	343	LYS
1	A	348	ARG
1	A	356	ASP
1	A	377	ASP
1	A	382	LEU
1	A	391	ILE
1	A	402	ARG
1	A	409	GLU
1	A	427	THR
1	A	430	LEU
1	A	432	GLU
1	A	433	MET
1	A	438	LEU
1	A	498	LYS
1	B	53	LEU
1	B	154	TRP
1	B	163	ASP
1	B	215	PRO
1	B	216	ASP
1	B	241	SER
1	B	249	ASP
1	B	251	GLU
1	B	261	MET
1	B	276	VAL
1	B	287	VAL
1	B	295	ASP
1	B	303	GLU
1	B	339	GLU
1	B	348	ARG
1	B	366	ARG
1	B	377	ASP
1	B	382	LEU
1	B	391	ILE
1	B	402	ARG
1	B	410	MET
1	B	419	ASN
1	B	427	THR

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Mol	Chain	Res	Type
1	B	432	GLU
1	B	433	MET
1	B	438	LEU
1	B	471	TYR
1	B	519	GLN
1	C	11	ASP
1	C	50	GLU
1	C	52	ASN
1	C	53	LEU
1	C	88	ASN
1	C	109	ARG
1	C	154	TRP
1	C	163	ASP
1	C	215	PRO
1	C	216	ASP
1	C	237	ARG
1	C	249	ASP
1	C	276	VAL
1	C	289	LYS
1	C	310	LYS
1	C	339	GLU
1	C	366	ARG
1	C	377	ASP
1	C	382	LEU
1	C	391	ILE
1	C	402	ARG
1	C	420	LYS
1	C	427	THR
1	C	430	LEU
1	C	432	GLU
1	C	433	MET
1	C	438	LEU
1	C	471	TYR

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	236	GLN
1	A	278	GLN
1	A	380	GLN
1	B	236	GLN
1	B	413	ASN

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Mol	Chain	Res	Type
1	B	475	ASN
1	C	52	ASN

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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	600	1	53,58,58	0.75	0	68,89,89	0.95	4 (5%)
2	FAD	B	600	1	53,58,58	0.64	0	68,89,89	0.68	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1	-	3/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	600	1	-	8/30/50/50	0/6/6/6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O2'-C2'-C1'	3.35	117.91	109.80
2	A	600	FAD	O3'-C3'-C4'	-2.35	103.13	108.81
2	A	600	FAD	P-O3P-PA	2.22	140.43	132.83
2	A	600	FAD	C4'-C3'-C2'	2.21	117.96	113.36
2	B	600	FAD	C5A-C6A-N6A	2.05	123.47	120.35

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C3'-C4'-C5'-O5'
2	A	600	FAD	O4'-C4'-C5'-O5'
2	B	600	FAD	C5'-O5'-P-O1P
2	B	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C2'-C3'-C4'-O4'
2	B	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	O3'-C3'-C4'-O4'

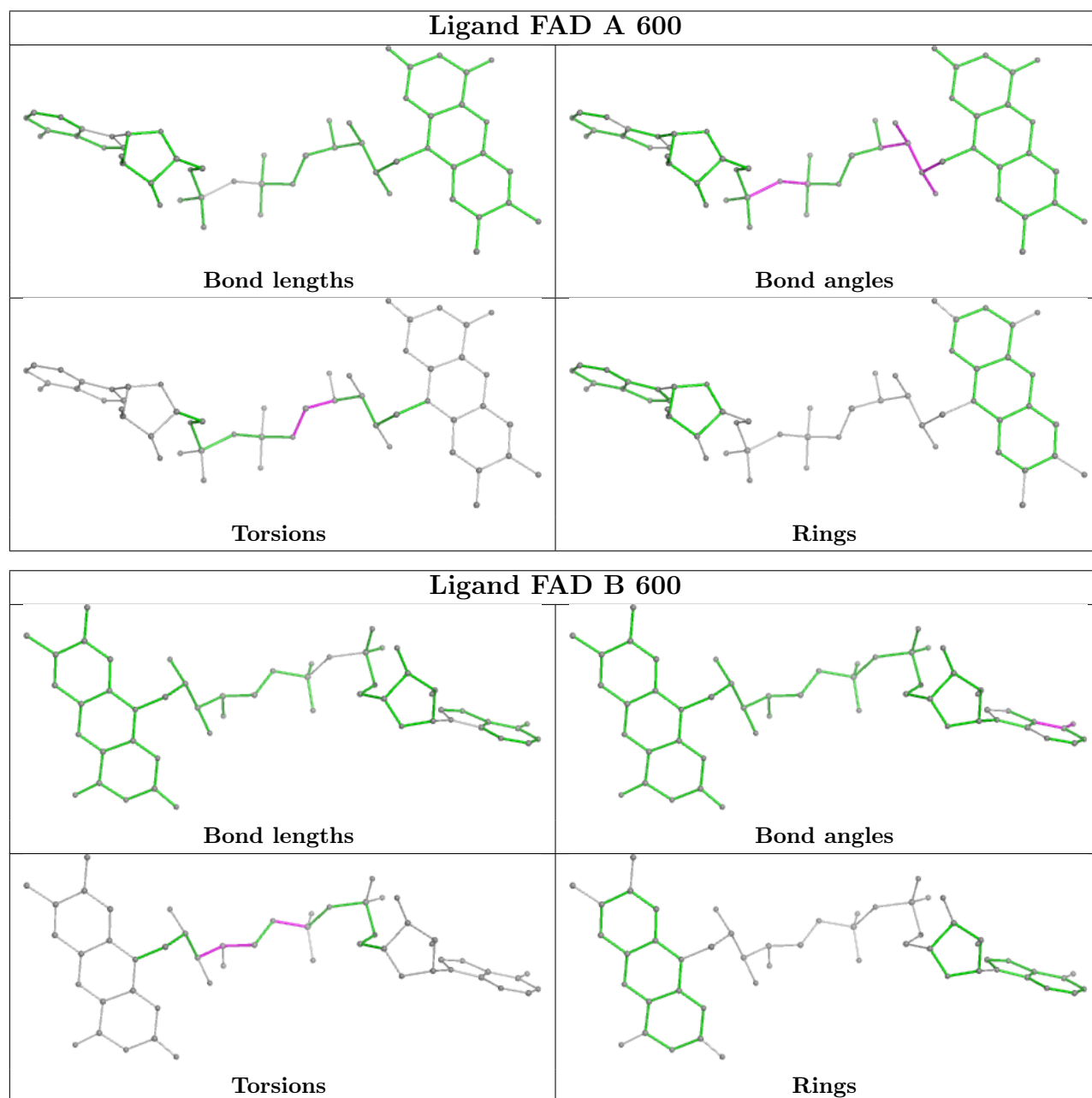
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	3	0
2	B	600	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [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	523/552 (94%)	-0.68	0	100 100	56, 84, 125, 161	0
1	B	521/552 (94%)	-0.47	2 (0%)	89 90	65, 109, 149, 170	0
1	C	515/552 (93%)	-0.42	2 (0%)	89 90	68, 104, 145, 183	0
All	All	1559/1656 (94%)	-0.52	4 (0%)	90 91	56, 99, 144, 183	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	49	ALA	2.3
1	C	326	PRO	2.3
1	B	359	GLY	2.3
1	B	2	THR	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](#)

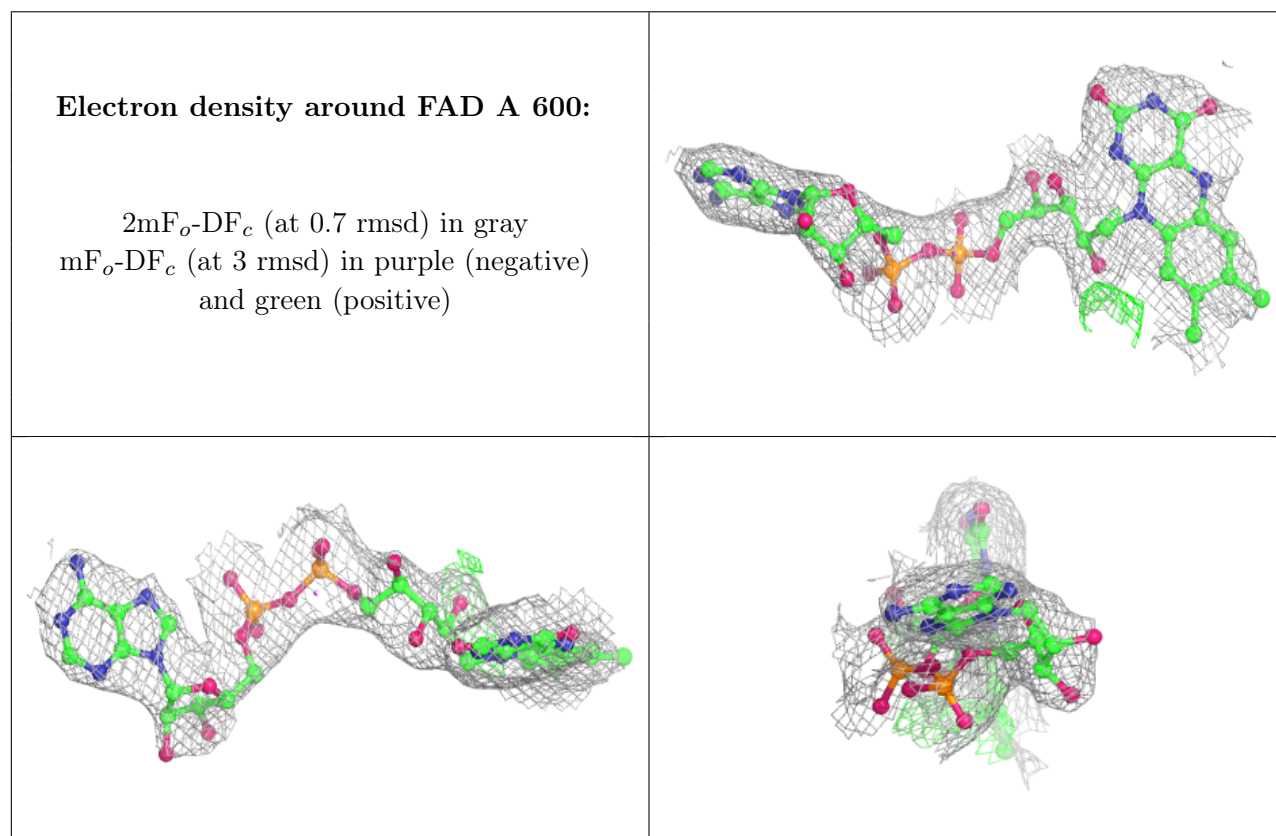
There are no monosaccharides in this entry.

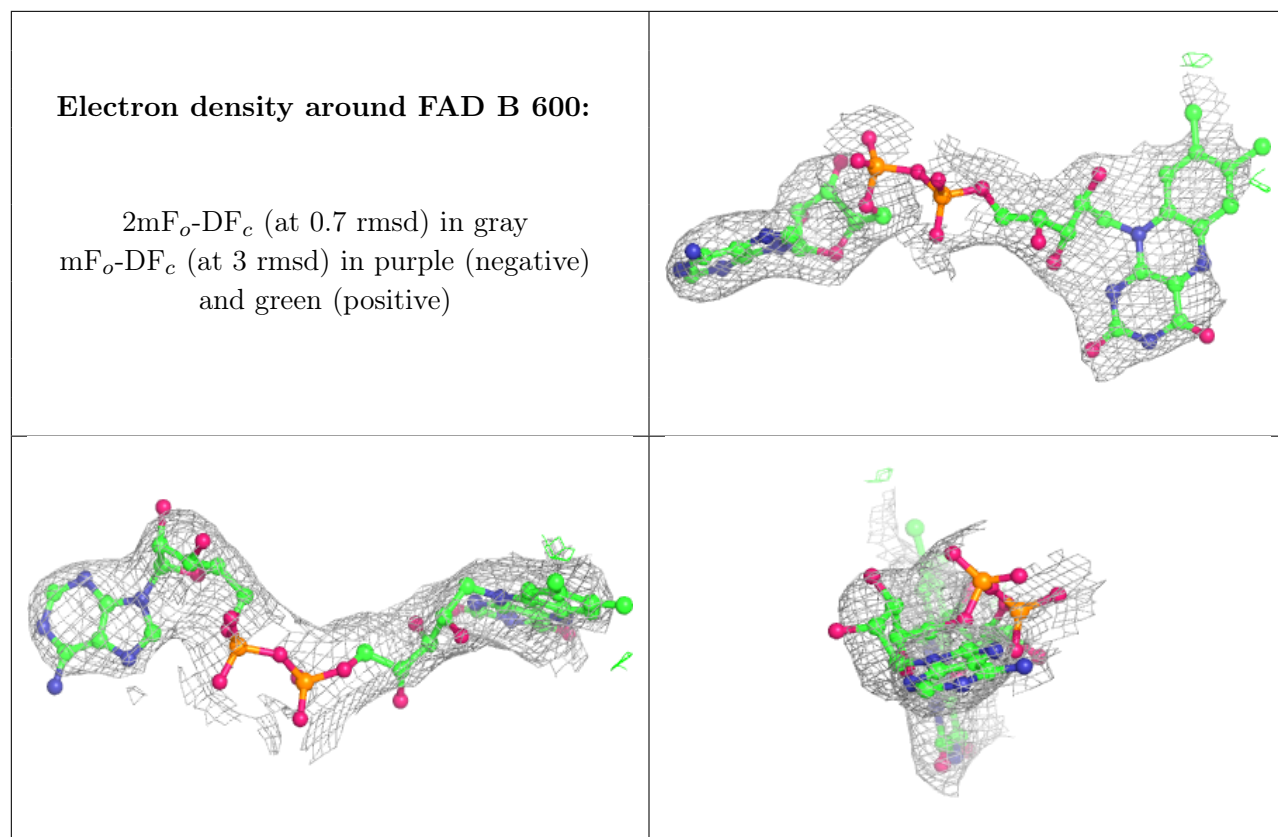
6.4 Ligands [i](#)

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
2	FAD	A	600	53/53	0.90	0.08	71,111,142,149	0
2	FAD	B	600	53/53	0.95	0.06	87,120,152,170	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.